



wwPDB EM Map/Model Validation Report ⓘ

May 5, 2016 – 10:19 PM EDT

PDB ID : 5FM1
EMDB ID: : EMD-1731
Title : Structure of gamma-tubulin small complex based on a cryo-EM map, chemical cross-links, and a remotely related structure
Authors : Greenberg, C.H.; Kollman, J.; Zelter, A.; Johnson, R.; MacCoss, M.J.; Davis, T.N.; Agard, D.A.; Sali, A.
Deposited on : 2015-10-30
Resolution : 8.00 Å(reported)

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

A user guide is available at

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

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-20027457

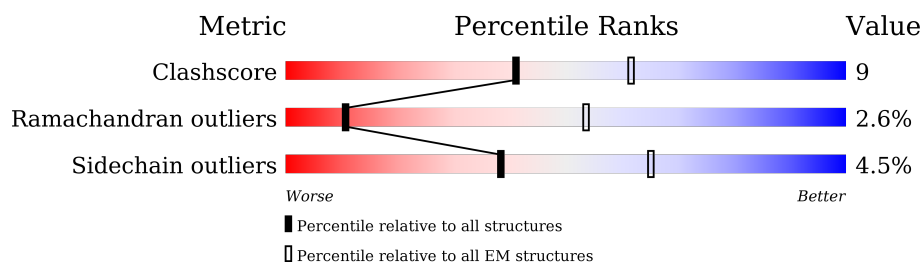
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 Å.

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




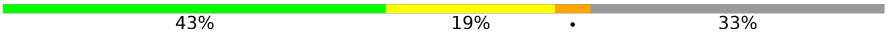
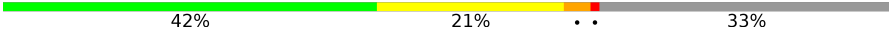

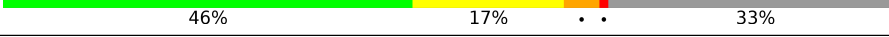
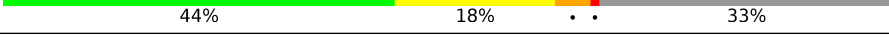
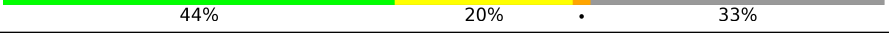
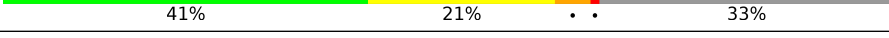
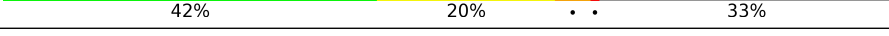
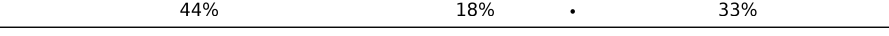
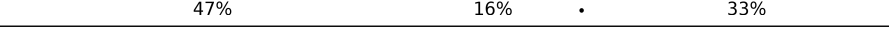
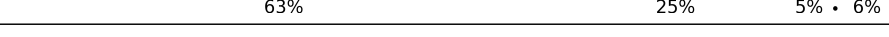

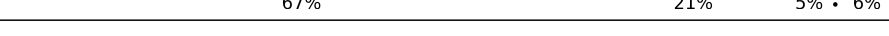


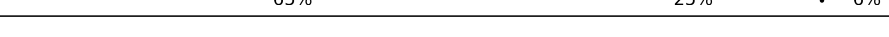

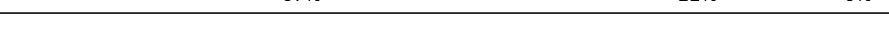






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1-A	823	
1	10-A	823	
1	2-A	823	
1	3-A	823	
1	4-A	823	
1	5-A	823	
1	6-A	823	
1	7-A	823	
1	8-A	823	
















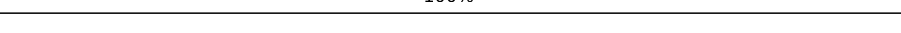
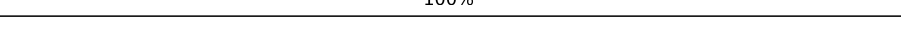
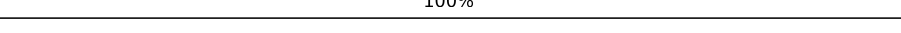
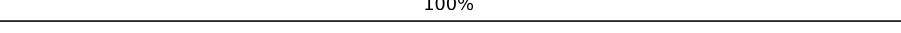
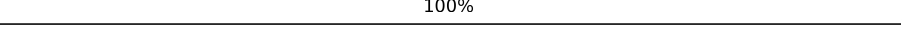
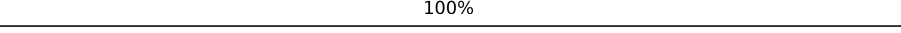
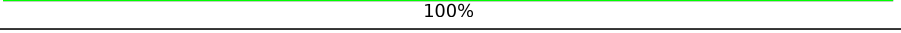
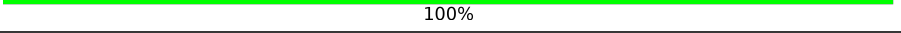
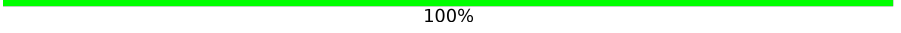
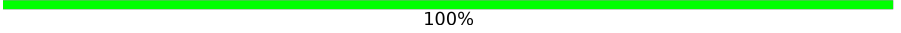
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Mol	Chain	Length	Quality of chain
1	9-A	823	
2	1-B	846	
2	10-B	846	
2	2-B	846	
2	3-B	846	
2	4-B	846	
2	5-B	846	
2	6-B	846	
2	7-B	846	
2	8-B	846	
2	9-B	846	
3	1-C	473	
3	1-D	473	
3	10-C	473	
3	10-D	473	
3	2-C	473	
3	2-D	473	
3	3-C	473	
3	3-D	473	
3	4-C	473	
3	4-D	473	
3	5-C	473	
3	5-D	473	
3	6-C	473	
3	6-D	473	


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Mol	Chain	Length	Quality of chain
3	7-C	473	 66%23%5%6%
3	7-D	473	 65%25%5%6%
3	8-C	473	 64%26%5%6%
3	8-D	473	 67%22%5%6%
3	9-C	473	 65%24%5%6%
3	9-D	473	 65%24%5%6%
4	1-E	44	 100%
4	1-F	44	 98%
4	10-E	44	 95%5%
4	10-F	44	 100%
4	2-E	44	 100%
4	2-F	44	 100%
4	3-E	44	 100%
4	3-F	44	 98%
4	4-E	44	 100%
4	4-F	44	 100%
4	5-E	44	 100%
4	5-F	44	 100%
4	6-E	44	 100%
4	6-F	44	 100%
4	7-E	44	 100%
4	7-F	44	 100%
4	8-E	44	 100%
4	8-F	44	 100%
4	9-E	44	 100%

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Mol	Chain	Length	Quality of chain
4	9-F	44	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 169380 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 SPINDLE POLE BODY COMPONENT SPC97.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	2-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	3-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	4-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	5-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	6-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	7-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	8-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	9-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		
1	10-A	575	Total	C	N	O	S	0	0
			4831	3110	806	889	26		

- Molecule 2 is a protein called SPINDLE POLE BODY COMPONENT SPC98.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	2-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	3-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	4-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	5-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	6-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	7-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	8-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	9-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		
2	10-B	565	Total	C	N	O	S	0	0
			4701	3058	775	853	15		

- Molecule 3 is a protein called TUBULIN GAMMA CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1-C	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	2-C	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	3-C	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	4-C	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	5-C	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	6-C	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	7-C	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	8-C	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	9-C	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	10-C	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	1-D	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	2-D	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	3-D	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	4-D	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	5-D	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	6-D	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	7-D	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	8-D	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	9-D	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		
3	10-D	445	Total	C	N	O	S	0	0
			3483	2179	591	696	17		

- Molecule 4 is a protein called SPINDLE POLE BODY COMPONENT 110.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	1-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	2-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	3-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	4-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	5-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	6-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	7-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	8-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	9-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	10-E	44	Total	C	N	O	0	0
			220	132	44	44		
4	1-F	44	Total	C	N	O	0	0
			220	132	44	44		
4	2-F	44	Total	C	N	O	0	0
			220	132	44	44		
4	3-F	44	Total	C	N	O	0	0
			220	132	44	44		

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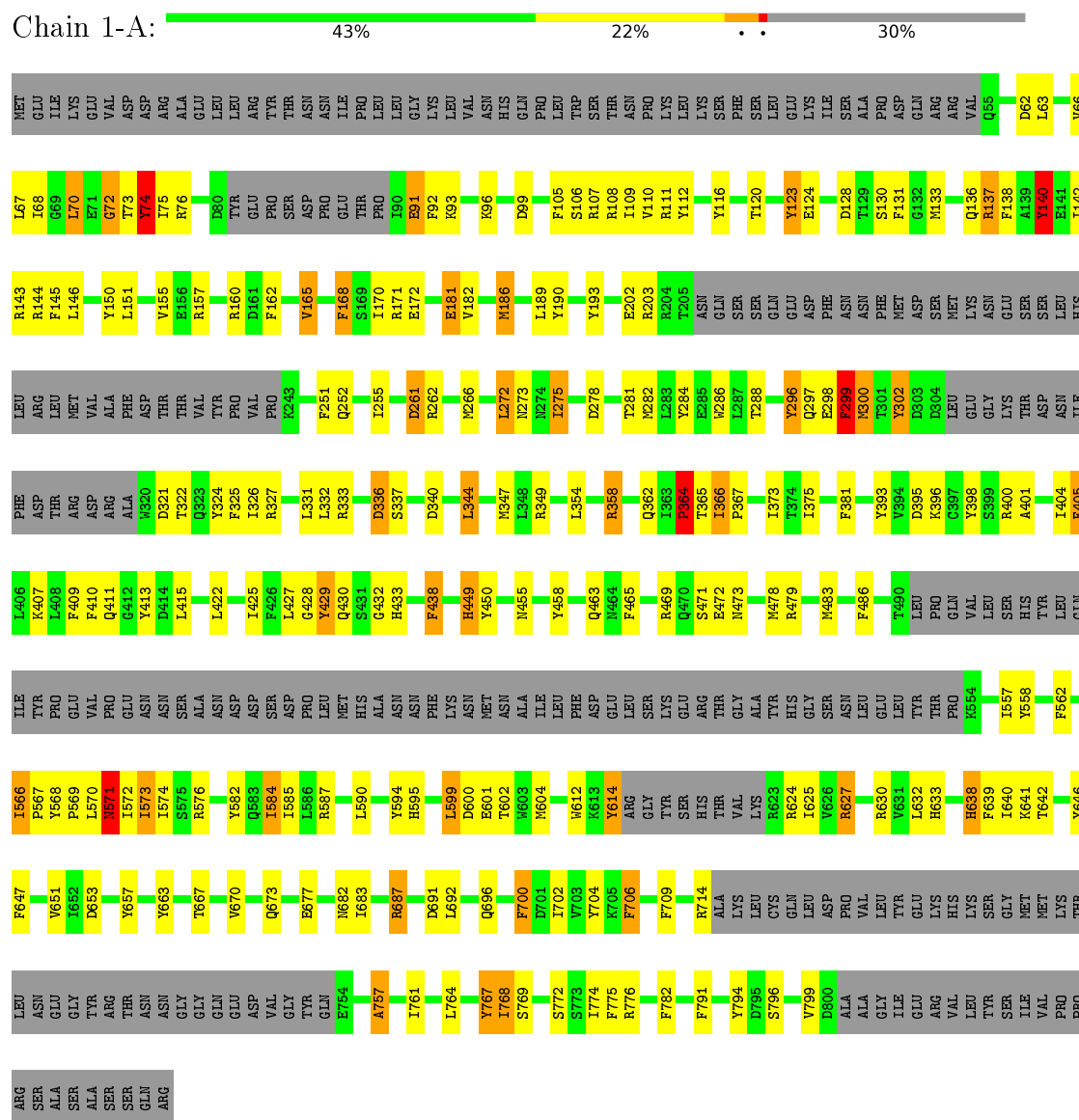
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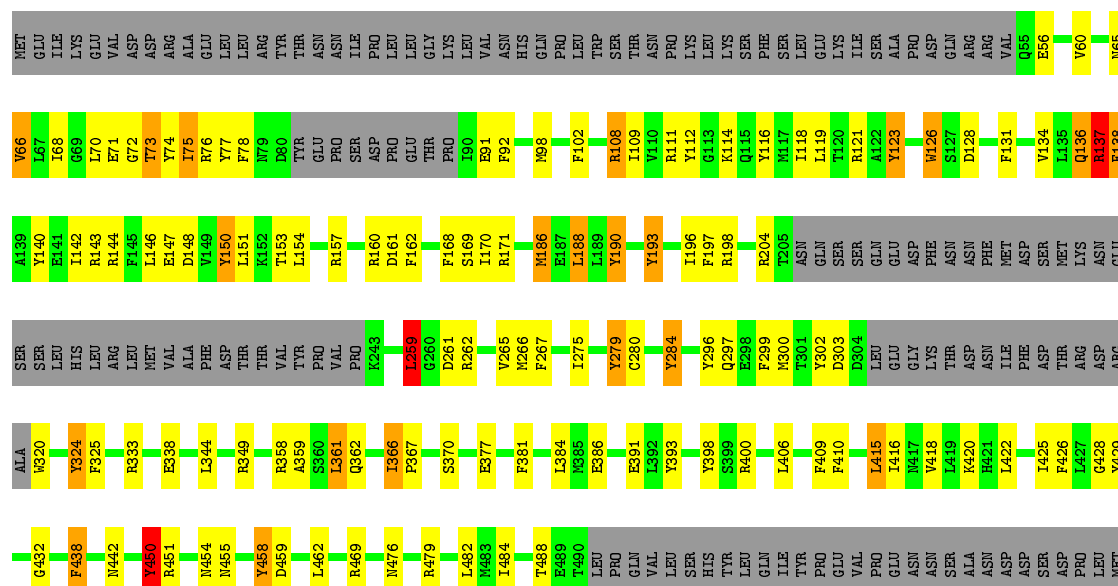
Mol	Chain	Residues	Atoms				AltConf	Trace
4	4-F	44	Total 220	C 132	N 44	O 44	0	0
4	5-F	44	Total 220	C 132	N 44	O 44	0	0
4	6-F	44	Total 220	C 132	N 44	O 44	0	0
4	7-F	44	Total 220	C 132	N 44	O 44	0	0
4	8-F	44	Total 220	C 132	N 44	O 44	0	0
4	9-F	44	Total 220	C 132	N 44	O 44	0	0
4	10-F	44	Total 220	C 132	N 44	O 44	0	0

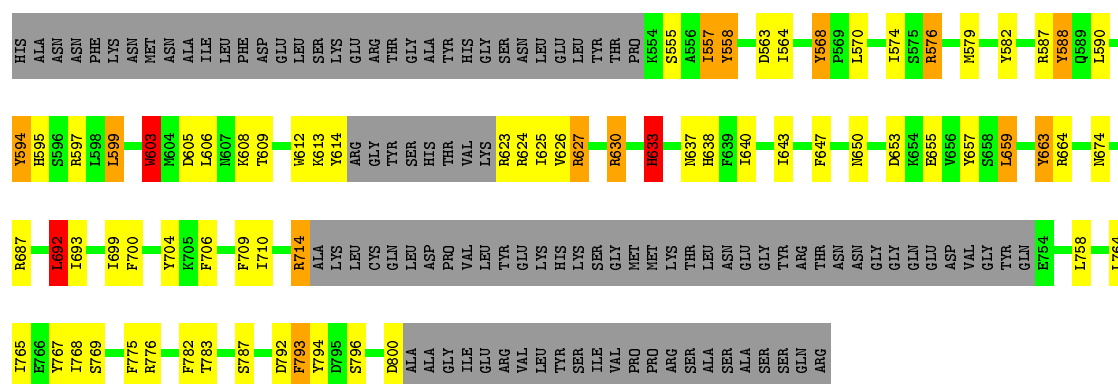
3 Residue-property plots

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: SPINDLE POLE BODY COMPONENT SPC97

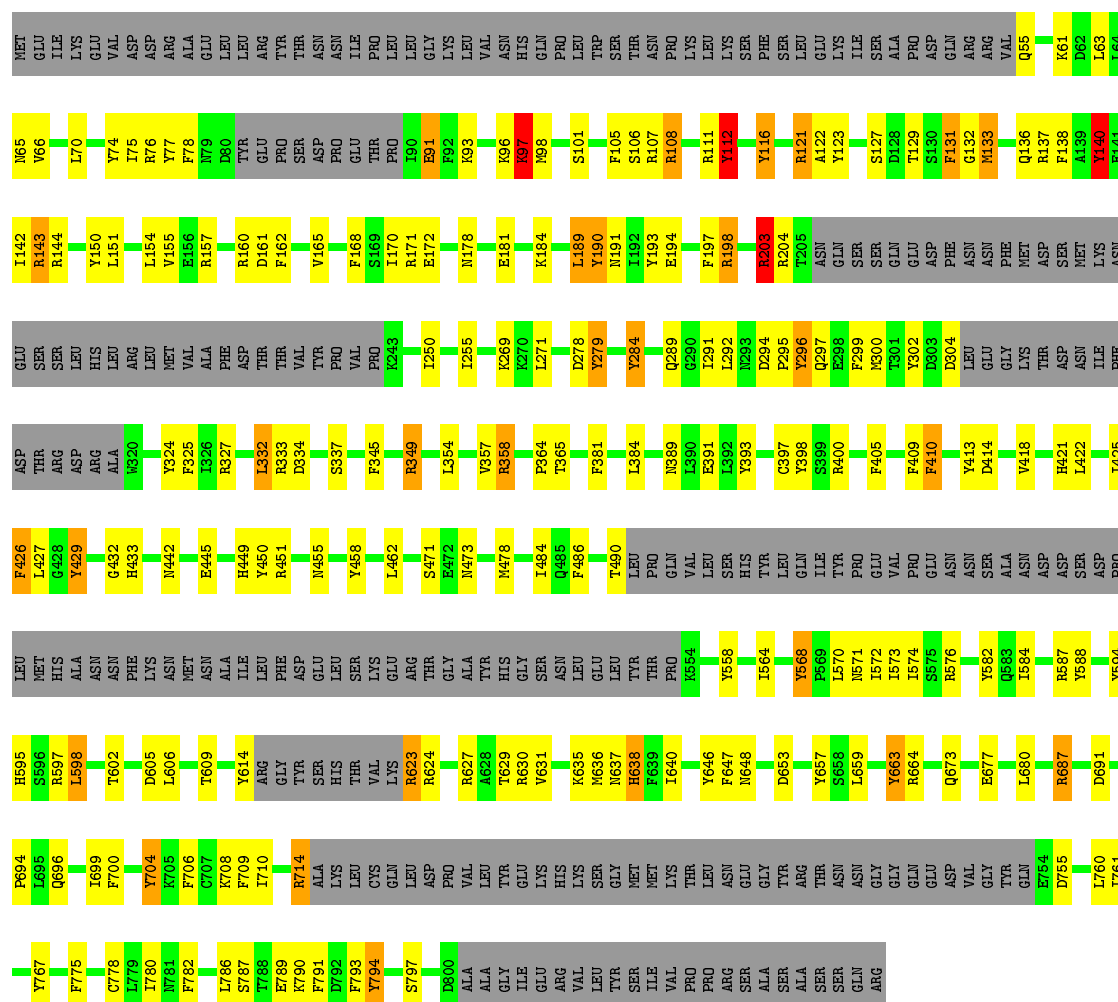






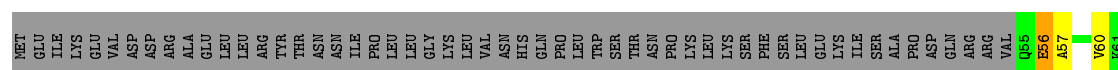
• Molecule 1: SPINDLE POLE BODY COMPONENT SPC97

Chain 7-A: 45% 21% 30%



• Molecule 1: SPINDLE POLE BODY COMPONENT SPC97

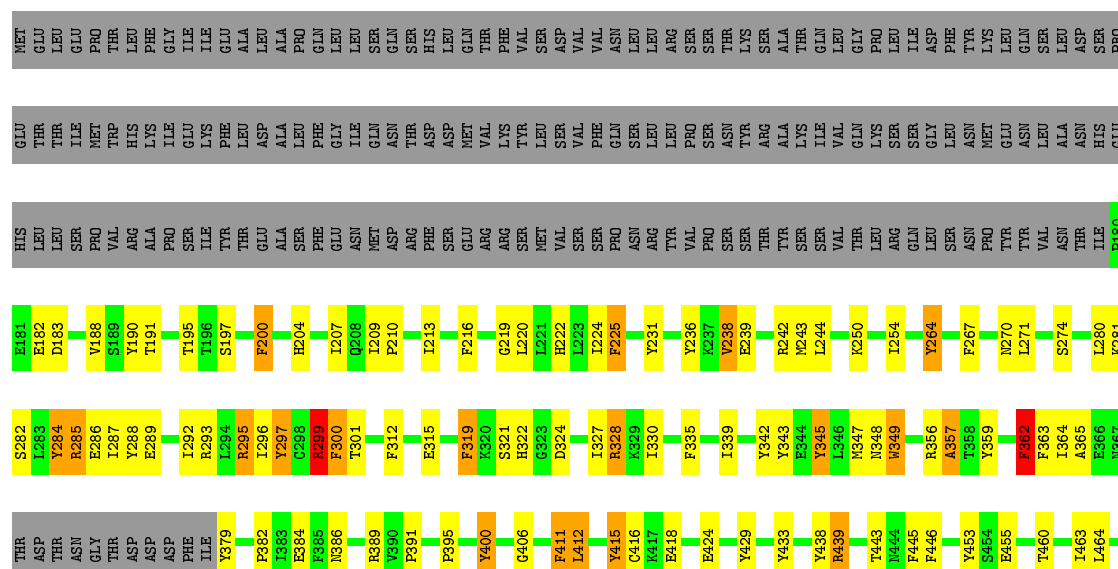
Chain 8-A: 45% 20% 30%

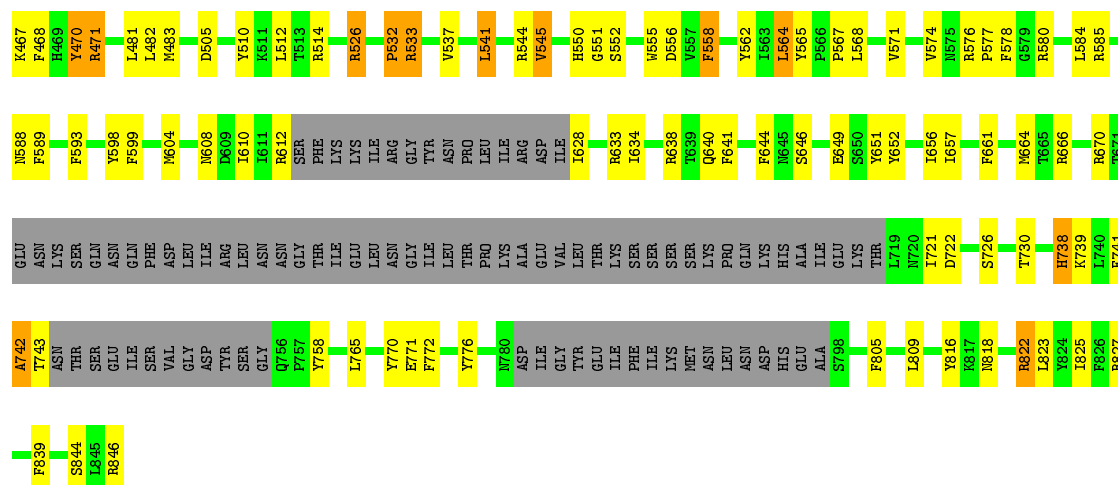






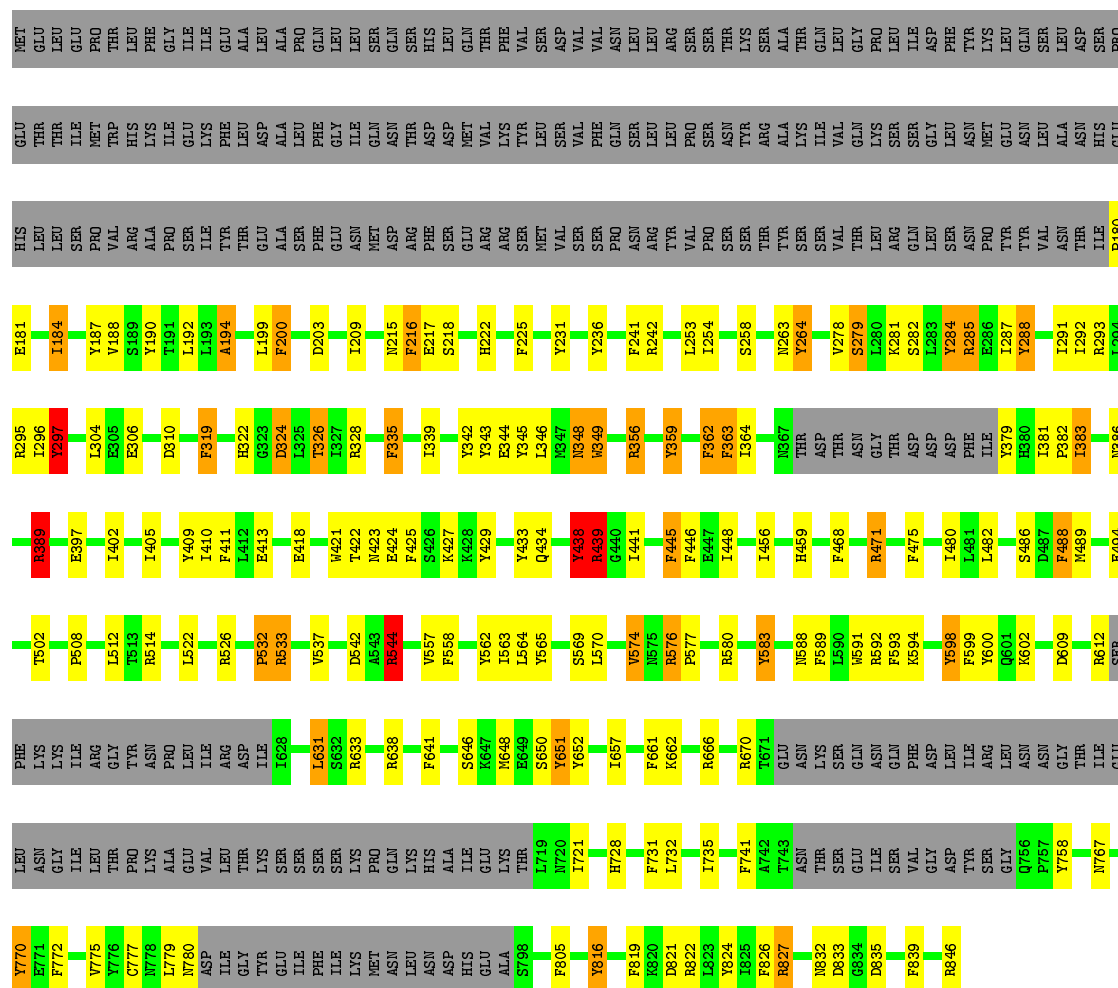
Chain 2-B:





• Molecule 2: SPINDLE POLE BODY COMPONENT SPC98

Chain 3-B: 46% 17% 33%



• Molecule 2: SPINDLE POLE BODY COMPONENT SPC98

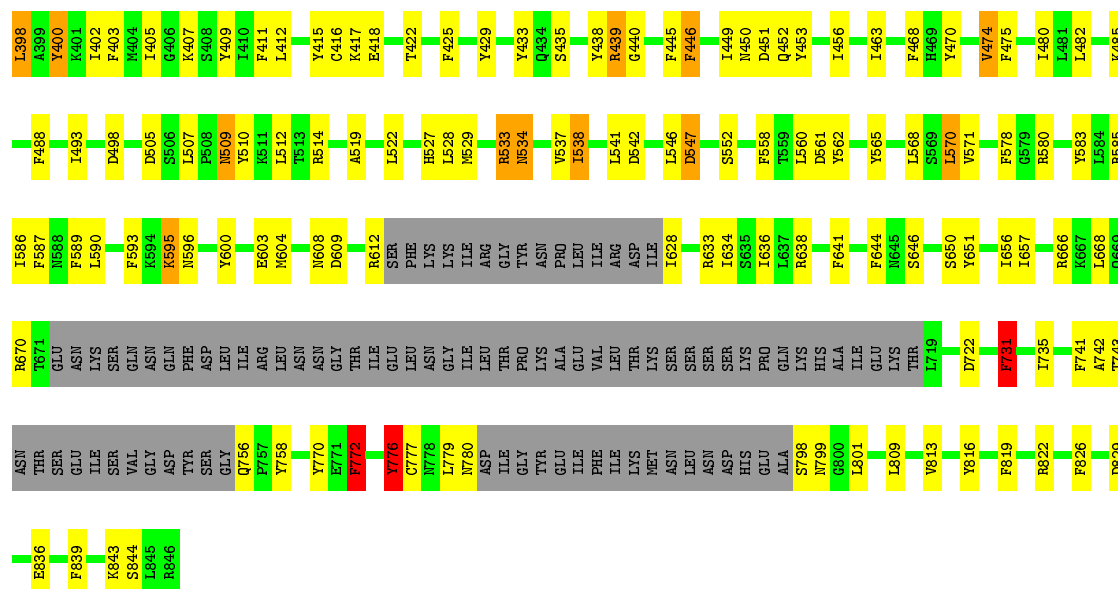
Chain 4-B: 44% 18% 33%

I812	H734	T665	R576	Y470	PHE	R285	HIS	GLU	MET
Y816	I735	T666	P577	B471	ILE	R286	LEU	THR	LEU
D821	K739	T671	R580	D472	Y379	Y288	SER	ILE	GLU
R822	L740	ASN	Y583	V473	N386	E289	PRO	MET	PRO
L823	F741	LVS	F583	F475	N387	T291	VAL	TRP	THR
Y824	A742	SER	L584	L480	E388	L292	ARG	HIS	LEU
L825	T743	GLN	R585	L481	R389	E295	ALA	LVS	PHE
F826	ASN	GLN	F586	L482	R390	L296	SER	ILE	GLY
R827	THR	GLN	F587	F483	P391	Y297	ILE	LVS	ILE
E837	SER	PHE	F588	Y483	A392	C298	THR	GLY	GLU
Y838	GLU	LEU	L590	F488	Y400	R299	LEU	LEU	ALA
R846	ILE	ASP	W591	K401	K401	F300	GLU	ASP	LEU
	SER	ILE	R592	L493	I402	E303	ALA	ALA	ALA
	VAL	ARG	F593	L507	I405	L304	SER	LEU	PRO
	GLY	LEU	R594	P508	Y409	E308	PHE	GLY	GLN
	ASP	ASN	K595		Y410	S218	ASN	ILE	LEU
	TYR	ASN			F411	E217	MET	GLN	SER
	SER	GLY	Y598	B514	L412	G219	ASP	ASN	GLN
	GLY	THR		W515		L220	ASP	THR	SER
	ILE	ILE	D609	L516		L221	ANG	THR	SER
	GLU	GLU	L610	L522	Y415	R222	PHE	ASP	LEU
	LEU	LEU	R612	S523		E322	SER	ASP	HIS
	ASN	ASN			E418	L223	GLU	MET	GLN
L765	GLY	GLY	SER		V419	G323	ARG	VAL	THR
L766	ILE	ILE	PHE	B526	Q434	D324	ARG	LVS	PHE
	LEU	LEU	LVS	H527	Q420	L325	SER	THR	VAL
Y770	THR	THR	LVS	L528	W421	A227	MET	LEU	SER
F771	PRO	PRO	ILE	W529	E424	R328	VAL	SER	ASP
F772	LVS	LVS	ARG			E328	SER	VAL	VAL
Y776	ALA	ALA	GLY	B533	F425	F335	SER	PHE	VAL
	GLU	GLU	TYR		S426	R237	PRO	GLN	ASN
	VAL	VAL	ASN	L538	K427	Y342	ASN	SER	LEU
H780	LEU	LEU	PRO	W539	R428		ANG	LEU	LEU
ASP	THR	THR	ILE	G540		Y345	TYR	LEU	ARG
ILE	LVS	LVS	ILE	L541	Y433	L346	VAL	PRO	SER
GLY	SER	SER	ARG		Q434	R347	PRO	SER	SER
TYR	SER	SER	ILE	B544		N348	ASN	THR	THR
GLU	SER	SER	ASP	W545	Y438	L349	SER	LVS	LVS
ILE	SER	SER	ILE	L546	R439	L350	THR	ARG	SER
PHE	LVS	LVS	L628			T351	ALA	ALA	ALA
ILE	PRO	PRO	R633	B550	F445	Y264	TYR	LVS	THR
LVS	GLN	GLN	L634		F446	L355	SER	LVS	THR
GLN	GLN	GLN	L635	W555	F447	R356	VAL	ILE	LEU
MET	LVS	LVS	S635	D556	I448		THR	VAL	GLN
ASN	HIS	HIS	I636	B557		Y359	LEU	GLN	GLY
LEU	ALA	ALA	L637	W557	Y453	E269	SER	LVS	PRO
ASN	ILE	ILE	R638	F558		N270	LEU	SER	LEU
ASP	GLU	GLU			S454		GLN	ILE	ILE
ASP	LVS	LVS	F641	Y562	E455	F363	LEU	GLY	ASP
HIS	LVS	LVS	F644	J563	I456		SER	LEU	PHE
GLU	THR	THR		L564			ASN	LEU	THR
ALA	L719	L719	F644	W565	H459	THR	ASN	ASN	ASN
	W720	W720	Y652	Y565	ASP	ASP	PRO	MET	LVS
	I721	I721			THR	THR	TYR	GLN	LEU
L801	H728	H728		L568	N460	GLY	VAL	GLN	LEU
F805			G655	W569	N461	THR	VAL	LEU	SER
			I656	L570	Q462		K281	ALA	LEU
	F731	F731	I657		I463	ASP	K282	ASN	ASP
N808	L732	L732	I657	W574	F468	ASP	L283	HIS	GLU
	T733	T733	M664	B575	H469	ASP	Y284	ILE	PRO

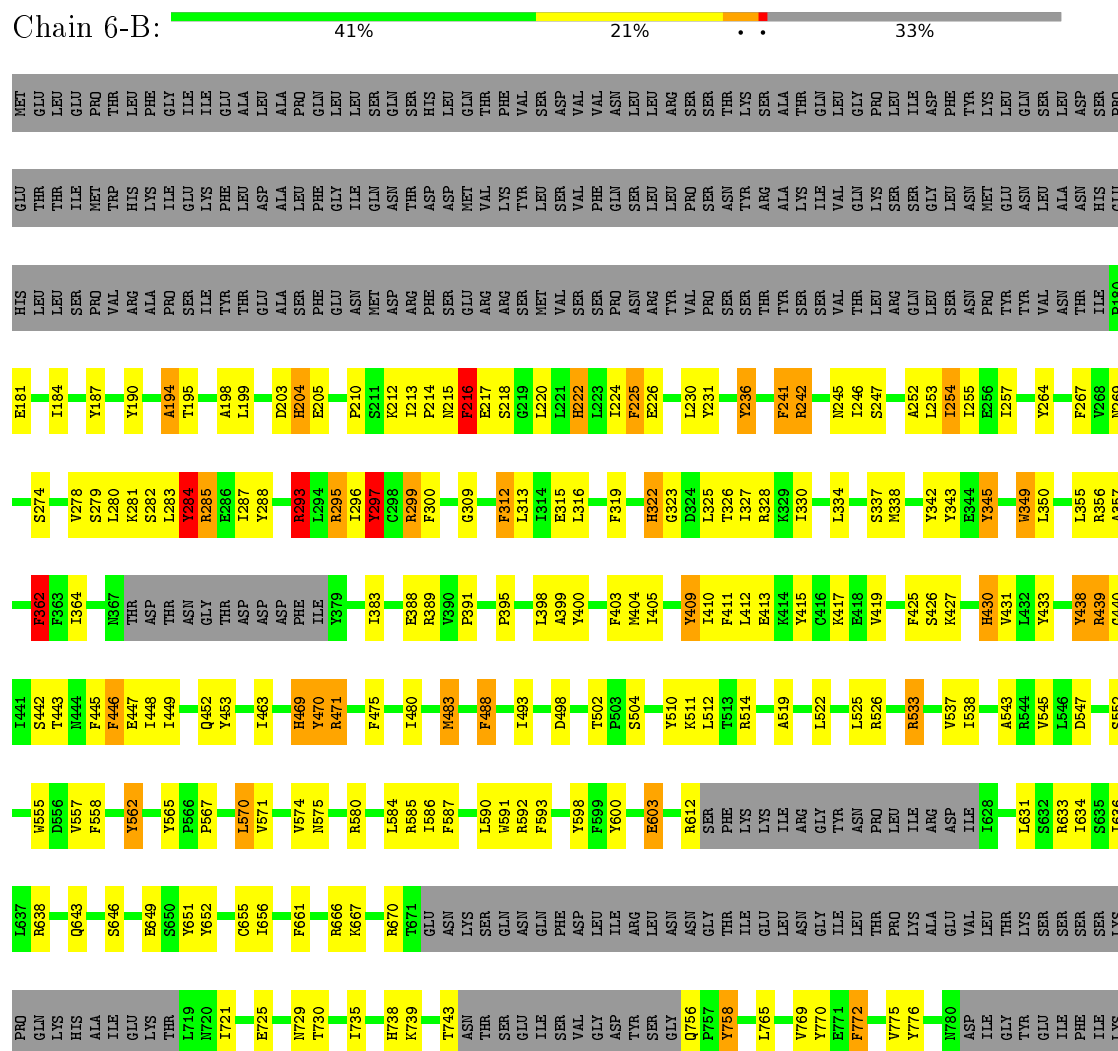
• Molecule 2: SPINDLE POLE BODY COMPONENT SPC98

Chain 5-B: 44% 20% 33%

R299	F300	T301	H302	T303	D310	T311	T314	E315	F319	G323	D324	T327	R328	T329	T339	Y342	Y343	E322	Y345	R356	A357	Y358	Y359	F363	L364	R367	T378	ASP	T379	ASN	GLY	T380	ASP	ASP	PHE	ILE	Y379	H380	L381	P382	F385	R389	F393	L394	P395	C298	P180										
D183			K186	Y187	V188	S189	Y190	T191		T195		F202		Q206	SER	PHE	GLY	P210	ASN	ASP	ARG	L220	L221	E222	L223	T224	F225		Y231		L234	F241	R242		L254	T257		Y264	F267		Y272		L280		Y284	R285		Y288	E289		R293	L294	R295	L296	Y297	C298	
HIS	LEU	LEU	SER	PRO	VAL	ARG	ALA	PRO	SER	ILE	TYR	THR	GLU	ALA	SER	PHE	GLY	ASN	MET	ASP	ARG	PHE	SER	GLU	ARG	SER	MET	VAL	SER	SER	SER	PHE	GLN	SER	LEU	LEU	VAL	THR	LEU	ARG	GLN	SER	LEU	LEU	GLY	ASP	PHE	ASN	PRO	TYR	THR	VAL	ASN	THR	ILE		
GLU	THR	THR	ILE	THR	TRP	LEU	LYS	ILE	GLU	PHE	LEU	ASP	ALA	LEU	LEU	PHE	GLY	ILE	GLN	ASN	THR	ASP	ASP	MET	GLN	THR	LYS	TYR	LEU	SER	ASP	PHE	VAL	VAL	GLN	SER	LEU	LEU	ARG	ALA	LYS	ILE	VAL	GLN	GLY	PRO	LEU	ILE	GLY	ASP	ASN	ALA	LEU	SER	GLU	GLY	HIS



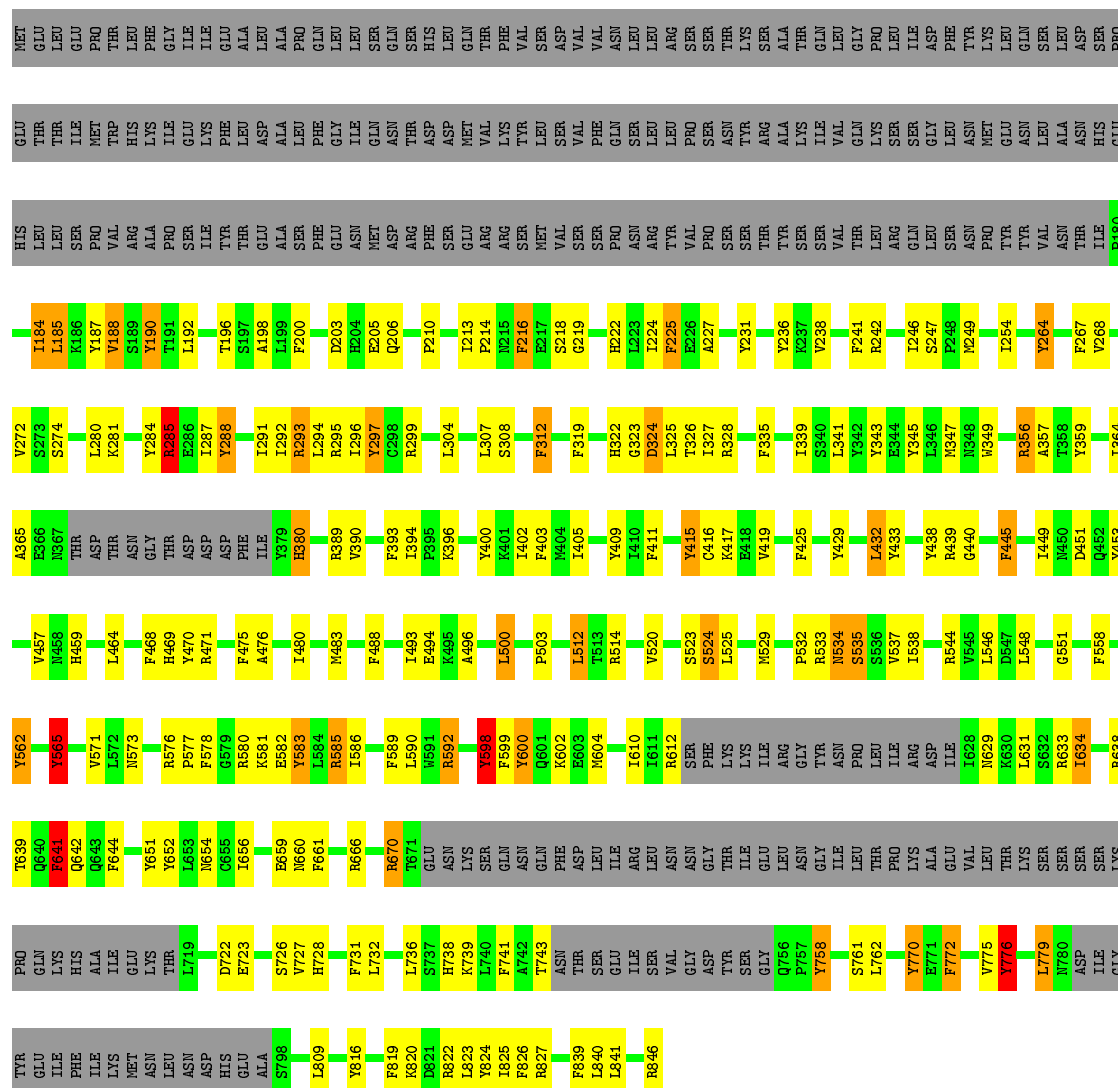
• Molecule 2: SPINDLE POLE BODY COMPONENT SPC98





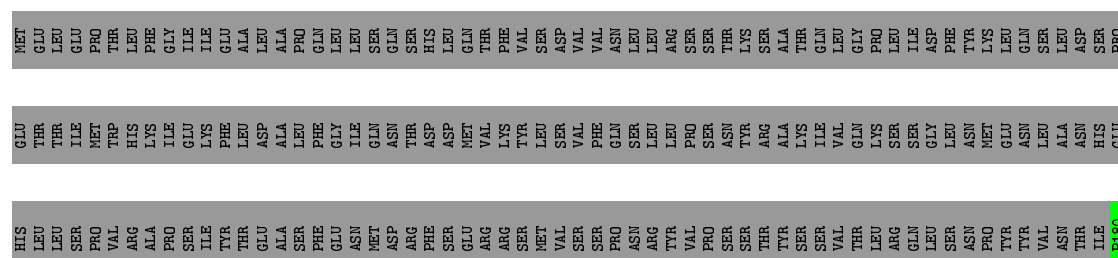
• Molecule 2: SPINDLE POLE BODY COMPONENT SPC98

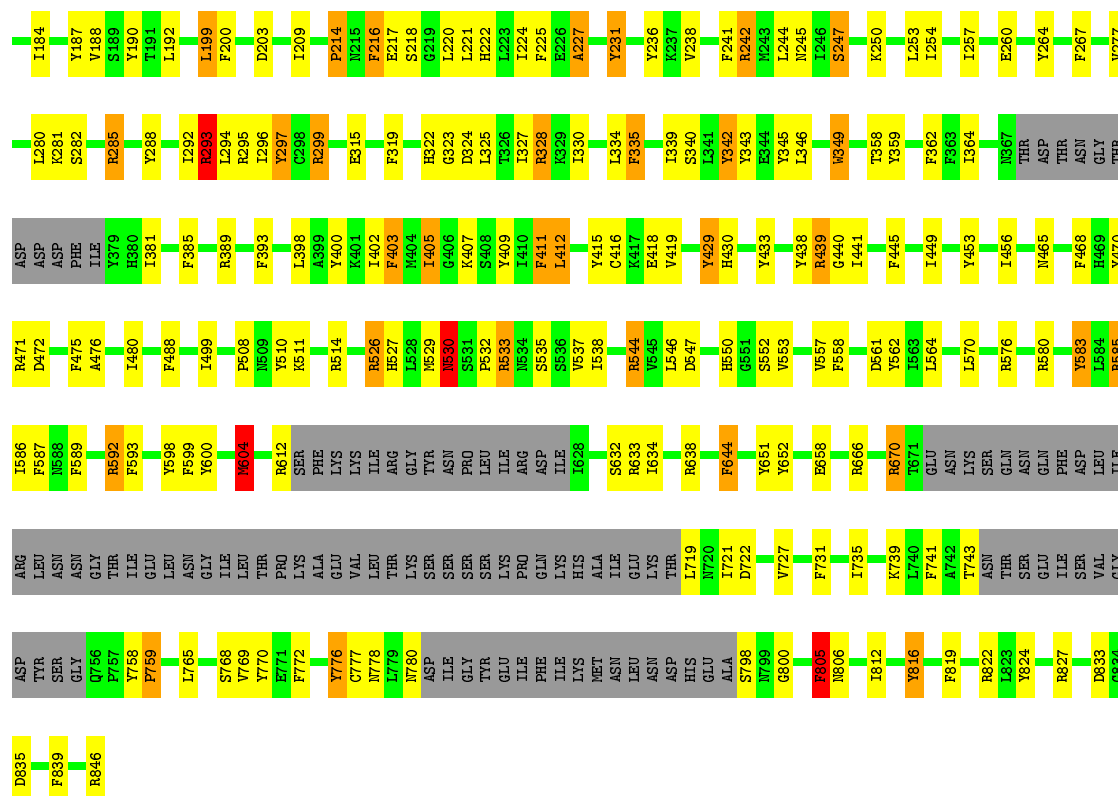
Chain 7-B: 42% 20% 33%



• Molecule 2: SPINDLE POLE BODY COMPONENT SPC98

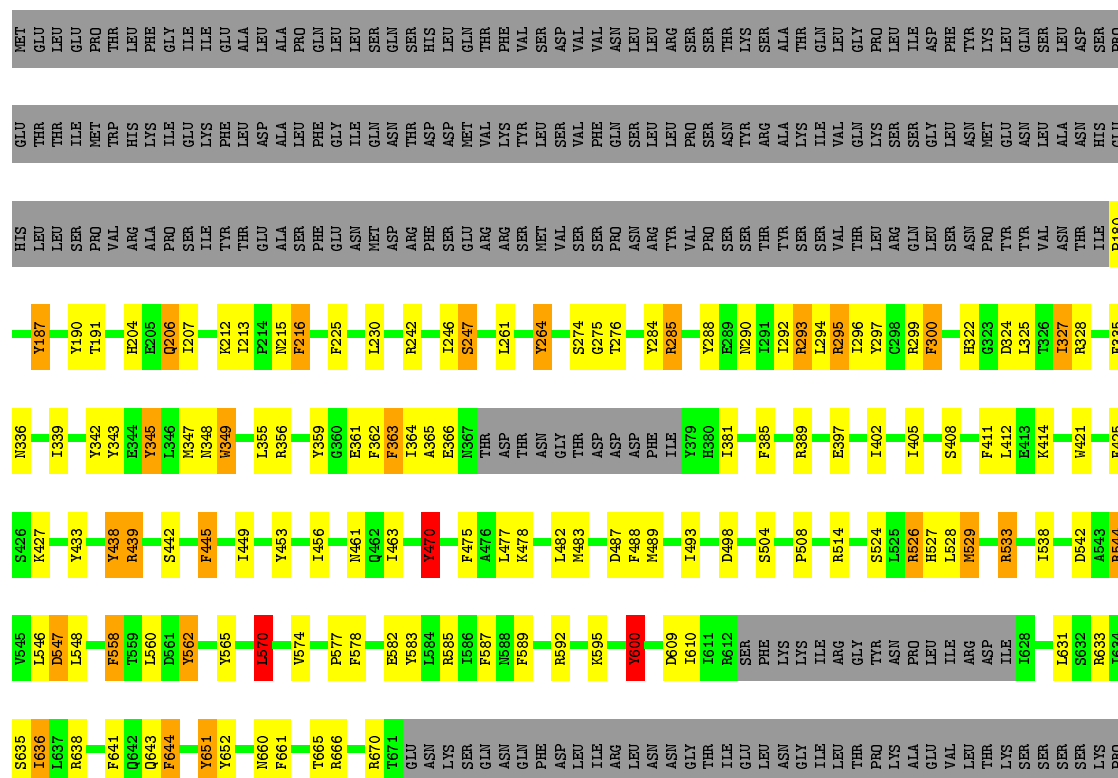
Chain 8-B: 44% 18% 33%

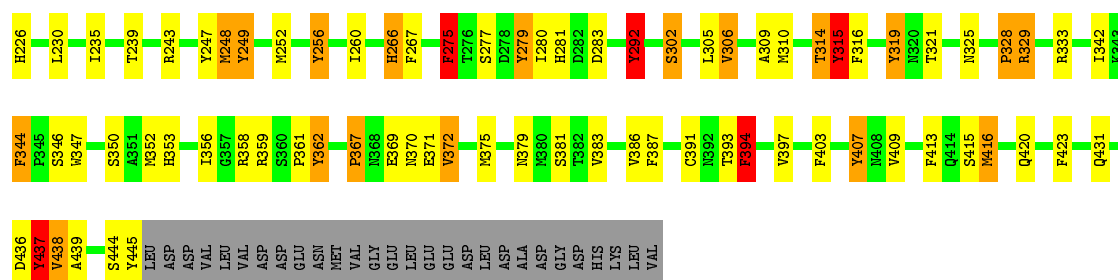




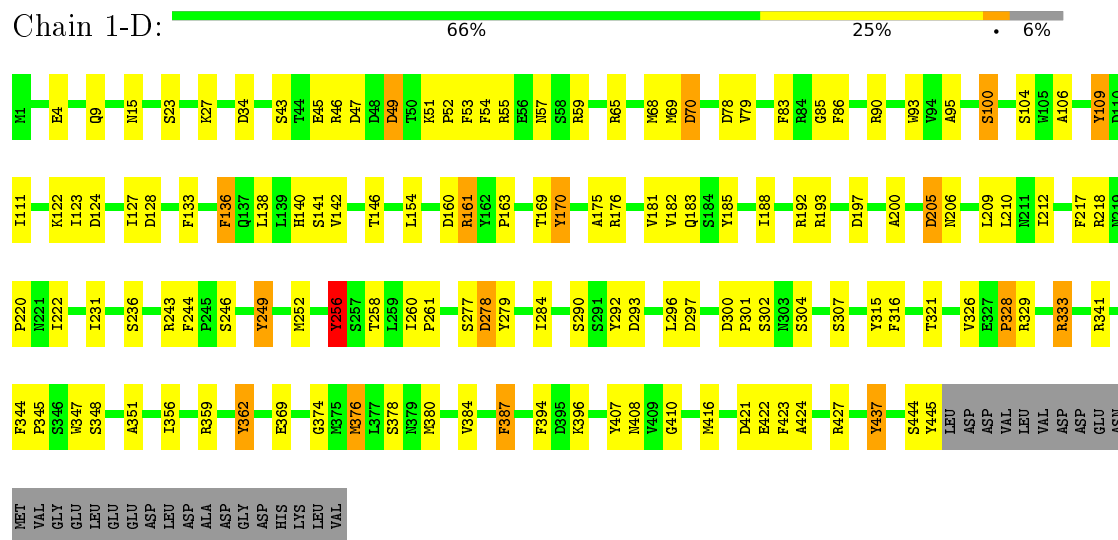
• Molecule 2: SPINDLE POLE BODY COMPONENT SPC98

Chain 9-B: 47% 16% 33%

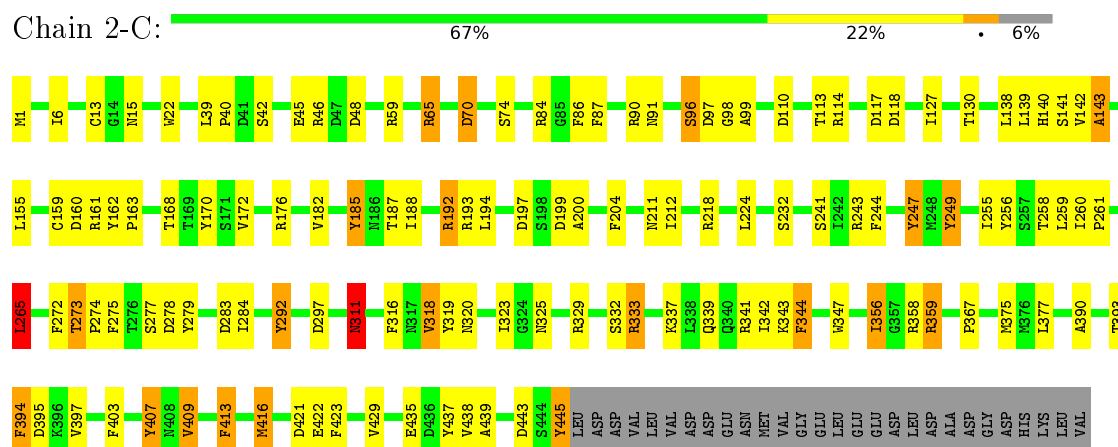




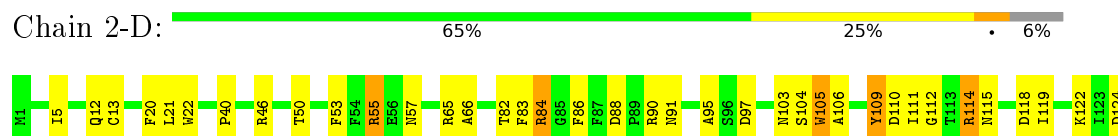
• Molecule 3: TUBULIN GAMMA CHAIN




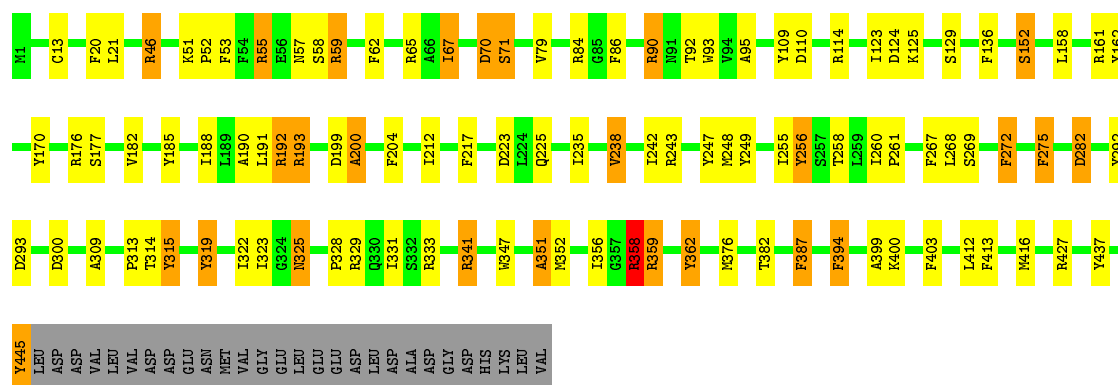
• Molecule 3: TUBULIN GAMMA CHAIN



• Molecule 3: TUBULIN GAMMA CHAIN

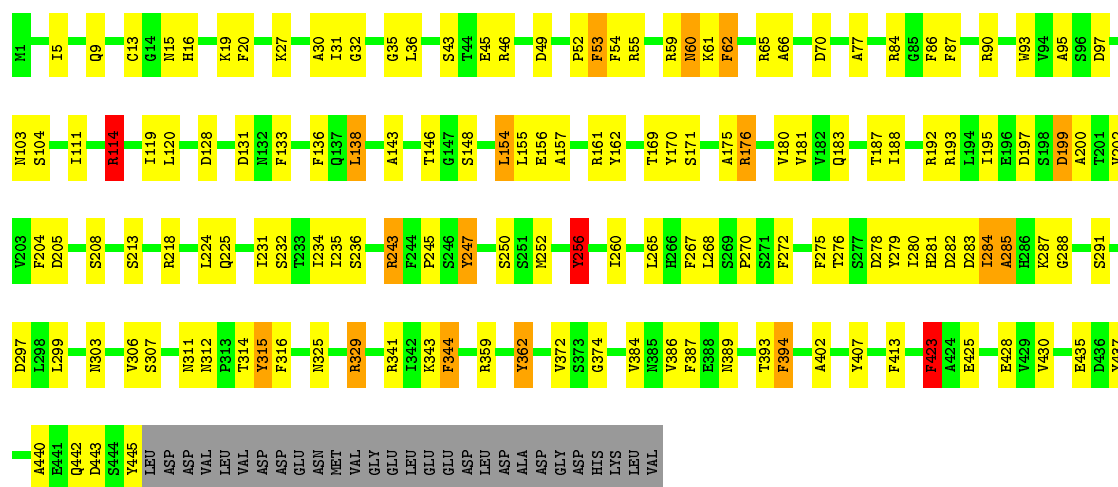


Chain 4-C:  72% 17% 5% 6%



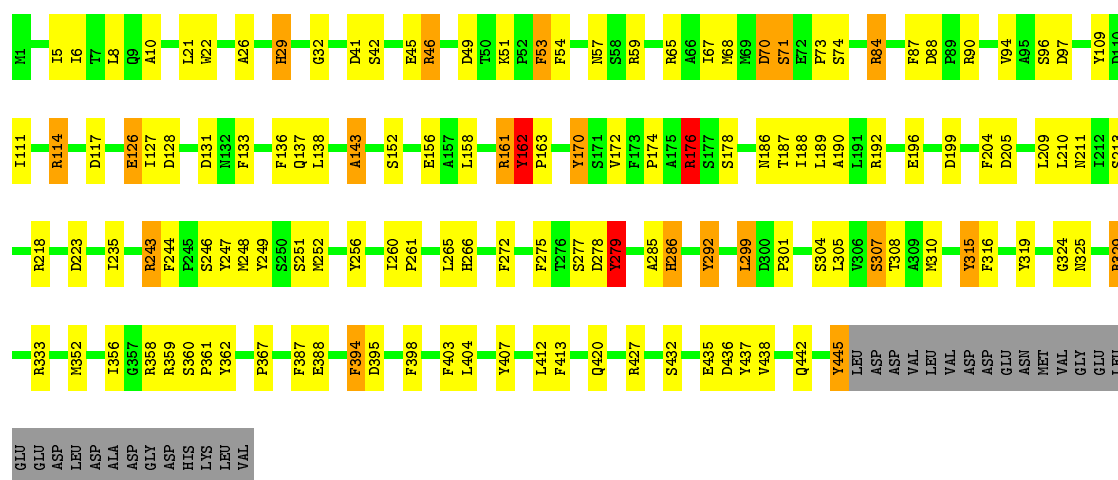
• Molecule 3: TUBULIN GAMMA CHAIN

Chain 4-D:  63% 27% 6%

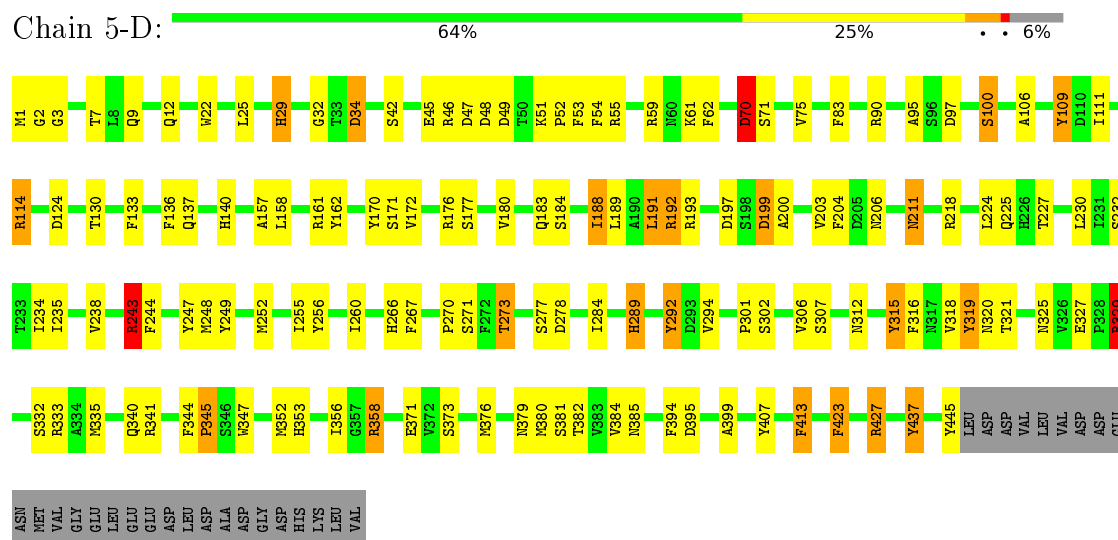


• Molecule 3: TUBULIN GAMMA CHAIN

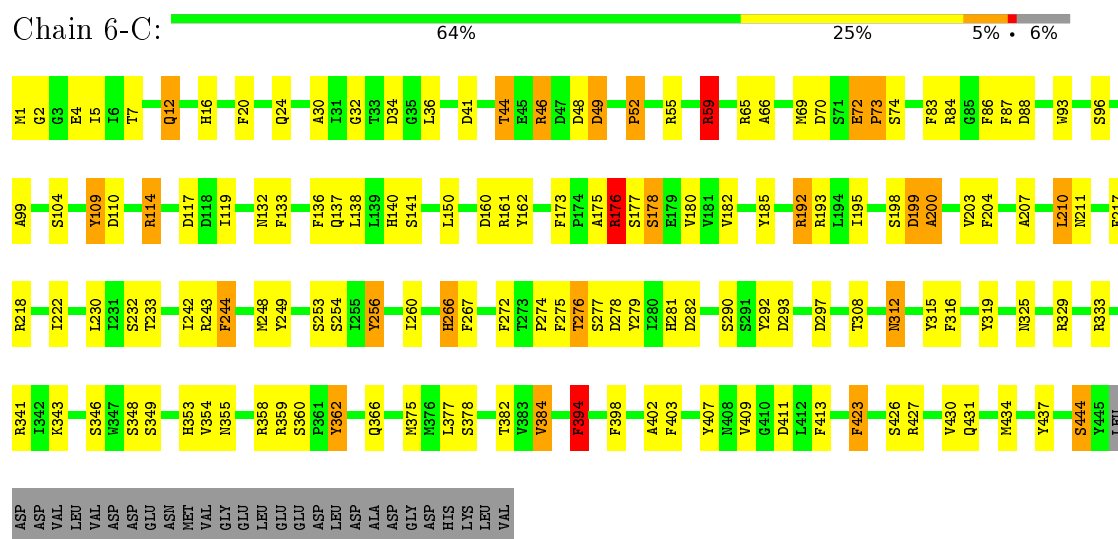
Chain 5-C:  65% 24% 6%



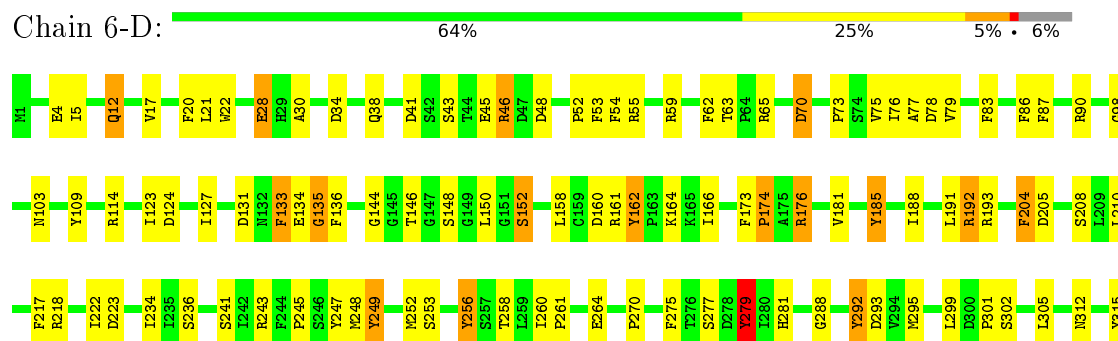
- Molecule 3: TUBULIN GAMMA CHAIN

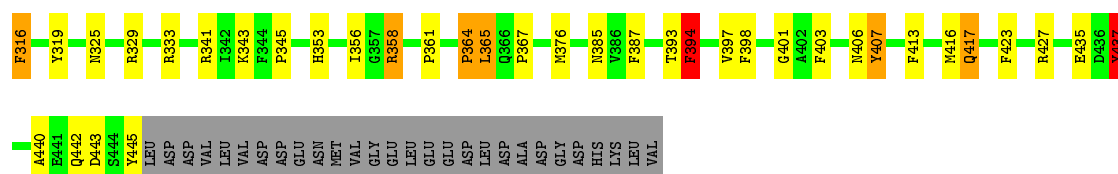


- Molecule 3: TUBULIN GAMMA CHAIN



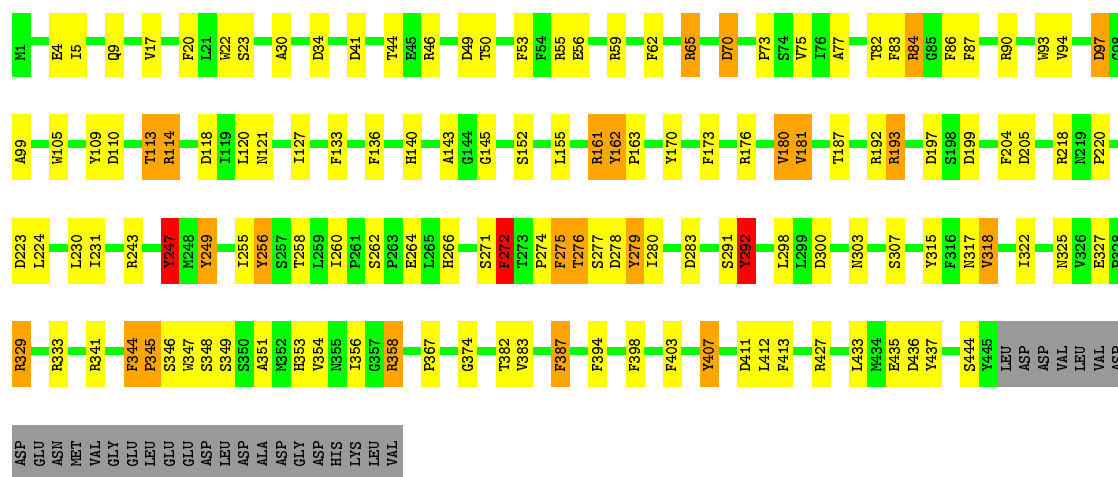
- Molecule 3: TUBULIN GAMMA CHAIN





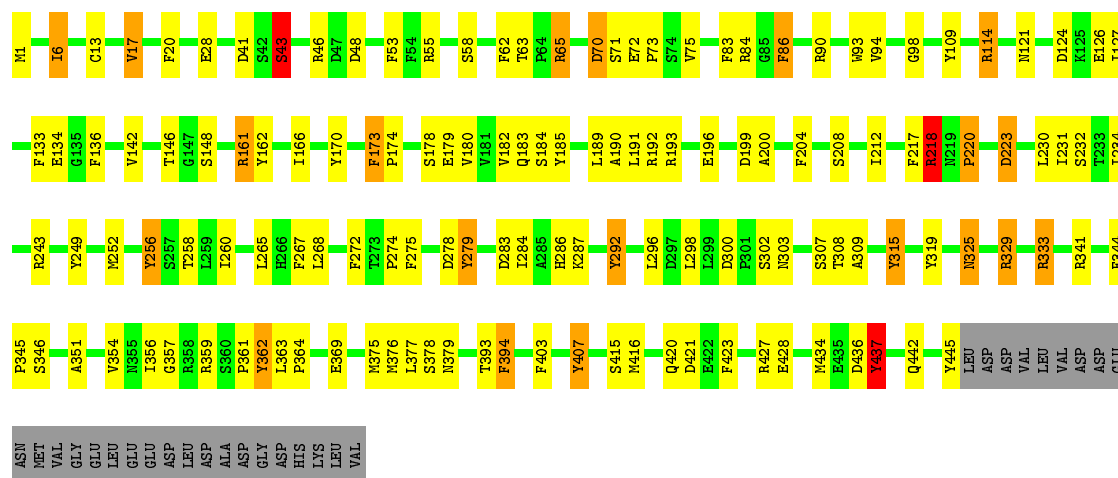
• Molecule 3: TUBULIN GAMMA CHAIN

Chain 7-C: 66% 23% 5% • 6%



• Molecule 3: TUBULIN GAMMA CHAIN

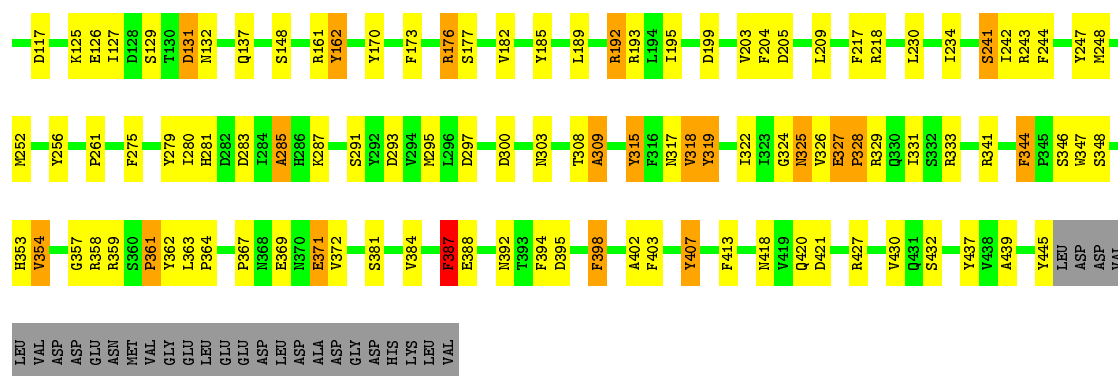
Chain 7-D: 65% 25% • • 6%



• Molecule 3: TUBULIN GAMMA CHAIN

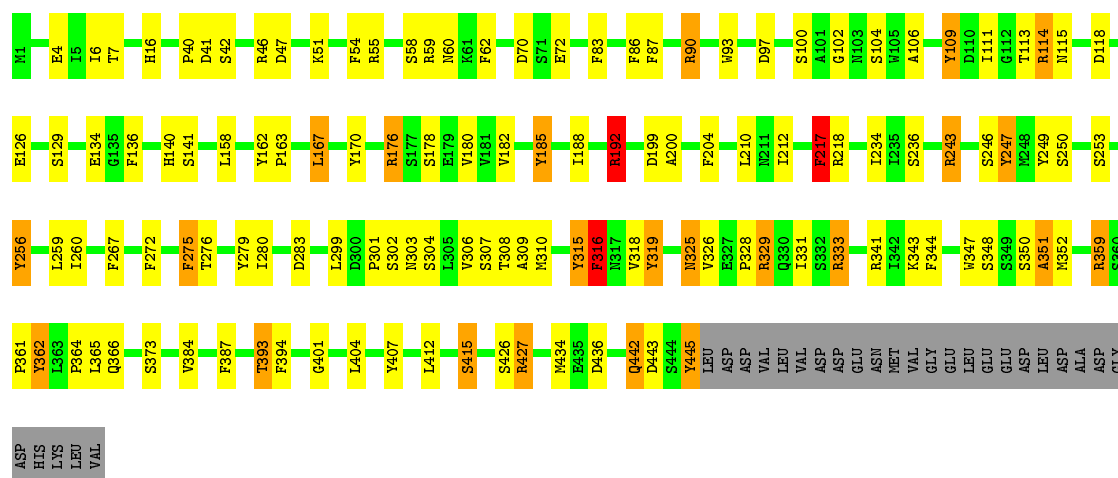
Chain 8-C: 64% 26% • 6%





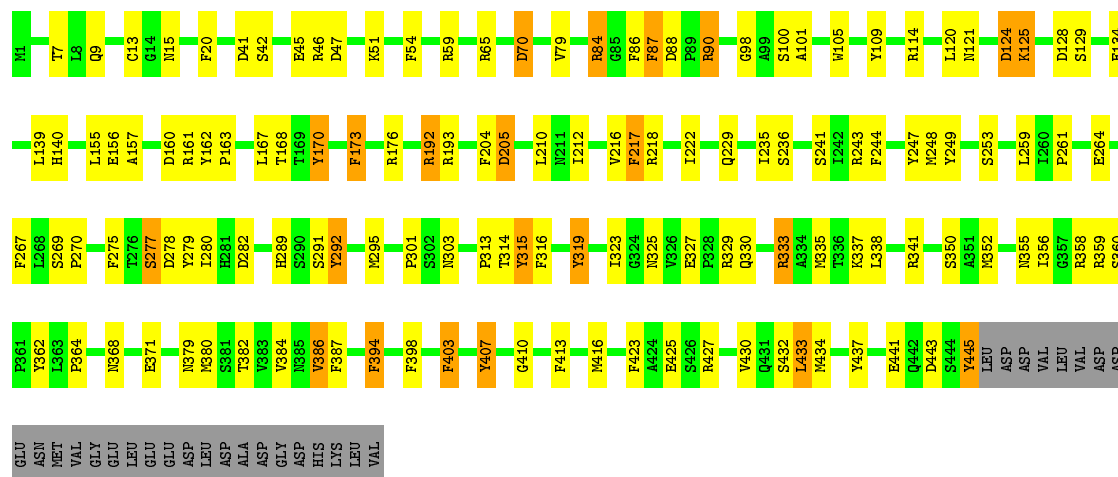
• Molecule 3: TUBULIN GAMMA CHAIN

Chain 8-D: 67% 22% 5% 6%

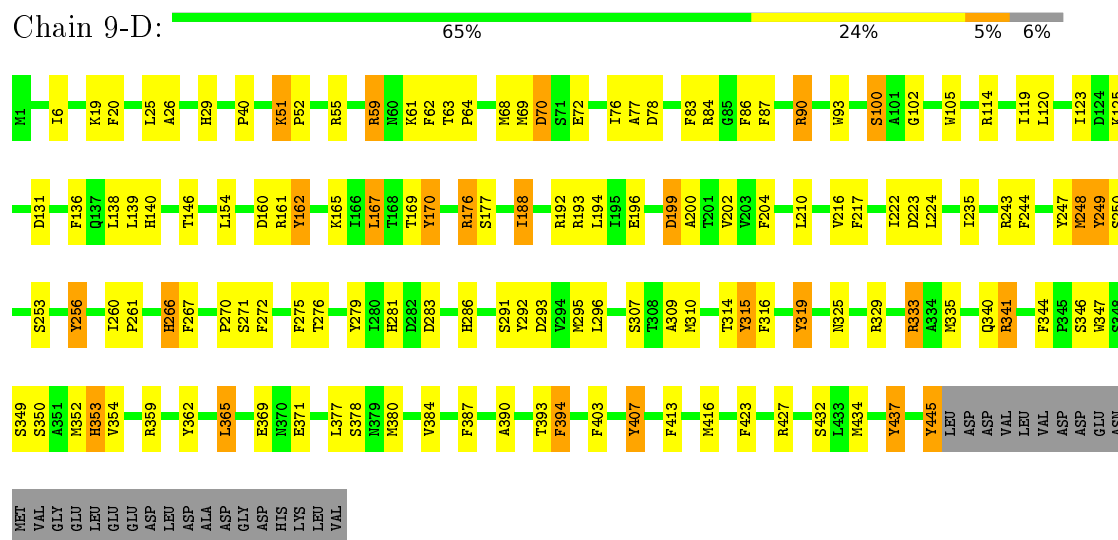


• Molecule 3: TUBULIN GAMMA CHAIN

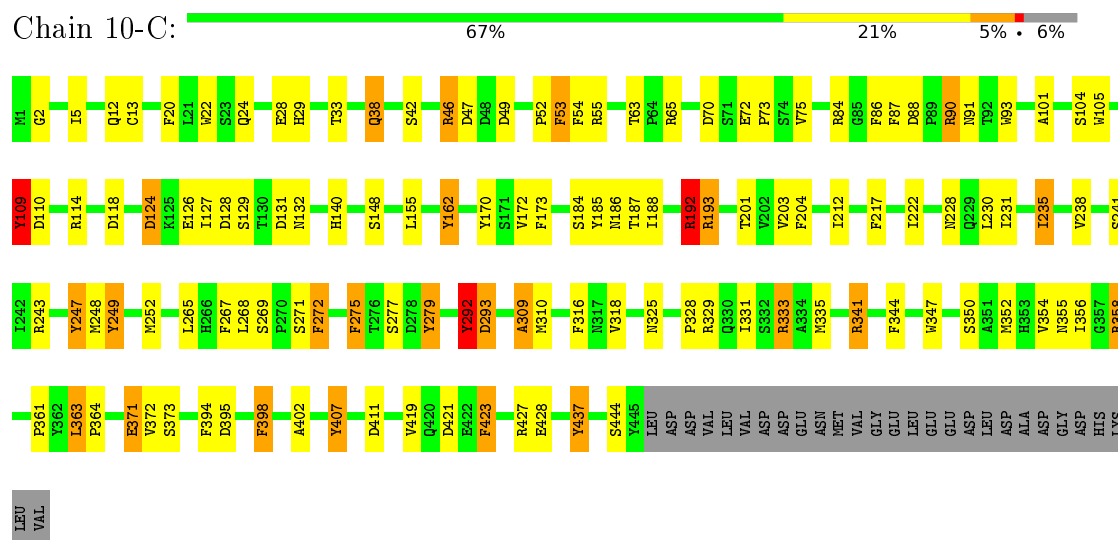
Chain 9-C: 65% 24% 5% 6%



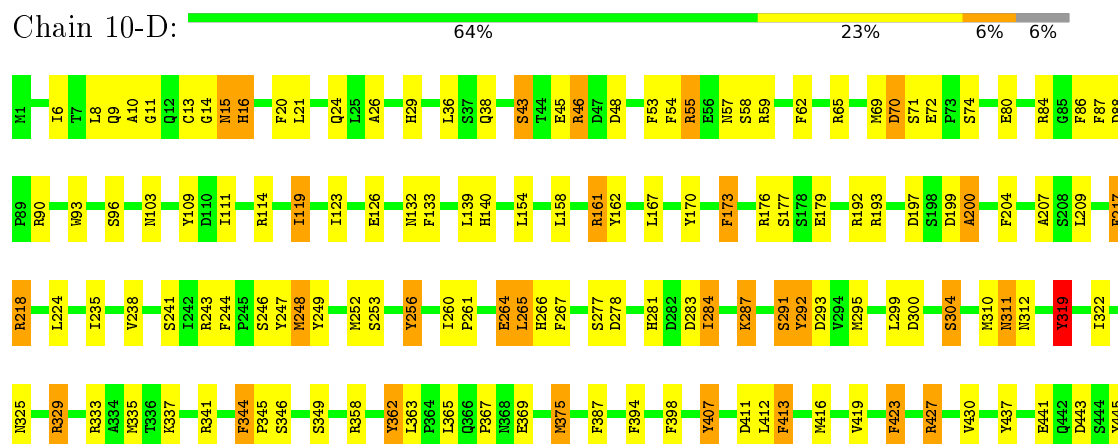
• Molecule 3: TUBULIN GAMMA CHAIN



• Molecule 3: TUBULIN GAMMA CHAIN



• Molecule 3: TUBULIN GAMMA CHAIN



LEU ASP ASP VAL LEU VAL ASP ASP GLU ASN MET VAL GLY LEU LEU GLU ASP LEU ASP ALA ASP GLY ASP HIS LEU VAL

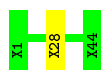
- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 1-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 1-F:  98%

 X1 X28 X44

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 2-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 2-F:  100%

There are no outlier residues recorded for this chain.

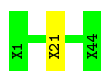
- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 3-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 3-F:  98%

 X1 X21 X44

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 4-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 4-F:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 5-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 5-F:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 6-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 6-F:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 7-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 7-F:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 8-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 8-F:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 9-E:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 9-F:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 10-E:  95% 5%



- Molecule 4: SPINDLE POLE BODY COMPONENT 110

Chain 10-F:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	WHOLE MICROGRAPH	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	60000	Depositor
Image detector	TVIPS TEMCAM-F816	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	1-A	1.71	38/4917 (0.8%)	2.02	155/6616 (2.3%)
1	10-A	1.75	47/4917 (1.0%)	2.05	150/6616 (2.3%)
1	2-A	1.77	53/4917 (1.1%)	1.95	137/6616 (2.1%)
1	3-A	1.69	39/4917 (0.8%)	1.95	144/6616 (2.2%)
1	4-A	1.75	55/4917 (1.1%)	1.99	142/6616 (2.1%)
1	5-A	1.73	45/4917 (0.9%)	1.96	127/6616 (1.9%)
1	6-A	1.77	59/4917 (1.2%)	1.99	132/6616 (2.0%)
1	7-A	1.74	42/4917 (0.9%)	2.03	143/6616 (2.2%)
1	8-A	1.75	45/4917 (0.9%)	1.99	130/6616 (2.0%)
1	9-A	1.72	47/4917 (1.0%)	1.97	132/6616 (2.0%)
2	1-B	1.74	49/4803 (1.0%)	2.00	139/6481 (2.1%)
2	10-B	1.74	46/4803 (1.0%)	1.93	132/6481 (2.0%)
2	2-B	1.76	53/4803 (1.1%)	1.93	115/6481 (1.8%)
2	3-B	1.74	54/4803 (1.1%)	1.98	129/6481 (2.0%)
2	4-B	1.74	50/4803 (1.0%)	1.93	123/6481 (1.9%)
2	5-B	1.75	44/4803 (0.9%)	2.01	137/6481 (2.1%)
2	6-B	1.75	50/4803 (1.0%)	2.01	138/6481 (2.1%)
2	7-B	1.75	49/4803 (1.0%)	1.94	130/6481 (2.0%)
2	8-B	1.73	40/4803 (0.8%)	1.96	118/6481 (1.8%)
2	9-B	1.72	33/4803 (0.7%)	1.98	134/6481 (2.1%)
3	1-C	1.71	22/3558 (0.6%)	1.96	95/4831 (2.0%)
3	1-D	1.72	36/3558 (1.0%)	1.93	99/4831 (2.0%)
3	10-C	1.74	32/3558 (0.9%)	1.98	100/4831 (2.1%)
3	10-D	1.74	35/3558 (1.0%)	1.93	90/4831 (1.9%)
3	2-C	1.72	23/3558 (0.6%)	2.00	104/4831 (2.2%)
3	2-D	1.70	30/3558 (0.8%)	1.96	89/4831 (1.8%)
3	3-C	1.70	30/3558 (0.8%)	1.94	96/4831 (2.0%)
3	3-D	1.73	25/3558 (0.7%)	1.92	81/4831 (1.7%)
3	4-C	1.71	27/3558 (0.8%)	2.00	83/4831 (1.7%)
3	4-D	1.76	35/3558 (1.0%)	2.02	110/4831 (2.3%)
3	5-C	1.74	34/3558 (1.0%)	1.95	92/4831 (1.9%)
3	5-D	1.69	23/3558 (0.6%)	1.89	72/4831 (1.5%)
3	6-C	1.77	42/3558 (1.2%)	1.95	93/4831 (1.9%)
3	6-D	1.72	36/3558 (1.0%)	1.99	98/4831 (2.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
3	7-C	1.75	44/3558 (1.2%)	2.01	96/4831 (2.0%)
3	7-D	1.70	28/3558 (0.8%)	1.94	99/4831 (2.0%)
3	8-C	1.73	28/3558 (0.8%)	1.93	99/4831 (2.0%)
3	8-D	1.72	31/3558 (0.9%)	1.92	83/4831 (1.7%)
3	9-C	1.73	39/3558 (1.1%)	2.02	109/4831 (2.3%)
3	9-D	1.69	32/3558 (0.9%)	1.99	94/4831 (1.9%)
All	All	1.73	1570/168360 (0.9%)	1.97	4569/227590 (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	1-A	0	19
1	10-A	0	20
1	2-A	0	16
1	3-A	0	15
1	4-A	0	16
1	5-A	0	18
1	6-A	0	24
1	7-A	0	19
1	8-A	0	21
1	9-A	0	19
2	1-B	0	25
2	10-B	0	25
2	2-B	0	18
2	3-B	0	17
2	4-B	0	21
2	5-B	0	7
2	6-B	0	19
2	7-B	0	23
2	8-B	0	28
2	9-B	0	15
3	1-C	0	15
3	1-D	0	9
3	10-C	0	11
3	10-D	0	17
3	2-C	0	9
3	2-D	0	6
3	3-C	0	16
3	3-D	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	4-C	0	13
3	4-D	0	13
3	5-C	0	8
3	5-D	0	10
3	6-C	0	12
3	6-D	1	8
3	7-C	0	9
3	7-D	0	11
3	8-C	0	9
3	8-D	0	14
3	9-C	0	8
3	9-D	0	14
All	All	1	609

All (1570) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-D	279	TYR	CG-CD1	10.47	1.52	1.39
3	4-D	43	SER	CA-CB	9.95	1.67	1.52
3	10-C	148	SER	CA-CB	9.75	1.67	1.52
3	1-D	341	ARG	NE-CZ	9.66	1.45	1.33
1	8-A	333	ARG	CZ-NH1	9.58	1.45	1.33
3	10-D	362	TYR	CB-CG	9.31	1.65	1.51
2	5-B	798	SER	CA-CB	9.30	1.66	1.52
1	9-A	74	TYR	CG-CD2	9.21	1.51	1.39
1	4-A	203	ARG	NE-CZ	9.07	1.44	1.33
3	6-C	349	SER	CA-CB	9.05	1.66	1.52
3	5-C	71	SER	CA-CB	8.97	1.66	1.52
3	3-D	84	ARG	CZ-NH1	8.91	1.44	1.33
3	4-D	84	ARG	CZ-NH2	8.87	1.44	1.33
2	8-B	562	TYR	CE2-CZ	8.84	1.50	1.38
3	6-D	319	TYR	CZ-OH	8.82	1.52	1.37
3	10-D	218	ARG	CD-NE	8.79	1.61	1.46
1	4-A	190	TYR	CE2-CZ	8.69	1.49	1.38
3	2-C	161	ARG	CZ-NH2	8.40	1.44	1.33
1	7-A	116	TYR	CE2-CZ	8.36	1.49	1.38
1	3-A	159	GLU	CB-CG	8.36	1.68	1.52
3	2-C	329	ARG	NE-CZ	8.35	1.44	1.33
2	2-B	190	TYR	CZ-OH	8.29	1.51	1.37
3	4-C	358	ARG	NE-CZ	8.18	1.43	1.33
2	5-B	389	ARG	NE-CZ	8.12	1.43	1.33
2	2-B	321	SER	CA-CB	8.09	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	10-D	74	SER	CA-CB	8.09	1.65	1.52
3	6-C	87	PHE	CG-CD1	8.06	1.50	1.38
1	4-A	144	ARG	CZ-NH2	8.04	1.43	1.33
1	10-A	127	SER	CA-CB	7.95	1.64	1.52
3	7-C	114	ARG	CZ-NH2	7.93	1.43	1.33
3	2-D	359	ARG	NE-CZ	7.92	1.43	1.33
2	5-B	666	ARG	NE-CZ	7.90	1.43	1.33
2	9-B	295	ARG	CZ-NH1	7.90	1.43	1.33
1	4-A	489	GLU	CG-CD	7.89	1.63	1.51
3	2-D	176	ARG	CD-NE	7.88	1.59	1.46
1	7-A	687	ARG	NE-CZ	7.86	1.43	1.33
2	8-B	552	SER	CA-CB	7.84	1.64	1.52
2	8-B	839	PHE	CG-CD2	7.83	1.50	1.38
3	9-C	176	ARG	NE-CZ	7.83	1.43	1.33
1	1-A	160	ARG	NE-CZ	7.83	1.43	1.33
3	9-C	176	ARG	CD-NE	7.83	1.59	1.46
3	8-C	53	PHE	CG-CD2	7.82	1.50	1.38
3	7-D	333	ARG	CZ-NH1	7.81	1.43	1.33
3	3-D	46	ARG	NE-CZ	7.80	1.43	1.33
3	4-D	114	ARG	CD-NE	7.77	1.59	1.46
1	3-A	76	ARG	NE-CZ	7.74	1.43	1.33
2	7-B	562	TYR	CG-CD2	7.73	1.49	1.39
1	6-A	687	ARG	CD-NE	7.73	1.59	1.46
3	2-D	55	ARG	CD-NE	7.71	1.59	1.46
1	7-A	112	TYR	CG-CD2	7.70	1.49	1.39
2	6-B	533	ARG	CZ-NH1	7.70	1.43	1.33
3	1-D	185	TYR	CE1-CZ	7.69	1.48	1.38
2	3-B	362	PHE	CG-CD1	7.69	1.50	1.38
1	9-A	327	ARG	NE-CZ	7.69	1.43	1.33
2	1-B	344	GLU	CG-CD	7.69	1.63	1.51
3	6-D	218	ARG	CD-NE	7.66	1.59	1.46
3	9-C	218	ARG	CZ-NH2	7.65	1.43	1.33
2	6-B	725	GLU	CD-OE1	7.65	1.34	1.25
2	5-B	438	TYR	CE2-CZ	7.63	1.48	1.38
1	6-A	391	GLU	CG-CD	7.62	1.63	1.51
2	4-B	288	TYR	CB-CG	-7.61	1.40	1.51
3	5-C	388	GLU	CD-OE2	7.61	1.34	1.25
2	9-B	439	ARG	CZ-NH2	7.60	1.43	1.33
2	7-B	670	ARG	CZ-NH2	7.59	1.43	1.33
1	5-A	398	TYR	CB-CG	7.55	1.62	1.51
1	10-A	140	TYR	CB-CG	7.55	1.62	1.51
1	4-A	358	ARG	CZ-NH1	7.54	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1-B	190	TYR	CE1-CZ	7.52	1.48	1.38
2	8-B	598	TYR	CB-CG	7.52	1.62	1.51
3	4-C	329	ARG	CD-NE	7.51	1.59	1.46
1	8-A	302	TYR	CE1-CZ	7.51	1.48	1.38
1	1-A	428	GLY	CA-C	-7.50	1.39	1.51
2	7-B	218	SER	CA-CB	7.49	1.64	1.52
3	2-C	193	ARG	CZ-NH1	7.47	1.42	1.33
1	8-A	623	ARG	NE-CZ	7.46	1.42	1.33
1	2-A	387	GLY	N-CA	-7.45	1.34	1.46
3	9-C	173	PHE	CB-CG	7.45	1.64	1.51
3	7-C	262	SER	CA-CB	7.45	1.64	1.52
3	4-D	13	CYS	CB-SG	7.44	1.94	1.82
3	5-C	324	GLY	CA-C	-7.44	1.40	1.51
2	6-B	439	ARG	CD-NE	7.44	1.59	1.46
2	1-B	274	SER	CA-CB	7.41	1.64	1.52
3	9-C	341	ARG	CZ-NH2	7.39	1.42	1.33
3	3-D	292	TYR	CG-CD1	7.36	1.48	1.39
2	3-B	282	SER	CA-CB	7.35	1.64	1.52
1	4-A	555	SER	CB-OG	7.35	1.51	1.42
1	3-A	337	SER	CA-CB	7.35	1.64	1.52
3	5-C	359	ARG	NE-CZ	7.33	1.42	1.33
3	3-C	37	SER	CB-OG	7.33	1.51	1.42
1	10-A	108	ARG	NE-CZ	7.32	1.42	1.33
2	4-B	438	TYR	CE2-CZ	7.32	1.48	1.38
1	5-A	632	LEU	CA-C	-7.31	1.33	1.52
2	5-B	210	PRO	N-CD	-7.31	1.37	1.47
3	10-D	304	SER	CB-OG	7.30	1.51	1.42
1	8-A	445	GLU	CG-CD	7.28	1.62	1.51
3	8-C	319	TYR	CE2-CZ	7.28	1.48	1.38
1	2-A	203	ARG	CZ-NH2	7.27	1.42	1.33
3	5-D	307	SER	CA-CB	7.27	1.63	1.52
1	10-A	773	SER	CA-CB	7.27	1.63	1.52
1	4-A	327	ARG	NE-CZ	7.26	1.42	1.33
1	5-A	116	TYR	CG-CD2	7.26	1.48	1.39
2	3-B	187	TYR	CG-CD2	7.24	1.48	1.39
3	9-D	243	ARG	NE-CZ	7.24	1.42	1.33
3	2-D	218	ARG	CZ-NH2	7.23	1.42	1.33
3	9-C	161	ARG	NE-CZ	7.23	1.42	1.33
2	6-B	242	ARG	CZ-NH1	7.23	1.42	1.33
1	7-A	101	SER	CA-CB	7.18	1.63	1.52
3	3-D	427	ARG	CD-NE	7.17	1.58	1.46
3	5-C	161	ARG	CZ-NH1	7.17	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	10-D	59	ARG	CZ-NH2	7.17	1.42	1.33
3	5-D	59	ARG	NE-CZ	7.15	1.42	1.33
3	9-C	358	ARG	NE-CZ	7.14	1.42	1.33
2	3-B	231	TYR	CZ-OH	7.14	1.50	1.37
3	8-D	129	SER	CA-CB	7.14	1.63	1.52
1	2-A	558	TYR	CE2-CZ	7.13	1.47	1.38
3	8-C	358	ARG	CD-NE	7.12	1.58	1.46
2	6-B	514	ARG	CZ-NH1	7.11	1.42	1.33
3	9-D	344	PHE	CG-CD2	7.11	1.49	1.38
1	6-A	714	ARG	NE-CZ	7.10	1.42	1.33
2	2-B	439	ARG	CD-NE	7.10	1.58	1.46
3	7-C	192	ARG	CZ-NH2	7.09	1.42	1.33
3	2-D	313	PRO	N-CD	-7.09	1.38	1.47
2	5-B	578	PHE	CG-CD1	7.09	1.49	1.38
1	10-A	171	ARG	CD-NE	7.09	1.58	1.46
3	9-D	55	ARG	NE-CZ	7.08	1.42	1.33
3	2-C	90	ARG	CD-NE	7.08	1.58	1.46
1	9-A	203	ARG	NE-CZ	7.08	1.42	1.33
2	6-B	409	TYR	CE2-CZ	7.07	1.47	1.38
2	1-B	578	PHE	CG-CD2	7.06	1.49	1.38
3	9-D	59	ARG	CZ-NH2	7.05	1.42	1.33
3	1-D	65	ARG	CZ-NH2	7.05	1.42	1.33
2	5-B	295	ARG	CZ-NH2	7.05	1.42	1.33
1	5-A	124	GLU	CG-CD	7.04	1.62	1.51
1	5-A	262	ARG	CZ-NH1	7.03	1.42	1.33
3	7-C	162	TYR	CE1-CZ	7.03	1.47	1.38
3	8-D	236	SER	CA-CB	7.02	1.63	1.52
1	2-A	279	TYR	CZ-OH	7.02	1.49	1.37
1	5-A	157	ARG	CD-NE	7.02	1.58	1.46
3	5-C	213	SER	CA-CB	7.02	1.63	1.52
2	2-B	533	ARG	NE-CZ	7.01	1.42	1.33
2	4-B	577	PRO	N-CD	-6.99	1.38	1.47
2	1-B	389	ARG	CZ-NH1	6.99	1.42	1.33
3	5-D	332	SER	CA-CB	6.98	1.63	1.52
1	9-A	181	GLU	CG-CD	6.98	1.62	1.51
3	9-D	341	ARG	CZ-NH1	6.98	1.42	1.33
2	2-B	666	ARG	CD-NE	6.98	1.58	1.46
1	10-A	202	GLU	CG-CD	6.97	1.62	1.51
1	2-A	466	GLU	CG-CD	6.97	1.62	1.51
2	2-B	514	ARG	CZ-NH1	6.96	1.42	1.33
2	6-B	846	ARG	CZ-NH1	6.96	1.42	1.33
3	7-D	218	ARG	NE-CZ	6.96	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7-C	145	GLY	CA-C	-6.96	1.40	1.51
2	5-B	583	TYR	CE2-CZ	6.95	1.47	1.38
1	3-A	486	PHE	CG-CD2	6.94	1.49	1.38
3	4-D	162	TYR	CZ-OH	6.94	1.49	1.37
1	7-A	107	ARG	CD-NE	6.93	1.58	1.46
3	2-D	90	ARG	NE-CZ	6.92	1.42	1.33
2	9-B	725	GLU	CD-OE2	6.92	1.33	1.25
2	6-B	565	TYR	CZ-OH	6.91	1.49	1.37
3	2-D	257	SER	CA-CB	6.91	1.63	1.52
1	9-A	106	SER	CA-CB	6.91	1.63	1.52
3	10-D	292	TYR	CE1-CZ	6.87	1.47	1.38
2	6-B	279	SER	CA-CB	6.86	1.63	1.52
2	2-B	552	SER	CA-CB	6.86	1.63	1.52
3	7-D	341	ARG	CZ-NH1	6.86	1.42	1.33
3	10-C	437	TYR	CE1-CZ	6.86	1.47	1.38
3	9-C	236	SER	CA-CB	6.85	1.63	1.52
3	9-D	176	ARG	NE-CZ	6.84	1.42	1.33
1	1-A	349	ARG	CZ-NH2	6.84	1.42	1.33
2	2-B	299	ARG	NE-CZ	6.83	1.42	1.33
2	5-B	345	TYR	CE1-CZ	6.83	1.47	1.38
3	3-D	108	GLY	N-CA	-6.82	1.35	1.46
3	6-C	315	TYR	CZ-OH	6.81	1.49	1.37
2	9-B	264	TYR	CZ-OH	6.81	1.49	1.37
1	8-A	195	GLU	CG-CD	6.80	1.62	1.51
1	3-A	775	PHE	CG-CD2	6.79	1.49	1.38
3	4-D	46	ARG	NE-CZ	6.79	1.41	1.33
2	5-B	433	TYR	CE2-CZ	6.77	1.47	1.38
1	6-A	280	CYS	CB-SG	6.77	1.93	1.82
1	6-A	558	TYR	CG-CD2	6.77	1.48	1.39
1	4-A	759	GLU	CG-CD	6.76	1.62	1.51
1	10-A	193	TYR	CE2-CZ	6.76	1.47	1.38
2	2-B	565	TYR	CE1-CZ	6.76	1.47	1.38
2	4-B	242	ARG	CZ-NH2	6.76	1.41	1.33
2	2-B	510	TYR	CG-CD1	6.75	1.48	1.39
2	7-B	638	ARG	NE-CZ	6.75	1.41	1.33
1	4-A	190	TYR	CB-CG	-6.75	1.41	1.51
3	2-D	348	SER	CB-OG	6.75	1.51	1.42
3	3-D	271	SER	CA-CB	6.74	1.63	1.52
1	10-A	143	ARG	NE-CZ	6.74	1.41	1.33
1	6-A	147	GLU	CG-CD	6.74	1.62	1.51
2	1-B	578	PHE	CE1-CZ	6.73	1.50	1.37
3	7-C	256	TYR	CE1-CZ	6.73	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	6-C	86	PHE	CE1-CZ	6.73	1.50	1.37
3	9-C	437	TYR	CG-CD1	6.73	1.48	1.39
2	10-B	565	TYR	CG-CD1	6.73	1.47	1.39
2	1-B	827	ARG	CZ-NH2	6.72	1.41	1.33
2	2-B	406	GLY	N-CA	-6.71	1.35	1.46
3	4-D	65	ARG	CZ-NH2	6.71	1.41	1.33
2	1-B	433	TYR	CG-CD2	6.71	1.47	1.39
2	3-B	424	GLU	CG-CD	-6.71	1.41	1.51
3	10-D	291	SER	CA-CB	6.71	1.63	1.52
1	9-A	479	ARG	CZ-NH2	6.71	1.41	1.33
1	2-A	429	TYR	CD2-CE2	6.70	1.49	1.39
2	6-B	638	ARG	NE-CZ	6.69	1.41	1.33
1	9-A	426	PHE	CG-CD2	6.69	1.48	1.38
1	4-A	116	TYR	CZ-OH	6.68	1.49	1.37
1	7-A	767	TYR	CE1-CZ	6.67	1.47	1.38
3	4-D	437	TYR	CG-CD2	6.67	1.47	1.39
2	7-B	772	PHE	CG-CD1	6.67	1.48	1.38
1	7-A	333	ARG	CZ-NH2	6.66	1.41	1.33
3	5-C	59	ARG	CZ-NH2	6.65	1.41	1.33
1	8-A	386	GLU	CD-OE2	6.65	1.32	1.25
2	10-B	641	PHE	CG-CD1	6.65	1.48	1.38
2	9-B	635	SER	CA-CB	6.64	1.62	1.52
1	1-A	116	TYR	CE2-CZ	6.64	1.47	1.38
2	1-B	533	ARG	CZ-NH1	6.64	1.41	1.33
1	9-A	141	GLU	CD-OE1	6.63	1.32	1.25
1	8-A	558	TYR	CE1-CZ	6.62	1.47	1.38
1	1-A	140	TYR	CE1-CZ	6.61	1.47	1.38
1	6-A	333	ARG	CZ-NH2	6.61	1.41	1.33
3	7-C	55	ARG	NE-CZ	6.61	1.41	1.33
1	6-A	160	ARG	NE-CZ	6.60	1.41	1.33
3	10-D	445	TYR	CE2-CZ	6.60	1.47	1.38
1	5-A	358	ARG	CZ-NH2	6.59	1.41	1.33
1	8-A	782	PHE	CG-CD1	6.59	1.48	1.38
3	9-D	432	SER	CA-CB	6.59	1.62	1.52
2	6-B	426	SER	CA-CB	6.59	1.62	1.52
3	7-D	193	ARG	CZ-NH2	6.59	1.41	1.33
2	7-B	288	TYR	CB-CG	6.59	1.61	1.51
3	8-C	388	GLU	CG-CD	6.58	1.61	1.51
1	10-A	776	ARG	NE-CZ	6.58	1.41	1.33
2	10-B	217	GLU	CG-CD	6.58	1.61	1.51
2	3-B	279	SER	CA-CB	6.58	1.62	1.52
3	2-C	319	TYR	CE1-CZ	6.57	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6-A	794	TYR	CG-CD2	6.57	1.47	1.39
2	2-B	726	SER	CA-CB	6.57	1.62	1.52
2	2-B	827	ARG	CZ-NH2	6.57	1.41	1.33
3	1-D	427	ARG	NE-CZ	6.56	1.41	1.33
1	4-A	124	GLU	CD-OE2	6.56	1.32	1.25
2	8-B	340	SER	CA-CB	6.56	1.62	1.52
3	4-C	176	ARG	CZ-NH1	6.56	1.41	1.33
2	7-B	308	SER	CA-CB	6.56	1.62	1.52
2	8-B	190	TYR	CG-CD2	6.55	1.47	1.39
3	8-D	192	ARG	CZ-NH2	6.55	1.41	1.33
2	1-B	429	TYR	CE2-CZ	6.54	1.47	1.38
2	7-B	438	TYR	CE2-CZ	6.54	1.47	1.38
2	1-B	725	GLU	CG-CD	6.53	1.61	1.51
2	7-B	524	SER	CA-CB	6.53	1.62	1.52
3	1-D	85	GLY	N-CA	-6.53	1.36	1.46
2	7-B	535	SER	CA-CB	6.53	1.62	1.52
1	8-A	664	ARG	CD-NE	6.53	1.57	1.46
1	9-A	797	SER	CA-CB	6.52	1.62	1.52
2	6-B	819	PHE	CG-CD1	6.52	1.48	1.38
3	10-C	241	SER	CA-CB	6.52	1.62	1.52
2	3-B	236	TYR	CG-CD2	6.51	1.47	1.39
3	10-D	14	GLY	N-CA	-6.51	1.36	1.46
3	3-D	78	ASP	CA-CB	6.50	1.68	1.53
2	6-B	816	TYR	CE1-CZ	6.48	1.47	1.38
2	5-B	438	TYR	CZ-OH	6.48	1.48	1.37
2	7-B	638	ARG	CZ-NH2	6.48	1.41	1.33
3	4-D	250	SER	CA-CB	6.48	1.62	1.52
2	6-B	447	GLU	CB-CG	6.48	1.64	1.52
3	3-D	109	TYR	CG-CD1	6.47	1.47	1.39
3	4-D	435	GLU	CD-OE1	-6.47	1.18	1.25
2	1-B	536	SER	CA-CB	6.47	1.62	1.52
3	4-C	269	SER	CA-CB	6.47	1.62	1.52
2	9-B	670	ARG	NE-CZ	6.46	1.41	1.33
1	10-A	576	ARG	NE-CZ	6.46	1.41	1.33
2	2-B	576	ARG	NE-CZ	6.46	1.41	1.33
2	4-B	285	ARG	CZ-NH2	6.46	1.41	1.33
3	9-C	192	ARG	CZ-NH2	6.46	1.41	1.33
3	10-C	427	ARG	CZ-NH1	6.45	1.41	1.33
2	7-B	644	PHE	CB-CG	-6.45	1.40	1.51
3	4-C	177	SER	CA-CB	6.45	1.62	1.52
2	9-B	187	TYR	CE2-CZ	6.45	1.47	1.38
3	6-C	253	SER	CA-CB	6.44	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5-A	143	ARG	NE-CZ	6.44	1.41	1.33
2	7-B	295	ARG	CZ-NH2	6.44	1.41	1.33
3	6-C	249	TYR	CG-CD2	6.44	1.47	1.39
3	9-D	114	ARG	CZ-NH1	6.43	1.41	1.33
2	4-B	652	TYR	CZ-OH	6.43	1.48	1.37
1	4-A	714	ARG	NE-CZ	6.43	1.41	1.33
2	1-B	447	GLU	CD-OE1	6.42	1.32	1.25
3	10-C	407	TYR	CG-CD1	6.42	1.47	1.39
3	4-D	46	ARG	CZ-NH1	6.42	1.41	1.33
2	3-B	379	TYR	CE2-CZ	6.42	1.46	1.38
1	5-A	203	ARG	CD-NE	6.41	1.57	1.46
2	2-B	770	TYR	CG-CD1	6.41	1.47	1.39
2	4-B	379	TYR	CZ-OH	6.40	1.48	1.37
3	10-C	114	ARG	CZ-NH2	6.40	1.41	1.33
3	10-D	329	ARG	CZ-NH1	6.40	1.41	1.33
2	8-B	345	TYR	CG-CD2	6.39	1.47	1.39
2	1-B	389	ARG	CD-NE	6.39	1.57	1.46
2	6-B	504	SER	CA-CB	6.39	1.62	1.52
2	8-B	822	ARG	NE-CZ	6.39	1.41	1.33
3	9-D	333	ARG	CZ-NH2	6.38	1.41	1.33
3	5-C	32	GLY	CA-C	-6.38	1.41	1.51
3	6-C	46	ARG	CZ-NH2	6.37	1.41	1.33
3	4-C	152	SER	CA-CB	6.37	1.62	1.52
1	5-A	630	ARG	CZ-NH2	6.37	1.41	1.33
1	9-A	160	ARG	NE-CZ	6.37	1.41	1.33
1	9-A	486	PHE	CG-CD2	6.37	1.48	1.38
3	9-D	272	PHE	CG-CD1	6.36	1.48	1.38
1	6-A	400	ARG	CZ-NH2	6.36	1.41	1.33
3	7-C	349	SER	CA-CB	6.36	1.62	1.52
3	3-C	315	TYR	CE2-CZ	6.36	1.46	1.38
2	4-B	471	ARG	CZ-NH1	6.36	1.41	1.33
3	4-C	59	ARG	CZ-NH2	6.36	1.41	1.33
3	6-C	341	ARG	CZ-NH2	6.35	1.41	1.33
2	10-B	295	ARG	CD-NE	6.35	1.57	1.46
2	1-B	670	ARG	CZ-NH2	6.35	1.41	1.33
3	7-C	193	ARG	NE-CZ	6.35	1.41	1.33
2	4-B	822	ARG	NE-CZ	6.35	1.41	1.33
1	7-A	576	ARG	NE-CZ	6.34	1.41	1.33
3	8-C	96	SER	CB-OG	-6.34	1.34	1.42
3	6-D	144	GLY	CA-C	-6.34	1.41	1.51
3	3-D	218	ARG	CZ-NH1	6.34	1.41	1.33
1	7-A	624	ARG	NE-CZ	6.34	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1-B	592	ARG	NE-CZ	6.33	1.41	1.33
1	10-A	286	TRP	CD2-CE3	-6.33	1.30	1.40
3	6-C	59	ARG	CZ-NH1	6.33	1.41	1.33
3	10-D	218	ARG	NE-CZ	6.33	1.41	1.33
2	3-B	544	ARG	CD-NE	6.32	1.57	1.46
2	9-B	361	GLU	CG-CD	6.32	1.61	1.51
2	3-B	827	ARG	NE-CZ	6.32	1.41	1.33
2	10-B	190	TYR	CZ-OH	6.32	1.48	1.37
3	1-C	319	TYR	CG-CD2	6.32	1.47	1.39
1	3-A	603	TRP	CB-CG	6.32	1.61	1.50
1	8-A	349	ARG	CD-NE	6.32	1.57	1.46
3	10-C	347	TRP	NE1-CE2	6.31	1.45	1.37
2	10-B	591	TRP	CZ2-CH2	6.31	1.49	1.37
2	7-B	633	ARG	NE-CZ	6.31	1.41	1.33
3	9-D	445	TYR	CG-CD1	6.30	1.47	1.39
3	2-D	437	TYR	CZ-OH	6.30	1.48	1.37
1	2-A	662	CYS	CB-SG	6.30	1.93	1.82
3	8-D	304	SER	CA-CB	6.30	1.62	1.52
3	6-D	437	TYR	CG-CD2	6.30	1.47	1.39
2	9-B	187	TYR	CE1-CZ	6.29	1.46	1.38
2	7-B	190	TYR	CZ-OH	6.29	1.48	1.37
3	10-D	358	ARG	CZ-NH2	6.29	1.41	1.33
1	5-A	611	SER	CB-OG	6.29	1.50	1.42
3	1-D	315	TYR	CE2-CZ	6.28	1.46	1.38
3	9-C	170	TYR	CZ-OH	6.28	1.48	1.37
3	1-D	359	ARG	CZ-NH2	6.28	1.41	1.33
3	1-D	378	SER	CA-CB	6.27	1.62	1.52
3	3-D	341	ARG	CD-NE	6.27	1.57	1.46
1	7-A	450	TYR	CZ-OH	6.27	1.48	1.37
2	7-B	267	PHE	CG-CD2	6.26	1.48	1.38
3	3-C	333	ARG	CZ-NH1	6.26	1.41	1.33
2	5-B	379	TYR	CG-CD2	6.26	1.47	1.39
3	10-D	193	ARG	CD-NE	6.26	1.57	1.46
3	4-C	362	TYR	CZ-OH	6.25	1.48	1.37
3	4-D	425	GLU	CD-OE2	6.25	1.32	1.25
3	1-C	437	TYR	CE1-CZ	6.25	1.46	1.38
3	3-C	198	SER	CA-CB	6.25	1.62	1.52
2	2-B	844	SER	CB-OG	6.25	1.50	1.42
3	7-C	444	SER	CA-CB	6.25	1.62	1.52
3	8-D	170	TYR	CG-CD1	6.25	1.47	1.39
1	4-A	558	TYR	CE2-CZ	6.24	1.46	1.38
3	7-D	178	SER	CB-OG	6.24	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3-B	293	ARG	NE-CZ	6.24	1.41	1.33
2	7-B	242	ARG	CZ-NH2	6.24	1.41	1.33
3	9-C	319	TYR	CE1-CZ	6.24	1.46	1.38
2	10-B	239	GLU	CG-CD	6.24	1.61	1.51
3	5-D	170	TYR	CG-CD2	6.23	1.47	1.39
3	5-C	218	ARG	CZ-NH1	6.23	1.41	1.33
1	5-A	469	ARG	NE-CZ	6.23	1.41	1.33
1	5-A	714	ARG	CZ-NH1	6.23	1.41	1.33
1	2-A	690	SER	CA-CB	6.23	1.62	1.52
2	3-B	264	TYR	CZ-OH	6.23	1.48	1.37
3	3-C	45	GLU	CG-CD	6.22	1.61	1.51
1	10-A	451	ARG	NE-CZ	6.22	1.41	1.33
3	6-C	378	SER	CA-CB	6.22	1.62	1.52
2	10-B	663	GLU	CD-OE2	6.22	1.32	1.25
2	1-B	600	TYR	CB-CG	6.22	1.60	1.51
2	3-B	569	SER	CA-CB	6.22	1.62	1.52
3	3-C	55	ARG	NE-CZ	6.22	1.41	1.33
1	4-A	131	PHE	CG-CD2	6.22	1.48	1.38
3	4-C	53	PHE	CG-CD1	6.22	1.48	1.38
2	5-B	264	TYR	CB-CG	6.22	1.60	1.51
3	7-C	329	ARG	CZ-NH1	6.22	1.41	1.33
1	4-A	582	TYR	CB-CG	6.21	1.60	1.51
3	4-D	344	PHE	CE2-CZ	6.21	1.49	1.37
3	7-C	192	ARG	CZ-NH1	6.21	1.41	1.33
2	6-B	299	ARG	NE-CZ	6.21	1.41	1.33
3	6-D	109	TYR	CG-CD1	6.21	1.47	1.39
3	3-C	319	TYR	CG-CD1	6.20	1.47	1.39
1	5-A	458	TYR	CZ-OH	6.20	1.48	1.37
1	6-A	769	SER	CA-CB	6.20	1.62	1.52
3	6-D	247	TYR	CZ-OH	6.19	1.48	1.37
1	1-A	687	ARG	CD-NE	6.19	1.56	1.46
1	8-A	798	SER	CA-CB	6.19	1.62	1.52
2	3-B	651	TYR	CE1-CZ	6.18	1.46	1.38
2	10-B	638	ARG	CZ-NH1	6.18	1.41	1.33
2	7-B	425	PHE	CE1-CZ	6.18	1.49	1.37
3	8-C	357	GLY	CA-C	-6.17	1.42	1.51
2	10-B	533	ARG	CZ-NH2	6.17	1.41	1.33
3	10-C	428	GLU	CD-OE2	6.17	1.32	1.25
1	2-A	279	TYR	CG-CD2	6.17	1.47	1.39
1	7-A	171	ARG	NE-CZ	6.17	1.41	1.33
1	2-A	262	ARG	CZ-NH2	6.17	1.41	1.33
1	2-A	198	ARG	CZ-NH2	6.17	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	8-D	55	ARG	CZ-NH1	6.15	1.41	1.33
3	9-D	371	GLU	CD-OE1	6.15	1.32	1.25
3	1-C	252	MET	CG-SD	6.14	1.97	1.81
1	3-A	203	ARG	CZ-NH2	6.14	1.41	1.33
2	4-B	816	TYR	CA-CB	6.14	1.67	1.53
3	8-D	114	ARG	NE-CZ	6.14	1.41	1.33
1	9-A	372	ASP	CB-CG	6.14	1.64	1.51
3	9-C	13	CYS	CB-SG	-6.14	1.71	1.82
1	3-A	766	GLU	CD-OE1	6.14	1.32	1.25
3	6-D	315	TYR	CE1-CZ	6.14	1.46	1.38
3	6-C	360	SER	CA-CB	6.13	1.62	1.52
3	8-C	59	ARG	CD-NE	6.13	1.56	1.46
2	1-B	360	GLY	CA-C	-6.13	1.42	1.51
2	4-B	264	TYR	CZ-OH	6.13	1.48	1.37
2	2-B	471	ARG	CZ-NH1	6.13	1.41	1.33
1	6-A	171	ARG	CZ-NH2	6.13	1.41	1.33
1	6-A	594	TYR	CG-CD1	6.13	1.47	1.39
1	2-A	144	ARG	CD-NE	6.12	1.56	1.46
2	10-B	583	TYR	CE2-CZ	6.12	1.46	1.38
3	1-D	141	SER	CA-CB	6.12	1.62	1.52
3	10-C	46	ARG	CZ-NH2	6.12	1.41	1.33
3	6-C	84	ARG	NE-CZ	6.11	1.41	1.33
2	10-B	280	LEU	CA-C	-6.11	1.37	1.52
3	6-C	193	ARG	CZ-NH2	6.11	1.41	1.33
1	3-A	593	GLN	CA-C	-6.11	1.37	1.52
3	7-D	437	TYR	CB-CG	-6.11	1.42	1.51
2	4-B	328	ARG	CZ-NH1	6.10	1.41	1.33
1	1-A	144	ARG	NE-CZ	6.10	1.41	1.33
2	5-B	633	ARG	CZ-NH2	6.10	1.41	1.33
3	8-C	407	TYR	CG-CD1	6.10	1.47	1.39
3	5-C	59	ARG	CD-NE	6.09	1.56	1.46
2	4-B	638	ARG	CZ-NH2	6.09	1.41	1.33
3	10-D	407	TYR	CG-CD2	6.08	1.47	1.39
3	6-C	218	ARG	CZ-NH2	6.08	1.41	1.33
3	6-C	232	SER	CA-CB	6.08	1.62	1.52
2	9-B	776	TYR	CE1-CZ	6.08	1.46	1.38
2	4-B	231	TYR	CB-CG	-6.08	1.42	1.51
3	4-C	46	ARG	NE-CZ	6.07	1.41	1.33
3	8-D	373	SER	CA-CB	6.07	1.62	1.52
3	7-C	344	PHE	CG-CD1	6.07	1.47	1.38
3	2-C	65	ARG	NE-CZ	6.06	1.41	1.33
2	4-B	273	SER	CA-CB	6.06	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6-B	226	GLU	CG-CD	6.06	1.61	1.51
3	3-D	144	GLY	CA-C	-6.05	1.42	1.51
3	8-D	350	SER	CA-CB	6.05	1.62	1.52
2	2-B	225	PHE	CG-CD1	6.05	1.47	1.38
1	2-A	358	ARG	NE-CZ	6.05	1.41	1.33
3	7-D	274	PRO	N-CA	-6.05	1.36	1.47
1	3-A	333	ARG	NE-CZ	6.04	1.41	1.33
2	9-B	299	ARG	CZ-NH1	6.04	1.41	1.33
2	10-B	345	TYR	CE1-CZ	6.04	1.46	1.38
1	4-A	320	TRP	NE1-CE2	6.04	1.45	1.37
1	5-A	627	ARG	NE-CZ	6.04	1.40	1.33
3	9-C	84	ARG	CZ-NH1	6.04	1.40	1.33
2	5-B	844	SER	CA-CB	6.03	1.62	1.52
2	6-B	439	ARG	NE-CZ	6.03	1.40	1.33
3	8-D	445	TYR	CG-CD1	6.03	1.47	1.39
1	2-A	263	SER	CA-CB	6.03	1.61	1.52
2	3-B	356	ARG	CD-NE	6.02	1.56	1.46
2	2-B	565	TYR	CG-CD2	6.02	1.47	1.39
3	4-D	161	ARG	CZ-NH2	6.02	1.40	1.33
2	8-B	439	ARG	NE-CZ	6.02	1.40	1.33
2	6-B	844	SER	CA-CB	6.02	1.61	1.52
3	6-D	301	PRO	N-CD	-6.02	1.39	1.47
3	6-D	401	GLY	CA-C	-6.02	1.42	1.51
3	1-C	346	SER	CA-CB	6.02	1.61	1.52
2	7-B	205	GLU	CB-CG	6.02	1.63	1.52
3	9-D	100	SER	CA-CB	6.01	1.61	1.52
2	2-B	182	GLU	CD-OE2	6.01	1.32	1.25
1	8-A	646	TYR	CB-CG	6.01	1.60	1.51
3	2-C	90	ARG	NE-CZ	6.01	1.40	1.33
3	7-C	4	GLU	CB-CG	6.00	1.63	1.52
3	4-D	341	ARG	CD-NE	6.00	1.56	1.46
1	1-A	325	PHE	CG-CD1	6.00	1.47	1.38
3	7-D	423	PHE	CB-CG	-6.00	1.41	1.51
1	4-A	77	TYR	CE2-CZ	6.00	1.46	1.38
3	10-D	11	GLY	N-CA	6.00	1.55	1.46
1	7-A	140	TYR	CE2-CZ	6.00	1.46	1.38
2	7-B	726	SER	CA-CB	6.00	1.61	1.52
1	4-A	198	ARG	CZ-NH2	5.99	1.40	1.33
2	8-B	393	PHE	CG-CD1	5.99	1.47	1.38
1	1-A	465	PHE	CB-CG	5.99	1.61	1.51
2	3-B	389	ARG	NE-CZ	5.99	1.40	1.33
3	5-D	373	SER	CA-CB	5.99	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2-B	846	ARG	CZ-NH2	5.98	1.40	1.33
3	8-C	114	ARG	CZ-NH1	5.98	1.40	1.33
2	2-B	646	SER	CA-C	-5.98	1.37	1.52
1	4-A	568	TYR	CE2-CZ	5.98	1.46	1.38
3	9-C	333	ARG	CD-NE	5.98	1.56	1.46
2	8-B	612	ARG	CZ-NH1	5.98	1.40	1.33
2	10-B	415	TYR	CG-CD2	5.98	1.47	1.39
3	10-D	349	SER	CA-CB	5.98	1.61	1.52
3	5-C	54	PHE	CE2-CZ	5.97	1.48	1.37
3	6-C	109	TYR	CE1-CZ	5.97	1.46	1.38
1	1-A	627	ARG	NE-CZ	5.96	1.40	1.33
3	7-C	152	SER	CA-CB	5.96	1.61	1.52
2	4-B	758	TYR	CE1-CZ	5.96	1.46	1.38
3	9-C	134	GLU	CD-OE2	5.96	1.32	1.25
3	10-C	84	ARG	CZ-NH1	5.96	1.40	1.33
3	2-D	46	ARG	CZ-NH1	5.95	1.40	1.33
3	3-C	333	ARG	CD-NE	5.95	1.56	1.46
2	2-B	738	HIS	CB-CG	-5.95	1.39	1.50
2	3-B	544	ARG	CZ-NH1	5.95	1.40	1.33
2	9-B	414	LYS	CA-CB	5.95	1.67	1.53
1	2-A	327	ARG	CD-NE	5.95	1.56	1.46
1	6-A	776	ARG	CZ-NH1	5.94	1.40	1.33
3	9-D	291	SER	CB-OG	5.94	1.50	1.42
1	2-A	438	PHE	CG-CD2	5.94	1.47	1.38
3	5-C	315	TYR	CB-CG	5.94	1.60	1.51
1	7-A	673	GLN	CG-CD	5.94	1.64	1.51
1	2-A	204	ARG	NE-CZ	5.94	1.40	1.33
3	2-C	114	ARG	CD-NE	5.94	1.56	1.46
2	5-B	300	PHE	CE1-CZ	5.94	1.48	1.37
1	1-A	327	ARG	CZ-NH2	5.93	1.40	1.33
3	1-C	62	PHE	CG-CD1	5.93	1.47	1.38
3	4-D	59	ARG	CD-NE	5.93	1.56	1.46
1	6-A	555	SER	CA-CB	5.93	1.61	1.52
3	4-D	374	GLY	CA-C	-5.93	1.42	1.51
2	7-B	231	TYR	CG-CD2	5.93	1.46	1.39
2	3-B	612	ARG	CZ-NH2	5.92	1.40	1.33
2	6-B	603	GLU	CD-OE1	5.92	1.32	1.25
3	10-C	341	ARG	CZ-NH2	5.92	1.40	1.33
3	4-D	35	GLY	CA-C	-5.92	1.42	1.51
1	9-A	284	TYR	CG-CD2	5.92	1.46	1.39
2	6-B	836	GLU	CD-OE2	5.92	1.32	1.25
3	1-C	192	ARG	NE-CZ	5.92	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	9-D	192	ARG	CZ-NH1	5.92	1.40	1.33
3	10-C	361	PRO	N-CD	-5.92	1.39	1.47
2	4-B	409	TYR	CZ-OH	5.91	1.47	1.37
2	1-B	356	ARG	NE-CZ	5.91	1.40	1.33
1	2-A	190	TYR	CG-CD1	5.91	1.46	1.39
3	5-C	84	ARG	CZ-NH2	5.91	1.40	1.33
3	3-D	109	TYR	CG-CD2	5.91	1.46	1.39
2	7-B	578	PHE	CG-CD1	5.91	1.47	1.38
1	7-A	587	ARG	CZ-NH2	5.90	1.40	1.33
1	8-A	171	ARG	CZ-NH2	5.90	1.40	1.33
1	10-A	137	ARG	CZ-NH1	5.90	1.40	1.33
1	2-A	594	TYR	CE1-CZ	5.89	1.46	1.38
3	2-C	87	PHE	CB-CG	-5.89	1.41	1.51
2	4-B	468	PHE	CE1-CZ	5.89	1.48	1.37
3	10-C	173	PHE	CG-CD1	5.89	1.47	1.38
3	2-C	218	ARG	CD-NE	5.89	1.56	1.46
2	6-B	205	GLU	CD-OE2	5.89	1.32	1.25
2	4-B	389	ARG	CD-NE	5.88	1.56	1.46
1	4-A	157	ARG	CZ-NH2	5.88	1.40	1.33
1	5-A	429	TYR	CZ-OH	5.88	1.47	1.37
2	2-B	483	MET	C-N	5.88	1.43	1.33
1	4-A	469	ARG	CZ-NH2	5.88	1.40	1.33
3	3-D	329	ARG	NE-CZ	5.88	1.40	1.33
2	7-B	345	TYR	CG-CD1	5.88	1.46	1.39
3	5-D	256	TYR	CZ-OH	5.87	1.47	1.37
2	1-B	638	ARG	NE-CZ	5.87	1.40	1.33
2	3-B	532	PRO	N-CD	-5.87	1.39	1.47
3	7-C	73	PRO	N-CD	-5.87	1.39	1.47
1	8-A	284	TYR	CZ-OH	5.87	1.47	1.37
3	7-C	266	HIS	CB-CG	5.86	1.60	1.50
1	10-A	284	TYR	CE2-CZ	5.86	1.46	1.38
2	5-B	328	ARG	NE-CZ	5.86	1.40	1.33
1	6-A	381	PHE	CG-CD1	5.86	1.47	1.38
3	9-C	65	ARG	CD-NE	5.86	1.56	1.46
3	1-C	177	SER	CA-CB	5.86	1.61	1.52
1	6-A	126	TRP	NE1-CE2	-5.86	1.29	1.37
3	10-D	192	ARG	CZ-NH1	5.86	1.40	1.33
1	1-A	413	TYR	CB-CG	-5.85	1.42	1.51
3	5-D	329	ARG	NE-CZ	5.85	1.40	1.33
3	9-D	250	SER	CA-CB	5.85	1.61	1.52
3	9-D	427	ARG	NE-CZ	5.85	1.40	1.33
3	7-C	176	ARG	CZ-NH2	5.85	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-C	359	ARG	CZ-NH1	5.85	1.40	1.33
3	1-C	46	ARG	CZ-NH1	5.84	1.40	1.33
2	5-B	670	ARG	NE-CZ	5.84	1.40	1.33
3	8-D	253	SER	CA-CB	5.84	1.61	1.52
1	10-A	339	GLU	CG-CD	5.84	1.60	1.51
2	6-B	798	SER	CA-CB	5.84	1.61	1.52
1	9-A	92	PHE	CB-CG	5.84	1.61	1.51
2	5-B	264	TYR	CE1-CZ	5.83	1.46	1.38
2	9-B	470	TYR	CB-CG	-5.83	1.43	1.51
2	3-B	359	TYR	CE2-CZ	5.83	1.46	1.38
1	9-A	458	TYR	CE1-CZ	5.83	1.46	1.38
3	1-D	421	ASP	CA-C	-5.82	1.37	1.52
3	9-D	315	TYR	CE2-CZ	5.82	1.46	1.38
2	6-B	514	ARG	NE-CZ	5.82	1.40	1.33
3	6-D	162	TYR	CG-CD1	5.82	1.46	1.39
1	8-A	400	ARG	CZ-NH1	5.82	1.40	1.33
2	5-B	839	PHE	CG-CD2	5.82	1.47	1.38
2	5-B	439	ARG	NE-CZ	5.82	1.40	1.33
2	8-B	412	LEU	CA-CB	5.82	1.67	1.53
3	2-D	193	ARG	NE-CZ	5.81	1.40	1.33
1	6-A	386	GLU	CD-OE1	5.81	1.32	1.25
2	10-B	242	ARG	CZ-NH2	5.81	1.40	1.33
1	2-A	143	ARG	CZ-NH1	5.81	1.40	1.33
3	2-D	236	SER	CB-OG	-5.81	1.34	1.42
3	6-D	59	ARG	CZ-NH1	5.81	1.40	1.33
1	1-A	286	TRP	CD2-CE2	5.81	1.48	1.41
3	3-D	162	TYR	CE2-CZ	5.81	1.46	1.38
1	4-A	393	TYR	CB-CG	5.81	1.60	1.51
3	4-D	53	PHE	CE1-CZ	5.81	1.48	1.37
2	7-B	565	TYR	CD2-CE2	5.81	1.48	1.39
1	10-A	107	ARG	CD-NE	5.81	1.56	1.46
3	6-C	407	TYR	CE1-CZ	5.81	1.46	1.38
3	1-C	381	SER	CB-OG	-5.80	1.34	1.42
3	8-C	241	SER	CA-CB	5.80	1.61	1.52
2	3-B	666	ARG	NE-CZ	5.80	1.40	1.33
3	10-C	373	SER	CA-CB	5.80	1.61	1.52
3	5-D	371	GLU	CG-CD	-5.80	1.43	1.51
1	7-A	144	ARG	CZ-NH2	5.80	1.40	1.33
1	2-A	690	SER	CB-OG	-5.79	1.34	1.42
3	2-C	292	TYR	CE2-CZ	5.79	1.46	1.38
3	3-C	243	ARG	NE-CZ	5.79	1.40	1.33
2	1-B	297	TYR	CE2-CZ	5.79	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5-A	687	ARG	CZ-NH2	5.79	1.40	1.33
3	10-D	53	PHE	CG-CD1	5.79	1.47	1.38
3	2-C	162	TYR	CG-CD1	5.78	1.46	1.39
2	3-B	824	TYR	CG-CD1	5.78	1.46	1.39
3	10-C	90	ARG	CZ-NH2	5.78	1.40	1.33
3	2-C	422	GLU	CG-CD	5.78	1.60	1.51
1	2-A	333	ARG	CZ-NH1	5.78	1.40	1.33
1	5-A	782	PHE	CG-CD2	5.78	1.47	1.38
3	1-C	59	ARG	NE-CZ	5.78	1.40	1.33
1	8-A	121	ARG	CZ-NH2	5.78	1.40	1.33
1	1-A	657	TYR	CG-CD2	5.77	1.46	1.39
2	1-B	260	GLU	CD-OE2	5.77	1.32	1.25
1	5-A	116	TYR	CZ-OH	5.77	1.47	1.37
3	10-C	371	GLU	CB-CG	5.77	1.63	1.52
3	7-D	287	LYS	C-N	5.77	1.43	1.33
3	1-D	161	ARG	CZ-NH1	5.77	1.40	1.33
1	6-A	612	TRP	CG-CD1	-5.76	1.28	1.36
3	7-D	184	SER	CA-CB	5.76	1.61	1.52
1	1-A	775	PHE	CG-CD2	5.76	1.47	1.38
2	2-B	356	ARG	NE-CZ	5.76	1.40	1.33
1	3-A	587	ARG	CZ-NH2	5.76	1.40	1.33
3	5-D	243	ARG	CZ-NH2	5.76	1.40	1.33
3	6-C	329	ARG	CZ-NH1	5.76	1.40	1.33
2	4-B	544	ARG	CZ-NH1	5.76	1.40	1.33
2	6-B	356	ARG	NE-CZ	5.76	1.40	1.33
3	6-C	192	ARG	CZ-NH2	5.75	1.40	1.33
2	7-B	592	ARG	NE-CZ	5.75	1.40	1.33
1	5-A	776	ARG	CZ-NH1	5.75	1.40	1.33
1	6-A	349	ARG	CD-NE	5.75	1.56	1.46
3	9-C	410	GLY	N-CA	-5.75	1.37	1.46
1	6-A	704	TYR	CE2-CZ	5.75	1.46	1.38
2	10-B	315	GLU	CG-CD	5.75	1.60	1.51
1	7-A	647	PHE	CG-CD1	5.75	1.47	1.38
2	7-B	819	PHE	CG-CD1	5.75	1.47	1.38
1	1-A	157	ARG	CZ-NH2	5.74	1.40	1.33
3	10-C	329	ARG	CD-NE	5.74	1.56	1.46
3	3-C	375	MET	N-CA	-5.74	1.34	1.46
1	5-A	714	ARG	CZ-NH2	5.74	1.40	1.33
3	6-D	258	THR	N-CA	-5.74	1.34	1.46
3	2-D	163	PRO	CA-C	-5.74	1.41	1.52
3	3-D	22	TRP	CD2-CE3	-5.74	1.31	1.40
2	8-B	285	ARG	CD-NE	5.74	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	10-C	325	ASN	CB-CG	5.73	1.64	1.51
1	9-A	279	TYR	CE2-CZ	5.73	1.46	1.38
3	5-C	394	PHE	CG-CD2	5.73	1.47	1.38
1	6-A	112	TYR	CG-CD1	5.73	1.46	1.39
1	7-A	413	TYR	CE1-CZ	5.73	1.46	1.38
3	6-D	329	ARG	NE-CZ	5.72	1.40	1.33
1	7-A	413	TYR	CG-CD1	5.72	1.46	1.39
3	10-C	350	SER	CA-CB	5.72	1.61	1.52
3	7-D	83	PHE	CG-CD1	5.72	1.47	1.38
1	4-A	630	ARG	CZ-NH1	5.72	1.40	1.33
3	10-C	55	ARG	CZ-NH1	5.72	1.40	1.33
1	3-A	714	ARG	CZ-NH2	5.71	1.40	1.33
2	10-B	267	PHE	CD2-CE2	5.71	1.50	1.39
2	3-B	592	ARG	NE-CZ	5.71	1.40	1.33
2	4-B	424	GLU	CD-OE1	-5.71	1.19	1.25
2	2-B	424	GLU	CB-CG	5.71	1.62	1.52
3	2-D	364	PRO	N-CD	-5.71	1.39	1.47
1	3-A	91	GLU	CD-OE2	5.71	1.31	1.25
1	10-A	451	ARG	CZ-NH1	5.71	1.40	1.33
3	6-C	359	ARG	NE-CZ	5.70	1.40	1.33
2	8-B	393	PHE	CB-CG	5.70	1.61	1.51
2	9-B	204	HIS	CB-CG	5.70	1.60	1.50
1	10-A	754	GLU	CD-OE1	5.70	1.31	1.25
3	6-D	114	ARG	CA-CB	5.70	1.66	1.53
3	7-C	358	ARG	NE-CZ	5.70	1.40	1.33
1	6-A	325	PHE	CG-CD1	5.69	1.47	1.38
1	6-A	630	ARG	CZ-NH2	5.69	1.40	1.33
2	9-B	819	PHE	CA-CB	5.69	1.66	1.53
3	9-D	346	SER	CA-CB	5.69	1.61	1.52
3	1-D	161	ARG	CZ-NH2	5.69	1.40	1.33
1	9-A	603	TRP	CD2-CE2	5.69	1.48	1.41
1	2-A	664	ARG	NE-CZ	5.69	1.40	1.33
3	7-D	232	SER	CB-OG	5.69	1.49	1.42
2	3-B	429	TYR	CE1-CZ	5.69	1.46	1.38
2	5-B	533	ARG	CZ-NH2	5.69	1.40	1.33
3	7-C	23	SER	CA-CB	5.69	1.61	1.52
3	9-D	87	PHE	CB-CG	-5.68	1.41	1.51
1	1-A	181	GLU	CD-OE1	5.68	1.31	1.25
1	10-A	587	ARG	NE-CZ	5.68	1.40	1.33
3	1-D	333	ARG	CZ-NH2	5.67	1.40	1.33
2	6-B	357	ALA	CA-CB	5.67	1.64	1.52
1	2-A	664	ARG	CZ-NH2	5.67	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6-A	479	ARG	CZ-NH2	5.67	1.40	1.33
3	10-D	264	GLU	CB-CG	5.67	1.62	1.52
3	8-C	244	PHE	CG-CD1	5.67	1.47	1.38
2	3-B	319	PHE	CE2-CZ	5.67	1.48	1.37
2	7-B	274	SER	CA-CB	5.67	1.61	1.52
3	10-C	269	SER	CA-CB	5.67	1.61	1.52
3	1-D	93	TRP	NE1-CE2	5.67	1.45	1.37
3	1-D	176	ARG	CZ-NH1	5.67	1.40	1.33
3	8-C	319	TYR	CB-CG	-5.67	1.43	1.51
2	9-B	335	PHE	CG-CD1	5.67	1.47	1.38
3	7-D	166	ILE	N-CA	-5.66	1.35	1.46
1	8-A	431	SER	CA-CB	5.66	1.61	1.52
1	3-A	339	GLU	CB-CG	5.66	1.62	1.52
3	5-C	126	GLU	CG-CD	5.66	1.60	1.51
3	6-D	135	GLY	CA-C	-5.66	1.42	1.51
1	3-A	193	TYR	CZ-OH	5.66	1.47	1.37
1	5-A	558	TYR	CE2-CZ	5.66	1.46	1.38
1	4-A	398	TYR	CZ-OH	5.65	1.47	1.37
2	7-B	761	SER	CA-CB	5.65	1.61	1.52
3	1-D	59	ARG	CZ-NH1	5.65	1.40	1.33
1	2-A	675	GLU	CG-CD	5.65	1.60	1.51
1	7-A	358	ARG	CZ-NH2	5.65	1.40	1.33
1	10-A	76	ARG	CZ-NH1	5.65	1.40	1.33
3	1-C	176	ARG	CZ-NH2	5.65	1.40	1.33
1	7-A	627	ARG	NE-CZ	5.65	1.40	1.33
2	9-B	827	ARG	CD-NE	5.65	1.56	1.46
2	4-B	574	VAL	CB-CG1	5.65	1.64	1.52
1	6-A	458	TYR	CD2-CE2	5.65	1.47	1.39
3	7-D	55	ARG	CZ-NH2	5.65	1.40	1.33
2	2-B	384	GLU	CB-CG	5.64	1.62	1.52
2	3-B	580	ARG	CZ-NH1	5.64	1.40	1.33
3	4-D	84	ARG	CD-NE	5.64	1.56	1.46
1	10-A	714	ARG	NE-CZ	5.64	1.40	1.33
1	8-A	279	TYR	CZ-OH	5.64	1.47	1.37
3	9-C	359	ARG	NE-CZ	5.64	1.40	1.33
1	9-A	286	TRP	NE1-CE2	5.64	1.44	1.37
3	7-C	387	PHE	CG-CD2	5.63	1.47	1.38
2	1-B	504	SER	CB-OG	-5.63	1.34	1.42
3	6-D	288	GLY	N-CA	-5.63	1.37	1.46
3	9-C	218	ARG	CD-NE	5.63	1.56	1.46
3	6-C	59	ARG	CD-NE	5.63	1.56	1.46
3	1-D	90	ARG	CD-NE	5.63	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7-B	731	PHE	CB-CG	5.63	1.60	1.51
3	7-D	445	TYR	CG-CD1	5.63	1.46	1.39
1	2-A	130	SER	CA-CB	5.62	1.61	1.52
3	10-D	243	ARG	NE-CZ	5.62	1.40	1.33
2	3-B	343	TYR	CB-CG	5.62	1.60	1.51
3	7-C	90	ARG	CD-NE	5.62	1.56	1.46
3	4-D	316	PHE	CG-CD2	5.62	1.47	1.38
1	5-A	582	TYR	CB-CG	-5.62	1.43	1.51
1	8-A	704	TYR	CE2-CZ	5.62	1.45	1.38
1	1-A	143	ARG	CZ-NH1	5.62	1.40	1.33
2	4-B	585	ARG	CZ-NH1	5.62	1.40	1.33
3	4-C	394	PHE	CB-CG	5.61	1.60	1.51
2	8-B	652	TYR	CE1-CZ	5.61	1.45	1.38
1	4-A	370	SER	CA-CB	5.61	1.61	1.52
2	4-B	612	ARG	CZ-NH2	5.61	1.40	1.33
3	6-D	152	SER	CA-CB	5.61	1.61	1.52
3	6-D	236	SER	CA-CB	5.61	1.61	1.52
2	8-B	670	ARG	CZ-NH2	5.61	1.40	1.33
2	1-B	587	PHE	CB-CG	5.61	1.60	1.51
2	3-B	822	ARG	CZ-NH2	5.61	1.40	1.33
1	1-A	74	TYR	CE1-CZ	5.61	1.45	1.38
3	2-D	355	ASN	CA-CB	5.61	1.67	1.53
1	4-A	123	TYR	CG-CD2	5.61	1.46	1.39
3	6-C	426	SER	CA-CB	5.61	1.61	1.52
1	7-A	150	TYR	CZ-OH	5.61	1.47	1.37
1	8-A	174	GLU	CG-CD	5.61	1.60	1.51
2	8-B	846	ARG	CZ-NH1	5.61	1.40	1.33
1	10-A	646	TYR	CG-CD1	5.61	1.46	1.39
2	10-B	409	TYR	CG-CD2	5.61	1.46	1.39
1	1-A	145	PHE	CE2-CZ	5.60	1.48	1.37
3	2-C	59	ARG	CZ-NH1	5.60	1.40	1.33
2	5-B	603	GLU	CD-OE1	5.60	1.31	1.25
2	6-B	231	TYR	CZ-OH	5.60	1.47	1.37
1	6-A	193	TYR	CE1-CZ	5.60	1.45	1.38
3	1-C	218	ARG	CZ-NH1	5.60	1.40	1.33
2	2-B	343	TYR	CE2-CZ	5.60	1.45	1.38
1	2-A	594	TYR	CE2-CZ	5.59	1.45	1.38
1	6-A	284	TYR	CG-CD2	5.59	1.46	1.39
2	1-B	638	ARG	CZ-NH2	5.59	1.40	1.33
3	10-D	217	PHE	CG-CD1	5.59	1.47	1.38
1	3-A	646	TYR	CE2-CZ	5.59	1.45	1.38
3	3-D	333	ARG	CZ-NH1	5.59	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7-C	264	GLU	CD-OE2	5.59	1.31	1.25
2	4-B	345	TYR	CZ-OH	5.58	1.47	1.37
2	5-B	580	ARG	CZ-NH2	5.58	1.40	1.33
3	5-D	247	TYR	CZ-OH	5.58	1.47	1.37
1	3-A	140	TYR	CD1-CE1	5.58	1.47	1.39
3	6-C	398	PHE	CG-CD2	5.58	1.47	1.38
3	6-C	427	ARG	CZ-NH2	5.58	1.40	1.33
1	7-A	704	TYR	CE2-CZ	5.58	1.45	1.38
2	8-B	415	TYR	CE2-CZ	5.58	1.45	1.38
2	8-B	553	VAL	CA-CB	5.58	1.66	1.54
1	9-A	150	TYR	CE2-CZ	5.58	1.45	1.38
3	2-D	204	PHE	CG-CD2	5.58	1.47	1.38
3	7-C	220	PRO	N-CD	-5.58	1.40	1.47
3	6-C	198	SER	CA-CB	5.58	1.61	1.52
1	2-A	687	ARG	NE-CZ	5.58	1.40	1.33
2	2-B	362	PHE	CB-CG	5.58	1.60	1.51
2	3-B	651	TYR	CG-CD2	5.58	1.46	1.39
3	4-C	190	ALA	CA-CB	5.58	1.64	1.52
1	7-A	76	ARG	NE-CZ	5.58	1.40	1.33
1	3-A	769	SER	CA-CB	5.57	1.61	1.52
1	6-A	377	GLU	CB-CG	5.57	1.62	1.52
1	8-A	190	TYR	CD2-CE2	5.57	1.47	1.39
3	5-C	162	TYR	CZ-OH	5.57	1.47	1.37
2	6-B	440	GLY	CA-C	-5.57	1.43	1.51
1	8-A	588	TYR	CZ-OH	5.57	1.47	1.37
1	5-A	704	TYR	CG-CD2	5.57	1.46	1.39
2	7-B	425	PHE	CG-CD1	5.57	1.47	1.38
3	9-C	371	GLU	CB-CG	5.57	1.62	1.52
1	6-A	92	PHE	CE1-CZ	5.56	1.48	1.37
2	2-B	544	ARG	NE-CZ	5.56	1.40	1.33
1	3-A	664	ARG	NE-CZ	5.56	1.40	1.33
1	5-A	776	ARG	CZ-NH2	5.56	1.40	1.33
1	6-A	594	TYR	CZ-OH	5.56	1.47	1.37
3	5-D	2	GLY	CA-C	-5.56	1.43	1.51
3	7-C	300	ASP	N-CA	-5.56	1.35	1.46
3	7-D	423	PHE	CE1-CZ	5.56	1.48	1.37
2	3-B	200	PHE	CG-CD1	5.55	1.47	1.38
3	7-C	143	ALA	C-N	5.55	1.43	1.33
3	9-C	327	GLU	CA-CB	5.55	1.66	1.53
2	10-B	475	PHE	CG-CD1	5.55	1.47	1.38
1	1-A	123	TYR	CE1-CZ	5.54	1.45	1.38
2	9-B	770	TYR	CZ-OH	5.54	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2-B	415	TYR	CB-CG	-5.54	1.43	1.51
1	3-A	130	SER	CA-CB	5.54	1.61	1.52
3	3-C	103	ASN	C-O	5.54	1.33	1.23
3	5-C	65	ARG	NE-CZ	5.54	1.40	1.33
2	1-B	837	GLU	CB-CG	5.54	1.62	1.52
3	1-C	84	ARG	CZ-NH2	5.54	1.40	1.33
2	10-B	646	SER	CA-CB	5.54	1.61	1.52
1	6-A	279	TYR	CZ-OH	5.54	1.47	1.37
2	7-B	523	SER	CA-CB	5.54	1.61	1.52
1	2-A	144	ARG	CZ-NH2	5.54	1.40	1.33
1	4-A	276	SER	CB-OG	-5.54	1.35	1.42
2	8-B	533	ARG	NE-CZ	5.54	1.40	1.33
3	3-C	84	ARG	CZ-NH2	5.53	1.40	1.33
1	5-A	77	TYR	CG-CD2	5.53	1.46	1.39
3	7-C	218	ARG	CZ-NH1	5.53	1.40	1.33
1	2-A	157	ARG	CZ-NH2	5.53	1.40	1.33
2	4-B	192	LEU	C-N	5.53	1.46	1.34
2	10-B	583	TYR	CE1-CZ	5.53	1.45	1.38
2	2-B	293	ARG	CD-NE	5.53	1.55	1.46
3	6-D	20	PHE	CG-CD2	5.53	1.47	1.38
1	9-A	203	ARG	CZ-NH2	5.53	1.40	1.33
1	2-A	181	GLU	CD-OE1	5.52	1.31	1.25
1	7-A	193	TYR	CE1-CZ	5.52	1.45	1.38
3	6-C	177	SER	CA-CB	5.52	1.61	1.52
2	10-B	660	ASN	CA-CB	5.52	1.67	1.53
1	2-A	333	ARG	CD-NE	5.52	1.55	1.46
1	7-A	105	PHE	CG-CD1	5.52	1.47	1.38
1	9-A	157	ARG	NE-CZ	5.52	1.40	1.33
3	9-D	253	SER	CA-CB	5.52	1.61	1.52
1	4-A	776	ARG	CZ-NH2	5.51	1.40	1.33
2	2-B	239	GLU	CD-OE2	5.51	1.31	1.25
3	8-D	246	SER	CA-CB	5.51	1.61	1.52
3	7-D	357	GLY	C-N	5.51	1.46	1.34
1	9-A	171	ARG	CZ-NH1	5.51	1.40	1.33
1	10-A	624	ARG	CZ-NH2	5.51	1.40	1.33
3	1-C	370	ASN	CA-CB	5.50	1.67	1.53
3	6-C	394	PHE	CG-CD1	5.50	1.47	1.38
2	7-B	433	TYR	CD1-CE1	5.50	1.47	1.39
2	6-B	846	ARG	CZ-NH2	5.50	1.40	1.33
1	5-A	190	TYR	CG-CD2	5.50	1.46	1.39
2	6-B	295	ARG	CZ-NH1	5.50	1.40	1.33
2	7-B	514	ARG	CZ-NH2	5.50	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-D	243	ARG	NE-CZ	5.50	1.40	1.33
3	9-D	154	LEU	CA-CB	5.50	1.66	1.53
2	10-B	288	TYR	CG-CD2	5.50	1.46	1.39
1	1-A	479	ARG	CZ-NH1	5.49	1.40	1.33
3	1-D	55	ARG	NE-CZ	5.49	1.40	1.33
2	5-B	562	TYR	CA-CB	5.49	1.66	1.53
2	8-B	400	TYR	CG-CD2	5.49	1.46	1.39
2	9-B	389	ARG	CZ-NH1	5.49	1.40	1.33
3	1-D	307	SER	CA-CB	5.49	1.61	1.52
1	9-A	776	ARG	CD-NE	5.49	1.55	1.46
3	10-C	55	ARG	CD-NE	5.49	1.55	1.46
1	8-A	204	ARG	CD-NE	5.49	1.55	1.46
1	5-A	575	SER	CA-CB	5.49	1.61	1.52
2	9-B	433	TYR	CZ-OH	5.48	1.47	1.37
2	1-B	228	GLY	C-N	5.48	1.46	1.34
2	7-B	439	ARG	NE-CZ	5.48	1.40	1.33
1	10-A	400	ARG	CZ-NH1	5.48	1.40	1.33
1	8-A	364	PRO	N-CA	5.48	1.56	1.47
3	10-C	109	TYR	CZ-OH	5.48	1.47	1.37
1	4-A	76	ARG	NE-CZ	5.48	1.40	1.33
1	4-A	143	ARG	CZ-NH1	5.48	1.40	1.33
2	4-B	526	ARG	CZ-NH1	5.48	1.40	1.33
2	6-B	299	ARG	CD-NE	5.48	1.55	1.46
3	6-D	241	SER	CB-OG	5.48	1.49	1.42
1	8-A	582	TYR	CZ-OH	5.48	1.47	1.37
2	10-B	349	TRP	NE1-CE2	5.48	1.44	1.37
2	9-B	488	PHE	CB-CG	5.47	1.60	1.51
2	10-B	578	PHE	CE1-CZ	5.47	1.47	1.37
1	2-A	687	ARG	CZ-NH2	5.47	1.40	1.33
1	7-A	157	ARG	CZ-NH1	5.47	1.40	1.33
1	10-A	623	ARG	CZ-NH2	5.47	1.40	1.33
3	10-D	72	GLU	C-N	5.47	1.44	1.34
3	9-C	398	PHE	CA-CB	5.47	1.66	1.53
3	1-D	437	TYR	CG-CD1	5.47	1.46	1.39
1	4-A	601	GLU	CD-OE1	5.47	1.31	1.25
3	8-D	348	SER	CA-CB	5.47	1.61	1.52
1	2-A	413	TYR	CG-CD1	5.47	1.46	1.39
3	5-C	319	TYR	CE2-CZ	5.47	1.45	1.38
3	4-C	445	TYR	CG-CD2	5.46	1.46	1.39
2	7-B	659	GLU	CG-CD	5.46	1.60	1.51
2	7-B	816	TYR	CG-CD1	5.46	1.46	1.39
3	7-D	28	GLU	CG-CD	5.46	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	8-D	118	ASP	CA-CB	5.46	1.66	1.53
3	8-C	161	ARG	CD-NE	5.46	1.55	1.46
3	2-C	356	ILE	C-N	5.46	1.42	1.33
3	3-C	65	ARG	NE-CZ	5.46	1.40	1.33
3	9-D	176	ARG	CZ-NH2	5.46	1.40	1.33
3	5-D	55	ARG	CZ-NH1	5.46	1.40	1.33
3	5-D	184	SER	CA-CB	5.46	1.61	1.52
1	2-A	450	TYR	CG-CD2	5.45	1.46	1.39
1	2-A	767	TYR	CG-CD1	5.45	1.46	1.39
2	3-B	335	PHE	CA-CB	5.45	1.66	1.53
2	5-B	438	TYR	CE1-CZ	-5.45	1.31	1.38
1	8-A	77	TYR	CZ-OH	5.45	1.47	1.37
1	8-A	759	GLU	CD-OE2	5.45	1.31	1.25
3	9-C	193	ARG	NE-CZ	5.45	1.40	1.33
1	4-A	794	TYR	CB-CG	5.45	1.59	1.51
2	1-B	526	ARG	CZ-NH2	5.44	1.40	1.33
2	7-B	583	TYR	CZ-OH	5.44	1.47	1.37
1	10-A	627	ARG	CZ-NH2	5.44	1.40	1.33
3	8-C	347	TRP	CE3-CZ3	5.44	1.47	1.38
1	9-A	278	ASP	CB-CG	5.44	1.63	1.51
1	9-A	299	PHE	CG-CD1	5.44	1.47	1.38
3	5-C	10	ALA	C-N	5.44	1.42	1.33
1	1-A	298	GLU	CD-OE1	5.44	1.31	1.25
2	5-B	772	PHE	CG-CD2	5.44	1.47	1.38
2	8-B	824	TYR	CG-CD2	5.43	1.46	1.39
2	2-B	526	ARG	CD-NE	5.43	1.55	1.46
3	3-C	237	SER	CA-CB	5.43	1.61	1.52
1	6-A	400	ARG	NE-CZ	5.43	1.40	1.33
3	6-D	333	ARG	CZ-NH1	5.43	1.40	1.33
3	5-D	341	ARG	CZ-NH1	5.43	1.40	1.33
3	6-D	435	GLU	CB-CG	5.43	1.62	1.52
2	1-B	258	SER	CB-OG	5.43	1.49	1.42
1	6-A	121	ARG	CD-NE	5.43	1.55	1.46
2	2-B	342	TYR	CE2-CZ	5.42	1.45	1.38
1	7-A	111	ARG	CG-CD	5.42	1.65	1.51
3	10-C	279	TYR	CE2-CZ	5.42	1.45	1.38
1	4-A	78	PHE	CD2-CE2	5.42	1.50	1.39
2	6-B	469	HIS	CB-CG	5.42	1.59	1.50
3	8-C	359	ARG	CZ-NH1	5.42	1.40	1.33
2	10-B	523	SER	CA-CB	5.42	1.61	1.52
1	4-A	143	ARG	NE-CZ	5.42	1.40	1.33
3	5-C	152	SER	CA-CB	5.42	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	10-B	612	ARG	CZ-NH1	5.42	1.40	1.33
2	4-B	225	PHE	CG-CD2	5.42	1.46	1.38
3	4-C	323	ILE	C-N	5.41	1.42	1.33
3	7-D	43	SER	CA-CB	5.41	1.61	1.52
2	5-B	293	ARG	CD-NE	5.41	1.55	1.46
2	7-B	776	TYR	CE1-CZ	5.41	1.45	1.38
3	2-C	243	ARG	CZ-NH2	5.41	1.40	1.33
1	6-A	262	ARG	CZ-NH1	5.41	1.40	1.33
1	3-A	108	ARG	CD-NE	5.41	1.55	1.46
2	3-B	565	TYR	CZ-OH	5.41	1.47	1.37
2	3-B	646	SER	CB-OG	-5.41	1.35	1.42
3	3-C	423	PHE	CG-CD1	5.41	1.46	1.38
3	5-C	367	PRO	N-CD	5.41	1.55	1.47
1	6-A	147	GLU	CD-OE1	5.41	1.31	1.25
3	7-C	62	PHE	CG-CD2	5.41	1.46	1.38
3	6-C	430	VAL	CB-CG1	5.41	1.64	1.52
1	2-A	576	ARG	CZ-NH1	5.40	1.40	1.33
3	1-D	170	TYR	CE2-CZ	5.40	1.45	1.38
1	2-A	193	TYR	CD2-CE2	5.40	1.47	1.39
2	2-B	342	TYR	CE1-CZ	5.40	1.45	1.38
3	3-D	394	PHE	CG-CD1	5.40	1.46	1.38
1	9-A	400	ARG	NE-CZ	5.40	1.40	1.33
2	10-B	826	PHE	CB-CG	5.40	1.60	1.51
3	2-D	185	TYR	CE1-CZ	5.40	1.45	1.38
3	6-C	319	TYR	CE2-CZ	5.40	1.45	1.38
1	9-A	398	TYR	CG-CD2	5.40	1.46	1.39
2	8-B	593	PHE	CG-CD2	5.40	1.46	1.38
1	10-A	320	TRP	CB-CG	5.40	1.59	1.50
3	1-C	319	TYR	CG-CD1	5.40	1.46	1.39
1	9-A	630	ARG	CZ-NH1	5.40	1.40	1.33
1	9-A	677	GLU	CD-OE2	5.40	1.31	1.25
3	7-D	73	PRO	CA-C	-5.40	1.42	1.52
2	10-B	758	TYR	CZ-OH	5.40	1.47	1.37
2	2-B	652	TYR	CE2-CZ	5.39	1.45	1.38
2	7-B	432	LEU	CA-CB	5.39	1.66	1.53
2	8-B	824	TYR	CG-CD1	5.39	1.46	1.39
1	3-A	320	TRP	CD2-CE3	-5.39	1.32	1.40
1	3-A	706	PHE	CA-CB	5.39	1.65	1.53
3	4-C	341	ARG	NE-CZ	5.39	1.40	1.33
1	6-A	144	ARG	CZ-NH1	5.39	1.40	1.33
2	2-B	526	ARG	CZ-NH2	5.39	1.40	1.33
2	6-B	533	ARG	CD-NE	5.39	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	8-D	83	PHE	CG-CD1	5.39	1.46	1.38
3	9-C	192	ARG	CZ-NH1	5.39	1.40	1.33
2	10-B	650	SER	CA-CB	5.39	1.61	1.52
3	5-C	196	GLU	CD-OE2	5.39	1.31	1.25
2	1-B	445	PHE	CG-CD1	5.38	1.46	1.38
3	4-C	161	ARG	NE-CZ	5.38	1.40	1.33
3	7-C	4	GLU	CG-CD	5.38	1.60	1.51
2	10-B	592	ARG	NE-CZ	5.38	1.40	1.33
3	3-C	346	SER	CA-CB	5.38	1.61	1.52
2	4-B	289	GLU	CD-OE1	5.38	1.31	1.25
3	1-C	415	SER	CA-CB	5.38	1.61	1.52
2	4-B	288	TYR	CE2-CZ	5.38	1.45	1.38
3	5-D	170	TYR	CE1-CZ	5.38	1.45	1.38
1	1-A	706	PHE	CE2-CZ	5.38	1.47	1.37
3	4-D	256	TYR	CG-CD2	5.38	1.46	1.39
2	5-B	776	TYR	CE1-CZ	5.38	1.45	1.38
3	8-D	243	ARG	CZ-NH2	5.38	1.40	1.33
2	1-B	286	GLU	CD-OE1	5.38	1.31	1.25
3	2-C	341	ARG	NE-CZ	5.38	1.40	1.33
1	10-A	413	TYR	CZ-OH	5.38	1.47	1.37
2	1-B	812	ILE	C-N	5.38	1.46	1.34
3	8-C	392	ASN	CB-CG	5.38	1.63	1.51
3	6-C	55	ARG	CD-NE	5.37	1.55	1.46
1	8-A	775	PHE	N-CA	-5.37	1.35	1.46
3	8-D	41	ASP	CB-CG	5.37	1.63	1.51
3	1-D	193	ARG	NE-CZ	5.37	1.40	1.33
3	2-D	112	GLY	N-CA	-5.37	1.38	1.46
2	9-B	600	TYR	CE1-CZ	5.37	1.45	1.38
3	1-C	279	TYR	CZ-OH	5.37	1.47	1.37
2	7-B	471	ARG	NE-CZ	5.37	1.40	1.33
3	3-C	383	VAL	CB-CG2	5.37	1.64	1.52
3	6-C	133	PHE	CE1-CZ	5.37	1.47	1.37
3	5-D	399	ALA	CA-CB	5.36	1.63	1.52
2	4-B	837	GLU	CG-CD	5.36	1.59	1.51
3	2-D	341	ARG	CZ-NH2	5.36	1.40	1.33
2	5-B	407	LYS	CA-CB	5.36	1.65	1.53
3	9-C	20	PHE	CE1-CZ	5.36	1.47	1.37
2	6-B	511	LYS	CA-CB	5.36	1.65	1.53
2	6-B	526	ARG	CD-NE	5.36	1.55	1.46
1	10-A	767	TYR	CE2-CZ	5.36	1.45	1.38
3	1-D	176	ARG	NE-CZ	5.36	1.40	1.33
3	4-C	67	ILE	CA-C	-5.36	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	10-A	675	GLU	CD-OE1	5.35	1.31	1.25
3	10-D	256	TYR	CG-CD1	5.35	1.46	1.39
3	9-C	380	MET	CA-C	-5.35	1.39	1.52
3	6-D	12	GLN	CA-CB	5.35	1.65	1.53
1	9-A	333	ARG	CZ-NH1	5.35	1.40	1.33
3	1-C	163	PRO	N-CD	-5.35	1.40	1.47
1	5-A	338	GLU	CD-OE2	5.35	1.31	1.25
3	7-C	407	TYR	CE2-CZ	5.35	1.45	1.38
2	9-B	592	ARG	CZ-NH1	5.35	1.40	1.33
2	1-B	837	GLU	CG-CD	-5.34	1.44	1.51
1	8-A	279	TYR	CG-CD2	5.34	1.46	1.39
1	8-A	630	ARG	CZ-NH1	5.34	1.40	1.33
3	10-C	243	ARG	CZ-NH1	5.34	1.40	1.33
3	4-D	53	PHE	CG-CD1	5.34	1.46	1.38
1	7-A	77	TYR	CD1-CE1	5.34	1.47	1.39
3	8-C	398	PHE	CG-CD1	5.34	1.46	1.38
1	2-A	479	ARG	CZ-NH1	5.34	1.40	1.33
3	9-C	292	TYR	CG-CD1	5.34	1.46	1.39
2	7-B	822	ARG	CZ-NH1	5.34	1.40	1.33
1	5-A	377	GLU	CG-CD	5.34	1.59	1.51
1	5-A	91	GLU	CD-OE1	-5.33	1.19	1.25
3	2-D	188	ILE	CA-CB	5.33	1.67	1.54
1	4-A	704	TYR	CE2-CZ	5.33	1.45	1.38
3	7-C	170	TYR	CG-CD2	5.33	1.46	1.39
2	2-B	285	ARG	CZ-NH2	5.33	1.40	1.33
1	6-A	479	ARG	CD-NE	5.33	1.55	1.46
1	6-A	116	TYR	CE1-CZ	5.33	1.45	1.38
1	5-A	465	PHE	CG-CD2	5.33	1.46	1.38
3	8-C	427	ARG	CZ-NH2	5.33	1.40	1.33
2	9-B	822	ARG	CZ-NH1	5.33	1.40	1.33
3	7-D	72	GLU	C-N	5.33	1.44	1.34
1	10-A	436	LEU	CA-CB	5.33	1.66	1.53
2	3-B	306	GLU	CD-OE1	5.32	1.31	1.25
1	10-A	262	ARG	CZ-NH2	5.32	1.40	1.33
1	2-A	380	ASP	N-CA	-5.32	1.35	1.46
3	10-D	394	PHE	CA-CB	5.32	1.65	1.53
1	3-A	489	GLU	CG-CD	5.32	1.59	1.51
2	3-B	297	TYR	CE1-CZ	5.32	1.45	1.38
2	6-B	300	PHE	CE2-CZ	5.32	1.47	1.37
3	8-D	275	PHE	CB-CG	-5.32	1.42	1.51
3	2-C	176	ARG	NE-CZ	5.32	1.40	1.33
1	7-A	664	ARG	CD-NE	5.32	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-A	714	ARG	CZ-NH1	5.32	1.40	1.33
2	10-B	741	PHE	CG-CD2	5.32	1.46	1.38
1	3-A	639	PHE	CG-CD2	5.32	1.46	1.38
1	6-A	603	TRP	CB-CG	5.32	1.59	1.50
3	6-D	302	SER	CB-OG	5.32	1.49	1.42
1	8-A	339	GLU	CD-OE1	5.32	1.31	1.25
1	10-A	402	ASN	CB-CG	5.32	1.63	1.51
3	1-C	444	SER	CA-CB	5.31	1.60	1.52
1	4-A	243	LYS	C-N	5.31	1.42	1.33
2	5-B	418	GLU	CD-OE1	5.31	1.31	1.25
3	10-D	132	ASN	CB-CG	5.31	1.63	1.51
3	8-D	279	TYR	CA-CB	5.31	1.65	1.53
3	6-C	290	SER	CB-OG	5.31	1.49	1.42
2	1-B	274	SER	CB-OG	5.31	1.49	1.42
2	6-B	612	ARG	CZ-NH2	5.31	1.40	1.33
1	1-A	131	PHE	CE1-CZ	5.31	1.47	1.37
1	1-A	772	SER	CA-CB	5.31	1.60	1.52
1	3-A	204	ARG	NE-CZ	5.31	1.40	1.33
3	6-D	86	PHE	CG-CD2	5.31	1.46	1.38
3	7-D	407	TYR	CE2-CZ	5.31	1.45	1.38
2	2-B	455	GLU	CD-OE1	5.30	1.31	1.25
1	3-A	251	PHE	CE2-CZ	5.30	1.47	1.37
3	4-C	55	ARG	NE-CZ	5.30	1.40	1.33
2	5-B	395	PRO	N-CD	-5.30	1.40	1.47
3	7-D	427	ARG	N-CA	-5.30	1.35	1.46
1	8-A	608	LYS	CD-CE	5.30	1.64	1.51
1	3-A	144	ARG	CZ-NH1	5.30	1.40	1.33
2	4-B	580	ARG	NE-CZ	5.30	1.40	1.33
3	4-C	93	TRP	CB-CG	5.30	1.59	1.50
2	8-B	598	TYR	CZ-OH	5.30	1.46	1.37
3	4-D	291	SER	CB-OG	5.30	1.49	1.42
1	9-A	185	GLN	CA-CB	5.30	1.65	1.53
3	2-C	70	ASP	CA-CB	5.29	1.65	1.53
2	2-B	231	TYR	CG-CD2	5.29	1.46	1.39
3	3-D	415	SER	CA-CB	5.29	1.60	1.52
3	3-D	428	GLU	CD-OE1	-5.29	1.19	1.25
2	4-B	295	ARG	CZ-NH1	5.29	1.40	1.33
3	3-C	23	SER	CA-CB	5.29	1.60	1.52
1	9-A	187	GLU	CB-CG	5.29	1.62	1.52
3	9-D	403	PHE	CG-CD2	5.29	1.46	1.38
1	1-A	124	GLU	CD-OE1	-5.29	1.19	1.25
2	1-B	258	SER	CA-CB	5.29	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-A	624	ARG	CZ-NH2	5.29	1.40	1.33
3	7-C	109	TYR	CB-CG	5.29	1.59	1.51
3	10-C	395	ASP	CA-CB	5.29	1.65	1.53
3	2-D	65	ARG	NE-CZ	5.28	1.40	1.33
2	3-B	846	ARG	CD-NE	5.28	1.55	1.46
1	9-A	469	ARG	CZ-NH2	5.28	1.40	1.33
2	10-B	585	ARG	CD-NE	5.28	1.55	1.46
3	10-D	369	GLU	CD-OE1	5.28	1.31	1.25
1	10-A	160	ARG	NE-CZ	5.28	1.40	1.33
3	2-D	90	ARG	CZ-NH2	5.28	1.40	1.33
3	7-C	271	SER	CA-CB	5.28	1.60	1.52
2	3-B	542	ASP	CB-CG	5.28	1.62	1.51
1	6-A	597	ARG	CZ-NH1	5.28	1.40	1.33
2	4-B	555	TRP	NE1-CE2	5.28	1.44	1.37
1	4-A	190	TYR	CG-CD1	5.28	1.46	1.39
1	6-A	108	ARG	CZ-NH1	5.28	1.40	1.33
2	2-B	567	PRO	N-CD	-5.27	1.40	1.47
1	4-A	171	ARG	CD-NE	5.27	1.55	1.46
3	10-D	111	ILE	C-N	5.27	1.42	1.33
2	3-B	344	GLU	CD-OE2	-5.27	1.19	1.25
1	4-A	284	TYR	CD1-CE1	5.27	1.47	1.39
1	10-A	700	PHE	CE1-CZ	5.27	1.47	1.37
3	1-D	59	ARG	CD-NE	5.27	1.55	1.46
3	4-D	162	TYR	CE2-CZ	5.27	1.45	1.38
3	5-C	413	PHE	CG-CD2	5.27	1.46	1.38
3	7-C	204	PHE	CG-CD1	5.27	1.46	1.38
3	8-D	47	ASP	CA-CB	5.27	1.65	1.53
3	8-D	141	SER	CA-CB	5.27	1.60	1.52
3	8-D	333	ARG	CD-NE	5.27	1.55	1.46
1	9-A	714	ARG	CD-NE	5.27	1.55	1.46
1	2-A	429	TYR	CE1-CZ	5.27	1.45	1.38
3	5-C	432	SER	CA-CB	5.27	1.60	1.52
3	4-C	71	SER	CB-OG	5.27	1.49	1.42
2	9-B	562	TYR	CB-CG	-5.27	1.43	1.51
3	6-D	367	PRO	N-CD	-5.26	1.40	1.47
1	10-A	558	TYR	CD2-CE2	5.26	1.47	1.39
2	3-B	670	ARG	NE-CZ	5.26	1.39	1.33
3	8-C	348	SER	CA-CB	5.26	1.60	1.52
2	3-B	356	ARG	CZ-NH2	5.26	1.39	1.33
2	3-B	421	TRP	CZ2-CH2	5.26	1.47	1.37
3	3-C	218	ARG	NE-CZ	5.26	1.39	1.33
3	6-D	176	ARG	NE-CZ	5.26	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	8-B	544	ARG	CZ-NH2	5.26	1.39	1.33
1	10-A	388	SER	N-CA	5.26	1.56	1.46
1	8-A	112	TYR	C-N	5.26	1.42	1.33
3	10-D	16	HIS	CG-CD2	5.26	1.44	1.35
3	4-C	400	LYS	C-N	5.25	1.42	1.33
2	1-B	300	PHE	CG-CD1	5.25	1.46	1.38
3	1-D	27	LYS	CD-CE	5.25	1.64	1.51
2	4-B	591	TRP	CZ2-CH2	5.25	1.47	1.37
1	5-A	707	CYS	CB-SG	5.25	1.91	1.82
2	5-B	470	TYR	CG-CD2	5.25	1.46	1.39
3	6-C	114	ARG	CD-NE	5.25	1.55	1.46
2	6-B	395	PRO	N-CD	-5.25	1.40	1.47
2	6-B	413	GLU	CD-OE2	5.25	1.31	1.25
1	9-A	143	ARG	CD-NE	5.25	1.55	1.46
3	1-D	133	PHE	CB-CG	-5.25	1.42	1.51
3	2-D	13	CYS	C-N	5.25	1.42	1.33
3	6-C	315	TYR	CD1-CE1	5.25	1.47	1.39
2	9-B	644	PHE	CG-CD2	5.25	1.46	1.38
3	1-D	4	GLU	CA-CB	5.25	1.65	1.53
2	1-B	425	PHE	CG-CD2	5.24	1.46	1.38
1	3-A	793	PHE	CG-CD2	5.24	1.46	1.38
2	6-B	297	TYR	CZ-OH	5.24	1.46	1.37
1	8-A	299	PHE	CG-CD2	5.24	1.46	1.38
3	8-D	176	ARG	NE-CZ	5.24	1.39	1.33
1	4-A	298	GLU	CD-OE1	5.24	1.31	1.25
3	5-C	74	SER	CA-CB	5.24	1.60	1.52
3	10-C	24	GLN	N-CA	-5.24	1.35	1.46
2	5-B	612	ARG	NE-CZ	5.24	1.39	1.33
1	6-A	148	ASP	CB-CG	5.24	1.62	1.51
3	6-D	77	ALA	CA-CB	5.24	1.63	1.52
3	3-C	358	ARG	CZ-NH1	5.24	1.39	1.33
3	6-D	174	PRO	N-CD	-5.24	1.40	1.47
2	7-B	580	ARG	NE-CZ	5.24	1.39	1.33
3	10-D	293	ASP	CA-CB	5.24	1.65	1.53
3	1-D	410	GLY	N-CA	-5.23	1.38	1.46
1	6-A	198	ARG	CZ-NH2	5.23	1.39	1.33
3	7-C	264	GLU	CD-OE1	5.23	1.31	1.25
3	9-C	430	VAL	CB-CG2	5.23	1.63	1.52
3	3-D	161	ARG	CD-NE	5.23	1.55	1.46
1	3-A	108	ARG	NE-CZ	5.23	1.39	1.33
2	9-B	558	PHE	CG-CD2	5.23	1.46	1.38
1	1-A	358	ARG	CZ-NH2	5.23	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-A	647	PHE	CG-CD2	5.22	1.46	1.38
2	4-B	426	SER	CA-CB	5.22	1.60	1.52
3	8-C	84	ARG	CD-NE	5.22	1.55	1.46
2	9-B	651	TYR	CG-CD2	5.22	1.46	1.39
2	1-B	494	GLU	CD-OE1	5.22	1.31	1.25
1	4-A	203	ARG	CD-NE	5.22	1.55	1.46
1	4-A	105	PHE	CG-CD2	5.22	1.46	1.38
3	4-C	176	ARG	NE-CZ	5.22	1.39	1.33
2	9-B	633	ARG	CZ-NH1	5.21	1.39	1.33
1	2-A	789	GLU	CD-OE2	5.21	1.31	1.25
1	6-A	111	ARG	CD-NE	5.21	1.55	1.46
3	2-C	170	TYR	CE1-CZ	5.21	1.45	1.38
3	3-C	190	ALA	CA-CB	5.21	1.63	1.52
1	6-A	704	TYR	CD2-CE2	5.21	1.47	1.39
1	9-A	121	ARG	CZ-NH2	5.21	1.39	1.33
3	10-C	437	TYR	CZ-OH	5.21	1.46	1.37
3	8-D	87	PHE	CG-CD1	5.21	1.46	1.38
3	6-C	218	ARG	CZ-NH1	5.21	1.39	1.33
3	3-C	249	TYR	CE2-CZ	5.20	1.45	1.38
3	3-D	176	ARG	CZ-NH1	5.20	1.39	1.33
3	5-C	403	PHE	CB-CG	5.20	1.60	1.51
3	6-D	264	GLU	CD-OE2	5.20	1.31	1.25
1	9-A	772	SER	N-CA	-5.20	1.35	1.46
3	9-C	291	SER	CA-CB	5.20	1.60	1.52
2	1-B	580	ARG	CZ-NH1	5.20	1.39	1.33
2	3-B	413	GLU	CD-OE1	5.20	1.31	1.25
2	10-B	284	TYR	CZ-OH	5.20	1.46	1.37
3	10-C	402	ALA	CA-CB	5.20	1.63	1.52
3	2-D	192	ARG	CZ-NH1	5.20	1.39	1.33
3	9-C	432	SER	CA-CB	5.20	1.60	1.52
1	1-A	381	PHE	CD2-CE2	5.20	1.49	1.39
2	4-B	418	GLU	CG-CD	5.20	1.59	1.51
3	5-D	53	PHE	CG-CD2	5.20	1.46	1.38
1	7-A	106	SER	CA-CB	5.20	1.60	1.52
3	8-C	176	ARG	CZ-NH1	5.20	1.39	1.33
2	4-B	770	TYR	CG-CD2	5.19	1.46	1.39
2	2-B	389	ARG	CZ-NH2	5.19	1.39	1.33
3	3-C	407	TYR	CZ-OH	5.19	1.46	1.37
2	8-B	600	TYR	CD1-CE1	5.19	1.47	1.39
2	2-B	670	ARG	CZ-NH2	5.19	1.39	1.33
1	3-A	262	ARG	NE-CZ	5.19	1.39	1.33
3	8-D	55	ARG	CZ-NH2	5.19	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5-B	836	GLU	CD-OE1	5.19	1.31	1.25
2	2-B	771	GLU	CD-OE1	5.19	1.31	1.25
3	2-D	83	PHE	CE1-CZ	5.19	1.47	1.37
3	5-C	174	PRO	CA-C	-5.19	1.42	1.52
2	2-B	770	TYR	CE1-CZ	5.19	1.45	1.38
1	5-A	113	GLY	CA-C	-5.18	1.43	1.51
2	8-B	632	SER	CA-CB	5.18	1.60	1.52
2	2-B	301	THR	C-N	5.18	1.46	1.34
3	5-C	427	ARG	CD-NE	5.18	1.55	1.46
3	5-C	84	ARG	CZ-NH1	5.18	1.39	1.33
1	7-A	623	ARG	CZ-NH2	5.18	1.39	1.33
3	7-C	348	SER	CA-CB	5.18	1.60	1.52
3	9-C	441	GLU	CG-CD	5.18	1.59	1.51
2	3-B	638	ARG	CZ-NH1	5.17	1.39	1.33
1	4-A	704	TYR	CE1-CZ	5.17	1.45	1.38
1	7-A	429	TYR	CA-CB	5.17	1.65	1.53
3	8-D	426	SER	CA-CB	5.17	1.60	1.52
1	2-A	108	ARG	CZ-NH2	5.17	1.39	1.33
2	2-B	470	TYR	CZ-OH	5.17	1.46	1.37
1	10-A	358	ARG	CZ-NH2	5.17	1.39	1.33
1	1-A	567	PRO	N-CD	5.17	1.55	1.47
1	4-A	450	TYR	CE2-CZ	5.17	1.45	1.38
1	9-A	116	TYR	CB-CG	-5.17	1.43	1.51
2	6-B	592	ARG	CD-NE	5.17	1.55	1.46
3	9-D	105	TRP	NE1-CE2	5.17	1.44	1.37
2	3-B	591	TRP	CD2-CE3	-5.17	1.32	1.40
3	5-C	256	TYR	CE1-CZ	5.17	1.45	1.38
2	6-B	255	ILE	N-CA	-5.17	1.36	1.46
2	8-B	238	VAL	CB-CG2	5.17	1.63	1.52
1	2-A	405	PHE	CG-CD1	5.17	1.46	1.38
3	4-D	287	LYS	C-N	5.17	1.42	1.33
2	8-B	576	ARG	NE-CZ	5.17	1.39	1.33
2	9-B	826	PHE	CG-CD1	5.17	1.46	1.38
1	2-A	428	GLY	N-CA	-5.16	1.38	1.46
2	3-B	638	ARG	CZ-NH2	5.16	1.39	1.33
3	3-C	74	SER	CA-CB	5.16	1.60	1.52
3	6-D	445	TYR	CE1-CZ	-5.16	1.31	1.38
3	1-D	53	PHE	CA-CB	5.16	1.65	1.53
2	2-B	389	ARG	NE-CZ	5.16	1.39	1.33
2	2-B	545	VAL	CB-CG1	5.16	1.63	1.52
2	6-B	282	SER	CA-CB	5.16	1.60	1.52
1	7-A	677	GLU	C-N	5.16	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1-B	663	GLU	CG-CD	5.16	1.59	1.51
2	6-B	580	ARG	NE-CZ	5.16	1.39	1.33
1	7-A	663	TYR	CZ-OH	5.16	1.46	1.37
2	10-B	346	LEU	N-CA	-5.16	1.36	1.46
1	10-A	116	TYR	CE1-CZ	5.16	1.45	1.38
1	2-A	286	TRP	CD2-CE3	5.16	1.48	1.40
1	6-A	576	ARG	CD-NE	5.16	1.55	1.46
3	6-D	329	ARG	CD-NE	5.16	1.55	1.46
3	9-C	241	SER	CA-CB	5.16	1.60	1.52
3	3-D	444	SER	CA-CB	5.15	1.60	1.52
2	7-B	776	TYR	CZ-OH	5.15	1.46	1.37
3	8-C	279	TYR	CE1-CZ	5.15	1.45	1.38
1	10-A	486	PHE	CG-CD2	5.15	1.46	1.38
1	3-A	112	TYR	CD1-CE1	5.15	1.47	1.39
3	4-D	208	SER	CA-CB	5.15	1.60	1.52
1	5-A	78	PHE	CG-CD2	5.15	1.46	1.38
3	6-C	427	ARG	NE-CZ	5.15	1.39	1.33
3	1-D	192	ARG	CD-NE	5.15	1.55	1.46
2	8-B	231	TYR	CG-CD1	5.15	1.45	1.39
3	8-D	51	LYS	C-N	5.15	1.44	1.34
3	1-C	359	ARG	NE-CZ	5.15	1.39	1.33
1	5-A	107	ARG	CD-NE	5.15	1.55	1.46
2	5-B	758	TYR	CZ-OH	5.15	1.46	1.37
1	7-A	74	TYR	CZ-OH	5.15	1.46	1.37
2	10-B	411	PHE	CA-C	-5.15	1.39	1.52
3	10-D	253	SER	CA-CB	5.15	1.60	1.52
2	5-B	777	CYS	CA-CB	5.15	1.65	1.53
2	8-B	798	SER	CA-CB	5.15	1.60	1.52
1	4-A	468	GLU	CD-OE1	5.14	1.31	1.25
3	9-C	423	PHE	CG-CD2	5.14	1.46	1.38
3	9-D	350	SER	CA-CB	5.14	1.60	1.52
1	10-A	68	ILE	C-N	5.14	1.42	1.33
3	5-D	109	TYR	CE2-CZ	5.14	1.45	1.38
3	5-D	423	PHE	CE1-CZ	5.14	1.47	1.37
3	9-D	275	PHE	CE1-CZ	5.14	1.47	1.37
1	5-A	56	GLU	CD-OE2	-5.14	1.20	1.25
3	8-D	415	SER	CA-CB	5.14	1.60	1.52
1	10-A	624	ARG	CZ-NH1	5.14	1.39	1.33
3	5-D	427	ARG	NE-CZ	5.14	1.39	1.33
1	9-A	612	TRP	CD1-NE1	-5.14	1.29	1.38
3	4-C	193	ARG	NE-CZ	5.13	1.39	1.33
3	8-D	341	ARG	CD-NE	5.13	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-A	404	ILE	C-N	5.13	1.45	1.34
3	5-C	359	ARG	CZ-NH2	5.13	1.39	1.33
2	7-B	483	MET	C-N	5.13	1.42	1.33
1	3-A	657	TYR	CG-CD1	5.13	1.45	1.39
2	3-B	190	TYR	CE2-CZ	5.13	1.45	1.38
3	4-C	243	ARG	CZ-NH2	5.13	1.39	1.33
1	7-A	127	SER	CA-CB	5.13	1.60	1.52
1	8-A	576	ARG	CD-NE	5.13	1.55	1.46
3	8-C	126	GLU	CG-CD	5.13	1.59	1.51
3	9-D	307	SER	CA-CB	5.13	1.60	1.52
1	10-A	126	TRP	CD2-CE3	-5.13	1.32	1.40
1	10-A	325	PHE	CE1-CZ	5.13	1.47	1.37
2	3-B	533	ARG	CA-CB	5.13	1.65	1.53
2	6-B	242	ARG	CZ-NH2	5.13	1.39	1.33
1	7-A	358	ARG	CZ-NH1	5.13	1.39	1.33
1	7-A	664	ARG	NE-CZ	5.13	1.39	1.33
1	2-A	99	ASP	CA-CB	5.13	1.65	1.53
1	6-A	320	TRP	NE1-CE2	-5.13	1.30	1.37
3	10-D	20	PHE	CE2-CZ	5.13	1.47	1.37
3	1-D	136	PHE	CE1-CZ	5.13	1.47	1.37
3	1-D	444	SER	CA-CB	5.13	1.60	1.52
2	5-B	822	ARG	CZ-NH1	5.13	1.39	1.33
3	6-C	316	PHE	CG-CD1	5.13	1.46	1.38
2	1-B	438	TYR	CB-CG	5.12	1.59	1.51
2	2-B	312	PHE	CG-CD2	5.12	1.46	1.38
1	4-A	56	GLU	CA-CB	5.12	1.65	1.53
1	3-A	558	TYR	CZ-OH	5.12	1.46	1.37
1	5-A	704	TYR	CD1-CE1	5.12	1.47	1.39
2	5-B	217	GLU	CG-CD	5.12	1.59	1.51
1	6-A	143	ARG	CZ-NH1	5.12	1.39	1.33
2	8-B	343	TYR	CB-CG	-5.12	1.44	1.51
3	7-D	378	SER	CA-CB	5.12	1.60	1.52
3	9-C	398	PHE	N-CA	-5.12	1.36	1.46
3	9-D	349	SER	CB-OG	-5.12	1.35	1.42
1	1-A	202	GLU	CG-CD	5.12	1.59	1.51
2	3-B	533	ARG	CD-NE	5.12	1.55	1.46
3	3-D	22	TRP	CZ2-CH2	5.12	1.47	1.37
1	9-A	566	ILE	CA-C	5.12	1.66	1.52
3	3-C	435	GLU	CD-OE1	5.12	1.31	1.25
1	6-A	325	PHE	CE2-CZ	5.12	1.47	1.37
2	8-B	580	ARG	NE-CZ	5.11	1.39	1.33
3	7-C	435	GLU	CD-OE2	5.11	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	10-D	193	ARG	CZ-NH1	5.11	1.39	1.33
3	1-D	362	TYR	CG-CD1	5.11	1.45	1.39
1	4-A	623	ARG	CZ-NH1	5.11	1.39	1.33
2	10-B	558	PHE	CB-CG	5.11	1.60	1.51
2	9-B	585	ARG	CZ-NH2	5.11	1.39	1.33
2	2-B	282	SER	CA-CB	5.11	1.60	1.52
1	9-A	171	ARG	NE-CZ	5.11	1.39	1.33
3	10-C	65	ARG	CZ-NH1	5.11	1.39	1.33
2	6-B	488	PHE	CG-CD1	5.11	1.46	1.38
3	6-C	266	HIS	CA-CB	-5.11	1.42	1.53
1	7-A	657	TYR	CG-CD1	5.11	1.45	1.39
1	8-A	576	ARG	NE-CZ	5.11	1.39	1.33
1	8-A	597	ARG	CZ-NH1	5.11	1.39	1.33
3	8-D	42	SER	C-N	5.11	1.45	1.34
2	10-B	393	PHE	CG-CD1	5.11	1.46	1.38
1	1-A	172	GLU	CD-OE2	5.10	1.31	1.25
2	5-B	510	TYR	CE1-CZ	5.10	1.45	1.38
3	6-D	65	ARG	CZ-NH1	5.10	1.39	1.33
3	1-D	387	PHE	CG-CD1	5.10	1.46	1.38
1	8-A	663	TYR	CG-CD2	5.10	1.45	1.39
2	1-B	293	ARG	CZ-NH1	5.10	1.39	1.33
2	3-B	592	ARG	CZ-NH1	5.10	1.39	1.33
2	6-B	756	GLN	CD-NE2	5.10	1.45	1.32
2	8-B	349	TRP	CD2-CE2	5.10	1.47	1.41
2	10-B	585	ARG	CZ-NH1	5.10	1.39	1.33
2	1-B	822	ARG	NE-CZ	5.10	1.39	1.33
3	1-C	247	TYR	CE2-CZ	5.10	1.45	1.38
3	5-D	161	ARG	NE-CZ	5.10	1.39	1.33
3	7-C	327	GLU	CD-OE1	-5.10	1.20	1.25
3	9-C	216	VAL	CA-CB	-5.10	1.44	1.54
2	10-B	514	ARG	CZ-NH2	5.10	1.39	1.33
1	2-A	630	ARG	CZ-NH1	5.09	1.39	1.33
3	6-C	267	PHE	C-N	5.09	1.45	1.34
3	7-C	345	PRO	CA-CB	-5.09	1.43	1.53
3	7-D	65	ARG	NE-CZ	5.09	1.39	1.33
1	10-A	381	PHE	CG-CD1	5.09	1.46	1.38
3	3-C	114	ARG	CD-NE	5.09	1.55	1.46
3	3-D	362	TYR	CG-CD1	5.09	1.45	1.39
1	5-A	597	ARG	NE-CZ	5.09	1.39	1.33
3	7-C	41	ASP	N-CA	-5.09	1.36	1.46
3	7-C	411	ASP	N-CA	-5.09	1.36	1.46
2	4-B	299	ARG	CZ-NH1	5.09	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7-C	133	PHE	CG-CD1	5.09	1.46	1.38
1	8-A	614	TYR	CD2-CE2	5.09	1.47	1.39
3	10-C	398	PHE	CB-CG	5.09	1.60	1.51
2	2-B	295	ARG	NE-CZ	5.09	1.39	1.33
2	8-B	800	GLY	CA-C	-5.09	1.43	1.51
2	4-B	388	GLU	CG-CD	5.08	1.59	1.51
3	4-D	171	SER	CA-CB	5.08	1.60	1.52
3	2-D	427	ARG	NE-CZ	5.08	1.39	1.33
2	3-B	471	ARG	CZ-NH2	5.08	1.39	1.33
3	8-C	129	SER	CA-CB	5.08	1.60	1.52
2	9-B	445	PHE	CB-CG	5.08	1.59	1.51
1	4-A	624	ARG	CD-NE	5.08	1.55	1.46
2	4-B	827	ARG	CZ-NH2	5.08	1.39	1.33
2	8-B	585	ARG	CZ-NH2	5.08	1.39	1.33
1	9-A	349	ARG	CD-NE	5.08	1.55	1.46
2	10-B	365	ALA	CA-CB	5.08	1.63	1.52
2	4-B	342	TYR	CZ-OH	5.08	1.46	1.37
3	4-C	275	PHE	CG-CD2	5.08	1.46	1.38
3	6-D	319	TYR	CA-CB	5.08	1.65	1.53
1	7-A	121	ARG	CD-NE	5.08	1.55	1.46
3	2-C	429	VAL	CB-CG1	5.08	1.63	1.52
1	6-A	204	ARG	CD-NE	5.08	1.55	1.46
2	6-B	770	TYR	CD1-CE1	5.08	1.47	1.39
2	7-B	187	TYR	CG-CD2	5.08	1.45	1.39
3	7-C	394	PHE	CE1-CZ	5.08	1.47	1.37
1	2-A	245	GLY	CA-C	-5.07	1.43	1.51
3	2-D	161	ARG	NE-CZ	5.07	1.39	1.33
3	3-C	72	GLU	CG-CD	5.07	1.59	1.51
2	5-B	475	PHE	CB-CG	5.07	1.59	1.51
1	6-A	655	GLU	CB-CG	5.07	1.61	1.52
1	2-A	134	VAL	CB-CG2	5.07	1.63	1.52
1	2-A	795	ASP	C-N	5.07	1.45	1.34
1	1-A	438	PHE	CG-CD2	5.07	1.46	1.38
2	1-B	533	ARG	CZ-NH2	5.07	1.39	1.33
2	7-B	585	ARG	NE-CZ	5.07	1.39	1.33
2	1-B	228	GLY	N-CA	5.07	1.53	1.46
2	3-B	295	ARG	CZ-NH1	5.07	1.39	1.33
3	6-C	200	ALA	CA-CB	5.07	1.63	1.52
1	7-A	327	ARG	CD-NE	5.07	1.55	1.46
1	3-A	555	SER	CB-OG	5.06	1.48	1.42
3	5-D	1	MET	C-N	5.06	1.42	1.33
1	6-A	137	ARG	CZ-NH2	5.06	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	10-D	411	ASP	CA-CB	5.06	1.65	1.53
2	4-B	488	PHE	CG-CD2	5.06	1.46	1.38
2	5-B	435	SER	CB-OG	-5.06	1.35	1.42
2	6-B	555	TRP	CD2-CE2	5.06	1.47	1.41
1	7-A	324	TYR	CE1-CZ	5.06	1.45	1.38
1	8-A	767	TYR	CG-CD2	5.06	1.45	1.39
3	8-C	84	ARG	C-N	5.06	1.42	1.33
2	1-B	293	ARG	NE-CZ	5.06	1.39	1.33
3	9-D	224	LEU	N-CA	-5.06	1.36	1.46
2	3-B	486	SER	CA-CB	5.06	1.60	1.52
1	4-A	160	ARG	CZ-NH1	5.06	1.39	1.33
3	1-C	46	ARG	NE-CZ	5.05	1.39	1.33
1	5-A	405	PHE	CG-CD2	5.05	1.46	1.38
3	5-C	90	ARG	CD-NE	5.05	1.55	1.46
1	6-A	324	TYR	CG-CD2	5.05	1.45	1.39
3	7-D	329	ARG	CZ-NH2	5.05	1.39	1.33
1	9-A	714	ARG	CZ-NH1	5.05	1.39	1.33
1	4-A	568	TYR	CG-CD2	5.05	1.45	1.39
1	6-A	398	TYR	CG-CD1	5.05	1.45	1.39
3	7-D	220	PRO	N-CD	-5.05	1.40	1.47
1	1-A	105	PHE	CG-CD1	5.05	1.46	1.38
1	2-A	160	ARG	CZ-NH1	5.05	1.39	1.33
1	8-A	646	TYR	CE2-CZ	5.05	1.45	1.38
1	9-A	630	ARG	NE-CZ	5.05	1.39	1.33
2	3-B	459	HIS	CB-CG	5.05	1.59	1.50
1	8-A	688	CYS	CA-CB	-5.05	1.42	1.53
2	10-B	768	SER	CA-CB	5.05	1.60	1.52
3	8-C	162	TYR	CZ-OH	5.05	1.46	1.37
1	9-A	458	TYR	CG-CD2	5.05	1.45	1.39
3	4-D	413	PHE	N-CA	-5.04	1.36	1.46
2	1-B	214	PRO	C-N	5.04	1.45	1.34
1	4-A	486	PHE	CE2-CZ	5.04	1.47	1.37
2	4-B	766	LEU	CA-CB	-5.04	1.42	1.53
3	4-D	307	SER	CA-CB	5.04	1.60	1.52
3	9-C	157	ALA	CA-CB	5.04	1.63	1.52
1	3-A	78	PHE	CG-CD2	5.04	1.46	1.38
1	5-A	576	ARG	CA-CB	5.04	1.65	1.53
2	4-B	533	ARG	CZ-NH2	5.04	1.39	1.33
3	4-D	270	PRO	CA-C	-5.04	1.42	1.52
1	6-A	284	TYR	CZ-OH	5.04	1.46	1.37
2	8-B	299	ARG	NE-CZ	5.04	1.39	1.33
1	10-A	324	TYR	CZ-OH	5.04	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-C	344	PHE	CG-CD1	5.04	1.46	1.38
1	4-A	168	PHE	N-CA	-5.04	1.36	1.46
3	5-C	356	ILE	C-N	5.04	1.42	1.33
3	9-C	170	TYR	CE1-CZ	5.04	1.45	1.38
3	10-D	80	GLU	CG-CD	5.04	1.59	1.51
3	5-C	445	TYR	CZ-OH	5.04	1.46	1.37
3	7-D	428	GLU	CD-OE2	5.04	1.31	1.25
3	8-D	250	SER	CA-CB	5.04	1.60	1.52
2	9-B	442	SER	CA-CB	5.04	1.60	1.52
2	1-B	345	TYR	CE2-CZ	5.03	1.45	1.38
3	4-C	114	ARG	CD-NE	5.03	1.55	1.46
3	4-D	162	TYR	CE1-CZ	5.03	1.45	1.38
3	6-C	333	ARG	NE-CZ	5.03	1.39	1.33
3	6-D	245	PRO	N-CD	5.03	1.54	1.47
2	8-B	405	ILE	CA-CB	-5.03	1.43	1.54
3	9-C	59	ARG	CD-NE	5.03	1.55	1.46
1	1-A	601	GLU	CG-CD	5.03	1.59	1.51
1	4-A	252	GLN	CG-CD	5.03	1.62	1.51
2	7-B	267	PHE	CE2-CZ	5.03	1.47	1.37
1	1-A	137	ARG	NE-CZ	5.03	1.39	1.33
3	4-C	192	ARG	CD-NE	5.03	1.55	1.46
2	8-B	638	ARG	CZ-NH1	5.03	1.39	1.33
3	3-C	267	PHE	CA-CB	5.03	1.65	1.53
3	8-C	329	ARG	CZ-NH1	5.03	1.39	1.33
1	3-A	645	GLU	CB-CG	5.03	1.61	1.52
3	4-D	288	GLY	CA-C	-5.03	1.43	1.51
1	5-A	126	TRP	CG-CD1	5.03	1.43	1.36
3	5-D	358	ARG	CD-NE	5.03	1.54	1.46
1	9-A	405	PHE	CG-CD2	5.03	1.46	1.38
2	10-B	328	ARG	NE-CZ	5.03	1.39	1.33
3	10-C	184	SER	CB-OG	-5.02	1.35	1.42
3	2-D	104	SER	CA-CB	5.02	1.60	1.52
2	3-B	181	GLU	CG-CD	5.02	1.59	1.51
3	4-D	156	GLU	CG-CD	5.02	1.59	1.51
1	5-A	77	TYR	CG-CD1	5.02	1.45	1.39
3	6-D	193	ARG	CZ-NH1	5.02	1.39	1.33
2	7-B	633	ARG	CZ-NH2	5.02	1.39	1.33
1	8-A	101	SER	CA-CB	5.02	1.60	1.52
2	10-B	259	GLU	CB-CG	5.02	1.61	1.52
2	7-B	356	ARG	CD-NE	5.02	1.54	1.46
1	9-A	349	ARG	CZ-NH1	5.02	1.39	1.33
2	4-B	816	TYR	CG-CD2	5.02	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6-B	649	GLU	CD-OE1	5.02	1.31	1.25
2	4-B	295	ARG	NE-CZ	5.02	1.39	1.33
3	4-D	176	ARG	CZ-NH1	5.02	1.39	1.33
2	5-B	638	ARG	CZ-NH1	5.02	1.39	1.33
3	9-D	346	SER	CB-OG	-5.02	1.35	1.42
3	9-D	407	TYR	CG-CD2	5.02	1.45	1.39
2	10-B	389	ARG	CZ-NH2	5.02	1.39	1.33
3	10-D	197	ASP	CB-CG	5.02	1.62	1.51
2	10-B	408	SER	CA-CB	5.02	1.60	1.52
1	1-A	624	ARG	CZ-NH2	5.01	1.39	1.33
1	2-A	609	THR	C-N	5.01	1.43	1.34
1	8-A	338	GLU	CB-CG	5.01	1.61	1.52
3	8-C	93	TRP	CG-CD1	-5.01	1.29	1.36
3	3-C	90	ARG	NE-CZ	5.01	1.39	1.33
3	6-C	2	GLY	N-CA	-5.01	1.38	1.46
3	7-C	427	ARG	CD-NE	5.01	1.54	1.46
1	10-A	484	ILE	CA-CB	-5.01	1.43	1.54
1	3-A	588	TYR	CD1-CE1	5.01	1.46	1.39
3	3-C	217	PHE	CE1-CZ	5.01	1.46	1.37
1	5-A	179	GLU	CG-CD	5.01	1.59	1.51
1	5-A	627	ARG	CZ-NH2	5.01	1.39	1.33
2	5-B	393	PHE	CG-CD1	5.01	1.46	1.38
1	6-A	78	PHE	CE2-CZ	5.01	1.46	1.37
2	1-B	612	ARG	CZ-NH2	5.01	1.39	1.33
3	2-D	218	ARG	CD-NE	5.01	1.54	1.46
3	3-D	179	GLU	CB-CG	5.01	1.61	1.52
3	1-D	54	PHE	CG-CD2	5.01	1.46	1.38
2	4-B	526	ARG	CZ-NH2	5.01	1.39	1.33
1	3-A	349	ARG	CZ-NH1	5.00	1.39	1.33
1	6-A	75	ILE	CA-C	-5.00	1.40	1.52
2	4-B	267	PHE	CA-CB	5.00	1.65	1.53
2	4-B	475	PHE	CG-CD2	5.00	1.46	1.38
1	6-A	409	PHE	CG-CD1	5.00	1.46	1.38

All (4569) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7-A	714	ARG	NE-CZ-NH1	20.47	130.54	120.30
2	9-B	343	TYR	CB-CG-CD2	-18.96	109.62	121.00
3	9-C	427	ARG	NE-CZ-NH2	-18.13	111.23	120.30
3	5-C	333	ARG	NE-CZ-NH1	18.03	129.32	120.30
3	7-C	84	ARG	NE-CZ-NH1	17.76	129.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	10-A	198	ARG	NE-CZ-NH1	17.71	129.15	120.30
1	10-A	198	ARG	NE-CZ-NH2	-17.70	111.45	120.30
1	8-A	479	ARG	NE-CZ-NH1	17.59	129.10	120.30
1	6-A	458	TYR	CB-CG-CD2	-17.54	110.48	121.00
2	1-B	446	PHE	CB-CG-CD2	17.02	132.72	120.80
1	4-A	587	ARG	NE-CZ-NH2	-16.94	111.83	120.30
2	10-B	433	TYR	CB-CG-CD2	-16.93	110.84	121.00
2	5-B	612	ARG	NE-CZ-NH2	-16.83	111.88	120.30
3	2-C	192	ARG	NE-CZ-NH2	-16.77	111.92	120.30
1	6-A	767	TYR	CB-CG-CD1	16.65	130.99	121.00
1	7-A	190	TYR	CB-CG-CD2	-16.61	111.03	121.00
3	2-C	272	PHE	CB-CG-CD2	-16.53	109.23	120.80
2	7-B	580	ARG	NE-CZ-NH2	-16.41	112.10	120.30
2	3-B	533	ARG	NE-CZ-NH2	-16.33	112.13	120.30
1	4-A	92	PHE	CB-CG-CD2	-16.32	109.37	120.80
3	2-D	204	PHE	CB-CG-CD1	16.23	132.16	120.80
3	7-C	114	ARG	NE-CZ-NH2	-16.23	112.19	120.30
1	1-A	614	TYR	CB-CG-CD1	-16.16	111.30	121.00
1	7-A	687	ARG	NE-CZ-NH2	-16.07	112.27	120.30
1	4-A	793	PHE	CB-CG-CD1	16.00	132.00	120.80
3	2-C	437	TYR	CB-CG-CD2	-15.96	111.42	121.00
3	10-C	46	ARG	NE-CZ-NH2	-15.88	112.36	120.30
2	2-B	651	TYR	CB-CG-CD2	-15.88	111.47	121.00
2	4-B	824	TYR	CB-CG-CD2	-15.88	111.47	121.00
3	7-C	84	ARG	NE-CZ-NH2	-15.87	112.36	120.30
1	4-A	92	PHE	CB-CG-CD1	15.80	131.86	120.80
1	5-A	588	TYR	CB-CG-CD1	15.77	130.46	121.00
2	6-B	267	PHE	CB-CG-CD1	15.61	131.73	120.80
2	5-B	385	PHE	CB-CG-CD2	-15.46	109.97	120.80
3	2-C	341	ARG	NE-CZ-NH2	-15.32	112.64	120.30
3	6-D	218	ARG	NE-CZ-NH2	-15.26	112.67	120.30
3	9-D	437	TYR	CB-CG-CD2	-15.25	111.85	121.00
1	10-A	144	ARG	NE-CZ-NH1	15.25	127.92	120.30
2	6-B	826	PHE	CB-CG-CD1	15.22	131.45	120.80
3	9-D	84	ARG	NE-CZ-NH1	15.22	127.91	120.30
3	2-C	243	ARG	NE-CZ-NH1	15.20	127.90	120.30
2	6-B	824	TYR	CB-CG-CD2	-15.16	111.91	121.00
2	1-B	816	TYR	CB-CG-CD2	-15.11	111.93	121.00
2	3-B	389	ARG	NE-CZ-NH2	-15.09	112.75	120.30
3	3-D	437	TYR	CB-CG-CD2	-14.95	112.03	121.00
2	2-B	589	PHE	CB-CG-CD1	14.81	131.17	120.80
1	7-A	77	TYR	CB-CG-CD2	-14.81	112.11	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3-B	438	TYR	CB-CG-CD2	-14.77	112.14	121.00
2	6-B	651	TYR	CB-CG-CD2	-14.69	112.19	121.00
2	8-B	576	ARG	NE-CZ-NH2	-14.66	112.97	120.30
2	8-B	544	ARG	NE-CZ-NH2	-14.64	112.98	120.30
1	10-A	426	PHE	CB-CG-CD2	-14.64	110.55	120.80
1	1-A	479	ARG	NE-CZ-NH2	-14.48	113.06	120.30
2	6-B	510	TYR	CB-CG-CD1	-14.47	112.32	121.00
2	10-B	599	PHE	CB-CG-CD1	14.45	130.91	120.80
3	9-C	358	ARG	NE-CZ-NH2	-14.39	113.11	120.30
1	2-A	76	ARG	NE-CZ-NH2	-14.30	113.15	120.30
1	6-A	767	TYR	CB-CG-CD2	-14.30	112.42	121.00
3	3-D	90	ARG	NE-CZ-NH2	-14.25	113.17	120.30
1	5-A	107	ARG	NE-CZ-NH2	-14.24	113.18	120.30
1	8-A	398	TYR	CB-CG-CD2	-14.24	112.46	121.00
1	3-A	102	PHE	CB-CG-CD2	-14.22	110.85	120.80
1	8-A	398	TYR	CB-CG-CD1	14.18	129.51	121.00
2	1-B	816	TYR	CB-CG-CD1	14.09	129.46	121.00
3	9-C	46	ARG	NE-CZ-NH1	14.05	127.33	120.30
3	9-D	279	TYR	CB-CG-CD2	-14.05	112.57	121.00
2	8-B	598	TYR	CB-CG-CD2	-14.03	112.58	121.00
2	4-B	345	TYR	CB-CG-CD2	-14.03	112.58	121.00
2	9-B	578	PHE	CB-CG-CD2	14.02	130.61	120.80
1	8-A	409	PHE	CB-CG-CD2	14.01	130.61	120.80
2	8-B	822	ARG	NE-CZ-NH2	-14.01	113.30	120.30
2	10-B	190	TYR	CB-CG-CD2	-13.98	112.61	121.00
1	10-A	116	TYR	CB-CG-CD2	-13.95	112.63	121.00
1	8-A	409	PHE	CB-CG-CD1	-13.94	111.04	120.80
2	5-B	580	ARG	NE-CZ-NH2	-13.88	113.36	120.30
2	6-B	242	ARG	NE-CZ-NH1	13.86	127.23	120.30
1	9-A	284	TYR	CB-CG-CD1	13.81	129.28	121.00
2	5-B	453	TYR	CB-CG-CD2	-13.75	112.75	121.00
2	10-B	343	TYR	CB-CG-CD2	-13.74	112.76	121.00
1	7-A	623	ARG	NE-CZ-NH2	-13.72	113.44	120.30
1	5-A	193	TYR	CB-CG-CD2	-13.67	112.80	121.00
2	6-B	651	TYR	CB-CG-CD1	13.63	129.18	121.00
1	8-A	776	ARG	NE-CZ-NH1	13.61	127.11	120.30
2	8-B	295	ARG	NE-CZ-NH2	-13.61	113.49	120.30
1	7-A	190	TYR	CB-CG-CD1	13.60	129.16	121.00
3	4-D	218	ARG	NE-CZ-NH1	13.59	127.10	120.30
3	2-D	218	ARG	NE-CZ-NH2	-13.56	113.52	120.30
3	10-C	185	TYR	CB-CG-CD2	-13.53	112.88	121.00
3	1-C	359	ARG	NE-CZ-NH1	13.52	127.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	775	PHE	CB-CG-CD1	13.51	130.26	120.80
1	2-A	204	ARG	NE-CZ-NH2	-13.48	113.56	120.30
3	10-C	247	TYR	CB-CG-CD1	-13.45	112.93	121.00
1	9-A	107	ARG	NE-CZ-NH2	-13.45	113.58	120.30
3	1-C	243	ARG	NE-CZ-NH2	-13.43	113.59	120.30
1	10-A	426	PHE	CB-CG-CD1	13.43	130.20	120.80
1	1-A	327	ARG	NE-CZ-NH1	13.37	126.99	120.30
2	3-B	816	TYR	CB-CG-CD1	13.34	129.00	121.00
2	5-B	293	ARG	NE-CZ-NH2	-13.32	113.64	120.30
1	9-A	74	TYR	CB-CG-CD2	13.31	128.99	121.00
2	5-B	385	PHE	CB-CG-CD1	13.30	130.11	120.80
1	2-A	782	PHE	CB-CG-CD1	-13.28	111.50	120.80
1	10-A	623	ARG	NE-CZ-NH1	13.26	126.93	120.30
1	4-A	582	TYR	CB-CG-CD2	-13.20	113.08	121.00
3	10-C	249	TYR	CB-CG-CD2	-13.14	113.12	121.00
1	3-A	646	TYR	CB-CG-CD1	13.06	128.84	121.00
1	2-A	393	TYR	CB-CG-CD2	-13.05	113.17	121.00
3	6-D	193	ARG	NE-CZ-NH2	-13.03	113.78	120.30
1	4-A	469	ARG	NE-CZ-NH2	-13.02	113.79	120.30
3	5-D	62	PHE	CB-CG-CD2	-13.02	111.68	120.80
1	9-A	327	ARG	NE-CZ-NH2	-13.02	113.79	120.30
3	4-D	362	TYR	CB-CG-CD2	-12.97	113.22	121.00
1	10-A	111	ARG	NE-CZ-NH1	12.97	126.78	120.30
2	5-B	562	TYR	CB-CG-CD1	-12.96	113.22	121.00
2	5-B	612	ARG	NE-CZ-NH1	12.95	126.77	120.30
3	9-C	445	TYR	CB-CG-CD2	-12.94	113.23	121.00
1	10-A	413	TYR	CB-CG-CD1	12.94	128.77	121.00
2	7-B	638	ARG	NE-CZ-NH2	-12.93	113.84	120.30
3	8-D	162	TYR	CB-CG-CD1	12.93	128.75	121.00
3	4-D	445	TYR	CB-CG-CD1	12.90	128.74	121.00
2	6-B	267	PHE	CB-CG-CD2	-12.90	111.77	120.80
3	10-D	423	PHE	CB-CG-CD2	-12.90	111.77	120.80
2	3-B	475	PHE	CB-CG-CD1	12.88	129.82	120.80
3	3-C	55	ARG	NE-CZ-NH1	-12.88	113.86	120.30
2	9-B	758	TYR	CB-CG-CD1	-12.86	113.28	121.00
2	9-B	816	TYR	CB-CG-CD2	-12.86	113.28	121.00
1	8-A	479	ARG	NE-CZ-NH2	-12.80	113.90	120.30
1	9-A	107	ARG	NE-CZ-NH1	12.80	126.70	120.30
2	6-B	190	TYR	CB-CG-CD2	-12.76	113.34	121.00
1	6-A	776	ARG	NE-CZ-NH2	-12.75	113.92	120.30
1	8-A	140	TYR	CB-CG-CD1	-12.75	113.35	121.00
2	5-B	300	PHE	CB-CG-CD1	-12.70	111.91	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-C	407	TYR	CB-CG-CD2	-12.69	113.39	121.00
3	8-D	176	ARG	NE-CZ-NH1	12.69	126.64	120.30
1	2-A	794	TYR	CB-CG-CD2	-12.68	113.39	121.00
1	4-A	349	ARG	NE-CZ-NH2	-12.68	113.96	120.30
1	6-A	381	PHE	CB-CG-CD1	12.67	129.67	120.80
2	8-B	225	PHE	CB-CG-CD2	-12.62	111.97	120.80
3	2-C	341	ARG	NE-CZ-NH1	12.61	126.61	120.30
1	7-A	144	ARG	NE-CZ-NH1	12.61	126.60	120.30
3	2-C	192	ARG	NE-CZ-NH1	12.53	126.56	120.30
1	6-A	144	ARG	NE-CZ-NH2	-12.51	114.04	120.30
1	9-A	121	ARG	NE-CZ-NH1	12.48	126.54	120.30
3	4-D	65	ARG	NE-CZ-NH1	12.47	126.53	120.30
3	7-D	437	TYR	CB-CG-CD2	-12.43	113.54	121.00
3	5-C	387	PHE	CB-CG-CD2	-12.39	112.13	120.80
3	2-D	204	PHE	CB-CG-CD2	-12.39	112.13	120.80
1	6-A	144	ARG	NE-CZ-NH1	12.34	126.47	120.30
1	2-A	324	TYR	CB-CG-CD2	-12.32	113.61	121.00
3	2-C	46	ARG	NE-CZ-NH1	12.30	126.45	120.30
2	6-B	312	PHE	CB-CG-CD1	12.27	129.39	120.80
1	8-A	794	TYR	CB-CG-CD2	-12.27	113.64	121.00
1	1-A	284	TYR	CB-CG-CD1	-12.27	113.64	121.00
1	5-A	588	TYR	CB-CG-CD2	-12.27	113.64	121.00
3	7-C	358	ARG	NE-CZ-NH2	-12.25	114.18	120.30
2	7-B	445	PHE	CB-CG-CD1	12.19	129.34	120.80
2	3-B	822	ARG	NE-CZ-NH1	12.14	126.37	120.30
2	10-B	562	TYR	CB-CG-CD2	-12.11	113.73	121.00
2	2-B	470	TYR	CB-CG-CD2	-12.11	113.74	121.00
2	9-B	666	ARG	NE-CZ-NH2	-12.11	114.25	120.30
2	4-B	592	ARG	NE-CZ-NH1	-12.10	114.25	120.30
1	10-A	469	ARG	NE-CZ-NH1	12.08	126.34	120.30
3	6-D	249	TYR	CB-CG-CD2	-12.08	113.75	121.00
1	6-A	623	ARG	NE-CZ-NH1	12.06	126.33	120.30
1	6-A	469	ARG	NE-CZ-NH1	12.05	126.32	120.30
2	7-B	470	TYR	CB-CG-CD2	12.02	128.21	121.00
3	10-C	341	ARG	NE-CZ-NH2	-12.00	114.30	120.30
1	3-A	160	ARG	NE-CZ-NH2	-11.99	114.30	120.30
3	7-C	55	ARG	NE-CZ-NH2	11.99	126.29	120.30
1	10-A	639	PHE	CB-CG-CD2	-11.99	112.41	120.80
1	4-A	582	TYR	CB-CG-CD1	11.96	128.18	121.00
2	2-B	651	TYR	CB-CG-CD1	11.95	128.17	121.00
2	9-B	285	ARG	NE-CZ-NH2	-11.95	114.32	120.30
1	10-A	116	TYR	CB-CG-CD1	11.93	128.16	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2-D	193	ARG	NE-CZ-NH1	11.93	126.26	120.30
2	7-B	514	ARG	NE-CZ-NH2	-11.93	114.34	120.30
1	7-A	171	ARG	NE-CZ-NH2	-11.89	114.35	120.30
2	1-B	429	TYR	CB-CG-CD1	11.89	128.13	121.00
2	6-B	190	TYR	CB-CG-CD1	11.89	128.13	121.00
2	10-B	468	PHE	CB-CG-CD1	11.88	129.12	120.80
1	10-A	479	ARG	NE-CZ-NH2	-11.84	114.38	120.30
2	3-B	343	TYR	CB-CG-CD2	11.84	128.10	121.00
3	4-C	319	TYR	CG-CD1-CE1	-11.80	111.86	121.30
3	9-C	403	PHE	CB-CG-CD1	11.80	129.06	120.80
2	2-B	285	ARG	NE-CZ-NH2	-11.77	114.41	120.30
2	1-B	343	TYR	CB-CG-CD2	-11.76	113.94	121.00
2	7-B	776	TYR	CB-CG-CD2	-11.73	113.96	121.00
3	4-C	267	PHE	CB-CG-CD1	-11.72	112.59	120.80
3	7-C	279	TYR	CB-CG-CD1	-11.69	113.99	121.00
1	5-A	279	TYR	CB-CG-CD1	-11.68	113.99	121.00
2	10-B	385	PHE	CB-CG-CD2	-11.66	112.64	120.80
3	10-D	109	TYR	CB-CG-CD2	-11.65	114.01	121.00
3	3-D	70	ASP	CB-CG-OD2	-11.63	107.83	118.30
2	1-B	471	ARG	NE-CZ-NH1	-11.63	114.49	120.30
1	1-A	714	ARG	NE-CZ-NH2	-11.62	114.49	120.30
1	4-A	333	ARG	NE-CZ-NH2	-11.61	114.50	120.30
1	1-A	465	PHE	CB-CG-CD2	-11.60	112.68	120.80
1	10-A	413	TYR	CB-CG-CD2	-11.58	114.05	121.00
3	8-C	387	PHE	CB-CG-CD2	-11.58	112.70	120.80
1	9-A	150	TYR	CB-CG-CD2	-11.55	114.07	121.00
1	4-A	469	ARG	NE-CZ-NH1	11.51	126.06	120.30
2	9-B	299	ARG	NE-CZ-NH1	11.51	126.05	120.30
1	10-A	458	TYR	CB-CG-CD2	-11.50	114.10	121.00
2	8-B	488	PHE	CB-CG-CD2	-11.49	112.76	120.80
3	2-C	170	TYR	CB-CG-CD2	-11.48	114.11	121.00
2	7-B	565	TYR	CB-CG-CD2	-11.48	114.11	121.00
1	8-A	116	TYR	CB-CG-CD1	-11.45	114.13	121.00
2	10-B	379	TYR	CB-CG-CD2	-11.44	114.14	121.00
1	9-A	646	TYR	CB-CG-CD1	11.44	127.86	121.00
3	9-D	333	ARG	NE-CZ-NH1	11.43	126.02	120.30
3	1-C	292	TYR	CB-CG-CD1	11.43	127.86	121.00
2	3-B	533	ARG	NE-CZ-NH1	11.42	126.01	120.30
2	2-B	846	ARG	NE-CZ-NH2	-11.40	114.60	120.30
2	1-B	526	ARG	NE-CZ-NH1	11.40	126.00	120.30
1	8-A	137	ARG	NE-CZ-NH1	11.39	126.00	120.30
3	9-C	413	PHE	CB-CG-CD2	-11.39	112.83	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4-C	427	ARG	NE-CZ-NH2	11.38	125.99	120.30
2	2-B	471	ARG	NE-CZ-NH1	11.38	125.99	120.30
3	10-C	20	PHE	CB-CG-CD2	-11.38	112.84	120.80
2	5-B	776	TYR	CB-CG-CD2	-11.37	114.18	121.00
3	1-D	387	PHE	CB-CG-CD1	11.36	128.75	120.80
2	1-B	641	PHE	CB-CG-CD1	-11.35	112.85	120.80
3	4-D	423	PHE	CB-CG-CD2	-11.34	112.86	120.80
3	5-C	333	ARG	NE-CZ-NH2	-11.31	114.64	120.30
3	5-D	427	ARG	NE-CZ-NH2	-11.31	114.65	120.30
3	9-D	204	PHE	CB-CG-CD2	-11.30	112.89	120.80
1	3-A	333	ARG	NE-CZ-NH1	-11.29	114.66	120.30
2	5-B	816	TYR	CB-CG-CD1	-11.29	114.23	121.00
3	10-D	54	PHE	CB-CG-CD1	-11.27	112.91	120.80
1	1-A	775	PHE	CB-CG-CD2	-11.27	112.91	120.80
1	7-A	458	TYR	CB-CG-CD2	-11.26	114.25	121.00
1	8-A	333	ARG	NE-CZ-NH2	11.24	125.92	120.30
2	9-B	822	ARG	NE-CZ-NH2	-11.24	114.68	120.30
3	5-D	278	ASP	CB-CG-OD2	-11.23	108.19	118.30
2	8-B	592	ARG	NE-CZ-NH2	-11.23	114.69	120.30
2	3-B	544	ARG	NE-CZ-NH2	-11.22	114.69	120.30
3	2-C	292	TYR	CB-CG-CD1	11.21	127.72	121.00
1	7-A	345	PHE	CB-CG-CD2	-11.20	112.96	120.80
3	2-D	217	PHE	CB-CG-CD1	11.20	128.64	120.80
1	4-A	349	ARG	NE-CZ-NH1	11.18	125.89	120.30
2	6-B	453	TYR	CB-CG-CD1	-11.18	114.29	121.00
3	9-C	445	TYR	CG-CD2-CE2	-11.18	112.36	121.30
2	2-B	593	PHE	CB-CG-CD2	-11.16	112.99	120.80
3	7-C	59	ARG	NE-CZ-NH2	11.15	125.87	120.30
1	9-A	381	PHE	CB-CG-CD2	-11.14	113.00	120.80
1	6-A	171	ARG	NE-CZ-NH2	-11.13	114.73	120.30
3	6-C	65	ARG	NE-CZ-NH2	-11.12	114.74	120.30
3	4-C	341	ARG	NE-CZ-NH1	11.11	125.86	120.30
2	2-B	285	ARG	NE-CZ-NH1	11.10	125.85	120.30
1	8-A	664	ARG	NE-CZ-NH2	-11.10	114.75	120.30
2	4-B	652	TYR	CB-CG-CD2	-11.10	114.34	121.00
1	2-A	112	TYR	CB-CG-CD2	-11.09	114.34	121.00
1	8-A	302	TYR	CB-CG-CD1	-11.08	114.35	121.00
3	2-D	292	TYR	CB-CG-CD2	11.08	127.65	121.00
3	6-D	218	ARG	NE-CZ-NH1	11.08	125.84	120.30
2	8-B	583	TYR	CB-CG-CD2	-11.08	114.35	121.00
3	3-D	65	ARG	NE-CZ-NH2	-11.05	114.77	120.30
3	7-C	358	ARG	NE-CZ-NH1	11.05	125.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	10-B	299	ARG	NE-CZ-NH2	11.03	125.82	120.30
3	7-D	193	ARG	NE-CZ-NH2	-11.03	114.78	120.30
1	10-A	105	PHE	CB-CG-CD2	-11.03	113.08	120.80
3	6-C	133	PHE	CB-CG-CD1	-11.02	113.08	120.80
3	7-D	315	TYR	CB-CG-CD1	11.02	127.61	121.00
1	7-A	709	PHE	CB-CG-CD2	11.02	128.51	120.80
3	10-C	427	ARG	NE-CZ-NH2	-11.01	114.79	120.30
2	3-B	805	PHE	CB-CG-CD1	10.99	128.49	120.80
2	9-B	514	ARG	NE-CZ-NH2	-10.98	114.81	120.30
2	1-B	433	TYR	CB-CG-CD1	10.96	127.58	121.00
1	6-A	458	TYR	CB-CG-CD1	10.96	127.57	121.00
1	6-A	296	TYR	CB-CG-CD1	10.95	127.57	121.00
3	4-D	256	TYR	CB-CG-CD2	-10.94	114.43	121.00
1	6-A	381	PHE	CB-CG-CD2	-10.94	113.14	120.80
1	8-A	400	ARG	NE-CZ-NH2	10.94	125.77	120.30
2	9-B	578	PHE	CB-CG-CD1	-10.94	113.15	120.80
3	4-D	315	TYR	CB-CG-CD2	-10.93	114.44	121.00
1	9-A	657	TYR	CB-CG-CD2	-10.92	114.45	121.00
3	7-D	315	TYR	CB-CG-CD2	-10.92	114.45	121.00
3	9-C	413	PHE	CB-CG-CD1	10.91	128.44	120.80
1	6-A	296	TYR	CB-CG-CD2	-10.91	114.46	121.00
2	10-B	345	TYR	CB-CG-CD2	-10.90	114.46	121.00
3	10-C	275	PHE	CB-CG-CD2	10.89	128.42	120.80
3	4-C	362	TYR	CB-CG-CD1	10.88	127.53	121.00
1	5-A	77	TYR	CB-CG-CD1	10.88	127.53	121.00
3	9-C	218	ARG	NE-CZ-NH2	-10.87	114.86	120.30
2	10-B	599	PHE	CB-CG-CD2	-10.87	113.19	120.80
3	2-D	218	ARG	NE-CZ-NH1	10.86	125.73	120.30
2	8-B	242	ARG	NE-CZ-NH2	-10.86	114.87	120.30
3	5-D	62	PHE	CB-CG-CD1	10.84	128.39	120.80
1	4-A	450	TYR	CB-CG-CD2	10.84	127.50	121.00
3	7-D	243	ARG	NE-CZ-NH2	-10.83	114.89	120.30
1	8-A	794	TYR	CB-CG-CD1	10.82	127.49	121.00
3	9-C	59	ARG	NE-CZ-NH2	10.80	125.70	120.30
3	10-D	362	TYR	CB-CG-CD2	-10.79	114.53	121.00
2	1-B	633	ARG	NE-CZ-NH1	10.78	125.69	120.30
3	3-D	114	ARG	NE-CZ-NH2	10.78	125.69	120.30
2	7-B	641	PHE	CB-CG-CD2	-10.76	113.27	120.80
2	5-B	514	ARG	NE-CZ-NH1	10.75	125.68	120.30
2	4-B	666	ARG	NE-CZ-NH1	10.75	125.67	120.30
2	8-B	816	TYR	CB-CG-CD2	-10.75	114.55	121.00
3	7-D	83	PHE	CB-CG-CD1	10.73	128.31	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	162	PHE	CB-CG-CD2	-10.71	113.31	120.80
1	2-A	588	TYR	CB-CG-CD1	-10.71	114.58	121.00
3	4-D	90	ARG	NE-CZ-NH2	-10.70	114.95	120.30
3	10-D	90	ARG	NE-CZ-NH1	10.70	125.65	120.30
3	4-D	394	PHE	CB-CG-CD2	-10.69	113.32	120.80
3	6-C	161	ARG	NE-CZ-NH2	10.68	125.64	120.30
3	7-D	341	ARG	NE-CZ-NH2	-10.67	114.96	120.30
3	7-D	375	MET	CG-SD-CE	-10.66	83.14	100.20
3	2-C	329	ARG	NE-CZ-NH1	-10.66	114.97	120.30
3	8-D	319	TYR	CB-CG-CD1	10.66	127.40	121.00
3	2-D	292	TYR	CB-CG-CD1	-10.65	114.61	121.00
2	8-B	583	TYR	CB-CG-CD1	10.64	127.39	121.00
2	7-B	652	TYR	CB-CG-CD2	-10.63	114.62	121.00
3	7-D	437	TYR	CB-CG-CD1	10.63	127.38	121.00
3	6-C	46	ARG	NE-CZ-NH2	-10.63	114.99	120.30
2	6-B	411	PHE	CB-CG-CD1	10.62	128.24	120.80
2	9-B	284	TYR	CB-CG-CD2	-10.60	114.64	121.00
3	10-C	90	ARG	NE-CZ-NH1	10.60	125.60	120.30
3	3-D	109	TYR	CB-CG-CD2	10.58	127.35	121.00
2	6-B	438	TYR	CB-CG-CD2	10.57	127.34	121.00
3	1-C	176	ARG	NE-CZ-NH2	-10.57	115.02	120.30
1	7-A	279	TYR	CB-CG-CD1	-10.57	114.66	121.00
3	10-D	218	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	5-A	793	PHE	CB-CG-CD2	10.56	128.19	120.80
3	7-C	329	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	5-A	160	ARG	NE-CZ-NH1	10.54	125.57	120.30
1	2-A	597	ARG	NE-CZ-NH2	-10.54	115.03	120.30
3	3-C	316	PHE	CB-CG-CD2	-10.54	113.42	120.80
3	3-D	54	PHE	CB-CG-CD1	10.54	128.18	120.80
1	7-A	381	PHE	CB-CG-CD1	10.52	128.16	120.80
2	3-B	475	PHE	CB-CG-CD2	-10.48	113.46	120.80
1	7-A	203	ARG	NE-CZ-NH1	-10.48	115.06	120.30
3	9-D	437	TYR	CB-CG-CD1	10.48	127.29	121.00
2	9-B	345	TYR	CB-CG-CD2	-10.47	114.72	121.00
1	5-A	438	PHE	CB-CG-CD1	10.47	128.13	120.80
1	5-A	77	TYR	CB-CG-CD2	-10.45	114.73	121.00
1	2-A	111	ARG	NE-CZ-NH2	-10.44	115.08	120.30
2	3-B	822	ARG	NE-CZ-NH2	-10.44	115.08	120.30
2	5-B	562	TYR	CB-CG-CD2	10.43	127.26	121.00
1	7-A	664	ARG	NE-CZ-NH2	-10.43	115.09	120.30
2	6-B	826	PHE	CB-CG-CD2	-10.42	113.50	120.80
3	8-D	217	PHE	CB-CG-CD2	-10.42	113.51	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9-B	652	TYR	CB-CG-CD1	10.41	127.24	121.00
2	4-B	824	TYR	CB-CG-CD1	10.40	127.24	121.00
1	8-A	623	ARG	NE-CZ-NH2	-10.39	115.10	120.30
3	6-C	427	ARG	NE-CZ-NH2	-10.38	115.11	120.30
3	9-D	407	TYR	CB-CG-CD2	-10.38	114.77	121.00
1	4-A	105	PHE	CB-CG-CD1	10.38	128.06	120.80
2	7-B	187	TYR	CG-CD2-CE2	-10.38	113.00	121.30
3	7-C	97	ASP	CB-CG-OD2	10.36	127.62	118.30
3	8-D	427	ARG	NE-CZ-NH1	10.35	125.47	120.30
3	9-D	279	TYR	CB-CG-CD1	10.34	127.21	121.00
1	10-A	588	TYR	CB-CG-CD2	-10.34	114.79	121.00
3	4-D	279	TYR	CB-CG-CD2	-10.34	114.80	121.00
2	6-B	295	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	7-A	714	ARG	NE-CZ-NH2	-10.32	115.14	120.30
3	4-C	256	TYR	CB-CG-CD2	-10.32	114.81	121.00
2	9-B	641	PHE	CB-CG-CD1	10.31	128.02	120.80
2	5-B	468	PHE	CB-CG-CD1	-10.31	113.58	120.80
1	10-A	302	TYR	CB-CG-CD2	-10.30	114.82	121.00
1	1-A	193	TYR	CB-CG-CD1	10.29	127.18	121.00
2	3-B	839	PHE	CB-CG-CD1	10.29	128.00	120.80
1	8-A	74	TYR	CB-CG-CD1	10.29	127.17	121.00
1	3-A	630	ARG	NE-CZ-NH1	10.28	125.44	120.30
1	3-A	646	TYR	CB-CG-CD2	-10.28	114.83	121.00
3	5-C	387	PHE	CB-CG-CD1	10.28	128.00	120.80
2	7-B	533	ARG	NE-CZ-NH2	-10.28	115.16	120.30
2	5-B	587	PHE	CB-CG-CD1	10.27	127.99	120.80
2	1-B	451	ASP	CB-CG-OD2	-10.27	109.06	118.30
3	4-D	362	TYR	CB-CG-CD1	10.25	127.15	121.00
2	1-B	190	TYR	CB-CG-CD1	10.24	127.14	121.00
1	7-A	405	PHE	CB-CG-CD2	-10.24	113.63	120.80
1	7-A	409	PHE	CB-CG-CD1	10.24	127.97	120.80
3	2-D	358	ARG	NE-CZ-NH1	10.23	125.42	120.30
3	10-D	300	ASP	CB-CG-OD1	10.22	127.50	118.30
3	2-D	192	ARG	NE-CZ-NH1	10.22	125.41	120.30
3	8-D	217	PHE	CB-CG-CD1	10.22	127.95	120.80
1	3-A	400	ARG	NE-CZ-NH2	-10.21	115.19	120.30
3	4-D	279	TYR	CB-CG-CD1	10.21	127.12	121.00
1	8-A	137	ARG	NE-CZ-NH2	-10.21	115.20	120.30
1	1-A	405	PHE	CB-CG-CD1	-10.20	113.66	120.80
1	1-A	123	TYR	CB-CG-CD2	10.20	127.12	121.00
3	9-C	218	ARG	NE-CZ-NH1	10.20	125.40	120.30
3	10-C	84	ARG	NE-CZ-NH1	10.19	125.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6-C	204	PHE	CB-CG-CD2	-10.16	113.69	120.80
1	3-A	111	ARG	NE-CZ-NH2	-10.16	115.22	120.30
3	9-D	86	PHE	CB-CG-CD1	10.16	127.91	120.80
2	6-B	580	ARG	NE-CZ-NH1	10.15	125.38	120.30
2	6-B	822	ARG	NE-CZ-NH1	10.15	125.38	120.30
2	10-B	190	TYR	CB-CG-CD1	10.13	127.08	121.00
3	4-D	267	PHE	CB-CG-CD1	-10.12	113.72	120.80
3	7-C	114	ARG	NE-CZ-NH1	10.12	125.36	120.30
3	1-D	53	PHE	CB-CG-CD2	-10.11	113.73	120.80
3	4-C	416	MET	CG-SD-CE	-10.11	84.03	100.20
2	7-B	203	ASP	CB-CG-OD2	-10.08	109.23	118.30
3	6-D	176	ARG	NE-CZ-NH1	10.08	125.34	120.30
1	9-A	393	TYR	CB-CG-CD2	-10.08	114.95	121.00
2	6-B	231	TYR	CB-CG-CD2	10.07	127.04	121.00
1	3-A	704	TYR	CB-CG-CD2	10.07	127.04	121.00
2	7-B	445	PHE	CB-CG-CD2	-10.06	113.75	120.80
3	8-D	279	TYR	CB-CG-CD1	-10.06	114.96	121.00
2	5-B	359	TYR	CB-CG-CD2	-10.05	114.97	121.00
1	7-A	302	TYR	CB-CG-CD1	-10.05	114.97	121.00
3	7-D	341	ARG	NE-CZ-NH1	10.05	125.33	120.30
3	5-C	53	PHE	CB-CG-CD1	-10.04	113.77	120.80
1	8-A	133	MET	CG-SD-CE	-10.04	84.13	100.20
3	6-D	161	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	7-A	451	ARG	NE-CZ-NH1	-10.04	115.28	120.30
1	3-A	588	TYR	CB-CG-CD2	-10.02	114.99	121.00
2	6-B	772	PHE	CB-CG-CD2	-10.02	113.78	120.80
2	8-B	242	ARG	NE-CZ-NH1	10.02	125.31	120.30
3	2-D	275	PHE	CB-CG-CD1	-10.01	113.79	120.80
2	6-B	284	TYR	CB-CG-CD1	-10.01	114.99	121.00
3	4-C	413	PHE	CB-CG-CD1	10.01	127.81	120.80
1	10-A	793	PHE	CB-CG-CD2	-9.98	113.81	120.80
2	2-B	585	ARG	NE-CZ-NH2	-9.98	115.31	120.30
2	10-B	468	PHE	CB-CG-CD2	-9.98	113.81	120.80
2	7-B	411	PHE	CB-CG-CD1	9.96	127.77	120.80
2	9-B	475	PHE	CB-CG-CD2	-9.96	113.83	120.80
3	8-D	109	TYR	CB-CG-CD1	9.96	126.97	121.00
3	7-C	333	ARG	NE-CZ-NH2	-9.96	115.32	120.30
3	9-C	407	TYR	CB-CG-CD2	-9.96	115.03	121.00
1	9-A	150	TYR	CB-CG-CD1	9.95	126.97	121.00
1	10-A	121	ARG	NE-CZ-NH2	-9.95	115.32	120.30
1	10-A	302	TYR	CB-CG-CD1	9.95	126.97	121.00
2	1-B	297	TYR	CB-CG-CD1	-9.93	115.04	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-C	394	PHE	CB-CG-CD1	9.93	127.75	120.80
1	2-A	108	ARG	NE-CZ-NH2	-9.92	115.34	120.30
2	6-B	453	TYR	CB-CG-CD2	9.91	126.95	121.00
3	4-D	93	TRP	CG-CD2-CE3	-9.91	124.98	133.90
3	4-D	55	ARG	NE-CZ-NH2	9.90	125.25	120.30
1	9-A	145	PHE	CB-CG-CD2	-9.90	113.87	120.80
1	8-A	74	TYR	CB-CG-CD2	-9.89	115.07	121.00
3	6-D	65	ARG	NE-CZ-NH1	-9.88	115.36	120.30
3	5-C	90	ARG	NE-CZ-NH2	-9.87	115.37	120.30
2	6-B	400	TYR	CB-CG-CD2	-9.87	115.08	121.00
1	1-A	791	PHE	CB-CG-CD1	-9.85	113.90	120.80
2	4-B	299	ARG	NE-CZ-NH2	-9.85	115.37	120.30
1	7-A	623	ARG	NE-CZ-NH1	9.85	125.23	120.30
3	3-D	62	PHE	CB-CG-CD1	9.85	127.69	120.80
3	5-C	204	PHE	CB-CG-CD1	9.84	127.69	120.80
1	10-A	624	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	10-A	78	PHE	CB-CG-CD1	9.83	127.68	120.80
3	6-D	413	PHE	CB-CG-CD1	-9.82	113.92	120.80
3	5-D	247	TYR	CB-CG-CD2	-9.82	115.11	121.00
2	5-B	345	TYR	CB-CG-CD2	-9.81	115.11	121.00
1	9-A	304	ASP	CB-CG-OD2	-9.80	109.48	118.30
2	1-B	415	TYR	CB-CG-CD2	-9.79	115.12	121.00
2	3-B	225	PHE	CB-CG-CD2	-9.79	113.95	120.80
3	6-D	204	PHE	CB-CG-CD1	-9.78	113.95	120.80
1	10-A	121	ARG	NE-CZ-NH1	9.78	125.19	120.30
2	1-B	514	ARG	NE-CZ-NH2	-9.77	115.42	120.30
3	8-C	387	PHE	CB-CG-CD1	9.77	127.64	120.80
2	1-B	446	PHE	CB-CG-CD1	-9.76	113.97	120.80
3	10-C	192	ARG	NE-CZ-NH1	-9.76	115.42	120.30
2	4-B	776	TYR	CB-CG-CD1	-9.75	115.15	121.00
1	1-A	614	TYR	CB-CG-CD2	9.74	126.85	121.00
2	9-B	285	ARG	NE-CZ-NH1	9.74	125.17	120.30
3	10-D	173	PHE	CB-CG-CD2	-9.74	113.98	120.80
1	7-A	279	TYR	CB-CG-CD2	9.72	126.83	121.00
1	1-A	302	TYR	CB-CG-CD1	9.72	126.83	121.00
1	5-A	327	ARG	NE-CZ-NH2	-9.71	115.44	120.30
3	6-D	54	PHE	CB-CG-CD1	9.71	127.60	120.80
1	1-A	74	TYR	CB-CG-CD1	-9.71	115.17	121.00
2	10-B	385	PHE	CB-CG-CD1	9.71	127.59	120.80
3	10-D	362	TYR	CB-CG-CD1	9.70	126.82	121.00
1	9-A	137	ARG	NE-CZ-NH1	9.68	125.14	120.30
3	7-C	193	ARG	NE-CZ-NH2	-9.68	115.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	8-D	170	TYR	CB-CG-CD1	-9.68	115.19	121.00
3	9-C	329	ARG	NE-CZ-NH2	-9.68	115.46	120.30
2	10-B	592	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	3-A	597	ARG	NE-CZ-NH2	-9.65	115.47	120.30
3	4-C	256	TYR	CB-CG-CD1	9.65	126.79	121.00
2	3-B	599	PHE	CB-CG-CD2	9.65	127.56	120.80
1	8-A	664	ARG	NE-CZ-NH1	9.65	125.12	120.30
3	8-C	49	ASP	CB-CG-OD1	9.65	126.98	118.30
3	3-D	55	ARG	NE-CZ-NH1	-9.63	115.48	120.30
2	7-B	284	TYR	CB-CG-CD1	-9.63	115.22	121.00
1	10-A	148	ASP	CB-CG-OD2	-9.63	109.63	118.30
1	2-A	261	ASP	CB-CG-OD2	-9.63	109.64	118.30
3	3-D	109	TYR	CB-CG-CD1	-9.63	115.22	121.00
2	4-B	664	MET	CG-SD-CE	-9.62	84.81	100.20
3	4-D	445	TYR	CB-CG-CD2	-9.62	115.23	121.00
1	6-A	320	TRP	CB-CG-CD2	-9.62	114.10	126.60
2	10-B	343	TYR	CB-CG-CD1	9.60	126.76	121.00
1	7-A	627	ARG	NE-CZ-NH2	-9.60	115.50	120.30
3	9-C	427	ARG	NE-CZ-NH1	9.59	125.10	120.30
2	8-B	187	TYR	CB-CG-CD2	-9.59	115.25	121.00
3	3-C	362	TYR	CB-CG-CD2	-9.59	115.25	121.00
3	5-C	247	TYR	CB-CG-CD2	-9.58	115.25	121.00
1	4-A	450	TYR	CB-CG-CD1	-9.58	115.25	121.00
3	3-D	445	TYR	CD1-CE1-CZ	-9.58	111.18	119.80
1	5-A	438	PHE	CB-CG-CD2	-9.57	114.10	120.80
1	2-A	709	PHE	CB-CG-CD2	-9.55	114.11	120.80
1	4-A	793	PHE	CB-CG-CD2	-9.55	114.12	120.80
1	9-A	657	TYR	CB-CG-CD1	9.55	126.73	121.00
2	8-B	415	TYR	CB-CG-CD2	-9.54	115.27	121.00
3	5-C	358	ARG	NE-CZ-NH1	9.54	125.07	120.30
2	2-B	295	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	10-A	775	PHE	CB-CG-CD2	-9.51	114.14	120.80
2	5-B	231	TYR	CB-CG-CD1	-9.51	115.30	121.00
3	4-C	223	ASP	CB-CG-OD2	-9.51	109.74	118.30
3	3-C	83	PHE	CB-CG-CD2	-9.50	114.15	120.80
3	4-D	218	ARG	NE-CZ-NH2	-9.50	115.55	120.30
2	3-B	236	TYR	CB-CG-CD2	-9.49	115.30	121.00
1	9-A	123	TYR	CB-CG-CD1	-9.49	115.30	121.00
1	10-A	588	TYR	CB-CG-CD1	9.49	126.70	121.00
3	1-D	243	ARG	NE-CZ-NH2	-9.49	115.55	120.30
3	8-C	359	ARG	NE-CZ-NH2	9.48	125.04	120.30
3	7-C	333	ARG	NE-CZ-NH1	9.47	125.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-A	663	TYR	CB-CG-CD2	-9.46	115.32	121.00
3	9-C	394	PHE	CB-CG-CD2	-9.47	114.17	120.80
1	3-A	324	TYR	CB-CG-CD1	-9.46	115.32	121.00
2	8-B	741	PHE	CB-CG-CD1	9.45	127.42	120.80
3	1-C	319	TYR	CB-CG-CD2	9.43	126.66	121.00
2	10-B	379	TYR	CB-CG-CD1	9.43	126.66	121.00
1	5-A	409	PHE	CB-CG-CD1	9.42	127.40	120.80
1	6-A	594	TYR	CG-CD1-CE1	-9.42	113.76	121.30
3	4-C	90	ARG	NE-CZ-NH2	-9.42	115.59	120.30
3	4-C	315	TYR	CB-CG-CD1	9.42	126.65	121.00
1	7-A	576	ARG	NE-CZ-NH2	-9.41	115.59	120.30
3	8-C	78	ASP	CB-CG-OD2	9.41	126.77	118.30
3	10-C	46	ARG	NE-CZ-NH1	9.40	125.00	120.30
2	3-B	846	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	7-A	587	ARG	NE-CZ-NH2	9.40	125.00	120.30
3	7-D	124	ASP	CB-CG-OD2	-9.39	109.84	118.30
3	10-C	275	PHE	CB-CG-CD1	-9.39	114.22	120.80
3	8-D	319	TYR	CB-CG-CD2	-9.38	115.37	121.00
2	5-B	345	TYR	CB-CG-CD1	9.38	126.63	121.00
3	5-D	124	ASP	CB-CG-OD1	9.38	126.75	118.30
2	3-B	514	ARG	NE-CZ-NH1	9.38	124.99	120.30
2	6-B	312	PHE	CB-CG-CD2	-9.38	114.23	120.80
3	8-C	90	ARG	NE-CZ-NH2	-9.38	115.61	120.30
3	1-D	423	PHE	CB-CG-CD1	-9.37	114.24	120.80
2	4-B	652	TYR	CB-CG-CD1	9.37	126.62	121.00
1	1-A	193	TYR	CB-CG-CD2	-9.37	115.38	121.00
3	1-C	90	ARG	NE-CZ-NH2	-9.36	115.62	120.30
2	3-B	335	PHE	CB-CG-CD2	-9.36	114.25	120.80
3	1-D	46	ARG	NE-CZ-NH1	-9.36	115.62	120.30
2	1-B	544	ARG	NE-CZ-NH2	9.35	124.97	120.30
3	4-D	193	ARG	NE-CZ-NH2	-9.34	115.63	120.30
3	4-D	20	PHE	CB-CG-CD2	9.34	127.34	120.80
1	9-A	145	PHE	CB-CG-CD1	9.33	127.33	120.80
2	3-B	293	ARG	NE-CZ-NH1	-9.33	115.63	120.30
2	2-B	593	PHE	CB-CG-CD1	9.32	127.32	120.80
1	1-A	150	TYR	CB-CG-CD2	-9.32	115.41	121.00
3	1-D	54	PHE	CB-CG-CD2	-9.32	114.28	120.80
3	2-D	275	PHE	CB-CG-CD2	9.31	127.32	120.80
2	2-B	284	TYR	CB-CG-CD1	-9.31	115.42	121.00
3	6-D	358	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	7-A	413	TYR	CB-CG-CD1	-9.30	115.42	121.00
3	4-C	282	ASP	CB-CG-OD2	-9.29	109.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	398	TYR	CB-CG-CD1	-9.28	115.43	121.00
2	5-B	409	TYR	CB-CG-CD2	-9.27	115.44	121.00
2	5-B	578	PHE	CB-CG-CD1	9.25	127.28	120.80
3	6-C	315	TYR	CB-CG-CD1	9.25	126.55	121.00
1	6-A	320	TRP	CB-CG-CD1	9.25	139.02	127.00
1	9-A	296	TYR	CB-CG-CD2	-9.25	115.45	121.00
3	1-C	55	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	3-A	438	PHE	CB-CG-CD2	-9.24	114.33	120.80
3	10-C	162	TYR	CB-CG-CD2	9.23	126.54	121.00
3	10-C	173	PHE	CB-CG-CD1	9.22	127.25	120.80
3	10-C	292	TYR	CB-CG-CD1	-9.21	115.47	121.00
2	4-B	285	ARG	NE-CZ-NH2	-9.21	115.69	120.30
2	9-B	533	ARG	NE-CZ-NH2	-9.21	115.69	120.30
1	10-A	663	TYR	CB-CG-CD2	-9.20	115.48	121.00
3	4-D	394	PHE	CB-CG-CD1	9.20	127.24	120.80
3	6-C	403	PHE	CB-CG-CD2	-9.19	114.36	120.80
3	2-D	131	ASP	CB-CG-OD2	9.19	126.57	118.30
1	4-A	624	ARG	NE-CZ-NH2	-9.19	115.71	120.30
2	4-B	433	TYR	CB-CG-CD1	9.18	126.51	121.00
3	6-D	114	ARG	NE-CZ-NH1	9.18	124.89	120.30
3	3-D	292	TYR	CB-CG-CD1	9.18	126.50	121.00
3	8-D	407	TYR	CB-CG-CD1	-9.18	115.50	121.00
2	3-B	599	PHE	CB-CG-CD1	-9.17	114.38	120.80
3	4-C	272	PHE	CB-CG-CD2	-9.16	114.39	120.80
2	8-B	604	MET	CG-SD-CE	-9.16	85.54	100.20
2	1-B	356	ARG	NE-CZ-NH2	-9.15	115.72	120.30
2	5-B	379	TYR	CB-CG-CD2	-9.15	115.51	121.00
1	2-A	333	ARG	NE-CZ-NH1	-9.15	115.73	120.30
3	4-C	249	TYR	CB-CG-CD1	9.15	126.49	121.00
2	6-B	293	ARG	NE-CZ-NH1	9.14	124.87	120.30
3	10-C	217	PHE	CB-CG-CD1	9.14	127.20	120.80
2	1-B	592	ARG	NE-CZ-NH2	-9.13	115.73	120.30
2	4-B	453	TYR	CB-CG-CD2	-9.12	115.53	121.00
2	8-B	816	TYR	CB-CG-CD1	9.12	126.47	121.00
2	8-B	190	TYR	CB-CG-CD1	9.11	126.46	121.00
3	5-D	316	PHE	CB-CG-CD2	-9.10	114.43	120.80
2	7-B	846	ARG	NE-CZ-NH2	-9.10	115.75	120.30
2	4-B	488	PHE	CB-CG-CD2	-9.09	114.44	120.80
1	7-A	597	ARG	NE-CZ-NH2	-9.09	115.75	120.30
3	3-D	65	ARG	NE-CZ-NH1	9.09	124.84	120.30
3	6-D	46	ARG	NE-CZ-NH2	-9.09	115.75	120.30
1	3-A	588	TYR	CB-CG-CD1	9.08	126.45	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4-C	86	PHE	CB-CG-CD1	9.08	127.16	120.80
1	5-A	400	ARG	NE-CZ-NH1	9.08	124.84	120.30
2	3-B	359	TYR	CB-CG-CD1	-9.08	115.55	121.00
1	8-A	410	PHE	CB-CG-CD2	-9.07	114.45	120.80
2	5-B	587	PHE	CB-CG-CD2	-9.06	114.46	120.80
3	2-C	256	TYR	CB-CG-CD2	-9.06	115.57	121.00
3	3-C	243	ARG	NE-CZ-NH2	-9.05	115.77	120.30
3	4-C	329	ARG	NE-CZ-NH1	9.05	124.83	120.30
3	10-C	114	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	8-A	62	ASP	CB-CG-OD2	-9.05	110.15	118.30
2	1-B	633	ARG	NE-CZ-NH2	-9.05	115.78	120.30
2	3-B	562	TYR	CB-CG-CD1	-9.05	115.57	121.00
2	1-B	652	TYR	CB-CG-CD2	-9.04	115.57	121.00
2	2-B	633	ARG	NE-CZ-NH1	9.04	124.82	120.30
2	9-B	652	TYR	CB-CG-CD2	-9.04	115.58	121.00
3	7-C	65	ARG	NE-CZ-NH2	9.04	124.82	120.30
3	8-D	249	TYR	CB-CG-CD1	-9.03	115.58	121.00
1	9-A	381	PHE	CB-CG-CD1	9.03	127.12	120.80
1	6-A	793	PHE	CB-CG-CD1	9.02	127.12	120.80
2	10-B	433	TYR	CB-CG-CD1	9.01	126.41	121.00
3	4-C	65	ARG	NE-CZ-NH2	-9.01	115.79	120.30
3	1-D	256	TYR	CB-CG-CD1	9.00	126.40	121.00
3	9-D	193	ARG	NE-CZ-NH2	-9.00	115.80	120.30
2	2-B	776	TYR	CB-CG-CD2	-8.99	115.61	121.00
3	6-D	192	ARG	NE-CZ-NH1	8.98	124.79	120.30
3	9-D	84	ARG	NE-CZ-NH2	-8.97	115.81	120.30
2	3-B	468	PHE	CB-CG-CD2	-8.97	114.52	120.80
1	7-A	709	PHE	CB-CG-CD1	-8.97	114.52	120.80
2	1-B	409	TYR	CB-CG-CD2	8.96	126.37	121.00
3	8-C	403	PHE	CB-CG-CD2	-8.95	114.53	120.80
1	10-A	140	TYR	CB-CG-CD2	-8.95	115.63	121.00
2	4-B	202	PHE	CB-CG-CD2	-8.95	114.53	120.80
1	5-A	582	TYR	CG-CD1-CE1	-8.94	114.15	121.30
3	4-C	114	ARG	NE-CZ-NH1	8.93	124.77	120.30
1	7-A	646	TYR	CB-CG-CD2	-8.93	115.64	121.00
1	10-A	204	ARG	NE-CZ-NH1	8.93	124.76	120.30
3	9-D	86	PHE	CB-CG-CD2	-8.92	114.56	120.80
2	10-B	293	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	8-A	76	ARG	NE-CZ-NH1	8.91	124.75	120.30
3	10-D	55	ARG	NE-CZ-NH1	8.91	124.75	120.30
2	1-B	598	TYR	CG-CD2-CE2	-8.90	114.18	121.30
1	7-A	116	TYR	CB-CG-CD1	-8.89	115.67	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	10-D	173	PHE	CB-CG-CD1	8.89	127.02	120.80
2	2-B	565	TYR	CB-CG-CD2	-8.89	115.67	121.00
3	6-C	41	ASP	CB-CG-OD2	8.88	126.29	118.30
3	2-C	437	TYR	CB-CG-CD1	8.88	126.33	121.00
2	10-B	816	TYR	CB-CG-CD1	8.87	126.33	121.00
3	6-C	20	PHE	CB-CG-CD2	-8.87	114.59	120.80
1	7-A	767	TYR	CB-CG-CD1	-8.87	115.68	121.00
2	8-B	822	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	5-A	409	PHE	CB-CG-CD2	-8.86	114.60	120.80
1	10-A	647	PHE	CB-CG-CD2	-8.86	114.60	120.80
1	9-A	775	PHE	CB-CG-CD2	-8.85	114.61	120.80
1	2-A	108	ARG	NE-CZ-NH1	-8.85	115.88	120.30
3	10-C	329	ARG	NE-CZ-NH2	-8.84	115.88	120.30
2	2-B	580	ARG	NE-CZ-NH2	-8.84	115.88	120.30
3	1-D	252	MET	CG-SD-CE	-8.83	86.07	100.20
2	8-B	544	ARG	NE-CZ-NH1	8.83	124.72	120.30
2	5-B	433	TYR	CB-CG-CD2	-8.82	115.71	121.00
2	6-B	295	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	4-A	630	ARG	NE-CZ-NH1	8.82	124.71	120.30
2	4-B	633	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	10-A	393	TYR	CB-CG-CD2	-8.81	115.71	121.00
2	3-B	770	TYR	CB-CG-CD2	-8.81	115.71	121.00
3	10-C	20	PHE	CB-CG-CD1	8.81	126.97	120.80
3	10-C	173	PHE	CB-CG-CD2	-8.81	114.63	120.80
2	1-B	558	PHE	CB-CG-CD1	-8.81	114.64	120.80
3	5-C	319	TYR	CB-CG-CD1	-8.80	115.72	121.00
2	1-B	400	TYR	CB-CG-CD1	-8.80	115.72	121.00
3	1-C	193	ARG	NE-CZ-NH2	-8.80	115.90	120.30
2	2-B	670	ARG	NE-CZ-NH2	-8.80	115.90	120.30
2	2-B	805	PHE	CB-CG-CD1	8.80	126.96	120.80
3	6-D	136	PHE	CG-CD2-CE2	-8.80	111.12	120.80
3	8-D	90	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	9-A	775	PHE	CB-CG-CD1	8.79	126.95	120.80
2	3-B	826	PHE	CB-CG-CD2	-8.78	114.66	120.80
3	1-C	93	TRP	CB-CG-CD2	-8.77	115.20	126.60
3	1-D	59	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	10-A	624	ARG	NE-CZ-NH2	-8.76	115.92	120.30
2	8-B	429	TYR	CB-CG-CD2	-8.75	115.75	121.00
1	10-A	782	PHE	CB-CG-CD2	8.75	126.92	120.80
3	6-D	248	MET	CG-SD-CE	-8.75	86.21	100.20
1	10-A	144	ARG	NE-CZ-NH2	-8.74	115.93	120.30
2	3-B	335	PHE	CB-CG-CD1	8.74	126.92	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3-B	600	TYR	CB-CG-CD1	8.73	126.24	121.00
3	10-C	279	TYR	CB-CG-CD1	8.73	126.24	121.00
3	2-C	110	ASP	CB-CG-OD2	8.72	126.15	118.30
2	3-B	342	TYR	CB-CG-CD1	8.72	126.23	121.00
3	9-C	249	TYR	CB-CG-CD2	-8.71	115.77	121.00
1	10-A	137	ARG	NE-CZ-NH1	-8.70	115.95	120.30
2	1-B	433	TYR	CB-CG-CD2	-8.70	115.78	121.00
2	7-B	293	ARG	NE-CZ-NH2	-8.70	115.95	120.30
3	9-C	87	PHE	CB-CG-CD2	-8.70	114.71	120.80
3	6-D	387	PHE	CB-CG-CD2	-8.69	114.71	120.80
2	3-B	821	ASP	CB-CG-OD2	8.69	126.12	118.30
1	7-A	782	PHE	CB-CG-CD2	-8.69	114.72	120.80
3	10-C	84	ARG	NE-CZ-NH2	-8.69	115.95	120.30
3	6-C	136	PHE	CB-CG-CD2	-8.69	114.72	120.80
2	5-B	359	TYR	CB-CG-CD1	8.68	126.21	121.00
3	7-C	411	ASP	CB-CG-OD1	8.67	126.11	118.30
3	4-C	358	ARG	NE-CZ-NH2	-8.67	115.97	120.30
3	1-C	279	TYR	CB-CG-CD2	8.67	126.20	121.00
3	9-D	362	TYR	CB-CG-CD2	-8.67	115.80	121.00
3	9-D	407	TYR	CB-CG-CD1	8.67	126.20	121.00
3	4-C	427	ARG	NE-CZ-NH1	-8.66	115.97	120.30
3	2-D	239	THR	CA-CB-CG2	-8.66	100.27	112.40
1	10-A	76	ARG	NE-CZ-NH2	-8.66	115.97	120.30
3	7-D	445	TYR	CB-CG-CD1	8.66	126.20	121.00
3	9-C	46	ARG	NE-CZ-NH2	-8.65	115.97	120.30
3	10-C	271	SER	N-CA-CB	8.65	123.48	110.50
3	7-D	333	ARG	NE-CZ-NH1	-8.65	115.98	120.30
2	7-B	819	PHE	CB-CG-CD1	8.63	126.84	120.80
3	4-C	437	TYR	CB-CG-CD1	-8.62	115.83	121.00
3	6-C	55	ARG	NE-CZ-NH1	8.62	124.61	120.30
2	7-B	411	PHE	CB-CG-CD2	-8.62	114.77	120.80
1	9-A	563	ASP	CB-CG-OD1	-8.62	110.55	118.30
1	8-A	639	PHE	CB-CG-CD2	-8.62	114.77	120.80
2	3-B	648	MET	CG-SD-CE	-8.61	86.42	100.20
3	4-D	90	ARG	NE-CZ-NH1	8.61	124.61	120.30
2	9-B	345	TYR	CB-CG-CD1	8.61	126.17	121.00
3	8-C	279	TYR	CB-CG-CD2	-8.61	115.83	121.00
1	5-A	582	TYR	CB-CG-CD1	-8.61	115.83	121.00
2	1-B	824	TYR	CB-CG-CD2	-8.60	115.84	121.00
1	5-A	345	PHE	CB-CG-CD2	-8.60	114.78	120.80
2	9-B	438	TYR	CB-CG-CD2	-8.60	115.84	121.00
3	8-D	315	TYR	CB-CG-CD2	8.59	126.16	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	409	PHE	CB-CG-CD1	8.59	126.81	120.80
1	4-A	398	TYR	CB-CG-CD2	-8.58	115.85	121.00
3	1-D	86	PHE	CB-CG-CD2	-8.58	114.79	120.80
2	8-B	805	PHE	CB-CG-CD2	-8.58	114.79	120.80
1	2-A	324	TYR	CB-CG-CD1	8.58	126.15	121.00
2	7-B	652	TYR	CB-CG-CD1	8.57	126.14	121.00
1	1-A	700	PHE	CB-CG-CD2	-8.55	114.81	120.80
2	6-B	236	TYR	CB-CG-CD1	-8.55	115.87	121.00
2	7-B	631	LEU	CB-CG-CD1	8.55	125.54	111.00
1	8-A	138	PHE	CB-CG-CD2	-8.55	114.81	120.80
2	1-B	578	PHE	CB-CG-CD1	8.55	126.78	120.80
2	6-B	319	PHE	CB-CG-CD2	-8.54	114.82	120.80
3	6-C	341	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	5-A	197	PHE	CB-CG-CD1	8.53	126.77	120.80
1	1-A	704	TYR	CB-CG-CD1	-8.53	115.88	121.00
2	9-B	583	TYR	CB-CG-CD2	8.53	126.12	121.00
1	2-A	614	TYR	CB-CG-CD1	8.52	126.11	121.00
1	9-A	405	PHE	CB-CG-CD1	-8.52	114.84	120.80
1	2-A	791	PHE	CB-CG-CD2	-8.52	114.84	120.80
3	7-D	359	ARG	NE-CZ-NH1	8.52	124.56	120.30
3	1-C	65	ARG	NE-CZ-NH1	-8.51	116.04	120.30
3	2-C	249	TYR	CB-CG-CD2	-8.51	115.89	121.00
2	7-B	770	TYR	CB-CG-CD1	8.51	126.11	121.00
1	10-A	775	PHE	CB-CG-CD1	8.51	126.76	120.80
1	4-A	409	PHE	CB-CG-CD1	8.50	126.75	120.80
3	10-D	114	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	9-A	327	ARG	NH1-CZ-NH2	8.49	128.74	119.40
3	1-D	243	ARG	NE-CZ-NH1	8.49	124.54	120.30
3	2-D	319	TYR	CB-CG-CD2	-8.49	115.91	121.00
2	6-B	562	TYR	CB-CG-CD1	8.48	126.09	121.00
2	8-B	488	PHE	CB-CG-CD1	8.48	126.73	120.80
3	3-C	48	ASP	CB-CG-OD1	-8.47	110.68	118.30
1	4-A	197	PHE	CB-CG-CD1	-8.47	114.87	120.80
1	3-A	102	PHE	CB-CG-CD1	8.47	126.73	120.80
3	3-D	344	PHE	CB-CG-CD2	-8.46	114.88	120.80
3	9-C	398	PHE	CB-CG-CD2	-8.46	114.88	120.80
3	3-C	78	ASP	CB-CG-OD2	-8.46	110.68	118.30
3	1-D	315	TYR	CB-CG-CD2	-8.46	115.92	121.00
1	1-A	278	ASP	CB-CG-OD2	-8.46	110.69	118.30
3	2-D	267	PHE	CB-CG-CD2	-8.45	114.88	120.80
2	4-B	297	TYR	CB-CG-CD2	-8.45	115.93	121.00
3	10-C	421	ASP	CB-CG-OD1	8.45	125.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	8-B	599	PHE	CB-CG-CD2	-8.44	114.89	120.80
1	7-A	767	TYR	CB-CG-CD2	8.44	126.07	121.00
3	8-C	131	ASP	CB-CG-OD1	-8.44	110.70	118.30
2	3-B	821	ASP	CB-CG-OD1	-8.44	110.71	118.30
1	2-A	123	TYR	CB-CG-CD2	-8.43	115.94	121.00
3	7-C	136	PHE	CB-CG-CD2	-8.43	114.90	120.80
3	4-D	59	ARG	NE-CZ-NH1	8.43	124.52	120.30
3	4-D	49	ASP	CB-CG-OD2	-8.43	110.71	118.30
1	8-A	663	TYR	CB-CG-CD1	8.42	126.05	121.00
1	1-A	190	TYR	CB-CG-CD1	8.42	126.05	121.00
1	1-A	349	ARG	NE-CZ-NH2	-8.42	116.09	120.30
2	9-B	805	PHE	CB-CG-CD2	8.42	126.69	120.80
3	10-C	292	TYR	CB-CG-CD2	8.41	126.05	121.00
1	10-A	429	TYR	CB-CG-CD2	-8.41	115.95	121.00
1	7-A	664	ARG	NE-CZ-NH1	8.41	124.51	120.30
3	2-C	117	ASP	CB-CG-OD1	-8.41	110.73	118.30
2	3-B	409	TYR	CG-CD2-CE2	-8.40	114.58	121.30
3	6-D	83	PHE	CB-CG-CD2	8.39	126.68	120.80
3	2-D	86	PHE	CB-CG-CD2	-8.39	114.92	120.80
3	2-D	90	ARG	NE-CZ-NH1	8.39	124.50	120.30
2	1-B	770	TYR	CG-CD2-CE2	-8.39	114.59	121.30
3	8-C	185	TYR	CG-CD1-CE1	8.38	128.00	121.30
1	5-A	704	TYR	CB-CG-CD2	-8.38	115.97	121.00
2	5-B	438	TYR	CB-CG-CD1	8.38	126.03	121.00
3	2-C	193	ARG	NE-CZ-NH2	8.37	124.48	120.30
2	9-B	363	PHE	CB-CG-CD1	8.37	126.66	120.80
3	9-D	90	ARG	NE-CZ-NH1	8.37	124.48	120.30
2	1-B	267	PHE	CB-CG-CD2	-8.36	114.95	120.80
3	6-C	375	MET	CG-SD-CE	-8.36	86.83	100.20
1	5-A	646	TYR	CB-CG-CD2	-8.36	115.99	121.00
3	1-D	387	PHE	CB-CG-CD2	-8.36	114.95	120.80
2	8-B	600	TYR	CG-CD1-CE1	-8.35	114.62	121.30
1	6-A	138	PHE	CB-CG-CD1	-8.34	114.96	120.80
2	9-B	651	TYR	CB-CG-CD2	-8.34	115.99	121.00
2	9-B	776	TYR	CB-CG-CD2	-8.34	115.99	121.00
3	4-C	192	ARG	NE-CZ-NH2	8.33	124.47	120.30
3	5-C	292	TYR	CB-CG-CD1	-8.33	116.00	121.00
3	7-C	292	TYR	CB-CG-CD1	8.33	126.00	121.00
3	7-C	205	ASP	CB-CG-OD2	-8.32	110.81	118.30
3	1-D	161	ARG	NE-CZ-NH1	-8.32	116.14	120.30
3	2-C	243	ARG	NE-CZ-NH2	-8.31	116.14	120.30
1	4-A	197	PHE	CB-CG-CD2	8.31	126.62	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6-B	816	TYR	CB-CG-CD2	-8.31	116.01	121.00
3	8-D	46	ARG	NE-CZ-NH1	8.31	124.45	120.30
3	4-D	282	ASP	CB-CG-OD2	-8.31	110.83	118.30
3	5-C	445	TYR	CB-CG-CD2	8.30	125.98	121.00
2	3-B	589	PHE	CB-CG-CD1	8.29	126.61	120.80
2	7-B	565	TYR	CB-CG-CD1	8.29	125.98	121.00
3	7-C	34	ASP	CB-CG-OD2	8.29	125.76	118.30
3	9-C	59	ARG	NE-CZ-NH1	-8.29	116.16	120.30
2	9-B	661	PHE	CB-CG-CD2	8.28	126.60	120.80
3	9-C	170	TYR	CB-CG-CD2	-8.28	116.03	121.00
1	5-A	193	TYR	CB-CG-CD1	8.27	125.96	121.00
2	8-B	389	ARG	NE-CZ-NH2	8.27	124.43	120.30
2	5-B	379	TYR	CB-CG-CD1	8.26	125.95	121.00
1	1-A	700	PHE	CB-CG-CD1	8.26	126.58	120.80
3	10-C	341	ARG	NE-CZ-NH1	8.26	124.43	120.30
2	4-B	433	TYR	CB-CG-CD2	-8.25	116.05	121.00
1	1-A	144	ARG	NE-CZ-NH1	-8.25	116.17	120.30
3	6-D	316	PHE	CB-CG-CD2	-8.25	115.03	120.80
2	9-B	770	TYR	CB-CG-CD1	-8.25	116.05	121.00
3	1-C	180	VAL	CA-CB-CG2	-8.24	98.53	110.90
3	3-C	217	PHE	CB-CG-CD2	-8.24	115.03	120.80
3	1-C	155	LEU	CB-CG-CD2	-8.24	96.99	111.00
1	6-A	266	MET	CG-SD-CE	-8.24	87.02	100.20
1	9-A	582	TYR	CB-CG-CD2	-8.24	116.06	121.00
2	10-B	475	PHE	CB-CG-CD2	-8.24	115.03	120.80
2	4-B	345	TYR	CB-CG-CD1	8.23	125.94	121.00
1	5-A	333	ARG	NE-CZ-NH2	-8.23	116.18	120.30
2	9-B	190	TYR	CB-CG-CD1	8.23	125.94	121.00
3	10-D	162	TYR	CB-CG-CD1	8.23	125.94	121.00
1	7-A	132	GLY	N-CA-C	-8.22	92.54	113.10
3	3-D	362	TYR	CG-CD1-CE1	-8.22	114.72	121.30
2	8-B	727	VAL	CA-CB-CG2	-8.22	98.57	110.90
1	10-A	458	TYR	CB-CG-CD1	8.21	125.92	121.00
3	1-D	329	ARG	NE-CZ-NH2	8.20	124.40	120.30
1	3-A	624	ARG	NE-CZ-NH2	-8.19	116.20	120.30
3	3-D	50	THR	CA-CB-CG2	-8.19	100.93	112.40
3	2-C	416	MET	CG-SD-CE	-8.19	87.10	100.20
1	6-A	193	TYR	CB-CG-CD2	-8.19	116.09	121.00
2	8-B	839	PHE	CB-CG-CD1	8.18	126.53	120.80
3	2-C	185	TYR	CB-CG-CD1	8.18	125.91	121.00
3	1-D	86	PHE	CB-CG-CD1	8.18	126.52	120.80
1	1-A	261	ASP	N-CA-CB	8.17	125.31	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-A	709	PHE	CB-CG-CD2	-8.17	115.08	120.80
3	7-C	344	PHE	CB-CG-CD2	8.16	126.52	120.80
1	3-A	108	ARG	NE-CZ-NH1	-8.16	116.22	120.30
2	5-B	435	SER	N-CA-CB	8.15	122.73	110.50
3	1-C	267	PHE	CB-CG-CD2	-8.15	115.10	120.80
1	3-A	465	PHE	CB-CG-CD2	-8.14	115.10	120.80
2	4-B	544	ARG	NE-CZ-NH2	8.14	124.37	120.30
2	3-B	446	PHE	CB-CG-CD1	-8.14	115.10	120.80
2	1-B	267	PHE	CB-CG-CD1	8.13	126.49	120.80
1	10-A	150	TYR	CB-CG-CD2	8.13	125.88	121.00
3	7-C	344	PHE	CB-CG-CD1	-8.12	115.11	120.80
2	9-B	731	PHE	CB-CG-CD2	-8.12	115.11	120.80
2	1-B	827	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	3-A	704	TYR	CB-CG-CD1	-8.12	116.13	121.00
2	3-B	593	PHE	CB-CG-CD1	8.12	126.48	120.80
3	5-C	87	PHE	CB-CG-CD1	-8.12	115.12	120.80
2	9-B	190	TYR	CB-CG-CD2	-8.12	116.13	121.00
3	6-D	41	ASP	CB-CG-OD1	-8.12	110.99	118.30
1	1-A	410	PHE	CB-CG-CD1	8.12	126.48	120.80
1	7-A	646	TYR	CB-CG-CD1	8.11	125.87	121.00
2	9-B	526	ARG	NE-CZ-NH1	8.11	124.36	120.30
3	9-C	168	THR	CA-CB-CG2	-8.11	101.05	112.40
1	7-A	782	PHE	CB-CG-CD1	8.10	126.47	120.80
3	1-D	380	MET	CG-SD-CE	-8.10	87.24	100.20
1	6-A	627	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	7-A	111	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	1-A	647	PHE	CB-CG-CD1	-8.10	115.13	120.80
1	1-A	299	PHE	CB-CG-CD1	-8.09	115.13	120.80
1	1-A	776	ARG	NE-CZ-NH1	-8.09	116.25	120.30
3	4-C	362	TYR	CB-CG-CD2	-8.09	116.15	121.00
2	1-B	598	TYR	CB-CG-CD2	-8.09	116.15	121.00
3	1-C	93	TRP	CB-CG-CD1	8.09	137.51	127.00
2	6-B	470	TYR	CB-CG-CD1	-8.09	116.15	121.00
1	5-A	791	PHE	CB-CG-CD1	8.08	126.46	120.80
3	8-D	247	TYR	CB-CG-CD2	-8.08	116.15	121.00
3	4-C	382	THR	CA-CB-CG2	-8.08	101.09	112.40
2	2-B	599	PHE	CB-CG-CD2	-8.08	115.14	120.80
1	6-A	458	TYR	CG-CD2-CE2	-8.08	114.84	121.30
1	10-A	614	TYR	CB-CG-CD1	-8.08	116.15	121.00
2	2-B	827	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	1-A	171	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	6-A	794	TYR	CB-CG-CD1	8.07	125.84	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4-B	225	PHE	CB-CG-CD1	8.06	126.44	120.80
3	5-D	437	TYR	CB-CG-CD2	-8.06	116.16	121.00
2	3-B	363	PHE	CB-CG-CD1	8.06	126.44	120.80
2	8-B	285	ARG	NE-CZ-NH2	-8.05	116.27	120.30
2	1-B	242	ARG	NE-CZ-NH2	-8.05	116.27	120.30
2	10-B	772	PHE	CB-CG-CD2	-8.05	115.17	120.80
2	8-B	741	PHE	CB-CG-CD2	-8.04	115.17	120.80
1	4-A	144	ARG	NE-CZ-NH1	-8.04	116.28	120.30
3	2-C	193	ARG	NE-CZ-NH1	-8.04	116.28	120.30
3	5-D	192	ARG	NE-CZ-NH1	8.04	124.32	120.30
2	2-B	638	ARG	NE-CZ-NH2	-8.04	116.28	120.30
2	1-B	241	PHE	CB-CG-CD1	8.04	126.42	120.80
3	1-C	316	PHE	CB-CG-CD2	8.03	126.42	120.80
2	4-B	190	TYR	CB-CG-CD2	-8.03	116.18	121.00
3	4-C	315	TYR	CB-CG-CD2	-8.03	116.18	121.00
1	7-A	137	ARG	NE-CZ-NH2	-8.03	116.28	120.30
2	6-B	231	TYR	CB-CG-CD1	-8.03	116.19	121.00
1	1-A	157	ARG	NE-CZ-NH2	-8.02	116.29	120.30
3	3-D	20	PHE	CB-CG-CD1	8.02	126.41	120.80
3	2-C	292	TYR	CG-CD2-CE2	8.02	127.71	121.30
3	9-D	423	PHE	CB-CG-CD1	-8.02	115.19	120.80
2	10-B	826	PHE	CB-CG-CD2	8.01	126.41	120.80
2	1-B	585	ARG	NE-CZ-NH2	-8.01	116.30	120.30
2	2-B	816	TYR	CB-CG-CD2	-8.01	116.20	121.00
1	6-A	112	TYR	CB-CG-CD2	-8.00	116.20	121.00
1	1-A	410	PHE	CB-CG-CD2	-8.00	115.20	120.80
2	9-B	600	TYR	CB-CG-CD1	7.99	125.79	121.00
2	4-B	827	ARG	NE-CZ-NH2	-7.98	116.31	120.30
2	2-B	297	TYR	CZ-CE2-CD2	7.98	126.98	119.80
3	1-C	407	TYR	CG-CD2-CE2	-7.97	114.92	121.30
2	5-B	300	PHE	CB-CG-CD2	7.97	126.38	120.80
2	3-B	411	PHE	CB-CG-CD2	7.97	126.38	120.80
2	10-B	409	TYR	CB-CG-CD2	-7.97	116.22	121.00
1	8-A	143	ARG	NE-CZ-NH2	7.97	124.29	120.30
3	10-C	162	TYR	CG-CD1-CE1	7.97	127.68	121.30
1	2-A	108	ARG	NH1-CZ-NH2	7.97	128.16	119.40
3	3-D	192	ARG	NE-CZ-NH1	-7.97	116.32	120.30
3	9-C	249	TYR	CB-CA-C	-7.97	94.46	110.40
1	10-A	658	SER	N-CA-CB	7.97	122.45	110.50
1	7-A	568	TYR	CB-CG-CD2	-7.96	116.22	121.00
1	2-A	148	ASP	CB-CG-OD1	7.96	125.46	118.30
2	10-B	453	TYR	CB-CG-CD2	7.96	125.78	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	8-D	310	MET	CG-SD-CE	-7.96	87.47	100.20
3	8-C	402	ALA	N-CA-CB	7.95	121.23	110.10
3	6-C	343	LYS	N-CA-CB	7.95	124.91	110.60
3	1-D	54	PHE	CB-CG-CD1	7.95	126.36	120.80
1	10-A	381	PHE	CB-CG-CD1	7.94	126.36	120.80
3	3-C	170	TYR	CG-CD2-CE2	7.93	127.65	121.30
2	9-B	190	TYR	CD1-CE1-CZ	7.93	126.94	119.80
1	7-A	161	ASP	CB-CG-OD2	-7.93	111.16	118.30
3	6-C	398	PHE	CB-CG-CD2	-7.93	115.25	120.80
2	3-B	805	PHE	CB-CG-CD2	-7.93	115.25	120.80
1	6-A	333	ARG	NE-CZ-NH1	7.92	124.26	120.30
2	8-B	651	TYR	CB-CG-CD1	7.92	125.75	121.00
1	5-A	458	TYR	CB-CG-CD1	-7.92	116.25	121.00
3	9-C	244	PHE	CB-CG-CD2	7.92	126.34	120.80
2	5-B	776	TYR	CB-CG-CD1	7.92	125.75	121.00
1	9-A	117	MET	CG-SD-CE	-7.92	87.53	100.20
2	3-B	839	PHE	CB-CG-CD2	-7.91	115.26	120.80
3	6-D	315	TYR	CB-CG-CD1	-7.91	116.25	121.00
1	7-A	143	ARG	NE-CZ-NH2	-7.91	116.34	120.30
2	8-B	225	PHE	CB-CG-CD1	7.91	126.34	120.80
1	9-A	190	TYR	CB-CG-CD1	7.91	125.74	121.00
1	3-A	663	TYR	CB-CG-CD1	-7.91	116.26	121.00
2	3-B	502	THR	CA-CB-CG2	-7.91	101.33	112.40
1	5-A	349	ARG	NE-CZ-NH2	-7.90	116.35	120.30
3	7-C	59	ARG	NH1-CZ-NH2	-7.90	110.71	119.40
1	8-A	709	PHE	CB-CG-CD2	-7.90	115.27	120.80
1	10-A	296	TYR	CB-CG-CD1	-7.90	116.26	121.00
3	6-C	427	ARG	NE-CZ-NH1	7.90	124.25	120.30
2	10-B	264	TYR	CB-CG-CD2	-7.90	116.26	121.00
1	5-A	278	ASP	N-CA-CB	7.89	124.81	110.60
2	7-B	295	ARG	NE-CZ-NH1	7.89	124.25	120.30
3	3-D	351	ALA	N-CA-CB	7.89	121.15	110.10
2	5-B	415	TYR	CB-CG-CD1	7.89	125.73	121.00
2	1-B	731	PHE	CB-CG-CD2	7.88	126.31	120.80
2	4-B	821	ASP	CB-CG-OD2	-7.87	111.22	118.30
3	6-C	413	PHE	CB-CG-CD2	7.87	126.31	120.80
3	9-C	403	PHE	CB-CG-CD2	-7.87	115.29	120.80
3	9-D	256	TYR	CB-CG-CD2	-7.87	116.28	121.00
3	5-C	90	ARG	NE-CZ-NH1	7.87	124.23	120.30
3	10-D	62	PHE	CB-CG-CD1	-7.87	115.29	120.80
1	4-A	372	ASP	CB-CG-OD1	7.87	125.38	118.30
1	5-A	111	ARG	NE-CZ-NH2	7.87	124.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7-A	429	TYR	CB-CG-CD2	-7.87	116.28	121.00
1	7-A	451	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	8-A	588	TYR	CB-CG-CD2	-7.87	116.28	121.00
3	3-C	176	ARG	NE-CZ-NH2	-7.87	116.37	120.30
2	6-B	288	TYR	CB-CG-CD1	-7.87	116.28	121.00
3	5-D	49	ASP	CB-CG-OD2	-7.85	111.23	118.30
3	9-D	114	ARG	NE-CZ-NH2	7.85	124.23	120.30
3	7-C	279	TYR	CB-CG-CD2	7.85	125.71	121.00
1	6-A	469	ARG	NE-CZ-NH2	-7.84	116.38	120.30
2	1-B	580	ARG	NE-CZ-NH2	7.84	124.22	120.30
1	8-A	111	ARG	NE-CZ-NH1	-7.84	116.38	120.30
2	8-B	585	ARG	NE-CZ-NH2	-7.84	116.38	120.30
3	10-D	176	ARG	NE-CZ-NH1	7.84	124.22	120.30
2	5-B	422	THR	CA-CB-CG2	-7.84	101.43	112.40
3	8-C	83	PHE	CB-CG-CD2	-7.83	115.32	120.80
2	10-B	583	TYR	CG-CD2-CE2	7.83	127.57	121.30
1	10-A	133	MET	CA-CB-CG	7.83	126.61	113.30
3	2-C	394	PHE	CB-CG-CD1	7.83	126.28	120.80
1	8-A	576	ARG	NE-CZ-NH1	7.83	124.21	120.30
2	9-B	583	TYR	CB-CG-CD1	-7.83	116.30	121.00
2	6-B	362	PHE	CB-CG-CD1	7.83	126.28	120.80
1	1-A	321	ASP	CB-CG-OD1	7.83	125.34	118.30
1	3-A	687	ARG	NE-CZ-NH1	7.83	124.21	120.30
2	6-B	824	TYR	CB-CG-CD1	7.83	125.70	121.00
2	7-B	470	TYR	CB-CG-CD1	-7.83	116.31	121.00
3	7-C	192	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	1-A	568	TYR	CB-CG-CD1	-7.82	116.31	121.00
3	10-C	192	ARG	NE-CZ-NH2	7.82	124.21	120.30
1	6-A	74	TYR	CB-CG-CD1	7.82	125.69	121.00
1	5-A	197	PHE	CB-CG-CD2	-7.82	115.33	120.80
2	9-B	190	TYR	CG-CD1-CE1	-7.82	115.05	121.30
3	10-D	84	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	5-A	198	ARG	NE-CZ-NH1	7.81	124.21	120.30
1	9-A	360	SER	CB-CA-C	-7.81	95.26	110.10
2	9-B	758	TYR	CG-CD1-CE1	-7.81	115.05	121.30
2	6-B	655	CYS	CA-CB-SG	7.81	128.06	114.00
1	4-A	451	ARG	NE-CZ-NH2	7.81	124.20	120.30
1	3-A	562	PHE	CB-CG-CD2	-7.81	115.34	120.80
1	9-A	76	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	4-A	112	TYR	CB-CG-CD2	-7.80	116.32	121.00
1	3-A	631	VAL	CA-CB-CG1	-7.80	99.19	110.90
3	3-C	83	PHE	CB-CG-CD1	7.80	126.26	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-A	143	ARG	NE-CZ-NH2	-7.80	116.40	120.30
2	6-B	470	TYR	CG-CD2-CE2	-7.80	115.06	121.30
2	9-B	483	MET	CG-SD-CE	-7.80	87.73	100.20
3	10-C	55	ARG	NE-CZ-NH2	-7.80	116.40	120.30
2	4-B	638	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	5-A	157	ARG	NE-CZ-NH2	-7.79	116.40	120.30
2	6-B	409	TYR	CB-CG-CD2	-7.79	116.33	121.00
2	7-B	819	PHE	CB-CG-CD2	-7.79	115.35	120.80
3	5-C	176	ARG	NE-CZ-NH2	-7.79	116.41	120.30
3	1-C	109	TYR	CB-CG-CD1	-7.79	116.33	121.00
3	1-C	394	PHE	CB-CG-CD2	-7.79	115.35	120.80
2	1-B	598	TYR	CG-CD1-CE1	-7.78	115.08	121.30
2	1-B	805	PHE	CB-CG-CD2	-7.78	115.35	120.80
1	7-A	426	PHE	CB-CG-CD2	-7.78	115.35	120.80
2	9-B	719	LEU	CB-CA-C	-7.78	95.42	110.20
2	9-B	670	ARG	NE-CZ-NH1	-7.77	116.42	120.30
2	2-B	576	ARG	NE-CZ-NH1	7.77	124.18	120.30
2	3-B	438	TYR	CB-CG-CD1	7.76	125.66	121.00
3	4-C	351	ALA	N-CA-CB	7.76	120.97	110.10
3	6-C	316	PHE	N-CA-CB	7.76	124.58	110.60
3	7-D	86	PHE	CB-CG-CD1	7.76	126.23	120.80
3	7-C	223	ASP	CB-CG-OD1	7.76	125.28	118.30
2	1-B	612	ARG	NE-CZ-NH2	-7.76	116.42	120.30
2	4-B	826	PHE	CB-CG-CD2	-7.75	115.37	120.80
2	9-B	206	GLN	N-CA-CB	7.75	124.56	110.60
1	2-A	704	TYR	CB-CG-CD1	7.75	125.65	121.00
2	1-B	236	TYR	CB-CG-CD2	-7.75	116.35	121.00
3	4-C	90	ARG	NE-CZ-NH1	7.75	124.17	120.30
2	5-B	589	PHE	CB-CG-CD1	7.75	126.22	120.80
3	6-D	329	ARG	NE-CZ-NH2	-7.75	116.43	120.30
3	8-D	329	ARG	NE-CZ-NH2	7.75	124.17	120.30
1	1-A	325	PHE	CB-CG-CD1	7.74	126.22	120.80
3	5-C	204	PHE	CB-CG-CD2	-7.74	115.38	120.80
3	9-C	167	LEU	CB-CG-CD1	7.74	124.16	111.00
1	6-A	588	TYR	CB-CG-CD2	-7.74	116.36	121.00
2	9-B	638	ARG	NE-CZ-NH2	-7.74	116.43	120.30
2	7-B	324	ASP	CB-CG-OD1	-7.74	111.33	118.30
1	5-A	767	TYR	CB-CG-CD2	-7.74	116.36	121.00
1	7-A	345	PHE	CB-CG-CD1	7.73	126.21	120.80
3	3-C	48	ASP	CB-CG-OD2	7.73	125.26	118.30
2	1-B	194	ALA	N-CA-CB	7.73	120.92	110.10
3	9-D	335	MET	CG-SD-CE	-7.73	87.83	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-C	302	SER	N-CA-CB	7.73	122.09	110.50
1	4-A	458	TYR	CG-CD1-CE1	-7.73	115.12	121.30
1	7-A	409	PHE	CB-CG-CD2	-7.72	115.39	120.80
3	4-C	387	PHE	CB-CG-CD1	7.72	126.20	120.80
2	8-B	335	PHE	CB-CG-CD1	-7.72	115.40	120.80
1	10-A	627	ARG	NE-CZ-NH1	-7.71	116.44	120.30
3	10-C	124	ASP	CB-CG-OD1	7.71	125.24	118.30
3	4-C	319	TYR	CD1-CE1-CZ	7.71	126.74	119.80
2	2-B	433	TYR	CG-CD1-CE1	7.70	127.46	121.30
1	7-A	284	TYR	CZ-CE2-CD2	7.70	126.73	119.80
1	9-A	398	TYR	CB-CG-CD2	7.70	125.62	121.00
1	1-A	111	ARG	NE-CZ-NH2	7.70	124.15	120.30
1	10-A	150	TYR	CB-CG-CD1	-7.70	116.38	121.00
3	10-C	110	ASP	CB-CG-OD1	-7.70	111.37	118.30
3	5-D	316	PHE	CB-CG-CD1	7.69	126.18	120.80
3	6-D	65	ARG	NE-CZ-NH2	7.69	124.14	120.30
1	7-A	327	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	1-A	429	TYR	CB-CG-CD2	-7.69	116.39	121.00
2	1-B	526	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	4-A	302	TYR	CB-CG-CD1	-7.68	116.39	121.00
2	3-B	816	TYR	CB-CG-CD2	-7.67	116.40	121.00
3	5-C	362	TYR	CB-CG-CD1	-7.67	116.40	121.00
3	10-C	293	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	6-A	116	TYR	CG-CD1-CE1	7.67	127.43	121.30
3	6-C	293	ASP	CB-CG-OD1	7.67	125.20	118.30
3	10-C	309	ALA	CB-CA-C	-7.67	98.60	110.10
2	5-B	328	ARG	NE-CZ-NH2	7.66	124.13	120.30
2	5-B	600	TYR	CB-CG-CD2	-7.66	116.41	121.00
1	9-A	143	ARG	NE-CZ-NH1	-7.66	116.47	120.30
1	10-A	162	PHE	CB-CG-CD2	-7.65	115.44	120.80
2	2-B	589	PHE	CB-CG-CD2	-7.65	115.44	120.80
2	5-B	758	TYR	CG-CD2-CE2	-7.65	115.18	121.30
3	2-C	445	TYR	CB-CG-CD1	7.65	125.59	121.00
1	5-A	597	ARG	NE-CZ-NH2	-7.64	116.48	120.30
2	8-B	190	TYR	CG-CD1-CE1	7.64	127.41	121.30
2	3-B	826	PHE	CB-CG-CD1	7.63	126.14	120.80
3	10-C	53	PHE	CB-CG-CD1	-7.63	115.46	120.80
1	4-A	429	TYR	CB-CG-CD1	7.63	125.58	121.00
2	7-B	731	PHE	CB-CG-CD2	-7.62	115.47	120.80
3	2-C	161	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	1-A	327	ARG	NE-CZ-NH2	-7.61	116.49	120.30
3	8-C	325	ASN	N-CA-CB	7.61	124.30	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-A	429	TYR	CB-CG-CD2	-7.61	116.44	121.00
3	3-C	386	VAL	CA-CB-CG1	7.61	122.31	110.90
1	10-A	706	PHE	CB-CG-CD2	-7.61	115.47	120.80
1	5-A	182	VAL	CA-CB-CG1	-7.60	99.50	110.90
2	7-B	533	ARG	NE-CZ-NH1	7.60	124.10	120.30
2	9-B	633	ARG	NE-CZ-NH2	-7.60	116.50	120.30
3	3-D	315	TYR	CB-CG-CD2	7.59	125.56	121.00
3	3-D	315	TYR	CB-CG-CD1	-7.59	116.44	121.00
2	9-B	529	MET	CG-SD-CE	-7.59	88.05	100.20
1	4-A	303	ASP	CB-CG-OD2	-7.59	111.47	118.30
3	4-D	247	TYR	CG-CD2-CE2	-7.59	115.23	121.30
3	9-C	398	PHE	CB-CG-CD1	7.58	126.11	120.80
2	8-B	562	TYR	CB-CG-CD1	7.58	125.55	121.00
1	1-A	300	MET	CA-CB-CG	7.58	126.19	113.30
1	9-A	80	ASP	CB-CG-OD2	7.58	125.12	118.30
2	3-B	526	ARG	NE-CZ-NH2	-7.58	116.51	120.30
2	1-B	400	TYR	CG-CD1-CE1	-7.58	115.24	121.30
3	9-C	278	ASP	CB-CG-OD1	-7.57	111.48	118.30
1	1-A	791	PHE	CB-CG-CD2	7.57	126.10	120.80
1	7-A	429	TYR	CB-CG-CD1	7.57	125.54	121.00
2	7-B	600	TYR	CB-CG-CD2	-7.57	116.46	121.00
3	8-C	53	PHE	CB-CG-CD2	7.57	126.10	120.80
1	1-A	92	PHE	CB-CG-CD1	-7.57	115.50	120.80
1	2-A	76	ARG	NE-CZ-NH1	7.56	124.08	120.30
3	10-C	279	TYR	CB-CG-CD2	-7.56	116.46	121.00
2	3-B	194	ALA	N-CA-CB	7.56	120.69	110.10
3	5-C	427	ARG	N-CA-CB	7.56	124.21	110.60
1	9-A	77	TYR	CB-CG-CD1	7.56	125.54	121.00
1	10-A	105	PHE	CB-CG-CD1	7.56	126.09	120.80
3	2-D	173	PHE	CB-CG-CD2	-7.55	115.51	120.80
1	6-A	370	SER	N-CA-CB	7.55	121.83	110.50
3	7-D	173	PHE	CB-CG-CD2	-7.55	115.52	120.80
3	7-D	427	ARG	CB-CA-C	-7.55	95.30	110.40
2	8-B	666	ARG	NE-CZ-NH1	-7.55	116.53	120.30
1	3-A	413	TYR	CB-CG-CD2	-7.54	116.47	121.00
2	8-B	633	ARG	NE-CZ-NH2	-7.54	116.53	120.30
2	10-B	312	PHE	CB-CG-CD2	-7.54	115.52	120.80
3	10-D	256	TYR	CB-CG-CD1	7.54	125.53	121.00
1	1-A	140	TYR	CB-CG-CD1	-7.54	116.48	121.00
1	7-A	77	TYR	CB-CG-CD1	7.54	125.52	121.00
3	4-D	285	ALA	N-CA-CB	7.53	120.65	110.10
1	10-A	562	PHE	CB-CG-CD2	7.53	126.07	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-B	638	ARG	NE-CZ-NH1	7.53	124.07	120.30
1	7-A	451	ARG	NH1-CZ-NH2	7.53	127.68	119.40
2	6-B	342	TYR	CG-CD2-CE2	-7.53	115.28	121.30
2	10-B	453	TYR	CB-CG-CD1	-7.52	116.49	121.00
2	3-B	343	TYR	CG-CD1-CE1	7.52	127.31	121.30
1	1-A	709	PHE	CB-CG-CD2	-7.51	115.54	120.80
3	2-D	217	PHE	CB-CG-CD2	-7.51	115.54	120.80
2	2-B	415	TYR	CB-CG-CD2	-7.51	116.50	121.00
3	5-D	315	TYR	CB-CG-CD2	7.51	125.51	121.00
3	6-C	282	ASP	CB-CG-OD2	7.51	125.06	118.30
3	4-D	161	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	5-A	623	ARG	NE-CZ-NH1	7.51	124.05	120.30
3	8-D	106	ALA	CB-CA-C	-7.51	98.84	110.10
3	9-C	315	TYR	CB-CG-CD2	-7.50	116.50	121.00
3	1-D	185	TYR	CD1-CE1-CZ	-7.50	113.05	119.80
2	6-B	562	TYR	CB-CG-CD2	-7.50	116.50	121.00
3	8-C	297	ASP	CB-CG-OD1	-7.50	111.55	118.30
2	5-B	638	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	3-A	76	ARG	NE-CZ-NH1	-7.49	116.55	120.30
2	4-B	225	PHE	CB-CG-CD2	-7.49	115.56	120.80
3	2-C	395	ASP	CB-CG-OD2	7.49	125.04	118.30
1	1-A	429	TYR	CG-CD1-CE1	-7.48	115.31	121.30
1	1-A	653	ASP	CB-CG-OD2	-7.48	111.57	118.30
3	7-C	133	PHE	CB-CG-CD2	-7.48	115.56	120.80
3	10-D	256	TYR	CB-CG-CD2	-7.48	116.51	121.00
1	4-A	321	ASP	CB-CG-OD1	7.48	125.03	118.30
3	1-D	218	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	2-A	107	ARG	NE-CZ-NH1	-7.47	116.56	120.30
3	9-C	86	PHE	CB-CG-CD2	7.47	126.03	120.80
1	10-A	657	TYR	CB-CG-CD1	-7.47	116.52	121.00
1	1-A	600	ASP	CB-CG-OD2	-7.47	111.58	118.30
2	3-B	819	PHE	CB-CG-CD2	7.47	126.03	120.80
2	2-B	312	PHE	CB-CG-CD1	-7.46	115.58	120.80
3	6-D	54	PHE	CB-CG-CD2	-7.46	115.58	120.80
3	8-C	283	ASP	CB-CG-OD2	-7.46	111.59	118.30
3	9-D	267	PHE	CB-CG-CD1	-7.46	115.58	120.80
3	10-C	185	TYR	CG-CD2-CE2	-7.46	115.33	121.30
1	3-A	98	MET	CG-SD-CE	-7.46	88.27	100.20
3	8-D	427	ARG	NE-CZ-NH2	-7.46	116.57	120.30
3	4-D	315	TYR	CB-CG-CD1	7.45	125.47	121.00
3	6-C	346	SER	N-CA-CB	7.45	121.67	110.50
3	8-D	243	ARG	NE-CZ-NH2	-7.45	116.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-C	170	TYR	CZ-CE2-CD2	-7.44	113.10	119.80
2	9-B	592	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	9-A	279	TYR	CB-CG-CD2	-7.44	116.54	121.00
1	10-A	284	TYR	CB-CG-CD1	7.44	125.46	121.00
2	1-B	389	ARG	NE-CZ-NH1	-7.43	116.58	120.30
1	5-A	73	THR	CA-CB-CG2	-7.43	101.99	112.40
3	3-C	90	ARG	NE-CZ-NH2	-7.43	116.58	120.30
3	4-C	300	ASP	CB-CG-OD1	-7.43	111.61	118.30
1	2-A	639	PHE	CB-CG-CD1	7.43	126.00	120.80
1	2-A	284	TYR	CB-CG-CD1	-7.42	116.55	121.00
2	8-B	343	TYR	CB-CG-CD1	7.42	125.45	121.00
1	1-A	186	MET	CG-SD-CE	-7.42	88.34	100.20
3	4-C	170	TYR	CB-CG-CD1	-7.42	116.55	121.00
1	6-A	450	TYR	CZ-CE2-CD2	-7.41	113.13	119.80
3	9-D	347	TRP	CE2-CD2-CE3	7.41	127.59	118.70
3	4-C	329	ARG	NE-CZ-NH2	-7.41	116.60	120.30
3	5-D	55	ARG	NE-CZ-NH2	-7.41	116.60	120.30
3	6-D	443	ASP	CB-CG-OD2	-7.41	111.63	118.30
3	3-D	160	ASP	CB-CG-OD1	7.40	124.96	118.30
3	3-D	20	PHE	CB-CG-CD2	-7.40	115.62	120.80
3	7-D	427	ARG	NE-CZ-NH1	7.39	124.00	120.30
3	1-C	243	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	4-A	137	ARG	NE-CZ-NH2	-7.39	116.60	120.30
2	5-B	826	PHE	CB-CG-CD1	7.39	125.97	120.80
1	1-A	349	ARG	NE-CZ-NH1	7.39	123.99	120.30
3	3-C	292	TYR	N-CA-CB	7.39	123.90	110.60
1	4-A	203	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	5-A	614	TYR	CB-CG-CD1	7.39	125.43	121.00
1	7-A	349	ARG	NE-CZ-NH2	-7.39	116.61	120.30
3	8-C	293	ASP	CB-CG-OD2	-7.38	111.66	118.30
3	6-C	256	TYR	CZ-CE2-CD2	-7.38	113.16	119.80
1	9-A	793	PHE	CB-CG-CD1	7.38	125.96	120.80
2	9-B	300	PHE	CB-CG-CD2	-7.38	115.64	120.80
1	8-A	395	ASP	CB-CG-OD2	7.38	124.94	118.30
3	9-D	316	PHE	CB-CG-CD1	-7.38	115.64	120.80
3	9-D	434	MET	CG-SD-CE	-7.38	88.40	100.20
2	6-B	284	TYR	CB-CG-CD2	7.38	125.42	121.00
1	4-A	588	TYR	CB-CG-CD2	-7.37	116.58	121.00
3	7-C	271	SER	N-CA-CB	7.37	121.56	110.50
1	9-A	334	ASP	CB-CG-OD1	-7.37	111.67	118.30
2	6-B	446	PHE	CB-CG-CD1	-7.37	115.64	120.80
2	10-B	526	ARG	NE-CZ-NH1	-7.37	116.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	10-B	585	ARG	NE-CZ-NH2	-7.37	116.62	120.30
3	6-C	359	ARG	NE-CZ-NH2	-7.37	116.62	120.30
2	1-B	312	PHE	CB-CG-CD1	7.36	125.95	120.80
2	9-B	845	LEU	CB-CG-CD2	7.36	123.52	111.00
3	9-C	267	PHE	CB-CG-CD2	7.36	125.95	120.80
3	4-D	65	ARG	NE-CZ-NH2	-7.36	116.62	120.30
2	6-B	533	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	7-A	471	SER	N-CA-C	-7.36	91.13	111.00
3	6-C	278	ASP	CB-CG-OD2	7.36	124.92	118.30
3	6-D	70	ASP	CB-CG-OD1	7.36	124.92	118.30
1	10-A	107	ARG	NE-CZ-NH1	7.36	123.98	120.30
2	2-B	670	ARG	NE-CZ-NH1	7.36	123.98	120.30
3	10-D	416	MET	CG-SD-CE	-7.36	88.43	100.20
2	4-B	241	PHE	CB-CG-CD2	-7.35	115.66	120.80
3	8-C	275	PHE	CB-CG-CD2	7.35	125.95	120.80
3	3-C	315	TYR	CB-CG-CD2	-7.35	116.59	121.00
2	4-B	666	ARG	NE-CZ-NH2	-7.35	116.63	120.30
3	7-D	20	PHE	CB-CG-CD1	7.35	125.94	120.80
2	1-B	816	TYR	CZ-CE2-CD2	-7.34	113.19	119.80
1	2-A	776	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	3-A	150	TYR	CG-CD1-CE1	-7.34	115.42	121.30
1	4-A	588	TYR	CB-CG-CD1	7.34	125.41	121.00
2	7-B	638	ARG	NE-CZ-NH1	7.34	123.97	120.30
2	4-B	826	PHE	CB-CG-CD1	7.34	125.94	120.80
2	2-B	470	TYR	CG-CD2-CE2	-7.34	115.43	121.30
3	1-C	319	TYR	CB-CG-CD1	-7.34	116.60	121.00
2	2-B	231	TYR	CB-CG-CD2	-7.34	116.60	121.00
3	3-C	351	ALA	N-CA-CB	7.34	120.37	110.10
1	6-A	410	PHE	CB-CG-CD1	7.34	125.94	120.80
2	10-B	284	TYR	CB-CG-CD2	-7.34	116.60	121.00
3	1-D	83	PHE	CB-CG-CD1	-7.33	115.67	120.80
1	8-A	687	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	9-A	609	THR	CA-CB-CG2	-7.33	102.14	112.40
3	2-D	249	TYR	CG-CD1-CE1	-7.32	115.44	121.30
1	6-A	794	TYR	CD1-CE1-CZ	7.32	126.39	119.80
1	1-A	646	TYR	CG-CD2-CE2	-7.32	115.44	121.30
2	6-B	488	PHE	CG-CD1-CE1	-7.32	112.75	120.80
1	2-A	636	MET	CG-SD-CE	-7.32	88.49	100.20
3	3-C	353	HIS	CA-CB-CG	7.32	126.05	113.60
3	4-D	59	ARG	NE-CZ-NH2	-7.31	116.64	120.30
2	5-B	505	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	3-A	775	PHE	CB-CG-CD1	7.31	125.92	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3-B	285	ARG	NE-CZ-NH2	7.31	123.95	120.30
2	5-B	829	ASP	CB-CG-OD2	7.31	124.88	118.30
3	2-D	84	ARG	NE-CZ-NH1	7.31	123.95	120.30
3	2-D	358	ARG	NE-CZ-NH2	-7.31	116.65	120.30
1	8-A	112	TYR	CB-CG-CD1	7.30	125.38	121.00
1	4-A	108	ARG	NE-CZ-NH1	7.30	123.95	120.30
3	5-C	190	ALA	N-CA-CB	7.30	120.33	110.10
1	3-A	775	PHE	CB-CG-CD2	-7.30	115.69	120.80
1	9-A	144	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	10-A	562	PHE	CB-CG-CD1	-7.30	115.69	120.80
1	9-A	706	PHE	CB-CG-CD1	-7.30	115.69	120.80
1	4-A	102	PHE	CB-CG-CD2	-7.29	115.69	120.80
1	10-A	337	SER	N-CA-CB	7.29	121.44	110.50
2	6-B	593	PHE	CB-CG-CD1	7.29	125.90	120.80
1	9-A	426	PHE	CB-CG-CD1	7.29	125.90	120.80
1	1-A	405	PHE	CB-CG-CD2	7.29	125.90	120.80
3	1-D	128	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	7-A	131	PHE	CB-CG-CD1	7.29	125.90	120.80
1	6-A	77	TYR	CB-CG-CD2	-7.28	116.63	121.00
3	2-D	437	TYR	CB-CG-CD1	-7.28	116.63	121.00
2	3-B	288	TYR	CB-CG-CD2	-7.28	116.63	121.00
3	8-C	87	PHE	CB-CG-CD2	-7.28	115.70	120.80
3	10-C	217	PHE	CB-CG-CD2	-7.28	115.70	120.80
2	2-B	730	THR	CA-CB-CG2	-7.28	102.21	112.40
2	9-B	514	ARG	NE-CZ-NH1	7.28	123.94	120.30
3	1-C	275	PHE	CB-CG-CD1	7.28	125.89	120.80
1	1-A	458	TYR	CB-CG-CD2	-7.27	116.64	121.00
3	7-D	333	ARG	NE-CZ-NH2	7.27	123.94	120.30
3	7-D	185	TYR	CB-CG-CD2	-7.27	116.64	121.00
1	3-A	603	TRP	CB-CG-CD1	-7.27	117.55	127.00
1	3-A	380	ASP	CB-CG-OD2	-7.27	111.76	118.30
3	8-D	106	ALA	N-CA-CB	7.27	120.28	110.10
3	3-D	55	ARG	NE-CZ-NH2	7.27	123.93	120.30
3	9-C	204	PHE	CB-CG-CD2	-7.26	115.72	120.80
1	1-A	131	PHE	CB-CG-CD2	-7.25	115.72	120.80
1	1-A	646	TYR	CB-CG-CD2	-7.25	116.65	121.00
1	10-A	393	TYR	CB-CG-CD1	7.25	125.35	121.00
1	1-A	160	ARG	NE-CZ-NH2	-7.25	116.68	120.30
3	3-D	244	PHE	CB-CG-CD1	-7.25	115.73	120.80
2	4-B	351	THR	CA-CB-CG2	-7.25	102.25	112.40
2	4-B	544	ARG	NE-CZ-NH1	-7.25	116.68	120.30
1	2-A	791	PHE	CB-CG-CD1	7.25	125.87	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6-D	358	ARG	NE-CZ-NH2	-7.24	116.68	120.30
3	7-D	243	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	3-A	162	PHE	CB-CG-CD1	-7.24	115.73	120.80
2	9-B	356	ARG	NE-CZ-NH1	7.24	123.92	120.30
3	5-D	225	GLN	N-CA-CB	7.24	123.63	110.60
3	10-D	300	ASP	CB-CG-OD2	-7.24	111.79	118.30
2	4-B	453	TYR	CB-CG-CD1	7.24	125.34	121.00
3	5-D	133	PHE	CB-CG-CD1	7.23	125.86	120.80
3	1-D	341	ARG	NE-CZ-NH2	-7.23	116.69	120.30
3	8-C	26	ALA	CB-CA-C	-7.23	99.26	110.10
2	7-B	544	ARG	NE-CZ-NH1	7.23	123.91	120.30
2	8-B	638	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	4-A	190	TYR	CB-CG-CD1	-7.22	116.67	121.00
3	4-D	329	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	6-A	161	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	8-A	349	ARG	NE-CZ-NH1	7.22	123.91	120.30
2	3-B	258	SER	N-CA-CB	7.22	121.33	110.50
3	3-C	445	TYR	CB-CG-CD2	7.22	125.33	121.00
3	4-D	95	ALA	CB-CA-C	-7.22	99.27	110.10
3	2-C	232	SER	N-CA-CB	7.22	121.32	110.50
2	2-B	362	PHE	CB-CG-CD1	7.21	125.85	120.80
3	8-D	162	TYR	CB-CG-CD2	-7.21	116.67	121.00
2	1-B	415	TYR	CB-CG-CD1	7.21	125.32	121.00
3	2-C	249	TYR	CB-CG-CD1	7.21	125.32	121.00
2	3-B	349	TRP	CG-CD2-CE3	-7.21	127.41	133.90
3	2-C	347	TRP	CE2-CD2-CG	-7.21	101.54	107.30
1	7-A	700	PHE	CB-CG-CD1	-7.20	115.76	120.80
1	7-A	74	TYR	CD1-CE1-CZ	7.20	126.28	119.80
1	4-A	776	ARG	NE-CZ-NH2	-7.20	116.70	120.30
3	5-D	244	PHE	CB-CG-CD1	-7.20	115.76	120.80
3	9-C	407	TYR	CG-CD1-CE1	-7.20	115.54	121.30
2	8-B	526	ARG	NE-CZ-NH1	7.20	123.90	120.30
2	10-B	514	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	10-A	110	VAL	O-C-N	-7.20	111.19	122.70
2	1-B	600	TYR	CB-CG-CD2	-7.19	116.69	121.00
3	9-D	120	LEU	CB-CG-CD1	7.19	123.22	111.00
1	3-A	60	VAL	CG1-CB-CG2	7.19	122.40	110.90
3	4-D	133	PHE	CB-CG-CD2	-7.19	115.77	120.80
3	6-C	244	PHE	CB-CG-CD2	-7.19	115.77	120.80
1	10-A	791	PHE	CB-CG-CD2	-7.18	115.77	120.80
2	2-B	510	TYR	CB-CG-CD1	7.18	125.31	121.00
2	5-B	561	ASP	CB-CG-OD1	-7.18	111.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-A	486	PHE	CB-CG-CD2	7.18	125.82	120.80
2	8-B	731	PHE	CB-CG-CD1	7.18	125.82	120.80
2	5-B	284	TYR	CB-CG-CD2	-7.17	116.69	121.00
2	5-B	295	ARG	NE-CZ-NH2	-7.17	116.71	120.30
3	9-D	390	ALA	N-CA-CB	7.17	120.14	110.10
3	7-D	394	PHE	CB-CG-CD2	-7.17	115.78	120.80
2	3-B	589	PHE	CB-CG-CD2	-7.17	115.78	120.80
1	3-A	663	TYR	CD1-CG-CD2	7.17	125.78	117.90
3	4-D	315	TYR	CD1-CE1-CZ	7.17	126.25	119.80
3	9-D	256	TYR	CB-CG-CD1	7.17	125.30	121.00
2	10-B	433	TYR	CG-CD1-CE1	-7.17	115.56	121.30
2	5-B	285	ARG	NE-CZ-NH1	7.17	123.88	120.30
3	9-C	124	ASP	CB-CG-OD2	7.17	124.75	118.30
1	1-A	558	TYR	CB-CG-CD2	-7.17	116.70	121.00
2	2-B	514	ARG	NE-CZ-NH1	-7.16	116.72	120.30
3	5-D	407	TYR	CB-CG-CD1	-7.16	116.70	121.00
3	3-C	319	TYR	CB-CG-CD1	7.16	125.29	121.00
1	2-A	174	GLU	N-CA-CB	7.16	123.48	110.60
2	3-B	342	TYR	CB-CG-CD2	-7.15	116.71	121.00
3	3-D	249	TYR	CB-CG-CD1	-7.15	116.71	121.00
1	4-A	458	TYR	CB-CG-CD1	-7.15	116.71	121.00
1	4-A	284	TYR	CB-CG-CD2	-7.15	116.71	121.00
1	8-A	358	ARG	NE-CZ-NH2	7.15	123.87	120.30
1	1-A	76	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	1-A	594	TYR	CB-CG-CD2	7.15	125.29	121.00
2	1-B	533	ARG	NE-CZ-NH1	-7.15	116.73	120.30
3	4-D	413	PHE	CB-CG-CD2	7.15	125.80	120.80
3	1-C	329	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	3-A	121	ARG	NE-CZ-NH1	-7.14	116.73	120.30
1	9-A	80	ASP	CB-CG-OD1	-7.14	111.87	118.30
1	9-A	193	TYR	CB-CG-CD2	-7.14	116.72	121.00
1	7-A	793	PHE	CB-CG-CD2	-7.14	115.80	120.80
1	4-A	443	MET	CG-SD-CE	-7.14	88.78	100.20
3	9-D	204	PHE	CB-CG-CD1	7.14	125.80	120.80
3	6-C	84	ARG	NE-CZ-NH1	7.13	123.87	120.30
3	10-D	217	PHE	CB-CG-CD2	-7.13	115.81	120.80
1	5-A	483	MET	CG-SD-CE	-7.13	88.79	100.20
2	6-B	389	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	1-A	131	PHE	O-C-N	-7.13	111.08	123.20
2	5-B	429	TYR	CZ-CE2-CD2	-7.13	113.38	119.80
1	7-A	663	TYR	N-CA-CB	7.13	123.43	110.60
1	5-A	458	TYR	CG-CD2-CE2	-7.12	115.60	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	627	ARG	NE-CZ-NH2	7.12	123.86	120.30
2	9-B	816	TYR	CB-CG-CD1	7.12	125.27	121.00
3	3-C	170	TYR	CB-CG-CD1	7.12	125.27	121.00
3	10-C	162	TYR	CB-CG-CD1	-7.12	116.73	121.00
2	8-B	599	PHE	CB-CG-CD1	7.12	125.78	120.80
2	6-B	833	ASP	CB-CG-OD2	7.11	124.70	118.30
2	7-B	425	PHE	CB-CG-CD1	7.11	125.78	120.80
3	6-C	341	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	7-A	647	PHE	CB-CG-CD1	7.11	125.78	120.80
1	10-A	409	PHE	CB-CG-CD1	7.11	125.78	120.80
1	2-A	296	TYR	CB-CG-CD1	-7.11	116.73	121.00
1	9-A	105	PHE	CB-CG-CD1	-7.10	115.83	120.80
2	3-B	362	PHE	CB-CG-CD2	-7.10	115.83	120.80
3	10-D	109	TYR	CB-CG-CD1	7.10	125.26	121.00
1	4-A	791	PHE	CB-CG-CD1	-7.10	115.83	120.80
2	10-B	600	TYR	CB-CG-CD1	-7.10	116.74	121.00
3	5-D	47	ASP	CB-CG-OD1	7.10	124.69	118.30
2	7-B	319	PHE	CB-CG-CD1	7.10	125.77	120.80
1	5-A	776	ARG	NE-CZ-NH2	7.09	123.85	120.30
2	7-B	494	GLU	N-CA-CB	7.09	123.37	110.60
2	4-B	545	VAL	CG1-CB-CG2	7.09	122.25	110.90
1	5-A	663	TYR	CB-CG-CD2	-7.09	116.75	121.00
1	4-A	381	PHE	CB-CG-CD1	7.08	125.76	120.80
3	6-D	193	ARG	NH1-CZ-NH2	7.08	127.19	119.40
1	2-A	691	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	7-A	74	TYR	CG-CD1-CE1	-7.08	115.64	121.30
2	4-B	445	PHE	CB-CG-CD2	-7.08	115.84	120.80
3	4-C	124	ASP	CB-CG-OD1	7.08	124.67	118.30
3	7-C	272	PHE	CB-CG-CD2	-7.07	115.85	120.80
1	1-A	465	PHE	CB-CG-CD1	7.07	125.75	120.80
3	5-C	279	TYR	CZ-CE2-CD2	-7.07	113.44	119.80
2	4-B	562	TYR	CG-CD1-CE1	-7.07	115.64	121.30
2	5-B	731	PHE	CB-CG-CD2	-7.07	115.85	120.80
3	2-C	344	PHE	CB-CG-CD1	7.06	125.74	120.80
1	9-A	382	ALA	N-CA-CB	7.06	119.99	110.10
3	4-D	93	TRP	CE2-CD2-CE3	7.05	127.16	118.70
2	5-B	425	PHE	CB-CG-CD2	-7.05	115.86	120.80
3	6-C	267	PHE	CB-CG-CD2	7.05	125.73	120.80
1	10-A	709	PHE	CB-CG-CD1	7.05	125.73	120.80
2	4-B	514	ARG	NE-CZ-NH1	-7.05	116.78	120.30
2	1-B	343	TYR	CG-CD1-CE1	-7.04	115.67	121.30
1	1-A	282	MET	CA-CB-CG	7.04	125.27	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	398	TYR	CG-CD2-CE2	-7.04	115.67	121.30
2	5-B	822	ARG	NE-CZ-NH1	7.04	123.82	120.30
3	5-C	170	TYR	CB-CG-CD2	-7.04	116.78	121.00
3	7-C	62	PHE	CB-CG-CD1	7.04	125.73	120.80
2	9-B	470	TYR	CB-CG-CD1	7.03	125.22	121.00
1	3-A	325	PHE	CB-CG-CD1	7.03	125.72	120.80
3	6-C	65	ARG	NE-CZ-NH1	7.03	123.81	120.30
2	7-B	438	TYR	CB-CG-CD2	7.03	125.22	121.00
3	8-D	170	TYR	CB-CG-CD2	7.03	125.22	121.00
3	8-D	299	LEU	CA-CB-CG	7.02	131.46	115.30
3	1-C	248	MET	CA-CB-CG	-7.02	101.36	113.30
3	6-D	75	VAL	CG1-CB-CG2	-7.02	99.67	110.90
3	7-C	341	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	5-A	582	TYR	CD1-CE1-CZ	7.02	126.12	119.80
1	6-A	410	PHE	CB-CG-CD2	-7.02	115.89	120.80
1	9-A	299	PHE	CB-CG-CD1	-7.02	115.89	120.80
2	10-B	515	VAL	CA-CB-CG1	7.02	121.43	110.90
2	4-B	285	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	6-A	647	PHE	CB-CG-CD1	7.02	125.71	120.80
1	4-A	413	TYR	CZ-CE2-CD2	-7.02	113.48	119.80
2	4-B	400	TYR	CB-CG-CD1	-7.01	116.79	121.00
3	5-D	47	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	7-A	129	THR	CA-CB-CG2	-7.01	102.58	112.40
1	8-A	261	ASP	CB-CG-OD2	-7.01	111.99	118.30
3	7-C	403	PHE	CB-CG-CD1	7.01	125.71	120.80
3	4-D	20	PHE	CB-CG-CD1	-7.01	115.89	120.80
3	1-D	297	ASP	CB-CG-OD2	7.01	124.61	118.30
2	8-B	562	TYR	CB-CG-CD2	-7.01	116.79	121.00
3	8-C	437	TYR	CG-CD1-CE1	-7.01	115.69	121.30
3	2-D	46	ARG	NE-CZ-NH2	-7.01	116.80	120.30
2	6-B	425	PHE	CB-CG-CD2	7.01	125.70	120.80
2	1-B	578	PHE	CB-CG-CD2	-7.00	115.90	120.80
3	6-D	83	PHE	CB-CG-CD1	-7.00	115.90	120.80
3	6-D	243	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	9-A	486	PHE	CB-CG-CD1	7.00	125.70	120.80
3	6-C	267	PHE	CB-CG-CD1	-6.99	115.91	120.80
1	6-A	66	VAL	CA-CB-CG2	-6.99	100.41	110.90
3	2-C	130	THR	CA-CB-CG2	-6.99	102.61	112.40
1	9-A	284	TYR	CD1-CG-CD2	-6.99	110.21	117.90
1	2-A	458	TYR	CB-CG-CD2	-6.99	116.81	121.00
1	2-A	764	LEU	CB-CG-CD2	6.99	122.88	111.00
3	4-D	297	ASP	CB-CG-OD1	6.99	124.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	10-A	284	TYR	CB-CG-CD2	-6.99	116.81	121.00
2	10-B	194	ALA	N-CA-CB	6.99	119.88	110.10
3	10-D	133	PHE	CB-CG-CD2	6.99	125.69	120.80
1	3-A	714	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	4-A	709	PHE	CB-CG-CD1	6.98	125.69	120.80
1	5-A	398	TYR	CG-CD1-CE1	-6.98	115.72	121.30
2	6-B	510	TYR	CB-CG-CD2	6.98	125.19	121.00
2	4-B	297	TYR	CB-CG-CD1	6.98	125.19	121.00
3	7-C	197	ASP	CB-CG-OD1	-6.98	112.02	118.30
2	8-B	342	TYR	CB-CG-CD2	-6.98	116.81	121.00
1	1-A	602	THR	CA-CB-CG2	-6.97	102.64	112.40
1	3-A	663	TYR	CG-CD2-CE2	-6.97	115.72	121.30
2	6-B	638	ARG	NE-CZ-NH2	-6.97	116.82	120.30
2	9-B	453	TYR	CB-CG-CD1	-6.97	116.82	121.00
3	8-C	308	THR	CA-CB-CG2	6.97	122.16	112.40
2	2-B	661	PHE	CB-CG-CD2	6.97	125.68	120.80
2	5-B	609	ASP	CB-CG-OD1	-6.97	112.03	118.30
3	9-D	170	TYR	CB-CG-CD2	6.97	125.18	121.00
3	2-D	272	PHE	CB-CG-CD1	-6.96	115.92	120.80
1	3-A	160	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	1-A	182	VAL	CA-CB-CG1	6.96	121.34	110.90
1	9-A	714	ARG	NE-CZ-NH1	-6.96	116.82	120.30
3	1-D	136	PHE	CB-CG-CD2	-6.95	115.93	120.80
2	5-B	731	PHE	CB-CG-CD1	6.95	125.67	120.80
3	6-C	46	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	8-A	588	TYR	CB-CG-CD1	6.95	125.17	121.00
3	10-C	131	ASP	CB-CG-OD2	6.95	124.56	118.30
3	2-D	362	TYR	CB-CG-CD2	-6.95	116.83	121.00
2	4-B	846	ARG	NE-CZ-NH2	-6.95	116.83	120.30
2	7-B	576	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	3-A	663	TYR	CG-CD1-CE1	-6.95	115.74	121.30
1	1-A	704	TYR	CD1-CG-CD2	6.95	125.54	117.90
1	9-A	474	PRO	N-CA-CB	6.95	111.64	103.30
3	4-D	430	VAL	CA-CB-CG2	-6.94	100.49	110.90
1	3-A	284	TYR	CB-CG-CD2	-6.94	116.84	121.00
1	3-A	663	TYR	CB-CG-CD2	-6.94	116.84	121.00
3	1-C	413	PHE	CB-CG-CD2	-6.93	115.95	120.80
1	4-A	116	TYR	CB-CG-CD2	-6.93	116.84	121.00
1	4-A	138	PHE	CB-CG-CD2	-6.93	115.95	120.80
3	9-C	170	TYR	CG-CD1-CE1	-6.93	115.75	121.30
1	5-A	646	TYR	CB-CG-CD1	6.93	125.16	121.00
3	7-C	292	TYR	CB-CG-CD2	-6.93	116.84	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	358	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	2-A	112	TYR	CG-CD2-CE2	-6.92	115.76	121.30
1	7-A	172	GLU	OE1-CD-OE2	6.92	131.61	123.30
3	1-C	292	TYR	CB-CG-CD2	-6.92	116.85	121.00
2	2-B	580	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	3-A	776	ARG	NE-CZ-NH2	-6.92	116.84	120.30
2	5-B	470	TYR	CG-CD1-CE1	6.92	126.83	121.30
2	7-B	299	ARG	NE-CZ-NH1	6.92	123.76	120.30
3	8-D	62	PHE	N-CA-CB	6.92	123.05	110.60
1	9-A	479	ARG	NE-CZ-NH2	-6.92	116.84	120.30
3	1-C	10	ALA	N-CA-CB	6.91	119.78	110.10
1	4-A	563	ASP	CB-CG-OD1	-6.91	112.08	118.30
2	7-B	294	LEU	CB-CG-CD2	6.91	122.75	111.00
2	8-B	429	TYR	N-CA-CB	6.91	123.04	110.60
2	10-B	555	TRP	CB-CG-CD1	6.91	135.99	127.00
2	3-B	425	PHE	CB-CG-CD1	6.91	125.64	120.80
1	1-A	647	PHE	CB-CG-CD2	6.91	125.64	120.80
3	8-C	185	TYR	CB-CG-CD2	6.91	125.15	121.00
2	3-B	562	TYR	CG-CD2-CE2	-6.91	115.77	121.30
3	8-C	437	TYR	CB-CG-CD1	-6.91	116.86	121.00
3	1-D	445	TYR	CB-CG-CD1	-6.91	116.86	121.00
3	1-D	161	ARG	NE-CZ-NH2	6.91	123.75	120.30
2	5-B	191	THR	CA-CB-CG2	-6.91	102.73	112.40
3	6-D	136	PHE	CZ-CE2-CD2	6.91	128.39	120.10
3	7-D	170	TYR	CB-CG-CD1	6.91	125.14	121.00
2	9-B	770	TYR	CB-CG-CD2	6.90	125.14	121.00
2	8-B	440	GLY	CA-C-O	6.90	133.01	120.60
3	9-C	387	PHE	CB-CG-CD1	6.90	125.63	120.80
2	4-B	728	HIS	N-CA-CB	6.89	123.01	110.60
2	4-B	776	TYR	CB-CG-CD2	6.89	125.14	121.00
3	6-C	398	PHE	CB-CG-CD1	6.89	125.63	120.80
2	7-B	839	PHE	CB-CG-CD1	6.89	125.63	120.80
3	8-D	162	TYR	CA-CB-CG	-6.89	100.31	113.40
3	9-C	362	TYR	CB-CG-CD2	-6.89	116.86	121.00
3	4-C	193	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	5-A	60	VAL	CA-CB-CG1	-6.89	100.57	110.90
2	6-B	288	TYR	CG-CD2-CE2	-6.89	115.79	121.30
3	5-C	59	ARG	NE-CZ-NH1	6.89	123.74	120.30
3	9-C	319	TYR	CB-CG-CD1	-6.89	116.87	121.00
1	10-A	438	PHE	CB-CG-CD2	6.89	125.62	120.80
1	2-A	782	PHE	CB-CG-CD2	6.88	125.62	120.80
2	5-B	267	PHE	CB-CG-CD1	6.88	125.62	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6-C	297	ASP	N-CA-CB	6.88	122.99	110.60
3	7-D	249	TYR	CZ-CE2-CD2	-6.88	113.60	119.80
1	1-A	704	TYR	CG-CD1-CE1	-6.88	115.80	121.30
1	2-A	160	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	2-A	193	TYR	N-CA-CB	6.88	122.98	110.60
1	2-A	193	TYR	CB-CG-CD1	-6.88	116.87	121.00
3	10-C	90	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	2-A	582	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	6-A	692	LEU	CB-CG-CD2	6.88	122.69	111.00
3	3-D	440	ALA	CB-CA-C	-6.87	99.79	110.10
1	7-A	427	LEU	N-CA-CB	6.87	124.14	110.40
3	1-C	218	ARG	NE-CZ-NH2	6.87	123.73	120.30
3	1-D	292	TYR	CB-CG-CD2	-6.87	116.88	121.00
2	1-B	363	PHE	CB-CG-CD2	-6.87	115.99	120.80
2	7-B	304	LEU	CB-CA-C	-6.87	97.16	110.20
2	4-B	300	PHE	CB-CG-CD1	-6.86	116.00	120.80
3	10-C	204	PHE	CB-CG-CD2	-6.86	116.00	120.80
1	4-A	365	THR	CA-CB-CG2	-6.86	102.79	112.40
2	2-B	400	TYR	CG-CD1-CE1	-6.86	115.81	121.30
1	6-A	638	HIS	N-CA-CB	6.85	122.93	110.60
1	7-A	198	ARG	NE-CZ-NH1	6.85	123.72	120.30
3	7-C	224	LEU	CB-CG-CD1	6.85	122.64	111.00
1	9-A	633	HIS	CA-CB-CG	6.85	125.24	113.60
1	10-A	112	TYR	CB-CG-CD2	-6.85	116.89	121.00
2	2-B	236	TYR	CB-CG-CD1	6.84	125.11	121.00
3	9-D	362	TYR	N-CA-CB	6.84	122.92	110.60
3	6-C	308	THR	CA-CB-CG2	-6.84	102.83	112.40
3	6-C	444	SER	N-CA-CB	6.84	120.76	110.50
2	5-B	505	ASP	CB-CG-OD1	6.84	124.45	118.30
1	9-A	102	PHE	CB-CG-CD1	-6.84	116.01	120.80
2	9-B	565	TYR	CB-CG-CD1	6.84	125.10	121.00
2	5-B	819	PHE	CB-CG-CD2	-6.83	116.02	120.80
3	7-D	354	VAL	CA-CB-CG2	-6.83	100.65	110.90
2	9-B	638	ARG	NE-CZ-NH1	6.83	123.72	120.30
3	10-D	267	PHE	CB-CG-CD2	6.83	125.58	120.80
1	7-A	627	ARG	NE-CZ-NH1	6.83	123.72	120.30
3	8-D	86	PHE	CB-CG-CD1	-6.83	116.02	120.80
2	9-B	758	TYR	CD1-CG-CD2	6.83	125.41	117.90
1	3-A	450	TYR	CB-CG-CD1	-6.83	116.91	121.00
2	3-B	363	PHE	CB-CG-CD2	-6.83	116.02	120.80
3	1-D	90	ARG	NE-CZ-NH2	6.82	123.71	120.30
2	6-B	772	PHE	CB-CG-CD1	6.82	125.58	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7-B	468	PHE	CB-CG-CD2	6.82	125.58	120.80
3	9-C	358	ARG	NE-CZ-NH1	6.82	123.71	120.30
3	6-C	173	PHE	CB-CG-CD2	-6.82	116.03	120.80
2	1-B	295	ARG	NE-CZ-NH1	6.82	123.71	120.30
3	8-C	437	TYR	CZ-CE2-CD2	-6.82	113.67	119.80
2	9-B	284	TYR	CB-CG-CD1	6.82	125.09	121.00
2	9-B	425	PHE	CB-CG-CD2	-6.82	116.03	120.80
3	10-C	55	ARG	NE-CZ-NH1	6.82	123.71	120.30
2	1-B	805	PHE	CB-CG-CD1	6.81	125.57	120.80
3	6-C	176	ARG	NE-CZ-NH2	-6.81	116.89	120.30
2	1-B	445	PHE	CB-CG-CD1	6.81	125.57	120.80
3	8-C	170	TYR	CB-CG-CD1	-6.81	116.91	121.00
1	7-A	204	ARG	NE-CZ-NH1	-6.81	116.90	120.30
3	3-C	315	TYR	CG-CD2-CE2	-6.80	115.86	121.30
1	6-A	140	TYR	CB-CG-CD1	6.80	125.08	121.00
1	6-A	614	TYR	CB-CG-CD1	-6.80	116.92	121.00
3	6-C	434	MET	CG-SD-CE	-6.80	89.31	100.20
1	3-A	299	PHE	CB-CG-CD2	-6.80	116.04	120.80
1	4-A	413	TYR	CG-CD2-CE2	6.80	126.74	121.30
3	3-C	59	ARG	NE-CZ-NH2	6.80	123.70	120.30
2	4-B	565	TYR	CB-CG-CD2	-6.80	116.92	121.00
2	1-B	600	TYR	CG-CD1-CE1	-6.79	115.86	121.30
2	4-B	227	ALA	CB-CA-C	-6.79	99.91	110.10
3	10-C	411	ASP	CB-CG-OD1	-6.79	112.19	118.30
1	3-A	145	PHE	CB-CG-CD2	-6.79	116.05	120.80
1	7-A	775	PHE	CB-CG-CD2	-6.79	116.05	120.80
2	6-B	337	SER	N-CA-CB	6.78	120.68	110.50
3	7-C	247	TYR	CB-CG-CD2	-6.78	116.93	121.00
3	2-C	86	PHE	CB-CG-CD1	-6.78	116.05	120.80
3	8-C	64	PRO	N-CA-CB	6.78	111.44	103.30
3	5-D	204	PHE	CB-CG-CD1	-6.78	116.05	120.80
2	8-B	587	PHE	CB-CG-CD1	-6.78	116.06	120.80
3	2-D	272	PHE	CB-CG-CD2	6.78	125.54	120.80
2	5-B	242	ARG	NE-CZ-NH2	-6.78	116.91	120.30
2	6-B	322	HIS	CA-CB-CG	6.78	125.12	113.60
2	8-B	293	ARG	NE-CZ-NH1	-6.78	116.91	120.30
2	9-B	805	PHE	CB-CG-CD1	-6.78	116.06	120.80
2	9-B	533	ARG	NE-CZ-NH1	6.77	123.69	120.30
2	2-B	301	THR	N-CA-CB	6.77	123.17	110.30
3	7-C	283	ASP	CB-CG-OD2	-6.77	112.21	118.30
3	9-D	217	PHE	CB-CG-CD1	6.77	125.54	120.80
2	3-B	349	TRP	CE2-CD2-CE3	6.77	126.82	118.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	190	TYR	CB-CG-CD2	-6.77	116.94	121.00
3	2-C	421	ASP	CB-CG-OD1	6.76	124.39	118.30
1	5-A	478	MET	CG-SD-CE	6.76	111.03	100.20
1	8-A	791	PHE	CB-CG-CD1	6.76	125.53	120.80
2	9-B	275	GLY	N-CA-C	-6.76	96.19	113.10
2	4-B	827	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	3-A	296	TYR	CB-CG-CD1	-6.76	116.94	121.00
1	6-A	594	TYR	CD1-CE1-CZ	6.76	125.88	119.80
3	6-D	20	PHE	CB-CG-CD1	6.76	125.53	120.80
1	4-A	324	TYR	CZ-CE2-CD2	6.76	125.88	119.80
2	7-B	475	PHE	CB-CG-CD1	6.76	125.53	120.80
3	1-D	292	TYR	CB-CG-CD1	6.75	125.05	121.00
1	2-A	473	ASN	N-CA-CB	6.75	122.75	110.60
2	3-B	438	TYR	CG-CD1-CE1	-6.75	115.90	121.30
2	5-B	295	ARG	NE-CZ-NH1	6.75	123.67	120.30
3	5-C	445	TYR	CG-CD1-CE1	6.75	126.70	121.30
1	4-A	767	TYR	CB-CG-CD1	-6.75	116.95	121.00
3	9-D	77	ALA	N-CA-CB	6.75	119.55	110.10
2	5-B	264	TYR	CB-CG-CD2	-6.75	116.95	121.00
1	2-A	558	TYR	CB-CG-CD2	-6.74	116.95	121.00
3	2-D	279	TYR	CG-CD2-CE2	6.74	126.69	121.30
2	6-B	403	PHE	CB-CG-CD1	-6.74	116.08	120.80
2	6-B	194	ALA	N-CA-CB	6.74	119.54	110.10
1	1-A	473	ASN	N-CA-CB	6.74	122.73	110.60
3	4-D	55	ARG	NE-CZ-NH1	-6.74	116.93	120.30
3	7-C	49	ASP	CB-CG-OD1	6.74	124.36	118.30
1	5-A	414	ASP	CB-CG-OD1	6.74	124.36	118.30
1	9-A	162	PHE	CB-CG-CD1	6.74	125.51	120.80
3	1-C	30	ALA	N-CA-CB	6.73	119.53	110.10
1	2-A	576	ARG	NE-CZ-NH1	-6.73	116.93	120.30
1	9-A	588	TYR	CB-CG-CD2	-6.73	116.96	121.00
2	9-B	769	VAL	CA-CB-CG2	-6.73	100.80	110.90
1	3-A	359	ALA	CB-CA-C	6.73	120.20	110.10
3	3-C	133	PHE	CB-CG-CD2	-6.73	116.09	120.80
3	9-C	350	SER	O-C-N	-6.73	111.93	122.70
1	1-A	667	THR	CA-CB-CG2	-6.73	102.98	112.40
3	4-C	84	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	6-A	609	THR	CA-CB-CG2	-6.73	102.98	112.40
3	2-C	437	TYR	CG-CD2-CE2	-6.73	115.92	121.30
3	4-D	128	ASP	CB-CA-C	-6.73	96.94	110.40
2	2-B	839	PHE	CB-CG-CD1	6.73	125.51	120.80
1	6-A	450	TYR	CB-CG-CD2	-6.73	116.96	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7-A	691	ASP	CB-CG-OD2	6.73	124.35	118.30
1	8-A	576	ARG	NH1-CZ-NH2	-6.73	112.00	119.40
1	2-A	639	PHE	CB-CG-CD2	-6.72	116.09	120.80
3	3-C	341	ARG	NE-CZ-NH1	6.72	123.66	120.30
3	8-C	65	ARG	NE-CZ-NH1	6.72	123.66	120.30
3	10-C	352	MET	CG-SD-CE	-6.72	89.45	100.20
1	3-A	148	ASP	CB-CA-C	-6.72	96.97	110.40
1	3-A	162	PHE	CB-CG-CD2	6.72	125.50	120.80
2	8-B	190	TYR	CD1-CE1-CZ	-6.72	113.75	119.80
3	9-D	87	PHE	CB-CG-CD1	-6.72	116.10	120.80
2	2-B	822	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	4-A	292	LEU	CB-CG-CD1	6.71	122.41	111.00
3	7-C	105	TRP	CG-CD2-CE3	-6.71	127.86	133.90
1	8-A	604	MET	CG-SD-CE	6.71	110.94	100.20
3	3-C	247	TYR	N-CA-CB	6.71	122.68	110.60
3	5-D	70	ASP	CB-CG-OD2	6.71	124.34	118.30
2	8-B	200	PHE	CB-CG-CD2	-6.71	116.10	120.80
3	8-D	315	TYR	CB-CG-CD1	-6.71	116.97	121.00
3	9-C	47	ASP	CB-CG-OD1	6.71	124.34	118.30
1	5-A	405	PHE	CB-CG-CD1	6.71	125.50	120.80
3	5-C	68	MET	CA-CB-CG	6.71	124.70	113.30
3	10-D	48	ASP	CB-CG-OD1	6.71	124.34	118.30
2	7-B	415	TYR	CB-CG-CD2	6.71	125.02	121.00
1	9-A	198	ARG	NE-CZ-NH1	-6.71	116.95	120.30
2	10-B	239	GLU	OE1-CD-OE2	6.71	131.35	123.30
3	2-C	84	ARG	NE-CZ-NH2	-6.70	116.95	120.30
3	8-D	243	ARG	CD-NE-CZ	-6.70	114.22	123.60
2	2-B	264	TYR	CG-CD2-CE2	-6.70	115.94	121.30
1	8-A	138	PHE	CB-CG-CD1	6.70	125.49	120.80
3	8-C	96	SER	CB-CA-C	-6.70	97.38	110.10
3	1-C	70	ASP	N-CA-CB	6.70	122.65	110.60
3	2-D	20	PHE	CG-CD1-CE1	-6.69	113.44	120.80
3	10-D	437	TYR	CB-CG-CD2	-6.69	116.98	121.00
1	3-A	755	ASP	CB-CG-OD2	6.69	124.32	118.30
1	5-A	799	VAL	CA-CB-CG2	6.69	120.93	110.90
1	8-A	357	VAL	CA-CB-CG1	6.68	120.92	110.90
2	1-B	300	PHE	CB-CG-CD2	6.68	125.47	120.80
3	4-D	232	SER	N-CA-CB	6.68	120.52	110.50
3	10-D	427	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	2-A	400	ARG	NE-CZ-NH2	-6.68	116.96	120.30
3	2-C	65	ARG	NE-CZ-NH2	-6.68	116.96	120.30
3	4-D	93	TRP	CH2-CZ2-CE2	6.68	124.08	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	10-A	687	ARG	NE-CZ-NH2	-6.68	116.96	120.30
3	10-D	217	PHE	CB-CG-CD1	6.68	125.47	120.80
3	3-C	341	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	5-A	107	ARG	NH1-CZ-NH2	6.67	126.74	119.40
2	10-B	805	PHE	CB-CG-CD1	6.67	125.47	120.80
1	7-A	413	TYR	CB-CG-CD2	6.67	125.00	121.00
3	1-D	34	ASP	CB-CA-C	-6.67	97.06	110.40
3	2-D	307	SER	N-CA-CB	6.67	120.51	110.50
3	2-D	375	MET	CG-SD-CE	-6.67	89.53	100.20
2	6-B	612	ARG	NE-CZ-NH2	-6.67	116.97	120.30
3	1-D	333	ARG	NE-CZ-NH2	-6.66	116.97	120.30
3	10-C	347	TRP	CB-CG-CD2	-6.66	117.94	126.60
1	1-A	630	ARG	NE-CZ-NH1	-6.66	116.97	120.30
3	9-C	247	TYR	CB-CG-CD1	6.66	125.00	121.00
3	9-C	160	ASP	CB-CG-OD2	-6.66	112.31	118.30
3	4-C	333	ARG	NE-CZ-NH1	-6.66	116.97	120.30
3	5-D	162	TYR	CB-CG-CD2	-6.66	117.01	121.00
3	6-D	185	TYR	CG-CD1-CE1	-6.66	115.98	121.30
3	5-C	46	ARG	NE-CZ-NH2	6.65	123.63	120.30
2	9-B	487	ASP	CB-CG-OD2	-6.65	112.31	118.30
3	9-D	177	SER	O-C-N	-6.65	112.06	122.70
2	6-B	438	TYR	CB-CG-CD1	-6.65	117.01	121.00
2	5-B	315	GLU	OE1-CD-OE2	6.65	131.28	123.30
2	2-B	411	PHE	N-CA-CB	6.65	122.56	110.60
1	4-A	193	TYR	CB-CG-CD1	6.65	124.99	121.00
1	6-A	663	TYR	CB-CG-CD1	6.65	124.99	121.00
2	9-B	633	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	5-A	638	HIS	CA-CB-CG	6.64	124.89	113.60
2	5-B	191	THR	N-CA-CB	6.64	122.92	110.30
1	9-A	123	TYR	CZ-CE2-CD2	6.64	125.78	119.80
2	7-B	433	TYR	CB-CG-CD2	-6.64	117.02	121.00
1	10-A	678	GLY	C-N-CA	6.64	136.25	122.30
1	6-A	709	PHE	CB-CG-CD1	6.64	125.45	120.80
1	8-A	279	TYR	CB-CG-CD2	6.64	124.98	121.00
2	10-B	773	VAL	CG1-CB-CG2	6.64	121.53	110.90
1	4-A	354	LEU	CB-CG-CD1	6.63	122.28	111.00
3	7-C	307	SER	N-CA-CB	6.63	120.45	110.50
2	9-B	644	PHE	N-CA-CB	-6.63	98.66	110.60
1	4-A	639	PHE	CB-CG-CD2	-6.63	116.16	120.80
3	5-C	251	SER	N-CA-CB	6.63	120.45	110.50
2	9-B	343	TYR	CD1-CG-CD2	6.63	125.20	117.90
1	1-A	601	GLU	OE1-CD-OE2	6.63	131.26	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5-B	425	PHE	CB-CG-CD1	6.63	125.44	120.80
3	6-C	411	ASP	CB-CG-OD2	-6.63	112.33	118.30
2	3-B	593	PHE	CB-CG-CD2	-6.63	116.16	120.80
2	5-B	509	ASN	CB-CG-OD1	-6.63	108.34	121.60
3	8-C	93	TRP	CD2-CE2-CZ2	-6.63	114.34	122.30
1	4-A	198	ARG	NE-CZ-NH2	-6.63	116.99	120.30
1	6-A	302	TYR	CB-CG-CD2	6.62	124.97	121.00
3	9-C	437	TYR	CD1-CE1-CZ	6.62	125.76	119.80
3	1-C	315	TYR	CZ-CE2-CD2	6.62	125.76	119.80
3	1-C	316	PHE	CB-CG-CD1	-6.62	116.16	120.80
2	5-B	272	VAL	CA-CB-CG2	-6.62	100.96	110.90
2	1-B	822	ARG	NE-CZ-NH1	6.62	123.61	120.30
3	5-C	88	ASP	CB-CG-OD2	-6.62	112.34	118.30
3	4-C	185	TYR	CB-CG-CD2	-6.62	117.03	121.00
1	10-A	180	THR	CA-CB-CG2	-6.62	103.13	112.40
1	10-A	582	TYR	CB-CG-CD2	-6.62	117.03	121.00
1	3-A	486	PHE	CB-CG-CD2	6.62	125.43	120.80
3	1-D	197	ASP	CB-CG-OD2	-6.62	112.35	118.30
3	4-D	31	ILE	C-N-CA	6.62	136.19	122.30
1	6-A	704	TYR	CB-CG-CD2	-6.62	117.03	121.00
2	1-B	731	PHE	CB-CG-CD1	-6.61	116.17	120.80
1	7-A	405	PHE	CB-CG-CD1	6.61	125.43	120.80
2	3-B	670	ARG	N-CA-CB	6.61	122.50	110.60
3	6-D	417	GLN	N-CA-CB	6.61	122.50	110.60
3	3-D	176	ARG	NE-CZ-NH2	6.61	123.61	120.30
3	4-D	413	PHE	CB-CG-CD1	-6.61	116.17	120.80
2	6-B	471	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	9-A	77	TYR	CB-CG-CD2	-6.61	117.03	121.00
2	3-B	264	TYR	CB-CG-CD2	-6.61	117.04	121.00
2	9-B	600	TYR	CD1-CE1-CZ	-6.61	113.86	119.80
3	9-D	26	ALA	N-CA-CB	6.61	119.35	110.10
3	3-C	319	TYR	CB-CG-CD2	-6.60	117.04	121.00
1	8-A	374	THR	CA-CB-CG2	-6.60	103.16	112.40
3	2-C	161	ARG	NE-CZ-NH2	-6.60	117.00	120.30
3	2-C	170	TYR	CB-CG-CD1	6.60	124.96	121.00
2	5-B	819	PHE	CB-CG-CD1	6.60	125.42	120.80
3	7-C	97	ASP	CB-CG-OD1	-6.60	112.36	118.30
3	2-D	82	THR	CA-CB-CG2	-6.59	103.17	112.40
3	6-C	243	ARG	NE-CZ-NH2	-6.59	117.00	120.30
3	9-C	160	ASP	CB-CG-OD1	6.59	124.23	118.30
3	8-D	387	PHE	CB-CG-CD2	-6.59	116.19	120.80
1	3-A	558	TYR	CB-CG-CD2	-6.59	117.05	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-C	247	TYR	CG-CD1-CE1	-6.59	116.03	121.30
1	7-A	157	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	4-A	594	TYR	CG-CD2-CE2	-6.59	116.03	121.30
2	8-B	600	TYR	CB-CG-CD1	-6.59	117.05	121.00
3	4-C	136	PHE	CB-CG-CD1	-6.58	116.19	120.80
3	7-D	86	PHE	CB-CG-CD2	-6.58	116.19	120.80
3	8-C	309	ALA	CB-CA-C	-6.58	100.23	110.10
1	3-A	755	ASP	CB-CG-OD1	-6.58	112.38	118.30
1	9-A	704	TYR	CB-CG-CD1	-6.58	117.05	121.00
2	9-B	609	ASP	CB-CG-OD2	6.58	124.22	118.30
2	2-B	359	TYR	CB-CG-CD2	-6.58	117.05	121.00
3	2-C	118	ASP	CB-CG-OD2	6.58	124.22	118.30
1	9-A	597	ARG	NE-CZ-NH1	6.58	123.59	120.30
3	10-C	267	PHE	CB-CG-CD2	-6.58	116.20	120.80
1	5-A	279	TYR	CG-CD1-CE1	-6.57	116.04	121.30
1	10-A	639	PHE	CB-CG-CD1	6.57	125.40	120.80
2	10-B	200	PHE	CB-CG-CD1	-6.57	116.20	120.80
3	5-D	247	TYR	CB-CG-CD1	6.57	124.94	121.00
3	6-D	279	TYR	CZ-CE2-CD2	6.57	125.71	119.80
3	3-C	17	VAL	CA-CB-CG2	6.57	120.75	110.90
1	1-A	344	LEU	CB-CG-CD1	6.57	122.16	111.00
2	2-B	468	PHE	CB-CG-CD1	6.57	125.40	120.80
1	1-A	321	ASP	CB-CG-OD2	-6.56	112.39	118.30
1	10-A	663	TYR	CB-CG-CD1	6.56	124.94	121.00
1	3-A	99	ASP	CB-CG-OD2	6.56	124.20	118.30
3	7-C	403	PHE	CB-CG-CD2	-6.56	116.21	120.80
3	8-C	348	SER	N-CA-CB	6.55	120.33	110.50
1	4-A	476	ASN	N-CA-CB	6.55	122.39	110.60
1	5-A	116	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	5-A	157	ARG	NE-CZ-NH1	6.55	123.58	120.30
2	4-B	244	LEU	CB-CG-CD1	6.55	122.14	111.00
3	7-C	86	PHE	CB-CG-CD1	6.55	125.39	120.80
3	3-D	110	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	4-A	203	ARG	NE-CZ-NH2	-6.55	117.03	120.30
3	4-D	272	PHE	CB-CG-CD1	6.55	125.39	120.80
1	9-A	324	TYR	CB-CG-CD1	6.55	124.93	121.00
2	10-B	505	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	3-A	438	PHE	CB-CG-CD1	6.55	125.38	120.80
1	7-A	429	TYR	CD1-CE1-CZ	-6.55	113.91	119.80
1	5-A	150	TYR	CB-CG-CD1	-6.54	117.07	121.00
3	6-C	354	VAL	CG1-CB-CG2	-6.54	100.43	110.90
2	3-B	612	ARG	NE-CZ-NH1	-6.54	117.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-A	772	SER	N-CA-CB	6.54	120.32	110.50
1	6-A	279	TYR	CB-CG-CD2	-6.54	117.08	121.00
3	10-D	69	MET	CG-SD-CE	-6.54	89.74	100.20
3	3-C	402	ALA	N-CA-CB	6.54	119.25	110.10
3	2-C	39	LEU	CB-CG-CD2	6.53	122.11	111.00
3	2-C	84	ARG	NE-CZ-NH1	6.53	123.57	120.30
3	9-C	20	PHE	CB-CG-CD2	-6.53	116.23	120.80
1	9-A	284	TYR	CG-CD1-CE1	6.53	126.53	121.30
2	8-B	778	ASN	N-CA-CB	6.53	122.35	110.60
1	9-A	251	PHE	CG-CD2-CE2	-6.53	113.62	120.80
3	9-D	90	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	5-A	121	ARG	CD-NE-CZ	-6.53	114.46	123.60
1	8-A	670	VAL	CG1-CB-CG2	6.53	121.35	110.90
1	9-A	646	TYR	CB-CG-CD2	-6.53	117.08	121.00
3	1-C	362	TYR	CB-CG-CD1	6.52	124.91	121.00
1	5-A	687	ARG	NE-CZ-NH2	6.52	123.56	120.30
2	10-B	835	ASP	CB-CG-OD1	6.52	124.17	118.30
3	3-D	173	PHE	CB-CG-CD1	6.52	125.36	120.80
3	5-C	65	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	8-A	576	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	3-A	568	TYR	CB-CG-CD1	-6.52	117.09	121.00
3	4-C	268	LEU	CB-CG-CD2	6.52	122.08	111.00
2	6-B	342	TYR	CB-CG-CD1	-6.52	117.09	121.00
2	9-B	225	PHE	CB-CG-CD2	6.52	125.36	120.80
3	6-D	41	ASP	CB-CG-OD2	6.51	124.16	118.30
3	7-D	302	SER	N-CA-CB	6.51	120.27	110.50
2	5-B	453	TYR	CB-CG-CD1	6.51	124.91	121.00
3	7-C	283	ASP	CB-CG-OD1	6.51	124.16	118.30
2	10-B	415	TYR	CB-CG-CD2	6.51	124.91	121.00
3	7-D	134	GLU	OE1-CD-OE2	6.51	131.11	123.30
2	5-B	529	MET	CG-SD-CE	-6.51	89.79	100.20
1	1-A	262	ARG	NE-CZ-NH1	-6.51	117.05	120.30
3	1-D	218	ARG	NE-CZ-NH1	6.51	123.55	120.30
2	2-B	438	TYR	CA-CB-CG	6.51	125.76	113.40
2	1-B	429	TYR	CG-CD2-CE2	6.50	126.50	121.30
2	3-B	758	TYR	CG-CD2-CE2	-6.50	116.10	121.30
3	3-D	162	TYR	CB-CG-CD2	-6.50	117.10	121.00
3	8-C	20	PHE	CB-CG-CD2	-6.50	116.25	120.80
1	5-A	333	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	6-A	384	LEU	CB-CG-CD2	6.50	122.05	111.00
3	4-C	249	TYR	CB-CG-CD2	-6.50	117.10	121.00
3	5-C	319	TYR	CB-CG-CD2	6.50	124.90	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4-B	409	TYR	CG-CD1-CE1	6.50	126.50	121.30
2	5-B	379	TYR	CD1-CE1-CZ	6.50	125.65	119.80
2	8-B	612	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	2-A	614	TYR	CB-CG-CD2	-6.50	117.10	121.00
1	3-A	365	THR	N-CA-CB	6.49	122.64	110.30
3	5-D	106	ALA	N-CA-CB	6.49	119.19	110.10
3	8-C	205	ASP	CB-CG-OD2	-6.49	112.46	118.30
3	10-C	309	ALA	N-CA-CB	6.49	119.19	110.10
3	1-D	47	ASP	CB-CG-OD2	-6.49	112.46	118.30
3	2-C	273	THR	CA-CB-CG2	-6.49	103.31	112.40
2	6-B	214	PRO	N-CA-CB	6.49	111.09	103.30
3	8-C	1	MET	CG-SD-CE	-6.49	89.82	100.20
2	10-B	362	PHE	CB-CG-CD2	6.49	125.34	120.80
3	1-C	109	TYR	CD1-CE1-CZ	-6.49	113.96	119.80
3	2-D	86	PHE	CB-CG-CD1	6.48	125.34	120.80
2	6-B	835	ASP	CB-CG-OD2	6.48	124.13	118.30
2	1-B	743	THR	CA-CB-CG2	-6.48	103.33	112.40
2	5-B	319	PHE	CB-CG-CD2	-6.48	116.26	120.80
3	6-C	193	ARG	NE-CZ-NH2	-6.48	117.06	120.30
2	10-B	830	LEU	CB-CG-CD2	6.48	122.02	111.00
2	5-B	231	TYR	CG-CD2-CE2	-6.48	116.12	121.30
3	1-D	316	PHE	CD1-CE1-CZ	-6.48	112.33	120.10
1	10-A	91	GLU	N-CA-CB	6.48	122.26	110.60
1	9-A	625	ILE	CA-CB-CG2	-6.47	97.95	110.90
1	1-A	74	TYR	CB-CG-CD2	6.47	124.88	121.00
2	7-B	525	LEU	CB-CG-CD2	6.47	122.00	111.00
1	1-A	273	ASN	N-CA-CB	6.47	122.25	110.60
2	1-B	245	ASN	N-CA-CB	6.47	122.25	110.60
1	6-A	160	ARG	CD-NE-CZ	6.47	132.66	123.60
1	8-A	568	TYR	CB-CG-CD1	-6.47	117.12	121.00
2	10-B	208	GLN	N-CA-CB	6.47	122.25	110.60
2	10-B	524	SER	N-CA-CB	6.47	120.20	110.50
3	4-D	66	ALA	CB-CA-C	-6.47	100.40	110.10
2	6-B	345	TYR	CB-CG-CD2	-6.47	117.12	121.00
2	5-B	415	TYR	CB-CG-CD2	-6.46	117.12	121.00
3	2-D	445	TYR	CB-CG-CD2	6.46	124.88	121.00
3	4-D	393	THR	CA-CB-CG2	6.46	121.44	112.40
1	7-A	594	TYR	CB-CG-CD2	-6.46	117.12	121.00
3	5-C	315	TYR	CB-CG-CD2	-6.46	117.12	121.00
3	1-C	387	PHE	CB-CG-CD1	6.46	125.32	120.80
2	5-B	288	TYR	CB-CG-CD2	6.46	124.87	121.00
2	5-B	666	ARG	NE-CZ-NH1	-6.46	117.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6-D	55	ARG	NE-CZ-NH2	6.46	123.53	120.30
2	10-B	666	ARG	NE-CZ-NH1	6.46	123.53	120.30
2	4-B	187	TYR	N-CA-CB	6.46	122.22	110.60
3	4-D	93	TRP	CD2-CE2-CZ2	-6.46	114.55	122.30
1	5-A	163	ASN	N-CA-CB	6.46	122.22	110.60
1	8-A	427	LEU	CB-CG-CD2	6.46	121.97	111.00
3	9-C	162	TYR	CB-CG-CD1	-6.46	117.13	121.00
3	5-D	227	THR	CA-CB-CG2	-6.45	103.36	112.40
3	1-C	309	ALA	N-CA-CB	6.45	119.13	110.10
3	4-C	114	ARG	NE-CZ-NH2	-6.45	117.07	120.30
3	2-D	441	GLU	N-CA-CB	6.45	122.21	110.60
2	5-B	356	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	3-A	372	ASP	CB-CG-OD2	6.45	124.10	118.30
3	6-C	249	TYR	CB-CG-CD1	6.45	124.87	121.00
2	10-B	450	ASN	N-CA-CB	6.45	122.21	110.60
1	5-A	296	TYR	CB-CG-CD2	-6.45	117.13	121.00
3	5-D	252	MET	CG-SD-CE	-6.45	89.89	100.20
3	2-D	413	PHE	CB-CG-CD2	6.45	125.31	120.80
1	10-A	349	ARG	NE-CZ-NH1	6.44	123.52	120.30
2	8-B	530	ASN	N-CA-CB	6.44	122.20	110.60
3	8-D	309	ALA	N-CA-CB	6.44	119.12	110.10
1	10-A	623	ARG	NH1-CZ-NH2	-6.44	112.32	119.40
3	10-D	58	SER	N-CA-CB	6.44	120.16	110.50
1	1-A	123	TYR	CB-CG-CD1	-6.44	117.14	121.00
3	1-C	59	ARG	NE-CZ-NH2	-6.44	117.08	120.30
2	4-B	400	TYR	CB-CG-CD2	6.44	124.86	121.00
3	6-D	398	PHE	CB-CG-CD1	-6.44	116.29	120.80
3	1-D	78	ASP	CB-CG-OD1	-6.44	112.51	118.30
1	7-A	755	ASP	CB-CG-OD2	-6.44	112.51	118.30
3	7-D	329	ARG	NE-CZ-NH2	-6.44	117.08	120.30
2	1-B	544	ARG	NE-CZ-NH1	-6.43	117.08	120.30
2	4-B	300	PHE	CB-CG-CD2	6.43	125.30	120.80
3	6-C	48	ASP	N-CA-CB	6.43	122.18	110.60
1	8-A	162	PHE	CB-CA-C	-6.43	97.53	110.40
2	3-B	741	PHE	CB-CG-CD1	6.43	125.30	120.80
3	3-D	386	VAL	CA-CB-CG2	-6.43	101.25	110.90
3	8-D	316	PHE	CB-CG-CD1	6.43	125.30	120.80
1	10-A	576	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	5-A	80	ASP	CB-CG-OD2	6.43	124.08	118.30
2	8-B	770	TYR	CG-CD1-CE1	6.43	126.44	121.30
3	9-D	316	PHE	CB-CG-CD2	6.42	125.30	120.80
1	3-A	597	ARG	NE-CZ-NH1	6.42	123.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4-B	593	PHE	CB-CG-CD2	-6.42	116.30	120.80
1	5-A	794	TYR	CB-CG-CD2	6.42	124.85	121.00
3	7-D	345	PRO	N-CA-CB	6.42	111.00	103.30
1	2-A	405	PHE	CB-CG-CD1	6.42	125.29	120.80
1	4-A	381	PHE	CB-CG-CD2	-6.42	116.31	120.80
1	8-A	57	ALA	CB-CA-C	-6.42	100.47	110.10
1	9-A	336	ASP	CB-CG-OD2	-6.42	112.53	118.30
2	6-B	488	PHE	CD1-CE1-CZ	6.42	127.80	120.10
1	7-A	755	ASP	CB-CG-OD1	6.41	124.07	118.30
2	2-B	644	PHE	CB-CG-CD1	6.41	125.29	120.80
3	2-D	362	TYR	CB-CG-CD1	6.41	124.84	121.00
1	4-A	663	TYR	CB-CG-CD2	-6.41	117.16	121.00
2	10-B	295	ARG	NE-CZ-NH2	-6.41	117.10	120.30
3	1-D	122	LYS	N-CA-CB	6.41	122.13	110.60
3	5-D	200	ALA	CB-CA-C	-6.41	100.49	110.10
3	8-C	275	PHE	CB-CG-CD1	-6.41	116.31	120.80
1	1-A	677	GLU	OE1-CD-OE2	-6.41	115.61	123.30
1	2-A	786	LEU	N-CA-CB	6.41	123.21	110.40
1	2-A	296	TYR	CG-CD1-CE1	-6.40	116.18	121.30
2	3-B	827	ARG	N-CA-CB	6.40	122.12	110.60
3	3-C	398	PHE	CB-CG-CD1	-6.40	116.32	120.80
3	7-D	162	TYR	CB-CG-CD1	6.40	124.84	121.00
1	1-A	284	TYR	CG-CD1-CE1	-6.40	116.18	121.30
1	1-A	296	TYR	CG-CD1-CE1	-6.40	116.18	121.30
1	7-A	381	PHE	CG-CD1-CE1	6.40	127.84	120.80
2	9-B	347	MET	CA-CB-CG	6.40	124.18	113.30
3	9-C	249	TYR	CB-CG-CD1	6.40	124.84	121.00
2	10-B	633	ARG	NE-CZ-NH1	6.40	123.50	120.30
3	4-D	437	TYR	CB-CG-CD2	6.40	124.84	121.00
1	6-A	123	TYR	CZ-CE2-CD2	6.40	125.56	119.80
1	7-A	490	THR	CA-CB-CG2	-6.40	103.44	112.40
3	1-C	436	ASP	N-CA-CB	6.40	122.12	110.60
3	5-C	307	SER	N-CA-CB	6.40	120.10	110.50
2	10-B	284	TYR	CG-CD1-CE1	-6.39	116.19	121.30
2	4-B	267	PHE	CB-CG-CD1	-6.39	116.33	120.80
2	5-B	445	PHE	CB-CG-CD1	-6.39	116.33	120.80
2	6-B	661	PHE	CB-CG-CD2	-6.39	116.33	120.80
3	4-D	136	PHE	CB-CG-CD2	-6.39	116.33	120.80
1	5-A	204	ARG	NE-CZ-NH2	-6.39	117.11	120.30
3	10-D	192	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	2-A	579	MET	CG-SD-CE	-6.39	89.97	100.20
2	8-B	250	LYS	N-CA-CB	6.39	122.10	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-A	336	ASP	N-CA-CB	6.39	122.10	110.60
3	2-D	114	ARG	NE-CZ-NH2	6.39	123.49	120.30
1	3-A	490	THR	N-CA-CB	6.39	122.44	110.30
3	3-C	403	PHE	N-CA-CB	6.39	122.10	110.60
2	6-B	525	LEU	CB-CG-CD1	6.39	121.86	111.00
3	8-C	369	GLU	OE1-CD-OE2	6.39	130.96	123.30
3	8-C	445	TYR	CG-CD1-CE1	-6.39	116.19	121.30
3	9-D	347	TRP	CE2-CD2-CG	-6.38	102.19	107.30
2	2-B	345	TYR	CB-CA-C	-6.38	97.64	110.40
1	8-A	428	GLY	N-CA-C	-6.38	97.14	113.10
3	4-C	192	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	6-A	153	THR	CA-CB-CG2	-6.38	103.47	112.40
1	6-A	769	SER	N-CA-CB	6.38	120.06	110.50
1	10-A	72	GLY	O-C-N	-6.38	112.50	122.70
3	5-C	42	SER	N-CA-CB	6.37	120.06	110.50
1	6-A	150	TYR	CB-CG-CD2	-6.37	117.18	121.00
2	10-B	470	TYR	CB-CG-CD1	6.37	124.82	121.00
1	1-A	393	TYR	CG-CD1-CE1	-6.37	116.20	121.30
2	5-B	593	PHE	CB-CG-CD2	-6.37	116.34	120.80
2	6-B	349	TRP	CZ3-CH2-CZ2	-6.37	113.95	121.60
1	9-A	600	ASP	CB-CA-C	-6.37	97.66	110.40
3	10-D	161	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	2-A	794	TYR	CG-CD2-CE2	-6.37	116.20	121.30
3	2-C	292	TYR	CD1-CG-CD2	-6.37	110.90	117.90
3	8-C	170	TYR	CG-CD1-CE1	-6.37	116.21	121.30
3	1-C	386	VAL	CG1-CB-CG2	6.37	121.08	110.90
3	3-C	328	PRO	N-CD-CG	6.37	112.75	103.20
2	8-B	429	TYR	CB-CG-CD1	6.37	124.82	121.00
2	10-B	393	PHE	CB-CG-CD2	-6.37	116.34	120.80
3	1-D	193	ARG	NE-CZ-NH2	6.36	123.48	120.30
3	9-D	136	PHE	CB-CG-CD2	6.36	125.25	120.80
3	10-D	437	TYR	CB-CG-CD1	6.36	124.82	121.00
3	8-D	275	PHE	CB-CG-CD2	6.36	125.25	120.80
1	1-A	594	TYR	CB-CG-CD1	-6.36	117.19	121.00
1	3-A	299	PHE	CB-CG-CD1	6.36	125.25	120.80
1	8-A	594	TYR	CZ-CE2-CD2	-6.36	114.08	119.80
3	10-D	423	PHE	CB-CG-CD1	6.36	125.25	120.80
2	7-B	216	PHE	CB-CG-CD1	-6.35	116.35	120.80
3	2-D	398	PHE	CB-CG-CD2	-6.35	116.35	120.80
3	5-C	435	GLU	N-CA-CB	6.35	122.03	110.60
1	8-A	609	THR	CA-CB-CG2	-6.35	103.51	112.40
2	9-B	585	ARG	NE-CZ-NH1	6.35	123.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-B	429	TYR	CB-CG-CD2	-6.35	117.19	121.00
2	2-B	216	PHE	CB-CG-CD1	-6.35	116.35	120.80
2	4-B	379	TYR	CB-CG-CD2	-6.35	117.19	121.00
1	9-A	76	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	1-A	409	PHE	CB-CG-CD2	-6.35	116.36	120.80
2	3-B	468	PHE	CB-CG-CD1	6.35	125.24	120.80
1	5-A	568	TYR	CB-CG-CD2	-6.35	117.19	121.00
1	7-A	116	TYR	N-CA-CB	6.35	122.03	110.60
3	7-C	394	PHE	CB-CG-CD2	-6.35	116.36	120.80
2	4-B	589	PHE	CB-CG-CD2	-6.34	116.36	120.80
3	4-D	27	LYS	CB-CA-C	-6.34	97.71	110.40
3	2-C	113	THR	CA-CB-CG2	-6.34	103.52	112.40
1	7-A	410	PHE	CB-CG-CD2	-6.34	116.36	120.80
1	7-A	414	ASP	N-CA-CB	6.34	122.02	110.60
2	7-B	415	TYR	CB-CG-CD1	-6.34	117.20	121.00
1	8-A	286	TRP	CB-CG-CD2	-6.34	118.36	126.60
3	8-C	421	ASP	CB-CG-OD1	-6.34	112.59	118.30
2	1-B	335	PHE	CB-CG-CD1	-6.34	116.36	120.80
3	1-D	278	ASP	CB-CG-OD2	6.34	124.00	118.30
1	10-A	140	TYR	CB-CG-CD1	6.34	124.80	121.00
3	5-D	197	ASP	CB-CG-OD2	-6.34	112.60	118.30
3	3-D	204	PHE	CB-CG-CD1	6.33	125.23	120.80
1	6-A	102	PHE	CB-CG-CD1	6.33	125.23	120.80
3	6-D	329	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	4-A	413	TYR	CG-CD1-CE1	-6.33	116.23	121.30
2	7-B	190	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	8-A	190	TYR	CG-CD2-CE2	-6.33	116.23	121.30
3	1-D	437	TYR	CB-CG-CD2	-6.33	117.20	121.00
2	7-B	583	TYR	CZ-CE2-CD2	-6.33	114.10	119.80
3	9-C	292	TYR	CB-CG-CD1	-6.33	117.20	121.00
3	2-D	140	HIS	N-CA-CB	6.33	121.99	110.60
3	7-C	223	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	9-A	767	TYR	N-CA-CB	6.33	121.99	110.60
2	9-B	180	PRO	CA-N-CD	-6.33	102.64	111.50
1	10-A	304	ASP	CB-CG-OD2	6.33	124.00	118.30
1	4-A	77	TYR	CB-CG-CD2	-6.33	117.20	121.00
3	7-D	283	ASP	CB-CG-OD1	6.33	123.99	118.30
1	8-A	102	PHE	CB-CG-CD2	-6.33	116.37	120.80
2	4-B	733	THR	CA-CB-CG2	-6.32	103.55	112.40
3	5-C	249	TYR	N-CA-CB	6.32	121.98	110.60
3	6-D	353	HIS	CA-CB-CG	6.32	124.35	113.60
3	5-C	398	PHE	CB-CG-CD1	6.32	125.22	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	782	PHE	CB-CG-CD1	-6.32	116.37	120.80
3	2-D	161	ARG	NE-CZ-NH2	6.32	123.46	120.30
3	6-C	407	TYR	CB-CG-CD1	-6.32	117.21	121.00
1	9-A	692	LEU	CB-CG-CD1	6.32	121.74	111.00
3	10-D	344	PHE	CB-CG-CD1	-6.32	116.38	120.80
2	6-B	245	ASN	N-CA-CB	6.31	121.96	110.60
2	1-B	403	PHE	CB-CG-CD1	6.31	125.22	120.80
1	4-A	431	SER	C-N-CA	6.31	135.55	122.30
2	5-B	498	ASP	CB-CG-OD1	-6.31	112.62	118.30
1	8-A	597	ARG	NE-CZ-NH1	6.31	123.45	120.30
2	9-B	445	PHE	CB-CG-CD2	-6.31	116.38	120.80
3	10-C	249	TYR	C-N-CA	6.31	137.47	121.70
3	10-D	90	ARG	NH1-CZ-NH2	-6.31	112.46	119.40
2	6-B	247	SER	N-CA-CB	6.31	119.96	110.50
2	7-B	264	TYR	CG-CD2-CE2	6.31	126.34	121.30
1	9-A	451	ARG	NE-CZ-NH2	-6.31	117.15	120.30
3	1-D	244	PHE	CB-CG-CD1	-6.30	116.39	120.80
2	3-B	772	PHE	CB-CG-CD2	-6.30	116.39	120.80
3	7-C	62	PHE	CB-CG-CD2	-6.30	116.39	120.80
1	5-A	410	PHE	CB-CA-C	-6.30	97.80	110.40
1	6-A	143	ARG	NE-CZ-NH1	6.30	123.45	120.30
3	7-C	161	ARG	NE-CZ-NH2	-6.30	117.15	120.30
2	10-B	555	TRP	CB-CG-CD2	-6.30	118.41	126.60
3	2-C	143	ALA	N-CA-CB	6.30	118.92	110.10
3	4-D	197	ASP	CB-CG-OD2	-6.30	112.63	118.30
3	7-C	181	VAL	N-CA-C	-6.30	94.00	111.00
3	3-C	306	VAL	CG1-CB-CG2	6.30	120.97	110.90
1	1-A	557	ILE	CA-CB-CG1	6.29	122.96	111.00
2	7-B	451	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	1-A	299	PHE	CB-CG-CD2	6.29	125.20	120.80
1	7-A	97	LYS	N-CA-CB	6.29	121.93	110.60
1	9-A	795	ASP	CB-CG-OD2	-6.29	112.64	118.30
3	6-C	203	VAL	CA-CB-CG2	-6.29	101.47	110.90
3	6-D	185	TYR	CB-CG-CD2	-6.29	117.23	121.00
3	1-C	352	MET	CA-CB-CG	6.29	123.99	113.30
2	1-B	285	ARG	NE-CZ-NH1	6.29	123.44	120.30
3	2-D	109	TYR	CB-CG-CD2	6.29	124.77	121.00
2	4-B	242	ARG	NE-CZ-NH2	-6.29	117.16	120.30
3	9-C	319	TYR	CG-CD1-CE1	-6.29	116.27	121.30
3	1-C	62	PHE	CB-CG-CD1	-6.28	116.40	120.80
3	5-D	243	ARG	NE-CZ-NH1	6.28	123.44	120.30
2	4-B	609	ASP	CB-CG-OD2	-6.28	112.65	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9-B	582	GLU	N-CA-CB	6.28	121.91	110.60
1	10-A	572	ILE	O-C-N	-6.28	112.66	122.70
2	9-B	343	TYR	CG-CD1-CE1	-6.28	116.28	121.30
1	6-A	787	SER	N-CA-CB	6.27	119.91	110.50
3	6-C	315	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	9-A	110	VAL	CG1-CB-CG2	-6.27	100.86	110.90
3	2-C	90	ARG	NE-CZ-NH2	-6.27	117.16	120.30
3	4-D	297	ASP	CB-CG-OD2	-6.27	112.65	118.30
3	7-D	190	ALA	N-CA-CB	6.27	118.88	110.10
3	10-D	267	PHE	CB-CG-CD1	-6.27	116.41	120.80
2	2-B	846	ARG	NE-CZ-NH1	6.27	123.44	120.30
3	10-D	15	ASN	CB-CA-C	-6.27	97.86	110.40
3	10-D	387	PHE	CB-CG-CD2	6.27	125.19	120.80
3	5-C	57	ASN	N-CA-CB	6.27	121.88	110.60
1	6-A	108	ARG	NE-CZ-NH1	-6.27	117.17	120.30
1	6-A	193	TYR	CB-CG-CD1	6.27	124.76	121.00
3	7-D	362	TYR	CB-CG-CD1	6.27	124.76	121.00
1	3-A	603	TRP	CB-CG-CD2	6.26	134.74	126.60
3	4-D	61	LYS	CB-CA-C	-6.26	97.88	110.40
1	5-A	273	ASN	CB-CA-C	-6.26	97.88	110.40
3	10-C	38	GLN	N-CA-C	-6.26	94.09	111.00
2	2-B	445	PHE	CB-CG-CD1	6.26	125.18	120.80
3	6-D	315	TYR	CD1-CE1-CZ	-6.26	114.17	119.80
3	9-C	101	ALA	C-N-CA	6.26	135.45	122.30
2	6-B	433	TYR	CZ-CE2-CD2	-6.26	114.17	119.80
2	8-B	216	PHE	CB-CG-CD1	-6.26	116.42	120.80
2	7-B	776	TYR	CB-CG-CD1	6.25	124.75	121.00
3	9-C	41	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	10-A	280	CYS	CA-CB-SG	-6.25	102.74	114.00
2	4-B	473	VAL	CG1-CB-CG2	6.25	120.90	110.90
3	5-C	128	ASP	CB-CG-OD2	6.25	123.92	118.30
2	4-B	446	PHE	CB-CG-CD2	-6.25	116.42	120.80
3	8-C	413	PHE	CB-CG-CD2	-6.25	116.42	120.80
2	4-B	598	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	7-A	144	ARG	NH1-CZ-NH2	-6.25	112.53	119.40
3	7-C	113	THR	CA-CB-CG2	-6.25	103.66	112.40
3	7-C	346	SER	N-CA-CB	6.25	119.87	110.50
2	9-B	641	PHE	CB-CG-CD2	-6.25	116.43	120.80
2	9-B	343	TYR	CB-CA-C	-6.24	97.91	110.40
1	9-A	443	MET	CG-SD-CE	-6.24	90.21	100.20
2	3-B	662	LYS	N-CA-CB	6.24	121.83	110.60
3	5-D	172	VAL	CA-CB-CG2	-6.24	101.54	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7-B	514	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	8-B	403	PHE	CB-CG-CD1	-6.24	116.43	120.80
3	8-C	281	HIS	N-CA-CB	6.24	121.83	110.60
2	3-B	576	ARG	NE-CZ-NH1	6.24	123.42	120.30
3	4-D	372	VAL	N-CA-C	-6.24	94.16	111.00
1	5-A	458	TYR	CZ-CE2-CD2	6.24	125.42	119.80
1	6-A	557	ILE	C-N-CA	6.24	137.29	121.70
1	9-A	333	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	1-A	251	PHE	CB-CG-CD2	-6.24	116.44	120.80
3	1-D	185	TYR	CG-CD1-CE1	6.24	126.29	121.30
3	5-D	325	ASN	N-CA-CB	6.24	121.83	110.60
3	9-D	247	TYR	CB-CG-CD2	6.24	124.74	121.00
2	10-B	533	ARG	NE-CZ-NH1	-6.24	117.18	120.30
3	10-D	335	MET	CG-SD-CE	-6.24	90.22	100.20
2	6-B	652	TYR	CB-CG-CD2	-6.23	117.26	121.00
3	5-C	360	SER	N-CA-CB	6.23	119.85	110.50
3	9-C	277	SER	N-CA-CB	6.23	119.85	110.50
2	1-B	288	TYR	CB-CG-CD1	-6.23	117.26	121.00
3	1-D	100	SER	N-CA-CB	6.23	119.84	110.50
2	5-B	772	PHE	CB-CG-CD1	6.23	125.16	120.80
3	10-C	22	TRP	CG-CD2-CE3	-6.23	128.29	133.90
2	5-B	651	TYR	CB-CG-CD2	-6.23	117.26	121.00
3	6-D	275	PHE	CB-CG-CD2	-6.23	116.44	120.80
2	10-B	772	PHE	CB-CG-CD1	6.23	125.16	120.80
2	3-B	770	TYR	CB-CG-CD1	6.23	124.74	121.00
2	6-B	557	VAL	CA-CB-CG1	-6.23	101.56	110.90
1	8-A	160	ARG	NE-CZ-NH1	6.23	123.41	120.30
3	1-D	316	PHE	CG-CD1-CE1	6.22	127.65	120.80
2	7-B	216	PHE	CZ-CE2-CD2	-6.22	112.63	120.10
2	9-B	343	TYR	CB-CG-CD1	6.22	124.73	121.00
3	9-D	293	ASP	CB-CG-OD1	6.22	123.90	118.30
1	2-A	117	MET	CG-SD-CE	-6.22	90.24	100.20
1	4-A	296	TYR	CA-CB-CG	-6.22	101.58	113.40
3	2-D	124	ASP	CB-CG-OD1	6.22	123.90	118.30
1	10-A	659	LEU	CB-CG-CD1	6.22	121.58	111.00
2	7-B	604	MET	CG-SD-CE	-6.22	90.25	100.20
3	4-C	359	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	6-B	409	TYR	CZ-CE2-CD2	-6.22	114.20	119.80
3	2-D	22	TRP	CG-CD2-CE3	-6.21	128.31	133.90
2	1-B	600	TYR	CD1-CE1-CZ	6.21	125.39	119.80
1	4-A	646	TYR	CB-CG-CD1	6.21	124.73	121.00
3	6-C	74	SER	N-CA-CB	6.21	119.82	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-C	59	ARG	NE-CZ-NH1	6.21	123.41	120.30
3	1-D	68	MET	CG-SD-CE	-6.21	90.26	100.20
1	2-A	99	ASP	CB-CG-OD1	6.21	123.89	118.30
1	5-A	627	ARG	NE-CZ-NH1	-6.21	117.19	120.30
3	6-C	83	PHE	CB-CG-CD1	-6.21	116.45	120.80
3	7-C	329	ARG	NH1-CZ-NH2	-6.21	112.57	119.40
3	7-D	170	TYR	CB-CG-CD2	-6.21	117.27	121.00
2	2-B	555	TRP	CB-CG-CD2	-6.21	118.53	126.60
2	3-B	600	TYR	CB-CG-CD2	-6.21	117.27	121.00
2	3-B	650	SER	N-CA-CB	6.21	119.81	110.50
2	6-B	362	PHE	CB-CG-CD2	-6.21	116.45	120.80
3	2-D	46	ARG	NE-CZ-NH1	6.21	123.40	120.30
2	6-B	652	TYR	CB-CG-CD1	6.21	124.72	121.00
3	8-C	407	TYR	CB-CG-CD1	-6.21	117.28	121.00
2	9-B	548	LEU	N-CA-CB	6.21	122.81	110.40
1	3-A	322	THR	CA-CB-CG2	-6.20	103.72	112.40
3	3-C	423	PHE	CB-CG-CD1	-6.20	116.46	120.80
1	10-A	57	ALA	N-CA-CB	6.20	118.78	110.10
1	1-A	483	MET	CG-SD-CE	-6.20	90.28	100.20
2	2-B	357	ALA	CB-CA-C	-6.20	100.80	110.10
2	10-B	457	VAL	CA-CB-CG1	-6.20	101.60	110.90
1	1-A	168	PHE	CB-CG-CD2	-6.20	116.46	120.80
1	1-A	651	VAL	CA-CB-CG2	-6.20	101.60	110.90
2	5-B	816	TYR	CG-CD2-CE2	-6.20	116.34	121.30
3	3-C	185	TYR	CG-CD2-CE2	-6.20	116.34	121.30
1	5-A	767	TYR	CB-CG-CD1	6.19	124.72	121.00
2	2-B	238	VAL	CA-CB-CG2	-6.19	101.61	110.90
1	4-A	657	TYR	CG-CD1-CE1	-6.19	116.35	121.30
1	3-A	190	TYR	CB-CG-CD2	-6.19	117.29	121.00
1	6-A	300	MET	CG-SD-CE	-6.19	90.30	100.20
2	6-B	514	ARG	NE-CZ-NH1	-6.19	117.20	120.30
2	7-B	741	PHE	CB-CG-CD2	-6.19	116.47	120.80
2	8-B	806	ASN	N-CA-CB	6.19	121.74	110.60
2	7-B	345	TYR	CG-CD2-CE2	-6.19	116.35	121.30
2	1-B	490	ASP	CB-CG-OD1	-6.19	112.73	118.30
2	9-B	242	ARG	NE-CZ-NH1	-6.19	117.21	120.30
3	2-C	278	ASP	N-CA-CB	6.18	121.73	110.60
1	3-A	656	VAL	CA-CB-CG1	-6.18	101.62	110.90
1	7-A	393	TYR	CB-CG-CD2	-6.18	117.29	121.00
3	5-C	299	LEU	CB-CG-CD2	6.18	121.51	111.00
3	6-C	104	SER	N-CA-CB	6.18	119.77	110.50
3	6-C	278	ASP	CB-CG-OD1	-6.18	112.74	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	451	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	9-B	670	ARG	NE-CZ-NH2	-6.18	117.21	120.30
2	10-B	264	TYR	CB-CG-CD1	6.18	124.71	121.00
1	1-A	203	ARG	N-CA-CB	6.18	121.72	110.60
3	1-C	267	PHE	CB-CG-CD1	6.18	125.13	120.80
3	4-D	87	PHE	CB-CA-C	-6.18	98.04	110.40
3	6-C	110	ASP	CB-CG-OD2	-6.18	112.74	118.30
3	8-D	249	TYR	CA-CB-CG	-6.18	101.66	113.40
3	3-C	370	ASN	N-CA-CB	6.18	121.72	110.60
3	6-D	59	ARG	NE-CZ-NH1	6.18	123.39	120.30
3	9-D	160	ASP	CB-CG-OD2	-6.18	112.74	118.30
2	5-B	328	ARG	CB-CA-C	-6.17	98.05	110.40
1	6-A	776	ARG	NE-CZ-NH1	6.17	123.39	120.30
2	6-B	299	ARG	NE-CZ-NH1	-6.17	117.21	120.30
3	7-C	398	PHE	CG-CD2-CE2	-6.17	114.01	120.80
2	7-B	500	LEU	CB-CG-CD2	6.17	121.50	111.00
1	8-A	345	PHE	CB-CG-CD2	-6.17	116.48	120.80
3	9-D	216	VAL	CA-CB-CG2	6.17	120.16	110.90
3	6-C	1	MET	CA-CB-CG	6.17	123.79	113.30
2	10-B	474	VAL	CA-CB-CG2	-6.17	101.64	110.90
3	4-C	109	TYR	CG-CD1-CE1	-6.17	116.36	121.30
1	7-A	473	ASN	N-CA-C	-6.17	94.34	111.00
3	3-C	217	PHE	CB-CG-CD1	6.17	125.12	120.80
3	8-C	341	ARG	NE-CZ-NH1	6.17	123.38	120.30
3	8-D	7	THR	CA-CB-CG2	-6.17	103.77	112.40
1	9-A	413	TYR	CB-CG-CD1	6.17	124.70	121.00
3	2-D	335	MET	CG-SD-CE	-6.16	90.34	100.20
2	9-B	585	ARG	NE-CZ-NH2	6.16	123.38	120.30
3	10-C	358	ARG	NE-CZ-NH1	-6.16	117.22	120.30
2	2-B	584	LEU	CB-CG-CD1	6.16	121.47	111.00
3	6-C	34	ASP	CB-CG-OD2	6.16	123.84	118.30
3	8-C	182	VAL	CA-CB-CG2	6.16	120.14	110.90
3	10-C	88	ASP	CB-CG-OD1	6.16	123.84	118.30
2	5-B	547	ASP	CB-CG-OD1	-6.16	112.76	118.30
3	6-D	407	TYR	CA-CB-CG	-6.16	101.70	113.40
3	7-D	249	TYR	CB-CG-CD2	-6.16	117.31	121.00
1	2-A	297	GLN	N-CA-CB	6.16	121.68	110.60
1	5-A	793	PHE	CG-CD2-CE2	6.16	127.57	120.80
2	6-B	343	TYR	CB-CG-CD2	-6.16	117.31	121.00
2	10-B	409	TYR	CB-CG-CD1	6.16	124.69	121.00
2	1-B	591	TRP	CE2-CD2-CG	-6.15	102.38	107.30
3	1-D	347	TRP	CZ3-CH2-CZ2	-6.15	114.22	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2-D	301	PRO	N-CD-CG	6.15	112.43	103.20
3	6-D	133	PHE	CB-CG-CD2	6.15	125.11	120.80
2	8-B	285	ARG	NE-CZ-NH1	6.15	123.38	120.30
2	10-B	342	TYR	CB-CG-CD1	-6.15	117.31	121.00
1	4-A	171	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	4-A	302	TYR	CB-CG-CD2	6.15	124.69	121.00
3	4-C	319	TYR	CB-CG-CD1	-6.15	117.31	121.00
1	9-A	74	TYR	CD1-CG-CD2	-6.15	111.14	117.90
2	9-B	827	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	10-A	112	TYR	CD1-CG-CD2	6.15	124.66	117.90
1	6-A	265	VAL	CA-CB-CG1	6.15	120.12	110.90
1	9-A	409	PHE	CB-CG-CD1	6.15	125.10	120.80
3	9-C	443	ASP	CB-CG-OD2	-6.15	112.77	118.30
3	1-C	83	PHE	CB-CG-CD2	-6.14	116.50	120.80
2	2-B	236	TYR	CB-CG-CD2	-6.14	117.31	121.00
3	7-C	199	ASP	CB-CG-OD2	6.14	123.83	118.30
3	9-D	315	TYR	CG-CD2-CE2	-6.14	116.39	121.30
2	1-B	356	ARG	NH1-CZ-NH2	6.14	126.16	119.40
3	6-D	413	PHE	CB-CG-CD2	6.14	125.10	120.80
2	9-B	297	TYR	CB-CG-CD1	-6.14	117.31	121.00
1	6-A	612	TRP	CE2-CD2-CG	-6.14	102.39	107.30
1	7-A	605	ASP	CB-CG-OD2	-6.14	112.77	118.30
2	5-B	558	PHE	CB-CG-CD1	6.14	125.10	120.80
3	7-C	5	ILE	CA-CB-CG1	6.14	122.67	111.00
3	7-D	319	TYR	CG-CD1-CE1	-6.14	116.39	121.30
3	6-D	48	ASP	CB-CG-OD2	6.14	123.82	118.30
1	4-A	190	TYR	CB-CG-CD2	6.13	124.68	121.00
3	5-C	170	TYR	CG-CD1-CE1	-6.13	116.39	121.30
2	2-B	776	TYR	CB-CG-CD1	6.13	124.68	121.00
3	2-C	283	ASP	CB-CG-OD2	-6.13	112.78	118.30
3	5-C	279	TYR	CG-CD2-CE2	6.13	126.20	121.30
3	4-C	170	TYR	CB-CG-CD2	6.13	124.68	121.00
2	6-B	433	TYR	CG-CD2-CE2	6.13	126.20	121.30
2	3-B	433	TYR	CG-CD2-CE2	6.13	126.20	121.30
1	5-A	614	TYR	CB-CG-CD2	-6.13	117.33	121.00
3	5-D	315	TYR	CB-CG-CD1	-6.13	117.32	121.00
3	7-C	437	TYR	CB-CG-CD2	-6.13	117.32	121.00
1	4-A	284	TYR	CB-CG-CD1	6.12	124.67	121.00
2	4-B	241	PHE	CB-CG-CD1	6.12	125.09	120.80
3	5-C	292	TYR	CB-CG-CD2	6.12	124.67	121.00
2	6-B	285	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	7-A	204	ARG	NE-CZ-NH2	6.12	123.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4-B	284	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	6-A	60	VAL	CG1-CB-CG2	6.12	120.69	110.90
2	6-B	584	LEU	CB-CG-CD2	6.12	121.40	111.00
2	7-B	312	PHE	CB-CG-CD1	6.12	125.08	120.80
3	3-D	82	THR	CA-CB-CG2	-6.12	103.84	112.40
1	2-A	393	TYR	CB-CG-CD1	6.12	124.67	121.00
3	4-C	53	PHE	CB-CG-CD2	6.12	125.08	120.80
2	7-B	236	TYR	CD1-CE1-CZ	6.12	125.30	119.80
1	1-A	653	ASP	CB-CG-OD1	6.11	123.80	118.30
2	2-B	598	TYR	CB-CG-CD1	-6.11	117.33	121.00
1	4-A	458	TYR	CD1-CG-CD2	6.11	124.63	117.90
1	4-A	767	TYR	CG-CD2-CE2	-6.11	116.41	121.30
1	6-A	418	VAL	CB-CA-C	-6.11	99.78	111.40
2	10-B	770	TYR	CD1-CE1-CZ	-6.11	114.30	119.80
2	9-B	294	LEU	CB-CA-C	-6.11	98.59	110.20
2	8-B	418	GLU	OE1-CD-OE2	6.11	130.63	123.30
2	9-B	470	TYR	CB-CG-CD2	-6.11	117.33	121.00
3	10-D	369	GLU	CB-CA-C	-6.11	98.19	110.40
3	10-D	413	PHE	O-C-N	-6.11	112.93	122.70
3	2-D	437	TYR	CB-CG-CD2	6.10	124.66	121.00
3	10-D	26	ALA	N-CA-CB	6.10	118.64	110.10
2	3-B	661	PHE	CB-CG-CD2	-6.10	116.53	120.80
1	7-A	122	ALA	N-CA-CB	6.10	118.64	110.10
1	4-A	594	TYR	CB-CG-CD1	-6.10	117.34	121.00
3	10-D	311	ASN	N-CA-CB	6.10	121.57	110.60
1	8-A	569	PRO	N-CA-CB	6.09	110.61	103.30
3	8-C	93	TRP	CE2-CD2-CG	-6.09	102.42	107.30
3	10-D	87	PHE	CB-CG-CD2	-6.09	116.53	120.80
2	2-B	365	ALA	N-CA-CB	6.09	118.63	110.10
3	5-C	161	ARG	NE-CZ-NH1	6.09	123.35	120.30
3	4-C	347	TRP	CD1-NE1-CE2	6.09	114.48	109.00
1	10-A	447	THR	N-CA-CB	6.09	121.87	110.30
3	10-C	155	LEU	CB-CG-CD2	6.09	121.36	111.00
3	4-D	136	PHE	CB-CG-CD1	6.09	125.06	120.80
2	9-B	216	PHE	CB-CG-CD1	6.09	125.06	120.80
2	7-B	585	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	4-A	398	TYR	CB-CG-CD1	6.08	124.65	121.00
1	1-A	150	TYR	CB-CG-CD1	6.08	124.65	121.00
1	5-A	451	ARG	NE-CZ-NH2	-6.08	117.26	120.30
3	8-C	315	TYR	CB-CG-CD2	6.08	124.65	121.00
3	7-C	118	ASP	CB-CG-OD2	-6.08	112.83	118.30
3	2-C	407	TYR	CB-CG-CD1	-6.08	117.35	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-C	316	PHE	N-CA-C	-6.08	94.59	111.00
1	1-A	340	ASP	CB-CG-OD1	6.08	123.77	118.30
1	8-A	204	ARG	NE-CZ-NH1	6.08	123.34	120.30
3	9-D	162	TYR	CB-CG-CD2	6.08	124.65	121.00
1	8-A	393	TYR	CG-CD2-CE2	-6.08	116.44	121.30
2	1-B	470	TYR	CG-CD2-CE2	6.07	126.16	121.30
3	3-D	105	TRP	CD1-CG-CD2	6.07	111.16	106.30
3	1-C	302	SER	CB-CA-C	-6.07	98.56	110.10
2	4-B	655	CYS	CA-CB-SG	6.07	124.93	114.00
1	1-A	160	ARG	NE-CZ-NH1	6.07	123.33	120.30
2	1-B	758	TYR	CA-C-N	6.07	134.10	117.10
1	2-A	129	THR	N-CA-C	-6.07	94.61	111.00
3	7-D	272	PHE	CB-CG-CD1	-6.07	116.55	120.80
2	5-B	641	PHE	CB-CG-CD1	6.07	125.05	120.80
1	8-A	405	PHE	CB-CG-CD2	-6.07	116.55	120.80
1	2-A	78	PHE	CB-CG-CD1	6.07	125.05	120.80
2	4-B	470	TYR	CB-CG-CD1	6.07	124.64	121.00
1	9-A	327	ARG	NE-CZ-NH1	-6.07	117.27	120.30
3	9-D	340	GLN	N-CA-CB	-6.07	99.68	110.60
3	1-C	48	ASP	O-C-N	-6.06	113.00	122.70
2	7-B	589	PHE	CG-CD2-CE2	-6.06	114.13	120.80
2	10-B	598	TYR	CG-CD1-CE1	-6.06	116.45	121.30
1	2-A	398	TYR	CZ-CE2-CD2	-6.06	114.35	119.80
1	3-A	358	ARG	NE-CZ-NH1	6.06	123.33	120.30
2	7-B	483	MET	CG-SD-CE	-6.06	90.51	100.20
3	1-C	358	ARG	N-CA-CB	6.06	121.50	110.60
1	3-A	198	ARG	NE-CZ-NH1	-6.06	117.27	120.30
3	5-C	84	ARG	NE-CZ-NH2	6.06	123.33	120.30
3	8-D	359	ARG	NE-CZ-NH2	6.06	123.33	120.30
2	4-B	638	ARG	NE-CZ-NH2	-6.05	117.27	120.30
2	7-B	779	LEU	CB-CG-CD1	6.05	121.29	111.00
3	10-C	193	ARG	NE-CZ-NH1	6.05	123.33	120.30
2	5-B	446	PHE	CB-CG-CD1	-6.05	116.56	120.80
2	4-B	633	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	5-A	105	PHE	CB-CG-CD2	-6.05	116.56	120.80
3	10-D	10	ALA	N-CA-CB	6.05	118.57	110.10
2	1-B	411	PHE	N-CA-CB	6.05	121.49	110.60
3	2-C	241	SER	N-CA-CB	6.05	119.57	110.50
3	4-D	180	VAL	CA-CB-CG2	-6.05	101.83	110.90
3	5-C	395	ASP	CB-CG-OD1	6.05	123.75	118.30
3	1-C	152	SER	N-CA-CB	6.05	119.57	110.50
2	5-B	409	TYR	CB-CG-CD1	6.05	124.63	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	10-D	111	ILE	CB-CA-C	-6.05	99.50	111.60
3	3-C	100	SER	N-CA-CB	6.05	119.57	110.50
3	3-D	105	TRP	CE2-CD2-CG	-6.05	102.46	107.30
3	5-C	329	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	6-A	663	TYR	CB-CA-C	-6.04	98.31	110.40
2	6-B	475	PHE	CB-CG-CD2	-6.04	116.57	120.80
2	8-B	315	GLU	OE1-CD-OE2	6.04	130.55	123.30
3	9-C	416	MET	CA-CB-CG	6.04	123.57	113.30
1	3-A	623	ARG	NE-CZ-NH1	-6.04	117.28	120.30
3	3-C	358	ARG	NE-CZ-NH2	6.04	123.32	120.30
2	6-B	819	PHE	CB-CG-CD2	-6.04	116.57	120.80
3	8-C	87	PHE	CB-CG-CD1	6.04	125.03	120.80
3	2-D	103	ASN	CA-CB-CG	-6.04	100.11	113.40
3	3-D	58	SER	N-CA-CB	6.04	119.56	110.50
1	6-A	279	TYR	CG-CD2-CE2	-6.04	116.47	121.30
3	9-C	100	SER	N-CA-CB	6.04	119.56	110.50
3	7-D	93	TRP	CB-CG-CD1	6.04	134.85	127.00
3	9-C	47	ASP	CB-CG-OD2	-6.04	112.87	118.30
3	3-C	243	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	5-A	787	SER	C-N-CA	6.04	136.79	121.70
1	7-A	289	GLN	CB-CA-C	-6.03	98.34	110.40
1	6-A	131	PHE	CB-CG-CD2	-6.03	116.58	120.80
3	3-C	249	TYR	CB-CG-CD1	-6.03	117.38	121.00
1	6-A	190	TYR	CB-CG-CD1	6.03	124.62	121.00
3	9-D	249	TYR	CG-CD2-CE2	-6.03	116.48	121.30
3	7-C	83	PHE	CZ-CE2-CD2	-6.03	112.87	120.10
3	7-D	307	SER	N-CA-CB	6.03	119.54	110.50
1	8-A	286	TRP	CB-CG-CD1	6.03	134.83	127.00
3	8-C	319	TYR	CB-CG-CD2	-6.02	117.39	121.00
1	1-A	108	ARG	NE-CZ-NH1	6.02	123.31	120.30
2	4-B	591	TRP	CB-CG-CD2	-6.02	118.78	126.60
1	6-A	663	TYR	CZ-CE2-CD2	6.02	125.22	119.80
3	9-C	335	MET	CG-SD-CE	-6.02	90.57	100.20
3	1-C	439	ALA	N-CA-CB	6.02	118.52	110.10
3	6-D	275	PHE	CB-CG-CD1	6.02	125.01	120.80
2	5-B	474	VAL	CA-CB-CG2	-6.02	101.88	110.90
1	5-A	787	SER	N-CA-CB	6.01	119.52	110.50
3	6-C	117	ASP	CB-CG-OD1	6.01	123.71	118.30
3	8-C	54	PHE	CB-CG-CD1	-6.01	116.59	120.80
2	1-B	408	SER	CB-CA-C	-6.01	98.68	110.10
3	6-D	406	ASN	N-CA-CB	-6.01	99.78	110.60
3	8-C	148	SER	N-CA-CB	6.01	119.52	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-A	465	PHE	CB-CG-CD2	-6.01	116.59	120.80
2	5-B	522	LEU	O-C-N	6.01	132.31	122.70
2	5-B	580	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	6-A	138	PHE	CB-CG-CD2	6.01	125.01	120.80
2	6-B	593	PHE	CB-CG-CD2	-6.01	116.59	120.80
3	6-D	293	ASP	CB-CA-C	-6.01	98.38	110.40
3	10-D	167	LEU	N-CA-CB	6.01	122.42	110.40
1	1-A	590	LEU	CB-CG-CD1	6.01	121.21	111.00
2	9-B	365	ALA	N-CA-C	-6.01	94.78	111.00
3	4-D	155	LEU	CB-CG-CD1	-6.00	100.79	111.00
3	4-D	275	PHE	CB-CG-CD1	-6.00	116.60	120.80
3	10-C	247	TYR	CB-CG-CD2	6.00	124.60	121.00
1	1-A	479	ARG	NH1-CZ-NH2	6.00	126.00	119.40
2	3-B	439	ARG	NE-CZ-NH1	6.00	123.30	120.30
2	5-B	224	ILE	N-CA-CB	6.00	124.61	110.80
3	5-D	292	TYR	CB-CG-CD2	-6.00	117.40	121.00
3	6-D	28	GLU	OE1-CD-OE2	6.00	130.50	123.30
1	7-A	597	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	2-A	712	SER	N-CA-CB	6.00	119.50	110.50
3	4-D	402	ALA	CB-CA-C	6.00	119.10	110.10
3	5-C	186	ASN	CB-CA-C	-6.00	98.39	110.40
1	7-A	606	LEU	CB-CG-CD1	6.00	121.20	111.00
1	9-A	785	GLU	N-CA-CB	6.00	121.40	110.60
3	10-C	91	ASN	CB-CA-C	-6.00	98.40	110.40
1	2-A	707	CYS	CA-CB-SG	-6.00	103.20	114.00
2	10-B	826	PHE	CG-CD2-CE2	6.00	127.40	120.80
2	3-B	242	ARG	NE-CZ-NH2	6.00	123.30	120.30
3	6-D	185	TYR	CD1-CE1-CZ	6.00	125.20	119.80
3	8-C	248	MET	CA-CB-CG	6.00	123.50	113.30
1	3-A	59	VAL	CA-CB-CG1	6.00	119.89	110.90
1	1-A	106	SER	N-CA-CB	6.00	119.49	110.50
1	6-A	488	THR	CA-CB-CG2	-5.99	104.01	112.40
3	1-C	20	PHE	N-CA-CB	5.99	121.38	110.60
3	1-C	333	ARG	NE-CZ-NH1	5.99	123.30	120.30
2	5-B	429	TYR	CG-CD1-CE1	-5.99	116.51	121.30
2	7-B	451	ASP	CB-CG-OD1	5.99	123.69	118.30
3	8-D	210	LEU	CB-CA-C	-5.99	98.82	110.20
3	9-D	380	MET	CG-SD-CE	-5.99	90.62	100.20
3	3-C	283	ASP	CB-CG-OD1	-5.99	112.91	118.30
2	7-B	577	PRO	CA-N-CD	-5.98	103.12	111.50
3	1-C	143	ALA	CB-CA-C	-5.98	101.12	110.10
3	2-D	91	ASN	CB-CA-C	-5.98	98.44	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2-B	295	ARG	N-CA-CB	5.98	121.36	110.60
3	2-D	285	ALA	N-CA-CB	5.98	118.47	110.10
3	7-C	170	TYR	CB-CG-CD2	5.98	124.59	121.00
1	9-A	123	TYR	CB-CG-CD2	5.98	124.59	121.00
2	9-B	299	ARG	NH1-CZ-NH2	-5.98	112.82	119.40
1	4-A	757	ALA	CB-CA-C	-5.98	101.14	110.10
1	6-A	568	TYR	CD1-CE1-CZ	-5.98	114.42	119.80
3	7-C	53	PHE	CD1-CE1-CZ	-5.98	112.93	120.10
3	1-D	200	ALA	N-CA-CB	5.98	118.47	110.10
2	4-B	598	TYR	CB-CG-CD1	5.97	124.58	121.00
3	9-D	114	ARG	NH1-CZ-NH2	-5.97	112.83	119.40
1	10-A	767	TYR	O-C-N	-5.97	113.14	122.70
2	10-B	770	TYR	CG-CD1-CE1	5.97	126.08	121.30
3	9-C	54	PHE	N-CA-CB	5.97	121.35	110.60
3	9-C	120	LEU	CB-CG-CD1	5.97	121.15	111.00
1	2-A	62	ASP	CB-CG-OD2	-5.97	112.93	118.30
3	4-D	243	ARG	NE-CZ-NH2	-5.97	117.31	120.30
3	7-D	403	PHE	N-CA-CB	5.97	121.35	110.60
3	8-C	19	LYS	N-CA-CB	-5.97	99.85	110.60
1	2-A	657	TYR	CB-CG-CD1	-5.97	117.42	121.00
3	5-D	191	LEU	CB-CG-CD1	5.97	121.15	111.00
3	9-C	315	TYR	CB-CG-CD1	5.97	124.58	121.00
2	8-B	441	ILE	CA-CB-CG2	-5.97	98.97	110.90
1	4-A	116	TYR	CB-CG-CD1	5.97	124.58	121.00
3	9-D	20	PHE	CB-CG-CD1	5.97	124.98	120.80
1	1-A	704	TYR	CG-CD2-CE2	-5.96	116.53	121.30
2	2-B	470	TYR	CD1-CG-CD2	5.96	124.46	117.90
3	2-D	133	PHE	CB-CG-CD2	-5.96	116.62	120.80
3	4-D	387	PHE	CB-CG-CD2	-5.96	116.62	120.80
2	10-B	558	PHE	CB-CG-CD2	-5.96	116.62	120.80
1	1-A	162	PHE	CB-CG-CD1	5.96	124.97	120.80
1	6-A	459	ASP	CB-CG-OD1	-5.96	112.93	118.30
2	4-B	652	TYR	N-CA-CB	5.96	121.33	110.60
2	9-B	769	VAL	CA-CB-CG1	5.96	119.84	110.90
3	8-D	129	SER	O-C-N	-5.96	113.17	122.70
1	1-A	296	TYR	CB-CG-CD2	-5.96	117.43	121.00
3	1-D	301	PRO	N-CA-CB	5.96	110.45	103.30
3	8-D	267	PHE	CB-CG-CD2	-5.95	116.63	120.80
2	1-B	231	TYR	CB-CG-CD2	5.95	124.57	121.00
3	2-D	347	TRP	CB-CG-CD1	5.95	134.74	127.00
3	10-C	162	TYR	CD1-CE1-CZ	-5.95	114.44	119.80
2	1-B	585	ARG	NE-CZ-NH1	5.95	123.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-D	347	TRP	CH2-CZ2-CE2	5.95	123.35	117.40
1	2-A	99	ASP	CB-CG-OD2	-5.95	112.94	118.30
2	2-B	644	PHE	CD1-CE1-CZ	5.95	127.24	120.10
1	4-A	800	ASP	CB-CG-OD1	5.95	123.66	118.30
3	4-C	110	ASP	N-CA-CB	5.95	121.31	110.60
1	10-A	602	THR	CA-CB-OG1	5.95	121.49	109.00
2	9-B	773	VAL	CA-CB-CG1	-5.95	101.98	110.90
1	10-A	714	ARG	NE-CZ-NH2	-5.95	117.33	120.30
3	4-C	55	ARG	NE-CZ-NH1	-5.95	117.33	120.30
2	9-B	397	GLU	OE1-CD-OE2	5.95	130.43	123.30
3	1-D	185	TYR	CB-CG-CD2	-5.94	117.43	121.00
3	9-C	162	TYR	CG-CD1-CE1	-5.94	116.55	121.30
2	3-B	609	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	5-A	345	PHE	CB-CG-CD1	5.94	124.96	120.80
2	5-B	826	PHE	CB-CG-CD2	-5.94	116.64	120.80
2	7-B	600	TYR	CB-CG-CD1	5.94	124.56	121.00
1	9-A	409	PHE	CB-CG-CD2	-5.94	116.64	120.80
2	9-B	488	PHE	CB-CG-CD2	5.94	124.96	120.80
3	4-D	146	THR	CA-CB-CG2	-5.94	104.08	112.40
3	5-D	319	TYR	CA-CB-CG	5.94	124.68	113.40
3	6-C	204	PHE	CB-CG-CD1	5.94	124.95	120.80
2	10-B	641	PHE	N-CA-CB	5.94	121.28	110.60
3	7-C	41	ASP	CB-CG-OD1	5.93	123.64	118.30
3	7-C	70	ASP	N-CA-CB	5.93	121.28	110.60
3	8-D	104	SER	CB-CA-C	-5.93	98.82	110.10
3	1-C	279	TYR	CB-CG-CD1	-5.93	117.44	121.00
2	4-B	236	TYR	CB-CG-CD2	5.93	124.56	121.00
3	2-C	403	PHE	N-CA-CB	5.93	121.28	110.60
1	3-A	204	ARG	NE-CZ-NH2	-5.93	117.33	120.30
3	9-C	269	SER	N-CA-CB	5.93	119.39	110.50
2	10-B	514	ARG	NE-CZ-NH1	5.93	123.26	120.30
3	2-D	347	TRP	CB-CG-CD2	-5.92	118.90	126.60
3	4-C	267	PHE	CD1-CG-CD2	5.92	126.00	118.30
1	9-A	431	SER	N-CA-CB	5.92	119.39	110.50
3	6-C	362	TYR	CB-CG-CD1	-5.92	117.45	121.00
1	3-A	79	ASN	N-CA-CB	5.92	121.26	110.60
2	4-B	199	LEU	CB-CG-CD1	5.92	121.06	111.00
1	8-A	168	PHE	CB-CG-CD2	5.92	124.95	120.80
1	4-A	456	ALA	N-CA-CB	5.92	118.39	110.10
3	4-C	347	TRP	CB-CG-CD2	-5.92	118.90	126.60
2	4-B	415	TYR	CB-CG-CD1	-5.92	117.45	121.00
3	5-D	199	ASP	CB-CG-OD1	-5.92	112.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7-B	580	ARG	NH1-CZ-NH2	5.92	125.91	119.40
2	8-B	295	ARG	NE-CZ-NH1	5.92	123.26	120.30
2	10-B	202	PHE	CB-CG-CD1	5.92	124.94	120.80
1	2-A	646	TYR	CB-CG-CD1	5.92	124.55	121.00
2	7-B	826	PHE	N-CA-CB	5.92	121.25	110.60
1	5-A	168	PHE	C-N-CA	5.92	136.49	121.70
3	5-D	267	PHE	CB-CG-CD1	-5.92	116.66	120.80
1	1-A	143	ARG	N-CA-CB	5.91	121.25	110.60
3	5-C	256	TYR	CG-CD1-CE1	-5.91	116.57	121.30
1	3-A	285	GLU	OE1-CD-OE2	5.91	130.39	123.30
3	3-D	162	TYR	CB-CG-CD1	5.91	124.55	121.00
1	4-A	478	MET	CG-SD-CE	5.91	109.65	100.20
1	8-A	333	ARG	NH1-CZ-NH2	-5.91	112.90	119.40
3	10-C	47	ASP	CB-CG-OD1	5.91	123.62	118.30
1	3-A	190	TYR	CB-CG-CD1	5.91	124.54	121.00
3	6-C	30	ALA	CB-CA-C	5.91	118.96	110.10
3	10-D	218	ARG	NH1-CZ-NH2	-5.91	112.90	119.40
3	4-D	268	LEU	CB-CG-CD1	5.91	121.04	111.00
1	6-A	344	LEU	CB-CG-CD1	5.91	121.04	111.00
3	7-D	124	ASP	CB-CG-OD1	5.91	123.61	118.30
2	9-B	427	LYS	CB-CA-C	-5.91	98.59	110.40
1	1-A	296	TYR	CD1-CE1-CZ	5.90	125.11	119.80
1	5-A	404	ILE	O-C-N	-5.90	113.25	122.70
1	8-A	302	TYR	CB-CG-CD2	5.90	124.54	121.00
2	3-B	583	TYR	CG-CD1-CE1	-5.90	116.58	121.30
1	5-A	190	TYR	CB-CG-CD1	5.90	124.54	121.00
3	5-D	133	PHE	CB-CG-CD2	-5.90	116.67	120.80
2	7-B	393	PHE	CB-CG-CD2	-5.90	116.67	120.80
2	1-B	400	TYR	CA-CB-CG	5.90	124.61	113.40
1	3-A	458	TYR	CB-CG-CD2	-5.90	117.46	121.00
3	3-C	49	ASP	CB-CG-OD1	5.90	123.61	118.30
2	5-B	415	TYR	N-CA-CB	5.90	121.22	110.60
1	8-A	339	GLU	N-CA-CB	-5.90	99.98	110.60
2	8-B	731	PHE	CB-CG-CD2	-5.90	116.67	120.80
3	5-C	192	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	8-A	681	THR	CA-CB-CG2	-5.90	104.14	112.40
3	5-C	96	SER	N-CA-CB	5.90	119.34	110.50
3	7-D	265	LEU	N-CA-C	-5.90	95.08	111.00
1	2-A	137	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	2-A	561	LYS	N-CA-CB	5.89	121.21	110.60
3	3-D	256	TYR	CB-CG-CD2	-5.89	117.46	121.00
3	8-C	285	ALA	N-CA-CB	5.89	118.35	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	171	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	1-A	398	TYR	CB-CG-CD2	5.89	124.54	121.00
1	6-A	168	PHE	CB-CG-CD2	5.89	124.92	120.80
2	6-B	565	TYR	CB-CG-CD1	5.89	124.53	121.00
3	10-D	310	MET	CB-CA-C	-5.89	98.62	110.40
3	1-D	376	MET	CG-SD-CE	-5.89	90.77	100.20
3	8-D	275	PHE	CB-CG-CD1	-5.89	116.68	120.80
3	2-D	344	PHE	CG-CD1-CE1	-5.89	114.32	120.80
1	9-A	171	ARG	NE-CZ-NH1	5.89	123.25	120.30
3	10-D	398	PHE	CB-CG-CD1	-5.89	116.68	120.80
3	5-D	180	VAL	CA-CB-CG2	-5.89	102.07	110.90
3	6-D	90	ARG	NE-CZ-NH2	-5.89	117.36	120.30
3	8-C	319	TYR	CG-CD2-CE2	-5.89	116.59	121.30
3	8-D	359	ARG	NH1-CZ-NH2	-5.89	112.92	119.40
3	2-D	232	SER	N-CA-CB	5.88	119.33	110.50
1	2-A	320	TRP	CG-CD2-CE3	-5.88	128.60	133.90
3	7-D	344	PHE	CB-CG-CD1	5.88	124.92	120.80
1	1-A	124	GLU	O-C-N	5.88	132.11	122.70
3	2-D	247	TYR	CB-CG-CD1	-5.88	117.47	121.00
3	2-D	279	TYR	CB-CG-CD2	5.88	124.53	121.00
2	6-B	195	THR	CA-CB-CG2	-5.88	104.17	112.40
3	7-C	4	GLU	N-CA-CB	5.88	121.19	110.60
1	10-A	451	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	6-A	587	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	3-A	462	LEU	CB-CG-CD2	5.88	121.00	111.00
1	3-A	587	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	6-B	293	ARG	NE-CZ-NH2	-5.88	117.36	120.30
3	6-D	78	ASP	CB-CG-OD1	-5.88	113.01	118.30
3	9-D	347	TRP	CD1-CG-CD2	5.88	111.00	106.30
3	1-D	163	PRO	N-CD-CG	5.88	112.01	103.20
1	8-A	322	THR	CA-CB-CG2	-5.88	104.17	112.40
2	3-B	319	PHE	CB-CG-CD2	-5.87	116.69	120.80
3	8-D	243	ARG	CB-CA-C	-5.87	98.65	110.40
1	9-A	168	PHE	CB-CG-CD1	-5.87	116.69	120.80
3	9-C	319	TYR	CB-CG-CD2	-5.87	117.47	121.00
2	1-B	293	ARG	NE-CZ-NH2	-5.87	117.36	120.30
3	2-C	74	SER	CB-CA-C	5.87	121.26	110.10
2	3-B	588	ASN	N-CA-CB	5.87	121.17	110.60
1	5-A	327	ARG	NE-CZ-NH1	5.87	123.23	120.30
3	5-D	25	LEU	CB-CG-CD2	5.87	120.98	111.00
2	1-B	773	VAL	CA-CB-CG2	-5.87	102.10	110.90
3	1-D	278	ASP	CB-CG-OD1	-5.87	113.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-C	63	THR	CA-CB-CG2	-5.87	104.18	112.40
3	5-D	238	VAL	CA-CB-CG2	-5.87	102.10	110.90
1	8-A	568	TYR	CB-CG-CD2	5.87	124.52	121.00
3	8-C	353	HIS	CA-CB-CG	5.87	123.58	113.60
1	4-A	450	TYR	CD1-CE1-CZ	5.87	125.08	119.80
2	10-B	827	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	2-A	271	LEU	CB-CG-CD2	5.86	120.97	111.00
1	3-A	347	MET	N-CA-CB	-5.86	100.05	110.60
1	4-A	173	LEU	CB-CG-CD2	5.86	120.96	111.00
2	7-B	758	TYR	CA-C-O	-5.86	107.79	120.10
3	9-D	136	PHE	CD1-CG-CD2	-5.86	110.68	118.30
3	1-D	49	ASP	C-N-CA	5.86	136.35	121.70
1	6-A	693	ILE	CA-C-N	5.86	133.51	117.10
3	5-C	277	SER	N-CA-CB	5.86	119.28	110.50
3	8-D	412	LEU	CB-CG-CD1	5.86	120.96	111.00
3	1-C	22	TRP	CB-CG-CD1	-5.86	119.39	127.00
2	5-B	519	ALA	N-CA-CB	5.86	118.30	110.10
2	4-B	592	ARG	NE-CZ-NH2	5.85	123.23	120.30
2	5-B	514	ARG	NE-CZ-NH2	-5.85	117.37	120.30
3	5-C	143	ALA	N-CA-CB	5.85	118.29	110.10
3	7-D	362	TYR	CA-CB-CG	5.85	124.52	113.40
3	8-C	185	TYR	CD1-CE1-CZ	-5.85	114.53	119.80
2	5-B	393	PHE	CB-CG-CD1	-5.85	116.70	120.80
3	2-C	15	ASN	CB-CA-C	-5.85	98.70	110.40
2	7-B	600	TYR	CG-CD1-CE1	-5.85	116.62	121.30
2	7-B	824	TYR	CB-CG-CD2	5.85	124.51	121.00
3	10-C	170	TYR	CG-CD1-CE1	-5.85	116.62	121.30
3	1-D	369	GLU	C-N-CA	5.84	136.31	121.70
3	2-C	204	PHE	CB-CG-CD1	5.84	124.89	120.80
3	7-D	393	THR	CA-CB-CG2	-5.84	104.22	112.40
1	2-A	576	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	2-A	624	ARG	NE-CZ-NH1	5.84	123.22	120.30
2	6-B	280	LEU	C-N-CA	5.84	136.30	121.70
2	7-B	264	TYR	CB-CG-CD2	5.84	124.50	121.00
2	7-B	295	ARG	NE-CZ-NH2	-5.84	117.38	120.30
2	7-B	666	ARG	NE-CZ-NH1	5.84	123.22	120.30
3	8-D	333	ARG	NE-CZ-NH2	-5.84	117.38	120.30
3	9-D	427	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	4-A	792	ASP	CB-CG-OD2	5.84	123.55	118.30
3	1-D	185	TYR	CB-CG-CD1	5.84	124.50	121.00
2	3-B	651	TYR	CB-CG-CD2	-5.84	117.50	121.00
2	4-B	470	TYR	CB-CG-CD2	-5.84	117.50	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4-D	359	ARG	CB-CA-C	-5.84	98.72	110.40
2	3-B	326	THR	CA-CB-CG2	-5.83	104.23	112.40
2	1-B	758	TYR	CB-CG-CD2	-5.83	117.50	121.00
2	1-B	827	ARG	NE-CZ-NH2	-5.83	117.38	120.30
3	2-C	110	ASP	CB-CG-OD1	-5.83	113.05	118.30
1	8-A	767	TYR	CA-CB-CG	-5.83	102.32	113.40
2	2-B	816	TYR	CB-CG-CD1	5.83	124.50	121.00
1	1-A	347	MET	CG-SD-CE	-5.83	90.87	100.20
3	1-C	372	VAL	CA-CB-CG1	-5.83	102.16	110.90
3	5-C	223	ASP	CB-CG-OD2	-5.83	113.05	118.30
2	7-B	840	LEU	CB-CG-CD1	5.83	120.91	111.00
2	9-B	544	ARG	N-CA-CB	5.83	121.09	110.60
1	9-A	148	ASP	CB-CG-OD2	-5.83	113.06	118.30
2	9-B	362	PHE	CB-CG-CD2	5.83	124.88	120.80
3	1-D	293	ASP	CB-CG-OD1	-5.82	113.06	118.30
3	3-C	278	ASP	CB-CG-OD2	5.82	123.54	118.30
1	4-A	160	ARG	NE-CZ-NH1	5.82	123.21	120.30
3	4-D	202	VAL	CA-CB-CG2	-5.82	102.17	110.90
2	5-B	195	THR	CA-CB-OG1	5.82	121.23	109.00
3	6-D	403	PHE	CB-CG-CD2	5.82	124.87	120.80
3	2-C	337	LYS	N-CA-CB	5.82	121.07	110.60
1	3-A	624	ARG	NE-CZ-NH1	5.82	123.21	120.30
2	8-B	227	ALA	N-CA-CB	5.82	118.24	110.10
2	1-B	343	TYR	CB-CG-CD1	5.82	124.49	121.00
3	5-D	100	SER	N-CA-CB	5.82	119.22	110.50
3	9-C	445	TYR	CZ-CE2-CD2	5.82	125.03	119.80
2	3-B	180	PRO	N-CA-CB	5.81	110.28	103.30
3	10-D	265	LEU	N-CA-C	-5.81	95.31	111.00
2	1-B	598	TYR	CZ-CE2-CD2	5.81	125.03	119.80
3	1-C	249	TYR	CB-CG-CD2	5.81	124.49	121.00
1	5-A	279	TYR	CD1-CG-CD2	5.81	124.29	117.90
2	5-B	542	ASP	N-CA-C	-5.81	95.32	111.00
2	6-B	181	GLU	CB-CA-C	-5.81	98.78	110.40
3	9-D	167	LEU	CB-CA-C	-5.81	99.16	110.20
1	2-A	105	PHE	CB-CG-CD1	-5.81	116.73	120.80
3	2-C	397	VAL	CA-CB-CG2	-5.81	102.19	110.90
1	4-A	451	ARG	NH1-CZ-NH2	-5.81	113.01	119.40
3	7-C	436	ASP	N-CA-CB	5.81	121.06	110.60
3	6-C	160	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	9-A	562	PHE	CB-CG-CD2	-5.80	116.74	120.80
2	1-B	359	TYR	CG-CD1-CE1	-5.80	116.66	121.30
1	10-A	178	ASN	C-N-CA	5.80	136.21	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	327	ARG	CG-CD-NE	-5.80	99.62	111.80
2	5-B	585	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	6-A	359	ALA	N-CA-CB	5.80	118.22	110.10
1	6-A	576	ARG	NE-CZ-NH2	-5.80	117.40	120.30
2	7-B	722	ASP	CB-CG-OD2	5.80	123.52	118.30
2	9-B	846	ARG	N-CA-CB	5.80	121.04	110.60
2	6-B	667	LYS	CB-CA-C	-5.80	98.80	110.40
3	7-D	41	ASP	CB-CG-OD1	5.80	123.52	118.30
1	5-A	344	LEU	CB-CG-CD1	5.80	120.86	111.00
2	10-B	542	ASP	CB-CG-OD1	5.80	123.52	118.30
2	10-B	772	PHE	CG-CD2-CE2	-5.80	114.42	120.80
3	10-C	118	ASP	CB-CG-OD2	5.80	123.52	118.30
1	4-A	639	PHE	CB-CG-CD1	5.80	124.86	120.80
3	9-C	362	TYR	CB-CG-CD1	5.80	124.48	121.00
1	4-A	443	MET	CA-CB-CG	5.79	123.15	113.30
1	3-A	76	ARG	NE-CZ-NH2	-5.79	117.40	120.30
3	3-C	161	ARG	CD-NE-CZ	-5.79	115.49	123.60
3	5-D	352	MET	CG-SD-CE	-5.79	90.93	100.20
1	1-A	137	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	3-A	599	LEU	CB-CG-CD1	5.79	120.85	111.00
3	3-D	110	ASP	CB-CG-OD1	5.79	123.51	118.30
1	10-A	594	TYR	CB-CG-CD1	-5.79	117.53	121.00
1	10-A	767	TYR	CB-CG-CD2	-5.79	117.53	121.00
1	1-A	150	TYR	CD1-CE1-CZ	-5.79	114.59	119.80
3	2-C	297	ASP	N-CA-CB	-5.79	100.18	110.60
1	1-A	393	TYR	CB-CG-CD1	-5.79	117.53	121.00
3	4-D	256	TYR	CG-CD1-CE1	-5.79	116.67	121.30
2	5-B	202	PHE	CB-CG-CD2	5.79	124.85	120.80
3	3-C	42	SER	N-CA-CB	5.79	119.18	110.50
3	7-C	407	TYR	CB-CG-CD2	-5.79	117.53	121.00
3	2-D	282	ASP	CB-CG-OD1	5.79	123.51	118.30
1	3-A	107	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	4-A	706	PHE	CG-CD1-CE1	-5.79	114.44	120.80
3	1-D	321	THR	CA-CB-CG2	5.78	120.50	112.40
2	6-B	319	PHE	CB-CG-CD1	5.78	124.85	120.80
3	5-D	437	TYR	CB-CG-CD1	5.78	124.47	121.00
1	8-A	140	TYR	CB-CG-CD2	5.78	124.47	121.00
2	3-B	438	TYR	CA-CB-CG	5.78	124.38	113.40
3	3-C	173	PHE	CB-CG-CD2	-5.78	116.76	120.80
3	3-D	132	ASN	CA-CB-CG	-5.78	100.69	113.40
3	5-C	211	ASN	N-CA-CB	5.78	121.00	110.60
3	6-C	192	ARG	NE-CZ-NH1	5.78	123.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-D	292	TYR	CG-CD1-CE1	-5.78	116.68	121.30
1	5-A	110	VAL	CA-CB-CG2	-5.78	102.24	110.90
2	8-B	221	LEU	CB-CG-CD1	5.78	120.82	111.00
3	10-C	347	TRP	CA-CB-CG	5.77	124.67	113.70
3	3-C	407	TYR	CA-CB-CG	-5.77	102.43	113.40
3	3-D	247	TYR	CZ-CE2-CD2	-5.77	114.61	119.80
3	5-C	436	ASP	CB-CG-OD2	5.77	123.50	118.30
3	8-D	118	ASP	CB-CG-OD1	-5.77	113.10	118.30
1	9-A	630	ARG	CD-NE-CZ	5.77	131.68	123.60
3	8-C	97	ASP	CB-CG-OD1	5.77	123.49	118.30
1	2-A	137	ARG	NE-CZ-NH2	-5.77	117.42	120.30
2	2-B	562	TYR	CB-CG-CD1	-5.77	117.54	121.00
3	6-D	181	VAL	O-C-N	-5.77	113.47	122.70
3	2-C	86	PHE	CZ-CE2-CD2	-5.77	113.18	120.10
3	3-D	56	GLU	N-CA-CB	5.77	120.98	110.60
3	7-D	53	PHE	CG-CD1-CE1	-5.77	114.46	120.80
1	9-A	644	MET	CG-SD-CE	-5.77	90.97	100.20
3	2-D	361	PRO	N-CA-CB	5.77	110.22	103.30
3	3-D	84	ARG	NE-CZ-NH1	-5.77	117.42	120.30
1	10-A	426	PHE	CB-CA-C	-5.77	98.87	110.40
3	5-C	22	TRP	CG-CD2-CE3	-5.76	128.71	133.90
1	6-A	714	ARG	NE-CZ-NH1	-5.76	117.42	120.30
3	7-D	142	VAL	CA-CB-CG1	-5.76	102.25	110.90
1	7-A	391	GLU	OE1-CD-OE2	5.76	130.22	123.30
3	1-D	49	ASP	CB-CG-OD2	-5.76	113.11	118.30
3	2-C	244	PHE	CD1-CE1-CZ	-5.76	113.19	120.10
2	5-B	284	TYR	N-CA-CB	5.76	120.97	110.60
3	6-D	387	PHE	CB-CG-CD1	5.76	124.83	120.80
3	8-D	97	ASP	CB-CG-OD1	5.76	123.49	118.30
2	9-B	731	PHE	CB-CG-CD1	5.76	124.83	120.80
1	2-A	140	TYR	CG-CD1-CE1	5.76	125.91	121.30
1	3-A	137	ARG	NE-CZ-NH2	-5.76	117.42	120.30
3	10-C	277	SER	CB-CA-C	-5.76	99.16	110.10
1	10-A	664	ARG	NE-CZ-NH1	5.76	123.18	120.30
3	6-D	48	ASP	N-CA-C	-5.76	95.46	111.00
1	8-A	76	ARG	NE-CZ-NH2	-5.76	117.42	120.30
2	8-B	342	TYR	CD1-CE1-CZ	-5.76	114.62	119.80
2	9-B	336	ASN	N-CA-CB	5.76	120.96	110.60
3	2-C	97	ASP	CB-CG-OD2	5.75	123.48	118.30
1	3-A	371	SER	N-CA-CB	5.75	119.13	110.50
3	4-D	97	ASP	CB-CA-C	-5.75	98.89	110.40
3	9-D	347	TRP	CD2-CE2-CZ2	-5.75	115.40	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	91	GLU	N-CA-CB	5.75	120.95	110.60
2	9-B	477	LEU	O-C-N	5.75	131.90	122.70
3	9-D	83	PHE	CB-CG-CD1	-5.75	116.77	120.80
2	10-B	297	TYR	CB-CG-CD2	5.75	124.45	121.00
3	1-C	20	PHE	CB-CA-C	-5.75	98.90	110.40
2	3-B	833	ASP	CB-CG-OD1	-5.75	113.12	118.30
2	6-B	470	TYR	CD1-CG-CD2	5.75	124.22	117.90
2	2-B	342	TYR	CG-CD1-CE1	-5.75	116.70	121.30
3	2-C	347	TRP	CB-CG-CD2	-5.75	119.13	126.60
3	7-D	359	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	9-A	393	TYR	CB-CG-CD1	5.75	124.45	121.00
3	7-D	161	ARG	CA-CB-CG	5.75	126.04	113.40
2	8-B	576	ARG	NH1-CZ-NH2	5.75	125.72	119.40
2	9-B	498	ASP	CB-CG-OD2	-5.75	113.13	118.30
2	9-B	585	ARG	NH1-CZ-NH2	-5.75	113.08	119.40
2	10-B	285	ARG	CD-NE-CZ	-5.75	115.56	123.60
3	6-C	249	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	8-A	105	PHE	CB-CG-CD2	-5.75	116.78	120.80
2	10-B	475	PHE	CB-CG-CD1	5.75	124.82	120.80
3	1-D	290	SER	N-CA-CB	-5.74	101.89	110.50
3	6-C	87	PHE	CB-CG-CD2	5.74	124.82	120.80
3	6-C	272	PHE	CB-CG-CD2	-5.74	116.78	120.80
3	8-D	279	TYR	CB-CG-CD2	5.74	124.45	121.00
1	10-A	203	ARG	NE-CZ-NH2	-5.74	117.43	120.30
2	6-B	411	PHE	CB-CG-CD2	-5.74	116.78	120.80
1	7-A	595	HIS	N-CA-CB	5.74	120.94	110.60
3	10-D	319	TYR	CG-CD1-CE1	5.74	125.89	121.30
3	3-C	239	THR	CA-CB-CG2	-5.74	104.36	112.40
3	3-D	36	LEU	O-C-N	-5.74	113.52	122.70
1	10-A	794	TYR	CG-CD2-CE2	5.74	125.89	121.30
2	1-B	562	TYR	CB-CG-CD1	5.74	124.44	121.00
2	8-B	411	PHE	CB-CG-CD1	5.74	124.82	120.80
1	1-A	324	TYR	CG-CD1-CE1	5.74	125.89	121.30
1	1-A	639	PHE	CB-CG-CD1	-5.74	116.79	120.80
3	2-C	22	TRP	CB-CG-CD1	-5.74	119.54	127.00
1	6-A	77	TYR	CZ-CE2-CD2	5.74	124.96	119.80
3	5-C	272	PHE	CB-CG-CD1	5.73	124.81	120.80
2	6-B	254	ILE	CA-CB-CG2	-5.73	99.43	110.90
3	6-D	17	VAL	CA-CB-CG1	-5.73	102.30	110.90
2	8-B	247	SER	N-CA-CB	5.73	119.10	110.50
3	5-C	158	LEU	CB-CG-CD2	5.73	120.74	111.00
3	7-C	155	LEU	O-C-N	-5.73	113.53	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-A	594	TYR	CB-CG-CD1	-5.73	117.56	121.00
2	8-B	833	ASP	CB-CA-C	-5.73	98.94	110.40
3	3-D	306	VAL	CA-CB-CG1	-5.73	102.31	110.90
3	4-C	445	TYR	CB-CG-CD1	-5.73	117.56	121.00
3	8-D	259	LEU	CB-CA-C	-5.73	99.31	110.20
3	6-C	292	TYR	CB-CG-CD2	5.73	124.44	121.00
1	7-A	358	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	1-A	364	PRO	CA-N-CD	-5.73	103.48	111.50
3	3-C	387	PHE	CB-CG-CD2	-5.73	116.79	120.80
2	10-B	276	THR	CA-CB-OG1	5.73	121.03	109.00
2	2-B	556	ASP	CB-CG-OD1	-5.73	113.15	118.30
1	4-A	576	ARG	CG-CD-NE	-5.73	99.78	111.80
1	5-A	793	PHE	CB-CG-CD1	-5.72	116.79	120.80
3	5-D	90	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	7-A	324	TYR	CD1-CE1-CZ	-5.72	114.65	119.80
2	8-B	409	TYR	CB-CG-CD2	-5.72	117.56	121.00
1	2-A	349	ARG	NE-CZ-NH2	5.72	123.16	120.30
3	3-D	165	LYS	N-CA-CB	5.72	120.90	110.60
1	6-A	116	TYR	CB-CG-CD1	5.72	124.43	121.00
1	8-A	171	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	1-B	470	TYR	CB-CG-CD2	5.72	124.43	121.00
1	6-A	796	SER	CB-CA-C	-5.72	99.23	110.10
1	2-A	612	TRP	CG-CD2-CE3	-5.72	128.75	133.90
3	3-D	344	PHE	N-CA-CB	5.72	120.89	110.60
1	4-A	302	TYR	CG-CD2-CE2	-5.72	116.73	121.30
2	9-B	838	LEU	CB-CG-CD2	5.72	120.72	111.00
3	2-C	118	ASP	CB-CG-OD1	-5.72	113.16	118.30
2	6-B	574	VAL	N-CA-C	-5.72	95.57	111.00
3	5-D	380	MET	CG-SD-CE	-5.71	91.06	100.20
2	2-B	722	ASP	CB-CA-C	-5.71	98.97	110.40
1	3-A	76	ARG	NH1-CZ-NH2	5.71	125.68	119.40
3	3-D	114	ARG	NH1-CZ-NH2	-5.71	113.12	119.40
3	10-C	316	PHE	CB-CG-CD2	5.71	124.80	120.80
1	3-A	276	SER	CB-CA-C	-5.71	99.25	110.10
2	9-B	421	TRP	CZ3-CH2-CZ2	-5.71	114.75	121.60
3	1-D	359	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	4-A	486	PHE	CB-CG-CD1	5.71	124.80	120.80
3	5-D	34	ASP	CB-CG-OD1	5.71	123.44	118.30
2	6-B	446	PHE	CB-CG-CD2	5.71	124.80	120.80
2	7-B	534	ASN	N-CA-C	-5.71	95.59	111.00
3	9-D	352	MET	CG-SD-CE	-5.71	91.07	100.20
3	4-D	16	HIS	CA-CB-CG	5.71	123.30	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	8-C	248	MET	CG-SD-CE	-5.71	91.07	100.20
3	2-D	193	ARG	NE-CZ-NH2	-5.70	117.45	120.30
2	4-B	295	ARG	CG-CD-NE	-5.70	99.82	111.80
3	4-D	278	ASP	CB-CG-OD2	-5.70	113.17	118.30
3	7-C	367	PRO	N-CA-CB	5.70	110.14	103.30
3	7-D	256	TYR	CB-CG-CD1	-5.70	117.58	121.00
3	8-C	357	GLY	N-CA-C	-5.70	98.84	113.10
3	8-D	178	SER	CB-CA-C	-5.70	99.27	110.10
3	10-D	197	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	1-A	165	VAL	N-CA-C	-5.70	95.60	111.00
3	6-D	305	LEU	CB-CG-CD2	5.70	120.69	111.00
3	8-C	93	TRP	NE1-CE2-CZ2	5.70	136.67	130.40
2	2-B	264	TYR	CB-CG-CD1	-5.70	117.58	121.00
3	7-D	309	ALA	N-CA-C	-5.70	95.61	111.00
3	2-C	272	PHE	CD1-CG-CD2	5.70	125.71	118.30
3	2-C	443	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	7-A	327	ARG	NH1-CZ-NH2	-5.70	113.13	119.40
1	9-A	793	PHE	CG-CD1-CE1	5.70	127.07	120.80
1	10-A	284	TYR	CG-CD1-CE1	5.70	125.86	121.30
3	2-C	333	ARG	NE-CZ-NH1	5.70	123.15	120.30
3	4-D	445	TYR	CG-CD1-CE1	5.70	125.86	121.30
2	1-B	593	PHE	CB-CG-CD2	-5.70	116.81	120.80
3	1-D	124	ASP	CB-CA-C	-5.70	99.01	110.40
1	2-A	167	ASN	N-CA-CB	5.70	120.85	110.60
1	4-A	604	MET	CG-SD-CE	-5.70	91.09	100.20
2	7-B	225	PHE	N-CA-CB	5.70	120.85	110.60
3	10-C	335	MET	CG-SD-CE	-5.69	91.09	100.20
3	10-D	200	ALA	N-CA-CB	5.69	118.07	110.10
3	1-C	423	PHE	CB-CG-CD2	5.69	124.78	120.80
2	3-B	494	GLU	OE1-CD-OE2	-5.69	116.47	123.30
2	7-B	236	TYR	CG-CD1-CE1	-5.69	116.75	121.30
2	2-B	197	SER	N-CA-CB	5.69	119.04	110.50
3	3-C	71	SER	N-CA-C	-5.69	95.64	111.00
2	7-B	599	PHE	CB-CG-CD2	-5.69	116.82	120.80
3	8-C	209	LEU	CB-CG-CD1	5.69	120.67	111.00
1	10-A	197	PHE	CB-CG-CD2	-5.69	116.82	120.80
1	2-A	296	TYR	CZ-CE2-CD2	-5.69	114.68	119.80
1	4-A	170	ILE	N-CA-C	5.69	126.36	111.00
3	9-D	393	THR	CA-CB-CG2	-5.69	104.44	112.40
2	10-B	510	TYR	CB-CG-CD1	-5.69	117.59	121.00
3	1-D	307	SER	N-CA-CB	5.69	119.03	110.50
3	8-C	279	TYR	CB-CG-CD1	5.69	124.41	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	646	TYR	CD1-CE1-CZ	-5.69	114.68	119.80
3	1-D	249	TYR	CG-CD2-CE2	-5.68	116.75	121.30
3	2-C	48	ASP	CB-CG-OD2	5.68	123.42	118.30
1	9-A	304	ASP	CB-CG-OD1	5.68	123.42	118.30
2	2-B	510	TYR	CD1-CG-CD2	-5.68	111.65	117.90
2	4-B	335	PHE	CB-CG-CD1	5.68	124.78	120.80
1	8-A	594	TYR	CG-CD1-CE1	-5.68	116.75	121.30
2	10-B	534	ASN	CA-CB-CG	-5.68	100.90	113.40
2	4-B	284	TYR	CG-CD2-CE2	-5.68	116.76	121.30
2	4-B	424	GLU	CA-CB-CG	5.68	125.89	113.40
2	4-B	824	TYR	CG-CD2-CE2	-5.68	116.76	121.30
3	5-C	161	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	2-A	160	ARG	CG-CD-NE	-5.68	99.88	111.80
2	1-B	598	TYR	CD1-CG-CD2	5.68	124.14	117.90
1	4-A	664	ARG	NE-CZ-NH1	5.68	123.14	120.30
3	10-C	395	ASP	CB-CG-OD2	-5.68	113.19	118.30
3	7-D	346	SER	CB-CA-C	5.67	120.88	110.10
2	8-B	319	PHE	CD1-CE1-CZ	5.67	126.91	120.10
2	10-B	801	LEU	CB-CG-CD2	5.67	120.65	111.00
1	1-A	70	LEU	CB-CA-C	-5.67	99.42	110.20
2	1-B	514	ARG	NE-CZ-NH1	5.67	123.14	120.30
2	1-B	652	TYR	CB-CG-CD1	5.67	124.40	121.00
2	2-B	467	LYS	N-CA-CB	5.67	120.81	110.60
3	5-D	395	ASP	CB-CG-OD1	5.67	123.41	118.30
3	7-C	110	ASP	CB-CA-C	-5.67	99.06	110.40
3	7-C	398	PHE	CB-CG-CD2	-5.67	116.83	120.80
3	9-C	316	PHE	CB-CG-CD1	5.67	124.77	120.80
3	2-D	149	GLY	O-C-N	-5.67	113.63	122.70
2	3-B	542	ASP	CB-CA-C	-5.67	99.07	110.40
3	3-C	182	VAL	CB-CA-C	-5.67	100.63	111.40
3	7-C	176	ARG	NE-CZ-NH2	-5.67	117.47	120.30
3	5-D	157	ALA	N-CA-CB	5.67	118.03	110.10
2	8-B	267	PHE	CB-CG-CD1	-5.67	116.83	120.80
3	1-D	315	TYR	CB-CG-CD1	5.66	124.40	121.00
1	7-A	96	LYS	O-C-N	5.66	131.76	122.70
1	8-A	143	ARG	CD-NE-CZ	-5.66	115.68	123.60
3	8-C	395	ASP	N-CA-CB	5.66	120.79	110.60
1	3-A	333	ARG	NH1-CZ-NH2	5.66	125.62	119.40
3	5-C	398	PHE	CB-CG-CD2	-5.66	116.84	120.80
3	6-D	43	SER	N-CA-CB	5.66	118.99	110.50
2	7-B	758	TYR	CA-C-N	5.66	132.94	117.10
2	10-B	342	TYR	CG-CD2-CE2	-5.66	116.77	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	10-D	333	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	1-A	696	GLN	CB-CA-C	-5.66	99.09	110.40
3	1-C	283	ASP	N-CA-CB	5.66	120.78	110.60
1	8-A	579	MET	CG-SD-CE	-5.66	91.15	100.20
1	8-A	791	PHE	CB-CG-CD2	-5.66	116.84	120.80
2	8-B	468	PHE	CB-CG-CD1	-5.66	116.84	120.80
2	10-B	769	VAL	N-CA-CB	5.66	123.94	111.50
2	5-B	310	ASP	CB-CG-OD1	5.66	123.39	118.30
2	7-B	347	MET	CA-CB-CG	5.66	122.92	113.30
3	1-C	416	MET	CG-SD-CE	-5.65	91.15	100.20
1	2-A	562	PHE	CB-CG-CD2	5.65	124.76	120.80
2	5-B	565	TYR	CG-CD1-CE1	-5.65	116.78	121.30
3	9-C	125	LYS	N-CA-CB	5.65	120.78	110.60
3	4-D	413	PHE	CZ-CE2-CD2	-5.65	113.32	120.10
1	7-A	791	PHE	CB-CG-CD2	-5.65	116.84	120.80
1	10-A	162	PHE	CB-CG-CD1	5.65	124.75	120.80
1	2-A	587	ARG	NE-CZ-NH2	-5.65	117.47	120.30
2	6-B	591	TRP	CB-CG-CD1	5.65	134.34	127.00
2	7-B	345	TYR	CZ-CE2-CD2	5.65	124.88	119.80
1	10-A	68	ILE	CB-CA-C	5.65	122.90	111.60
3	4-C	314	THR	CA-CB-CG2	-5.65	104.49	112.40
2	10-B	587	PHE	CB-CG-CD1	-5.65	116.85	120.80
3	10-C	87	PHE	CB-CG-CD2	-5.65	116.85	120.80
3	4-D	306	VAL	CA-CB-CG2	-5.65	102.43	110.90
3	8-C	94	VAL	CG1-CB-CG2	5.65	119.93	110.90
2	10-B	649	GLU	OE1-CD-OE2	5.65	130.08	123.30
3	3-C	319	TYR	CA-CB-CG	5.64	124.12	113.40
1	7-A	429	TYR	CG-CD2-CE2	-5.64	116.78	121.30
3	7-D	376	MET	CB-CA-C	-5.64	99.11	110.40
1	10-A	794	TYR	N-CA-CB	5.64	120.76	110.60
1	2-A	121	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	2-B	544	ARG	NE-CZ-NH2	-5.64	117.48	120.30
3	3-C	358	ARG	N-CA-CB	5.64	120.76	110.60
1	4-A	800	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	9-A	118	ILE	N-CA-CB	5.64	123.78	110.80
3	9-D	354	VAL	CA-C-O	5.64	131.95	120.10
2	5-B	829	ASP	CB-CG-OD1	-5.64	113.22	118.30
3	8-C	177	SER	N-CA-CB	5.64	118.96	110.50
2	6-B	343	TYR	CG-CD1-CE1	-5.64	116.79	121.30
2	7-B	365	ALA	CB-CA-C	-5.64	101.64	110.10
2	10-B	211	SER	O-C-N	5.64	131.72	122.70
1	3-A	70	LEU	CB-CG-CD1	5.64	120.58	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4-B	587	PHE	CB-CG-CD2	-5.64	116.85	120.80
3	8-D	46	ARG	NH1-CZ-NH2	-5.64	113.20	119.40
1	10-A	600	ASP	CB-CG-OD1	-5.64	113.23	118.30
1	10-A	800	ASP	CB-CG-OD1	-5.64	113.23	118.30
3	10-C	47	ASP	N-CA-C	-5.64	95.78	111.00
1	3-A	71	GLU	OE1-CD-OE2	5.63	130.06	123.30
1	5-A	711	LYS	N-CA-CB	5.63	120.74	110.60
3	5-D	124	ASP	CB-CG-OD2	-5.63	113.23	118.30
3	6-D	316	PHE	CB-CG-CD1	5.63	124.74	120.80
3	9-C	359	ARG	NE-CZ-NH2	5.63	123.12	120.30
3	4-C	437	TYR	CB-CG-CD2	5.63	124.38	121.00
3	6-D	34	ASP	CB-CG-OD2	-5.63	113.23	118.30
3	8-D	344	PHE	CB-CG-CD2	5.63	124.74	120.80
1	2-A	385	MET	CG-SD-CE	-5.63	91.20	100.20
3	4-C	315	TYR	N-CA-C	-5.63	95.81	111.00
3	8-D	109	TYR	CB-CG-CD2	-5.63	117.62	121.00
2	4-B	558	PHE	CB-CG-CD2	-5.63	116.86	120.80
3	9-C	384	VAL	CG1-CB-CG2	5.63	119.90	110.90
1	3-A	134	VAL	CA-CB-CG2	-5.62	102.46	110.90
2	3-B	594	LYS	O-C-N	-5.62	113.70	122.70
2	2-B	284	TYR	CG-CD2-CE2	-5.62	116.80	121.30
3	3-C	58	SER	N-CA-CB	5.62	118.94	110.50
1	4-A	286	TRP	CE2-CD2-CG	-5.62	102.80	107.30
1	6-A	769	SER	CB-CA-C	-5.62	99.41	110.10
2	1-B	651	TYR	CB-CG-CD2	-5.62	117.63	121.00
3	1-D	59	ARG	CG-CD-NE	-5.62	100.00	111.80
2	2-B	225	PHE	CB-CG-CD1	-5.62	116.87	120.80
2	2-B	300	PHE	CB-CG-CD1	5.62	124.74	120.80
1	4-A	623	ARG	NE-CZ-NH2	5.62	123.11	120.30
3	2-C	421	ASP	CB-CG-OD2	-5.62	113.24	118.30
3	3-C	157	ALA	N-CA-CB	5.62	117.97	110.10
3	5-D	211	ASN	N-CA-CB	5.62	120.72	110.60
1	6-A	128	ASP	CB-CG-OD1	5.62	123.36	118.30
1	7-A	691	ASP	CB-CG-OD1	-5.62	113.24	118.30
1	2-A	284	TYR	CB-CA-C	-5.62	99.16	110.40
3	2-D	95	ALA	N-CA-CB	5.62	117.97	110.10
1	3-A	767	TYR	CG-CD2-CE2	-5.62	116.81	121.30
3	5-C	247	TYR	CD1-CG-CD2	5.62	124.08	117.90
2	10-B	237	LYS	CB-CA-C	-5.62	99.16	110.40
2	8-B	389	ARG	NE-CZ-NH1	-5.62	117.49	120.30
2	9-B	335	PHE	CG-CD1-CE1	-5.62	114.62	120.80
3	9-C	360	SER	N-CA-C	-5.62	95.83	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	10-B	187	TYR	CB-CG-CD2	5.62	124.37	121.00
1	4-A	630	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	3-A	296	TYR	CB-CG-CD2	5.61	124.37	121.00
3	5-C	109	TYR	CB-CG-CD2	-5.61	117.63	121.00
3	5-D	413	PHE	CB-CG-CD2	-5.61	116.87	120.80
1	3-A	465	PHE	CB-CG-CD1	5.61	124.73	120.80
3	6-C	292	TYR	CB-CG-CD1	-5.61	117.63	121.00
1	5-A	437	LYS	CB-CA-C	-5.61	99.18	110.40
1	6-A	409	PHE	CG-CD2-CE2	5.61	126.97	120.80
2	7-B	641	PHE	CG-CD2-CE2	-5.61	114.63	120.80
3	9-D	413	PHE	CB-CG-CD1	-5.61	116.87	120.80
1	1-A	682	ASN	CA-CB-CG	-5.61	101.06	113.40
3	3-C	274	PRO	N-CA-CB	-5.61	96.43	102.60
3	5-D	224	LEU	CB-CG-CD1	-5.61	101.46	111.00
1	7-A	189	LEU	CB-CG-CD2	5.61	120.53	111.00
2	2-B	231	TYR	CB-CG-CD1	5.61	124.36	121.00
3	1-D	249	TYR	CB-CG-CD2	-5.61	117.64	121.00
1	2-A	60	VAL	CA-CB-CG1	5.61	119.31	110.90
3	7-D	376	MET	CG-SD-CE	-5.61	91.23	100.20
1	1-A	336	ASP	CB-CG-OD1	-5.60	113.26	118.30
3	9-D	271	SER	N-CA-CB	5.60	118.91	110.50
1	2-A	410	PHE	CB-CG-CD1	-5.60	116.88	120.80
1	8-A	143	ARG	NE-CZ-NH1	-5.60	117.50	120.30
2	8-B	592	ARG	NH1-CZ-NH2	5.60	125.56	119.40
1	10-A	144	ARG	CD-NE-CZ	-5.60	115.76	123.60
1	5-A	706	PHE	CB-CA-C	-5.60	99.20	110.40
1	6-A	792	ASP	CB-CG-OD1	5.60	123.34	118.30
1	9-A	286	TRP	CG-CD1-NE1	5.60	115.70	110.10
1	10-A	700	PHE	CB-CG-CD2	-5.60	116.88	120.80
1	7-A	397	CYS	CA-CB-SG	-5.60	103.92	114.00
1	7-A	636	MET	CA-CB-CG	5.60	122.82	113.30
2	3-B	821	ASP	N-CA-CB	5.60	120.67	110.60
2	6-B	269	ASN	O-C-N	-5.60	113.75	122.70
3	1-C	423	PHE	CD1-CE1-CZ	5.59	126.81	120.10
1	4-A	334	ASP	CB-CG-OD2	5.59	123.33	118.30
3	7-D	65	ARG	NE-CZ-NH1	-5.59	117.50	120.30
3	7-D	445	TYR	CB-CG-CD2	-5.59	117.64	121.00
1	8-A	427	LEU	N-CA-CB	5.59	121.59	110.40
3	1-C	73	PRO	N-CA-CB	5.59	110.01	103.30
3	5-C	407	TYR	CG-CD2-CE2	-5.59	116.83	121.30
2	4-B	721	ILE	O-C-N	-5.59	113.75	122.70
3	7-C	87	PHE	CZ-CE2-CD2	-5.59	113.39	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	8-B	658	GLU	OE1-CD-OE2	5.59	130.01	123.30
2	4-B	528	LEU	CB-CG-CD2	5.59	120.50	111.00
3	4-C	92	THR	CA-CB-CG2	-5.59	104.58	112.40
3	4-D	440	ALA	N-CA-CB	5.59	117.92	110.10
2	3-B	297	TYR	CB-CG-CD1	5.59	124.35	121.00
2	3-B	409	TYR	CZ-CE2-CD2	5.59	124.83	119.80
3	3-D	48	ASP	N-CA-CB	5.59	120.66	110.60
3	10-D	241	SER	N-CA-CB	5.59	118.88	110.50
2	1-B	824	TYR	CB-CG-CD1	5.58	124.35	121.00
3	3-D	302	SER	N-CA-CB	5.58	118.88	110.50
3	8-C	439	ALA	N-CA-CB	5.58	117.92	110.10
2	3-B	670	ARG	NE-CZ-NH1	5.58	123.09	120.30
3	3-C	315	TYR	CZ-CE2-CD2	5.58	124.82	119.80
2	5-B	488	PHE	CB-CG-CD1	5.58	124.71	120.80
2	6-B	502	THR	CA-CB-CG2	-5.58	104.59	112.40
2	7-B	599	PHE	CB-CG-CD1	5.58	124.71	120.80
3	4-C	275	PHE	CB-CG-CD2	5.58	124.71	120.80
2	5-B	589	PHE	CB-CG-CD2	-5.58	116.89	120.80
1	2-A	62	ASP	CB-CG-OD1	5.58	123.32	118.30
3	6-D	87	PHE	N-CA-CB	5.58	120.64	110.60
1	2-A	440	THR	OG1-CB-CG2	-5.58	97.18	110.00
1	3-A	99	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	3-A	409	PHE	CB-CG-CD2	-5.58	116.90	120.80
3	3-D	232	SER	N-CA-CB	5.58	118.86	110.50
3	6-C	272	PHE	CB-CG-CD1	5.58	124.70	120.80
3	7-D	41	ASP	CB-CG-OD2	-5.58	113.28	118.30
3	7-D	53	PHE	CB-CG-CD1	-5.58	116.90	120.80
3	8-C	327	GLU	N-CA-CB	5.58	120.64	110.60
3	3-C	233	THR	CA-CB-CG2	5.57	120.20	112.40
1	4-A	410	PHE	N-CA-CB	5.57	120.63	110.60
3	4-D	204	PHE	N-CA-CB	5.57	120.63	110.60
1	6-A	296	TYR	CZ-CE2-CD2	5.57	124.82	119.80
1	8-A	116	TYR	CB-CG-CD2	5.57	124.34	121.00
3	4-D	54	PHE	CB-CG-CD1	5.57	124.70	120.80
2	5-B	816	TYR	CD1-CG-CD2	5.57	124.03	117.90
3	5-D	75	VAL	CB-CA-C	-5.57	100.82	111.40
2	1-B	282	SER	N-CA-CB	5.57	118.85	110.50
3	6-C	110	ASP	CB-CG-OD1	5.57	123.31	118.30
3	6-C	207	ALA	CB-CA-C	-5.57	101.75	110.10
3	9-D	292	TYR	CG-CD2-CE2	-5.57	116.84	121.30
2	1-B	769	VAL	CA-CB-CG1	5.57	119.25	110.90
1	2-A	287	LEU	CB-CG-CD2	5.57	120.47	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	143	ARG	NE-CZ-NH1	5.57	123.08	120.30
2	3-B	411	PHE	CB-CG-CD1	-5.57	116.90	120.80
1	5-A	657	TYR	CB-CG-CD2	5.57	124.34	121.00
2	1-B	629	ASN	CB-CA-C	-5.57	99.27	110.40
2	4-B	363	PHE	CB-CG-CD1	-5.57	116.90	120.80
2	7-B	200	PHE	CG-CD2-CE2	5.57	126.92	120.80
3	8-D	54	PHE	CB-CG-CD2	-5.57	116.90	120.80
3	9-C	387	PHE	CB-CG-CD2	-5.57	116.91	120.80
1	5-A	385	MET	CG-SD-CE	-5.56	91.30	100.20
3	5-C	445	TYR	CD1-CG-CD2	-5.56	111.78	117.90
1	6-A	197	PHE	CB-CG-CD1	-5.56	116.91	120.80
3	8-D	90	ARG	NE-CZ-NH2	-5.56	117.52	120.30
3	9-D	217	PHE	CZ-CE2-CD2	-5.56	113.42	120.10
3	5-D	22	TRP	CD1-CG-CD2	-5.56	101.85	106.30
3	5-D	83	PHE	CG-CD1-CE1	5.56	126.92	120.80
2	8-B	570	LEU	CB-CG-CD2	5.56	120.46	111.00
1	9-A	320	TRP	CE2-CD2-CG	5.56	111.75	107.30
2	7-B	288	TYR	CZ-CE2-CD2	5.56	124.81	119.80
2	6-B	283	LEU	CB-CG-CD1	-5.56	101.55	111.00
3	6-D	160	ASP	CB-CA-C	-5.56	99.28	110.40
3	9-C	315	TYR	CG-CD1-CE1	-5.56	116.85	121.30
3	1-C	325	ASN	N-CA-CB	5.56	120.61	110.60
2	3-B	359	TYR	CG-CD1-CE1	-5.56	116.85	121.30
3	7-C	53	PHE	CG-CD1-CE1	5.56	126.91	120.80
3	7-D	292	TYR	CD1-CE1-CZ	5.56	124.80	119.80
1	8-A	294	ASP	CB-CA-C	-5.56	99.28	110.40
3	8-C	218	ARG	NE-CZ-NH1	5.56	123.08	120.30
3	8-D	325	ASN	N-CA-CB	5.56	120.60	110.60
3	5-D	114	ARG	NE-CZ-NH1	5.55	123.08	120.30
3	8-C	78	ASP	CB-CG-OD1	-5.55	113.30	118.30
3	9-D	64	PRO	N-CA-CB	5.55	109.96	103.30
1	1-A	700	PHE	N-CA-CB	5.55	120.59	110.60
2	3-B	200	PHE	CB-CG-CD2	-5.55	116.91	120.80
3	3-C	293	ASP	N-CA-CB	5.55	120.59	110.60
2	4-B	390	VAL	CA-CB-CG1	5.55	119.23	110.90
1	3-A	349	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	6-A	768	ILE	CB-CA-C	5.55	122.70	111.60
2	6-B	526	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	8-A	62	ASP	CB-CG-OD1	5.55	123.29	118.30
2	8-B	824	TYR	CG-CD2-CE2	-5.55	116.86	121.30
3	8-D	393	THR	CA-CB-CG2	-5.55	104.63	112.40
1	10-A	111	ARG	NH1-CZ-NH2	-5.55	113.30	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5-B	242	ARG	N-CA-CB	5.55	120.59	110.60
3	7-C	249	TYR	CD1-CE1-CZ	5.55	124.79	119.80
3	7-D	6	ILE	N-CA-CB	5.55	123.56	110.80
3	1-D	396	LYS	CB-CA-C	-5.55	99.31	110.40
1	2-A	775	PHE	N-CA-CB	5.55	120.58	110.60
2	8-B	722	ASP	CB-CG-OD1	-5.55	113.31	118.30
3	8-D	436	ASP	CB-CG-OD1	5.55	123.29	118.30
3	8-C	185	TYR	CD1-CG-CD2	-5.54	111.80	117.90
1	1-A	558	TYR	CB-CG-CD1	5.54	124.33	121.00
3	3-C	421	ASP	CB-CG-OD1	-5.54	113.31	118.30
2	2-B	347	MET	CG-SD-CE	-5.54	91.33	100.20
1	1-A	604	MET	CG-SD-CE	-5.54	91.34	100.20
3	3-D	437	TYR	CB-CG-CD1	5.54	124.32	121.00
1	5-A	467	LEU	CB-CG-CD1	5.54	120.42	111.00
1	2-A	465	PHE	CB-CG-CD1	-5.54	116.92	120.80
1	8-A	160	ARG	NH1-CZ-NH2	-5.54	113.31	119.40
2	8-B	839	PHE	CB-CG-CD2	-5.54	116.92	120.80
3	8-C	204	PHE	CG-CD1-CE1	-5.54	114.71	120.80
1	9-A	251	PHE	O-C-N	-5.54	113.84	122.70
3	10-C	407	TYR	CA-CB-CG	-5.54	102.88	113.40
3	1-D	70	ASP	N-CA-CB	5.54	120.57	110.60
2	3-B	777	CYS	CA-CB-SG	-5.54	104.03	114.00
1	5-A	246	ALA	N-CA-CB	5.54	117.85	110.10
1	6-A	653	ASP	CB-CG-OD1	-5.54	113.32	118.30
1	8-A	395	ASP	CB-CG-OD1	-5.54	113.32	118.30
1	8-A	469	ARG	NE-CZ-NH2	-5.54	117.53	120.30
3	9-D	192	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	5-B	288	TYR	CD1-CE1-CZ	-5.53	114.82	119.80
3	4-D	131	ASP	CB-CA-C	-5.53	99.34	110.40
2	7-B	238	VAL	CA-CB-CG2	5.53	119.20	110.90
2	5-B	435	SER	CB-CA-C	-5.53	99.59	110.10
3	5-C	279	TYR	CB-CG-CD1	5.53	124.32	121.00
1	7-A	91	GLU	CA-CB-CG	5.53	125.57	113.40
2	10-B	565	TYR	CB-CG-CD1	-5.53	117.68	121.00
1	6-A	150	TYR	CD1-CE1-CZ	-5.53	114.82	119.80
1	7-A	337	SER	N-CA-CB	5.53	118.79	110.50
3	2-D	344	PHE	CB-CG-CD1	-5.53	116.93	120.80
3	3-C	292	TYR	CB-CG-CD1	5.53	124.32	121.00
1	8-A	612	TRP	CH2-CZ2-CE2	5.53	122.92	117.40
2	8-B	835	ASP	CB-CG-OD1	5.53	123.27	118.30
2	3-B	631	LEU	CB-CG-CD1	5.52	120.39	111.00
2	4-B	264	TYR	CG-CD2-CE2	-5.52	116.88	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	91	GLU	N-CA-CB	5.52	120.54	110.60
3	2-C	377	LEU	CB-CA-C	-5.52	99.71	110.20
1	5-A	421	HIS	CA-CB-CG	-5.52	104.21	113.60
2	9-B	439	ARG	NE-CZ-NH1	5.52	123.06	120.30
3	1-C	247	TYR	CB-CG-CD1	5.52	124.31	121.00
1	6-A	415	LEU	O-C-N	-5.52	113.87	122.70
3	9-D	59	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	2-A	111	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	2-A	335	CYS	N-CA-CB	5.52	120.54	110.60
3	5-D	249	TYR	CD1-CE1-CZ	5.52	124.77	119.80
1	8-A	461	LEU	CB-CA-C	-5.52	99.72	110.20
2	3-B	242	ARG	NH1-CZ-NH2	-5.52	113.33	119.40
3	7-D	279	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	8-A	776	ARG	NE-CZ-NH2	-5.52	117.54	120.30
3	9-C	295	MET	CG-SD-CE	-5.52	91.37	100.20
3	9-D	244	PHE	CB-CG-CD2	-5.52	116.94	120.80
1	2-A	759	GLU	OE1-CD-OE2	5.52	129.92	123.30
1	6-A	594	TYR	CB-CG-CD2	-5.52	117.69	121.00
2	1-B	238	VAL	N-CA-CB	5.51	123.63	111.50
1	5-A	337	SER	N-CA-CB	5.51	118.77	110.50
3	4-D	389	ASN	N-CA-CB	5.51	120.52	110.60
2	6-B	555	TRP	CB-CG-CD2	-5.51	119.43	126.60
3	1-C	328	PRO	N-CD-CG	5.51	111.47	103.20
1	3-A	614	TYR	CB-CG-CD1	-5.51	117.69	121.00
2	3-B	348	ASN	N-CA-CB	5.51	120.52	110.60
1	4-A	700	PHE	CB-CG-CD1	5.51	124.66	120.80
1	8-A	286	TRP	CH2-CZ2-CE2	5.51	122.91	117.40
2	9-B	757	PRO	N-CA-CB	5.51	109.91	103.30
1	1-A	757	ALA	CB-CA-C	-5.51	101.84	110.10
1	3-A	469	ARG	NE-CZ-NH2	5.51	123.06	120.30
3	4-D	314	THR	CA-CB-CG2	-5.51	104.69	112.40
3	6-D	416	MET	CA-CB-CG	5.51	122.67	113.30
3	10-C	355	ASN	N-CA-C	-5.51	96.12	111.00
3	10-D	8	LEU	N-CA-CB	5.51	121.42	110.40
3	5-D	176	ARG	NE-CZ-NH2	-5.51	117.55	120.30
3	10-C	344	PHE	CD1-CE1-CZ	5.51	126.71	120.10
3	10-D	312	ASN	CA-CB-CG	-5.51	101.28	113.40
3	2-C	172	VAL	CA-CB-CG2	5.51	119.16	110.90
1	3-A	636	MET	CG-SD-CE	-5.51	91.39	100.20
3	4-D	384	VAL	CG1-CB-CG2	5.51	119.71	110.90
1	7-A	98	MET	CG-SD-CE	-5.51	91.39	100.20
1	8-A	123	TYR	N-CA-CB	5.51	120.51	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	10-B	411	PHE	CB-CG-CD2	-5.51	116.95	120.80
1	3-A	140	TYR	CB-CA-C	-5.50	99.39	110.40
1	1-A	146	LEU	CB-CG-CD2	5.50	120.36	111.00
1	1-A	252	GLN	CG-CD-OE1	-5.50	110.59	121.60
2	1-B	497	ASN	CB-CA-C	-5.50	99.39	110.40
3	2-C	162	TYR	CB-CG-CD1	5.50	124.30	121.00
1	5-A	450	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	5-A	703	VAL	CA-CB-CG2	-5.50	102.64	110.90
3	5-C	248	MET	CG-SD-CE	-5.50	91.40	100.20
2	6-B	252	ALA	O-C-N	5.50	131.51	122.70
3	2-D	362	TYR	C-N-CA	5.50	135.46	121.70
1	3-A	77	TYR	CG-CD2-CE2	-5.50	116.90	121.30
3	6-C	173	PHE	CB-CG-CD1	5.50	124.65	120.80
2	7-B	816	TYR	CD1-CE1-CZ	5.50	124.75	119.80
3	9-C	7	THR	CA-CB-CG2	-5.50	104.70	112.40
2	10-B	580	ARG	NE-CZ-NH2	-5.50	117.55	120.30
3	10-C	109	TYR	CD1-CE1-CZ	-5.50	114.85	119.80
3	1-D	59	ARG	NH1-CZ-NH2	-5.50	113.35	119.40
3	10-C	341	ARG	CD-NE-CZ	5.50	131.30	123.60
2	7-B	634	ILE	CA-CB-CG2	5.50	121.89	110.90
3	10-D	93	TRP	CG-CD2-CE3	-5.50	128.95	133.90
2	1-B	561	ASP	CB-CG-OD2	5.50	123.25	118.30
2	4-B	591	TRP	CA-CB-CG	5.50	124.14	113.70
1	7-A	381	PHE	CD1-CG-CD2	-5.50	111.16	118.30
1	3-A	281	THR	N-CA-CB	5.49	120.74	110.30
3	5-D	302	SER	N-CA-CB	5.49	118.74	110.50
3	8-C	83	PHE	CB-CG-CD1	5.49	124.65	120.80
1	10-A	763	LYS	N-CA-CB	5.49	120.49	110.60
3	10-D	365	LEU	CB-CG-CD2	5.49	120.34	111.00
3	2-C	311	ASN	N-CA-C	-5.49	96.17	111.00
3	4-D	199	ASP	O-C-N	-5.49	113.91	122.70
3	6-D	217	PHE	CB-CG-CD1	5.49	124.64	120.80
3	9-D	93	TRP	CH2-CZ2-CE2	5.49	122.89	117.40
3	3-C	55	ARG	NH1-CZ-NH2	5.49	125.44	119.40
1	7-A	160	ARG	NE-CZ-NH2	-5.49	117.56	120.30
3	8-D	41	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	6-A	451	ARG	NE-CZ-NH1	-5.49	117.56	120.30
2	9-B	816	TYR	CG-CD1-CE1	-5.49	116.91	121.30
1	3-A	128	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	3-A	296	TYR	CD1-CE1-CZ	5.49	124.74	119.80
3	4-D	312	ASN	N-CA-CB	5.49	120.47	110.60
2	5-B	651	TYR	CB-CG-CD1	5.49	124.29	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	8-D	167	LEU	CB-CG-CD1	5.49	120.32	111.00
3	9-D	416	MET	CG-SD-CE	5.49	108.98	100.20
1	1-A	429	TYR	CD1-CE1-CZ	5.48	124.73	119.80
3	1-C	160	ASP	CB-CG-OD1	-5.48	113.37	118.30
3	3-D	382	THR	N-CA-CB	5.48	120.72	110.30
3	5-D	193	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	5-A	184	LYS	CA-CB-CG	5.48	125.45	113.40
2	2-B	628	ILE	CA-CB-CG1	5.48	121.40	111.00
1	3-A	64	LEU	CB-CG-CD2	-5.48	101.69	111.00
1	4-A	670	VAL	CA-CB-CG1	-5.48	102.69	110.90
1	5-A	126	TRP	CE3-CZ3-CH2	-5.48	115.18	121.20
2	10-B	816	TYR	CG-CD2-CE2	5.48	125.68	121.30
1	6-A	563	ASP	CB-CG-OD2	-5.47	113.37	118.30
3	8-D	247	TYR	CB-CA-C	-5.47	99.45	110.40
3	10-C	373	SER	C-N-CA	-5.47	110.80	122.30
1	5-A	454	ASN	CB-CG-OD1	-5.47	110.66	121.60
3	5-D	162	TYR	CZ-CE2-CD2	-5.47	114.88	119.80
3	7-C	315	TYR	CG-CD2-CE2	5.47	125.68	121.30
1	4-A	576	ARG	NE-CZ-NH1	5.47	123.03	120.30
2	5-B	288	TYR	CG-CD1-CE1	5.47	125.68	121.30
3	7-C	180	VAL	CG1-CB-CG2	-5.47	102.15	110.90
2	1-B	565	TYR	CG-CD1-CE1	-5.47	116.93	121.30
3	6-C	293	ASP	CB-CG-OD2	-5.47	113.38	118.30
3	6-D	181	VAL	CA-CB-CG1	-5.47	102.70	110.90
2	7-B	544	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	8-A	111	ARG	NE-CZ-NH2	5.47	123.03	120.30
2	8-B	546	LEU	N-CA-CB	5.47	121.33	110.40
1	10-A	587	ARG	NE-CZ-NH2	5.47	123.03	120.30
3	10-C	170	TYR	CB-CG-CD2	-5.47	117.72	121.00
3	7-C	298	LEU	CB-CG-CD1	5.46	120.29	111.00
3	4-C	413	PHE	CB-CA-C	-5.46	99.47	110.40
3	3-D	244	PHE	CB-CG-CD2	5.46	124.62	120.80
1	6-A	624	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	6-B	225	PHE	N-CA-CB	5.46	120.43	110.60
2	6-B	225	PHE	CB-CA-C	5.46	121.32	110.40
3	3-D	249	TYR	CG-CD1-CE1	-5.46	116.93	121.30
1	6-A	706	PHE	CB-CG-CD1	-5.46	116.98	120.80
1	8-A	126	TRP	CB-CG-CD1	5.46	134.09	127.00
3	9-C	279	TYR	N-CA-CB	5.46	120.42	110.60
3	9-C	379	ASN	N-CA-C	-5.46	96.27	111.00
2	2-B	195	THR	CA-CB-CG2	-5.46	104.76	112.40
3	4-D	276	THR	CA-CB-CG2	-5.46	104.76	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6-D	48	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	3-A	112	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	3-A	409	PHE	CB-CG-CD1	5.45	124.62	120.80
3	10-C	187	THR	CA-CB-CG2	-5.45	104.77	112.40
3	6-D	109	TYR	CB-CG-CD1	-5.45	117.73	121.00
1	9-A	381	PHE	CG-CD1-CE1	-5.45	114.80	120.80
2	9-B	574	VAL	CA-CB-CG1	-5.45	102.72	110.90
1	10-A	700	PHE	CG-CD2-CE2	-5.45	114.80	120.80
3	1-C	191	LEU	CB-CG-CD1	5.45	120.26	111.00
3	2-C	343	LYS	N-CA-CB	5.45	120.41	110.60
1	6-A	599	LEU	CB-CG-CD2	-5.45	101.74	111.00
3	6-C	384	VAL	CG1-CB-CG2	5.45	119.62	110.90
2	7-B	328	ARG	NE-CZ-NH1	5.45	123.03	120.30
2	7-B	589	PHE	CZ-CE2-CD2	5.45	126.64	120.10
3	10-D	54	PHE	CG-CD1-CE1	-5.45	114.81	120.80
3	1-C	168	THR	N-CA-C	-5.45	96.29	111.00
1	3-A	124	GLU	C-N-CA	5.45	135.31	121.70
3	3-C	162	TYR	CB-CG-CD1	-5.45	117.73	121.00
3	3-D	285	ALA	N-CA-CB	5.45	117.72	110.10
2	4-B	349	TRP	CG-CD2-CE3	-5.45	129.00	133.90
2	4-B	741	PHE	CB-CG-CD2	-5.45	116.99	120.80
3	8-D	341	ARG	NE-CZ-NH2	-5.45	117.58	120.30
3	1-D	69	MET	CG-SD-CE	-5.44	91.49	100.20
2	5-B	303	HIS	N-CA-CB	5.44	120.40	110.60
3	5-C	279	TYR	CA-CB-CG	5.44	123.74	113.40
1	9-A	299	PHE	CG-CD1-CE1	-5.44	114.81	120.80
1	9-A	656	VAL	CG1-CB-CG2	5.44	119.61	110.90
1	2-A	261	ASP	CB-CG-OD1	5.44	123.20	118.30
3	6-C	182	VAL	CA-CB-CG1	-5.44	102.74	110.90
2	8-B	644	PHE	CB-CG-CD1	5.44	124.61	120.80
3	10-C	63	THR	CA-CB-CG2	-5.44	104.78	112.40
3	1-D	362	TYR	CB-CG-CD1	5.44	124.27	121.00
3	2-C	197	ASP	CB-CG-OD2	5.44	123.20	118.30
1	5-A	393	TYR	CB-CG-CD2	-5.44	117.74	121.00
3	6-D	427	ARG	NE-CZ-NH2	-5.44	117.58	120.30
2	7-B	464	LEU	CB-CG-CD2	5.44	120.25	111.00
1	8-A	92	PHE	CB-CG-CD2	-5.44	116.99	120.80
3	8-C	344	PHE	CZ-CE2-CD2	-5.44	113.57	120.10
1	10-A	626	VAL	CG1-CB-CG2	-5.44	102.20	110.90
2	10-B	482	LEU	CB-CG-CD1	5.44	120.25	111.00
2	1-B	435	SER	N-CA-CB	5.44	118.66	110.50
3	2-C	143	ALA	CB-CA-C	-5.44	101.94	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-C	294	VAL	CA-CB-CG1	-5.44	102.74	110.90
3	9-C	243	ARG	O-C-N	-5.44	114.00	122.70
3	9-D	194	LEU	CB-CA-C	-5.44	99.87	110.20
3	10-D	411	ASP	CB-CG-OD2	5.44	123.19	118.30
2	2-B	200	PHE	CB-CG-CD1	-5.44	116.99	120.80
2	2-B	384	GLU	CA-CB-CG	5.44	125.36	113.40
3	5-C	67	ILE	C-N-CA	5.44	135.29	121.70
3	9-D	378	SER	N-CA-CB	5.43	118.65	110.50
1	2-A	794	TYR	CB-CG-CD1	5.43	124.26	121.00
2	4-B	587	PHE	CB-CG-CD1	5.43	124.60	120.80
2	6-B	274	SER	C-N-CA	5.43	133.71	122.30
3	9-C	90	ARG	NE-CZ-NH2	-5.43	117.58	120.30
2	1-B	206	GLN	O-C-N	5.43	131.39	122.70
3	3-C	329	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	5-A	697	LEU	CB-CA-C	-5.43	99.88	110.20
3	5-C	352	MET	CG-SD-CE	-5.43	91.51	100.20
1	7-A	588	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	9-A	62	ASP	CB-CG-OD1	-5.43	113.41	118.30
1	4-A	261	ASP	N-CA-CB	5.43	120.37	110.60
3	4-C	62	PHE	N-CA-CB	5.43	120.37	110.60
2	7-B	571	VAL	CA-CB-CG1	-5.43	102.76	110.90
2	9-B	293	ARG	NE-CZ-NH2	-5.43	117.58	120.30
3	10-D	21	LEU	CB-CG-CD2	5.43	120.23	111.00
2	2-B	362	PHE	CB-CG-CD2	-5.43	117.00	120.80
2	7-B	723	GLU	OE1-CD-OE2	5.43	129.81	123.30
3	8-D	434	MET	CA-CB-CG	5.43	122.53	113.30
3	2-D	246	SER	N-CA-CB	5.43	118.64	110.50
1	6-A	302	TYR	CB-CG-CD1	-5.43	117.75	121.00
3	9-C	192	ARG	NE-CZ-NH1	5.43	123.01	120.30
2	1-B	728	HIS	CA-CB-CG	5.42	122.82	113.60
1	2-A	612	TRP	CB-CG-CD1	5.42	134.05	127.00
3	4-D	443	ASP	CB-CG-OD1	-5.42	113.42	118.30
3	5-D	335	MET	N-CA-CB	-5.42	100.84	110.60
2	4-B	483	MET	CG-SD-CE	-5.42	91.52	100.20
3	3-C	136	PHE	CA-CB-CG	-5.42	100.89	113.90
1	4-A	56	GLU	OE1-CD-OE2	5.42	129.81	123.30
3	9-C	386	VAL	CA-CB-CG2	5.42	119.03	110.90
1	5-A	198	ARG	NE-CZ-NH2	-5.42	117.59	120.30
3	5-D	211	ASN	C-N-CA	5.42	135.25	121.70
2	8-B	362	PHE	CB-CG-CD2	-5.42	117.01	120.80
2	6-B	587	PHE	CD1-CG-CD2	-5.42	111.26	118.30
3	9-C	87	PHE	CG-CD2-CE2	-5.42	114.84	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-C	173	PHE	CB-CG-CD2	5.42	124.59	120.80
2	4-B	514	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	5-A	267	PHE	CB-CG-CD2	-5.42	117.01	120.80
2	5-B	534	ASN	N-CA-C	-5.42	96.37	111.00
3	6-C	83	PHE	CG-CD1-CE1	-5.42	114.84	120.80
3	8-C	319	TYR	CG-CD1-CE1	-5.42	116.97	121.30
1	2-A	398	TYR	CB-CG-CD2	-5.42	117.75	121.00
2	6-B	439	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	10-A	336	ASP	N-CA-CB	5.42	120.35	110.60
3	10-C	162	TYR	CG-CD2-CE2	-5.41	116.97	121.30
3	6-C	199	ASP	CB-CG-OD1	-5.41	113.43	118.30
3	2-D	279	TYR	CD1-CG-CD2	-5.41	111.95	117.90
1	7-A	413	TYR	CZ-CE2-CD2	5.41	124.67	119.80
3	10-D	293	ASP	CB-CG-OD2	5.41	123.17	118.30
3	8-C	41	ASP	CB-CG-OD1	5.41	123.17	118.30
3	2-D	319	TYR	CB-CG-CD1	5.41	124.24	121.00
3	7-D	58	SER	N-CA-CB	5.41	118.61	110.50
2	8-B	652	TYR	CB-CG-CD2	-5.41	117.76	121.00
1	10-A	148	ASP	CB-CG-OD1	5.41	123.17	118.30
1	2-A	204	ARG	NH1-CZ-NH2	5.40	125.34	119.40
1	8-A	304	ASP	CB-CG-OD1	5.40	123.16	118.30
2	8-B	343	TYR	CZ-CE2-CD2	5.40	124.66	119.80
1	1-A	782	PHE	O-C-N	5.40	131.34	122.70
2	6-B	819	PHE	CB-CG-CD1	5.40	124.58	120.80
3	7-D	218	ARG	NE-CZ-NH2	-5.40	117.60	120.30
2	8-B	236	TYR	CB-CA-C	-5.40	99.60	110.40
3	1-D	445	TYR	CB-CG-CD2	5.40	124.24	121.00
1	2-A	489	GLU	O-C-N	5.40	131.34	122.70
3	6-D	217	PHE	CB-CG-CD2	-5.40	117.02	120.80
3	9-C	279	TYR	CB-CG-CD2	5.40	124.24	121.00
1	7-A	778	CYS	CB-CA-C	-5.40	99.60	110.40
3	10-C	87	PHE	CB-CG-CD1	5.40	124.58	120.80
1	1-A	663	TYR	CG-CD2-CE2	5.40	125.62	121.30
1	4-A	698	GLN	CB-CA-C	-5.40	99.61	110.40
3	4-D	224	LEU	O-C-N	-5.40	114.06	122.70
1	7-A	63	LEU	O-C-N	-5.40	114.06	122.70
3	7-C	347	TRP	CB-CG-CD2	-5.40	119.58	126.60
3	7-D	136	PHE	CB-CG-CD2	-5.40	117.02	120.80
3	10-C	395	ASP	CB-CG-OD1	5.40	123.16	118.30
3	1-D	217	PHE	CB-CG-CD2	-5.40	117.02	120.80
3	3-C	176	ARG	NE-CZ-NH1	5.40	123.00	120.30
3	6-C	49	ASP	CB-CG-OD2	-5.40	113.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-A	77	TYR	CG-CD2-CE2	-5.39	116.98	121.30
2	8-B	719	LEU	CB-CG-CD1	5.39	120.17	111.00
1	10-A	92	PHE	CB-CG-CD2	-5.39	117.02	120.80
2	10-B	542	ASP	CB-CG-OD2	-5.39	113.44	118.30
2	1-B	319	PHE	CB-CG-CD1	5.39	124.58	120.80
1	2-A	169	SER	C-N-CA	5.39	135.18	121.70
2	7-B	582	GLU	OE1-CD-OE2	-5.39	116.83	123.30
3	7-C	173	PHE	CB-CG-CD1	-5.39	117.03	120.80
2	6-B	242	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	7-A	297	GLN	N-CA-CB	5.39	120.30	110.60
1	7-A	365	THR	N-CA-CB	5.39	120.54	110.30
1	9-A	791	PHE	CB-CG-CD1	-5.39	117.03	120.80
2	2-B	532	PRO	N-CA-C	5.39	126.11	112.10
3	4-C	20	PHE	CB-CG-CD2	-5.39	117.03	120.80
3	4-C	57	ASN	N-CA-CB	5.39	120.30	110.60
3	6-D	256	TYR	CD1-CE1-CZ	5.39	124.65	119.80
1	7-A	486	PHE	CZ-CE2-CD2	-5.39	113.63	120.10
2	9-B	288	TYR	CB-CG-CD1	5.39	124.23	121.00
3	2-C	168	THR	N-CA-CB	5.39	120.54	110.30
3	8-D	256	TYR	CA-CB-CG	5.39	123.64	113.40
2	2-B	670	ARG	CB-CA-C	-5.39	99.62	110.40
2	4-B	816	TYR	CD1-CG-CD2	-5.39	111.97	117.90
3	4-D	236	SER	N-CA-CB	5.39	118.58	110.50
3	6-C	375	MET	CB-CA-C	-5.39	99.63	110.40
3	9-D	377	LEU	CB-CA-C	-5.39	99.97	110.20
2	10-B	651	TYR	CB-CG-CD1	5.39	124.23	121.00
3	5-D	273	THR	CA-CB-CG2	-5.38	104.86	112.40
1	6-A	136	GLN	CG-CD-OE1	-5.38	110.83	121.60
3	9-C	42	SER	N-CA-CB	5.38	118.58	110.50
1	10-A	400	ARG	NE-CZ-NH2	5.38	122.99	120.30
2	3-B	422	THR	CA-CB-CG2	-5.38	104.86	112.40
3	6-C	44	THR	CA-CB-CG2	-5.38	104.86	112.40
3	6-D	103	ASN	N-CA-CB	5.38	120.29	110.60
2	9-B	216	PHE	CG-CD1-CE1	5.38	126.72	120.80
3	4-C	65	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	7-A	630	ARG	NE-CZ-NH1	5.38	122.99	120.30
3	7-D	252	MET	CG-SD-CE	-5.38	91.59	100.20
3	1-D	90	ARG	CA-CB-CG	5.38	125.23	113.40
3	2-C	59	ARG	NE-CZ-NH2	5.38	122.99	120.30
3	2-D	106	ALA	N-CA-CB	5.38	117.63	110.10
2	3-B	203	ASP	C-N-CA	5.38	135.14	121.70
1	4-A	58	LEU	CB-CG-CD2	5.38	120.14	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6-B	415	TYR	CB-CG-CD1	5.38	124.23	121.00
1	10-A	258	ASN	CB-CA-C	5.38	121.16	110.40
1	10-A	285	GLU	CB-CG-CD	-5.38	99.68	114.20
2	10-B	776	TYR	CD1-CE1-CZ	-5.38	114.96	119.80
3	3-D	392	ASN	N-CA-CB	5.38	120.28	110.60
1	7-A	648	ASN	N-CA-CB	5.38	120.28	110.60
2	7-B	242	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	8-A	596	SER	CB-CA-C	-5.38	99.89	110.10
3	3-C	78	ASP	CB-CG-OD1	5.38	123.14	118.30
2	9-B	247	SER	N-CA-CB	5.38	118.56	110.50
2	9-B	670	ARG	NH1-CZ-NH2	5.38	125.31	119.40
3	1-C	347	TRP	CD1-CG-CD2	-5.37	102.00	106.30
3	5-D	271	SER	N-CA-CB	5.37	118.56	110.50
3	6-C	279	TYR	CB-CG-CD1	-5.37	117.78	121.00
3	9-D	347	TRP	CB-CG-CD2	-5.37	119.61	126.60
1	10-A	398	TYR	CG-CD2-CE2	5.37	125.60	121.30
3	1-C	95	ALA	N-CA-CB	5.37	117.62	110.10
2	2-B	545	VAL	CA-CB-CG1	-5.37	102.84	110.90
3	7-D	403	PHE	CG-CD1-CE1	-5.37	114.89	120.80
1	10-A	558	TYR	CB-CG-CD1	5.37	124.22	121.00
3	10-C	124	ASP	CB-CG-OD2	-5.37	113.47	118.30
3	8-C	413	PHE	CB-CG-CD1	5.37	124.56	120.80
2	10-B	363	PHE	CB-CG-CD2	-5.37	117.04	120.80
2	1-B	200	PHE	CB-CG-CD2	-5.37	117.04	120.80
3	4-D	170	TYR	CB-CG-CD1	-5.37	117.78	121.00
2	5-B	813	VAL	CG1-CB-CG2	-5.37	102.31	110.90
3	8-D	185	TYR	CD1-CE1-CZ	-5.37	114.97	119.80
1	8-A	324	TYR	CA-CB-CG	-5.37	103.20	113.40
1	4-A	714	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	5-A	624	ARG	CA-CB-CG	5.37	125.20	113.40
2	5-B	560	LEU	CB-CG-CD1	5.37	120.12	111.00
1	7-A	304	ASP	CB-CG-OD2	5.37	123.13	118.30
2	3-B	263	ASN	N-CA-CB	5.36	120.25	110.60
1	5-A	602	THR	CA-CB-CG2	-5.36	104.89	112.40
2	5-B	741	PHE	CB-CG-CD1	5.36	124.56	120.80
2	2-B	357	ALA	N-CA-CB	5.36	117.61	110.10
3	1-D	217	PHE	CB-CG-CD1	5.36	124.55	120.80
2	3-B	304	LEU	CB-CA-C	-5.36	100.02	110.20
1	5-A	364	PRO	N-CA-CB	5.36	109.73	103.30
2	5-B	485	LYS	N-CA-C	-5.36	96.52	111.00
1	9-A	422	LEU	O-C-N	-5.36	114.12	122.70
2	9-B	542	ASP	N-CA-CB	5.36	120.25	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	10-B	492	LEU	CB-CG-CD1	5.36	120.11	111.00
2	1-B	671	THR	CA-CB-CG2	-5.36	104.90	112.40
1	5-A	785	GLU	N-CA-CB	5.36	120.25	110.60
1	10-A	104	THR	CA-CB-CG2	-5.36	104.90	112.40
3	1-C	275	PHE	N-CA-CB	5.36	120.24	110.60
3	1-D	23	SER	N-CA-CB	5.36	118.54	110.50
2	5-B	538	ILE	O-C-N	5.36	131.27	122.70
2	9-B	212	LYS	N-CA-CB	5.36	120.24	110.60
3	10-C	331	ILE	CA-CB-CG1	5.36	121.18	111.00
1	7-A	184	LYS	CB-CA-C	-5.36	99.69	110.40
2	7-B	532	PRO	N-CD-CG	5.36	111.23	103.20
3	5-C	292	TYR	CB-CA-C	5.35	121.11	110.40
1	8-A	266	MET	CG-SD-CE	-5.35	91.63	100.20
3	10-D	176	ARG	NH1-CZ-NH2	-5.35	113.51	119.40
3	1-D	249	TYR	CA-CB-CG	-5.35	103.23	113.40
1	2-A	203	ARG	NE-CZ-NH2	-5.35	117.62	120.30
3	2-D	110	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	3-A	200	ILE	CA-CB-CG1	5.35	121.17	111.00
2	3-B	389	ARG	NH1-CZ-NH2	5.35	125.29	119.40
3	3-C	358	ARG	NH1-CZ-NH2	-5.35	113.51	119.40
1	5-A	657	TYR	CB-CG-CD1	-5.35	117.79	121.00
1	6-A	162	PHE	N-CA-CB	5.35	120.24	110.60
1	6-A	297	GLN	N-CA-CB	5.35	120.23	110.60
3	6-D	343	LYS	N-CA-CB	5.35	120.23	110.60
3	8-C	381	SER	N-CA-CB	5.35	118.53	110.50
3	8-D	93	TRP	C-N-CA	5.35	135.08	121.70
3	1-C	438	VAL	CA-CB-CG1	5.35	118.93	110.90
1	3-A	80	ASP	CB-CG-OD1	5.35	123.11	118.30
2	3-B	609	ASP	CB-CG-OD1	5.35	123.11	118.30
1	4-A	119	LEU	CB-CG-CD2	-5.35	101.91	111.00
3	4-C	399	ALA	O-C-N	5.35	131.26	122.70
3	8-C	347	TRP	CG-CD1-NE1	5.35	115.45	110.10
3	8-D	62	PHE	CB-CA-C	-5.35	99.70	110.40
1	9-A	288	THR	O-C-N	-5.35	114.14	122.70
1	1-A	571	ASN	N-CA-CB	5.35	120.22	110.60
3	4-C	293	ASP	CB-CG-OD1	-5.35	113.49	118.30
2	1-B	471	ARG	NH1-CZ-NH2	5.35	125.28	119.40
2	8-B	759	PRO	N-CA-CB	5.35	109.72	103.30
1	3-A	483	MET	CG-SD-CE	-5.34	91.65	100.20
1	3-A	664	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	3-A	707	CYS	CA-CB-SG	5.34	123.62	114.00
2	5-B	363	PHE	CB-CG-CD2	5.34	124.54	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7-A	418	VAL	CB-CA-C	-5.34	101.25	111.40
1	5-A	257	GLU	C-N-CA	5.34	135.06	121.70
3	2-C	142	VAL	CA-CB-CG1	-5.34	102.89	110.90
3	3-D	185	TYR	CG-CD1-CE1	5.34	125.57	121.30
2	4-B	276	THR	CA-CB-CG2	-5.34	104.92	112.40
2	7-B	319	PHE	CB-CG-CD2	-5.34	117.06	120.80
1	8-A	562	PHE	CB-CG-CD1	5.34	124.54	120.80
1	10-A	288	THR	CA-CB-CG2	-5.34	104.92	112.40
2	3-B	598	TYR	CG-CD2-CE2	-5.34	117.03	121.30
3	3-D	38	GLN	C-N-CA	5.34	135.05	121.70
1	4-A	112	TYR	CB-CG-CD1	5.34	124.20	121.00
2	4-B	816	TYR	CB-CG-CD1	5.34	124.20	121.00
2	6-B	315	GLU	CB-CG-CD	-5.34	99.78	114.20
3	7-C	291	SER	N-CA-CB	5.34	118.51	110.50
1	8-A	340	ASP	CB-CG-OD1	5.34	123.11	118.30
3	9-D	276	THR	N-CA-C	-5.34	96.58	111.00
3	1-D	220	PRO	N-CA-CB	5.34	109.70	103.30
3	6-D	440	ALA	CB-CA-C	-5.34	102.09	110.10
3	7-D	109	TYR	CB-CG-CD1	-5.34	117.80	121.00
2	1-B	276	THR	CA-CB-CG2	-5.34	104.93	112.40
3	1-D	408	ASN	N-CA-CB	5.34	120.21	110.60
2	2-B	576	ARG	N-CA-CB	5.34	120.21	110.60
3	2-C	329	ARG	NH1-CZ-NH2	5.34	125.27	119.40
1	4-A	558	TYR	CD1-CE1-CZ	5.34	124.60	119.80
2	5-B	799	ASN	C-N-CA	5.34	133.50	122.30
1	10-A	400	ARG	NE-CZ-NH1	5.34	122.97	120.30
3	5-C	29	HIS	CA-CB-CG	5.33	122.67	113.60
2	10-B	770	TYR	CB-CG-CD2	5.33	124.20	121.00
3	8-D	407	TYR	CB-CG-CD2	5.33	124.20	121.00
3	10-C	235	ILE	O-C-N	-5.33	114.17	122.70
1	3-A	591	VAL	CA-CB-CG1	5.33	118.89	110.90
3	3-C	329	ARG	CD-NE-CZ	-5.33	116.14	123.60
3	2-C	1	MET	CG-SD-CE	-5.33	91.67	100.20
1	3-A	330	VAL	CA-CB-CG2	-5.33	102.91	110.90
3	6-C	230	LEU	CB-CG-CD2	-5.33	101.94	111.00
1	4-A	146	LEU	CB-CG-CD2	5.33	120.06	111.00
2	9-B	225	PHE	CZ-CE2-CD2	5.33	126.49	120.10
2	1-B	591	TRP	CE2-CD2-CE3	5.33	125.09	118.70
3	2-C	344	PHE	N-CA-CB	5.33	120.19	110.60
2	4-B	611	ILE	N-CA-C	-5.33	96.62	111.00
2	7-B	188	VAL	N-CA-CB	5.33	123.22	111.50
3	7-D	223	ASP	N-CA-C	5.33	125.38	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	10-B	312	PHE	CB-CG-CD1	5.33	124.53	120.80
3	10-D	244	PHE	N-CA-CB	5.33	120.18	110.60
1	2-A	121	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	3-A	187	GLU	N-CA-CB	5.32	120.18	110.60
1	5-A	374	THR	N-CA-CB	5.32	120.42	110.30
2	8-B	776	TYR	CA-CB-CG	5.32	123.52	113.40
1	9-A	333	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	10-A	413	TYR	CD1-CE1-CZ	-5.32	115.01	119.80
3	3-D	99	ALA	N-CA-CB	5.32	117.55	110.10
3	1-D	424	ALA	N-CA-CB	5.32	117.55	110.10
3	3-D	218	ARG	NE-CZ-NH2	-5.32	117.64	120.30
3	10-D	430	VAL	N-CA-CB	5.32	123.21	111.50
3	2-D	105	TRP	CD1-NE1-CE2	-5.32	104.21	109.00
3	2-C	272	PHE	CG-CD2-CE2	-5.32	114.95	120.80
3	3-C	256	TYR	CZ-CE2-CD2	-5.32	115.01	119.80
3	5-C	407	TYR	CE1-CZ-CE2	5.32	128.31	119.80
1	8-A	688	CYS	CA-CB-SG	-5.32	104.43	114.00
1	10-A	130	SER	CB-CA-C	5.32	120.20	110.10
2	10-B	186	LYS	CA-CB-CG	5.32	125.10	113.40
3	10-D	278	ASP	CB-CG-OD1	5.32	123.08	118.30
1	1-A	281	THR	O-C-N	-5.32	114.19	122.70
3	5-C	275	PHE	CB-CG-CD2	-5.32	117.08	120.80
2	6-B	585	ARG	NE-CZ-NH1	-5.32	117.64	120.30
3	7-C	358	ARG	CD-NE-CZ	-5.32	116.16	123.60
1	9-A	777	LYS	N-CA-CB	5.32	120.17	110.60
1	10-A	179	GLU	N-CA-CB	5.32	120.17	110.60
1	4-A	138	PHE	CG-CD2-CE2	-5.31	114.95	120.80
2	4-B	472	ASP	CB-CG-OD2	5.31	123.08	118.30
3	7-C	49	ASP	CB-CG-OD2	-5.31	113.52	118.30
3	7-D	173	PHE	CB-CG-CD1	5.31	124.52	120.80
3	1-D	329	ARG	NE-CZ-NH1	-5.31	117.64	120.30
3	4-D	275	PHE	CG-CD2-CE2	-5.31	114.96	120.80
2	6-B	284	TYR	CZ-CE2-CD2	-5.31	115.02	119.80
1	7-A	284	TYR	CG-CD2-CE2	-5.31	117.05	121.30
3	7-D	62	PHE	CB-CG-CD1	5.31	124.52	120.80
2	9-B	345	TYR	CZ-CE2-CD2	-5.31	115.02	119.80
3	1-D	205	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	8-A	400	ARG	CB-CA-C	-5.31	99.78	110.40
1	6-A	783	THR	CA-CB-CG2	-5.31	104.97	112.40
2	6-B	519	ALA	N-CA-CB	5.31	117.53	110.10
3	6-C	266	HIS	CB-CA-C	-5.31	99.78	110.40
3	10-C	33	THR	CA-CB-CG2	-5.31	104.97	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	10-D	43	SER	N-CA-C	-5.31	96.66	111.00
1	3-A	426	PHE	CB-CG-CD1	-5.31	117.08	120.80
1	4-A	274	ASN	N-CA-CB	5.31	120.15	110.60
3	4-D	272	PHE	CB-CG-CD2	-5.31	117.08	120.80
3	7-D	421	ASP	CB-CG-OD2	5.31	123.08	118.30
1	8-A	429	TYR	CG-CD1-CE1	5.31	125.55	121.30
3	8-D	247	TYR	CG-CD2-CE2	-5.31	117.05	121.30
3	10-D	365	LEU	CB-CA-C	-5.31	100.12	110.20
2	1-B	637	LEU	CB-CG-CD2	5.31	120.02	111.00
3	3-D	376	MET	CG-SD-CE	-5.31	91.71	100.20
3	9-C	114	ARG	O-C-N	5.31	131.19	122.70
2	1-B	451	ASP	CB-CG-OD1	5.30	123.07	118.30
2	1-B	502	THR	CA-CB-CG2	-5.30	104.97	112.40
1	2-A	128	ASP	N-CA-CB	5.30	120.15	110.60
3	9-D	68	MET	CG-SD-CE	-5.30	91.71	100.20
2	9-B	288	TYR	CB-CG-CD2	-5.30	117.82	121.00
2	10-B	819	PHE	CB-CG-CD1	5.30	124.51	120.80
3	1-C	315	TYR	CG-CD2-CE2	-5.30	117.06	121.30
3	4-D	84	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	5-B	453	TYR	CZ-CE2-CD2	-5.30	115.03	119.80
2	7-B	488	PHE	CB-CG-CD1	5.30	124.51	120.80
2	8-B	409	TYR	CG-CD1-CE1	-5.30	117.06	121.30
3	8-C	117	ASP	C-N-CA	5.30	134.95	121.70
3	10-D	407	TYR	CG-CD2-CE2	-5.30	117.06	121.30
3	1-C	239	THR	O-C-N	-5.30	114.22	122.70
3	1-C	407	TYR	CB-CG-CD2	-5.30	117.82	121.00
3	4-D	278	ASP	CB-CG-OD1	5.30	123.07	118.30
3	5-C	407	TYR	CD1-CG-CD2	5.30	123.73	117.90
2	6-B	483	MET	CA-CB-CG	5.30	122.31	113.30
3	6-C	355	ASN	N-CA-CB	5.30	120.14	110.60
2	7-B	775	VAL	CA-CB-CG2	-5.30	102.95	110.90
3	7-C	161	ARG	NE-CZ-NH1	5.30	122.95	120.30
3	10-C	203	VAL	CA-CB-CG2	-5.30	102.95	110.90
3	2-D	244	PHE	CB-CG-CD1	5.30	124.51	120.80
3	8-D	176	ARG	NE-CZ-NH2	-5.30	117.65	120.30
3	5-C	172	VAL	N-CA-C	-5.30	96.70	111.00
3	6-C	211	ASN	N-CA-CB	5.30	120.13	110.60
3	6-D	279	TYR	N-CA-CB	5.30	120.13	110.60
2	8-B	508	PRO	CA-N-CD	-5.30	104.08	111.50
3	8-C	95	ALA	N-CA-CB	5.30	117.52	110.10
2	8-B	236	TYR	CB-CG-CD1	-5.29	117.82	121.00
3	3-C	387	PHE	CG-CD2-CE2	-5.29	114.98	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4-B	202	PHE	CD1-CE1-CZ	5.29	126.45	120.10
2	4-B	555	TRP	CB-CG-CD2	-5.29	119.72	126.60
1	5-A	485	GLN	N-CA-CB	5.29	120.13	110.60
1	10-A	149	VAL	CA-CB-CG2	5.29	118.84	110.90
2	2-B	649	GLU	CA-CB-CG	5.29	125.04	113.40
2	2-B	822	ARG	NE-CZ-NH1	5.29	122.95	120.30
2	4-B	202	PHE	CB-CG-CD1	5.29	124.50	120.80
1	5-A	800	ASP	CB-CG-OD2	-5.29	113.54	118.30
3	8-C	407	TYR	CG-CD1-CE1	-5.29	117.07	121.30
2	10-B	565	TYR	CB-CG-CD2	5.29	124.17	121.00
3	2-C	318	VAL	CB-CA-C	-5.29	101.35	111.40
2	3-B	557	VAL	CG1-CB-CG2	5.29	119.36	110.90
3	3-C	161	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	6-A	303	ASP	N-CA-CB	5.29	120.12	110.60
2	2-B	386	ASN	CA-CB-CG	-5.29	101.77	113.40
3	2-C	316	PHE	N-CA-C	-5.29	96.72	111.00
3	6-D	223	ASP	N-CA-CB	5.29	120.12	110.60
3	3-D	282	ASP	N-CA-CB	5.29	120.11	110.60
1	6-A	597	ARG	O-C-N	-5.29	114.24	122.70
3	8-D	308	THR	CA-CB-CG2	-5.29	105.00	112.40
1	9-A	692	LEU	CB-CA-C	-5.29	100.16	110.20
3	9-D	384	VAL	O-C-N	-5.29	114.24	122.70
1	10-A	286	TRP	CA-CB-CG	5.29	123.74	113.70
1	4-A	200	ILE	N-CA-CB	5.28	122.95	110.80
3	8-D	319	TYR	CA-CB-CG	5.28	123.44	113.40
3	9-C	156	GLU	CG-CD-OE1	-5.28	107.73	118.30
1	10-A	791	PHE	CG-CD2-CE2	-5.28	114.99	120.80
3	4-D	138	LEU	CB-CG-CD2	-5.28	102.02	111.00
1	1-A	120	THR	CA-CB-CG2	-5.28	105.01	112.40
3	1-C	431	GLN	CB-CA-C	-5.28	99.84	110.40
2	2-B	652	TYR	CG-CD2-CE2	5.28	125.52	121.30
3	2-C	138	LEU	CB-CG-CD1	5.28	119.98	111.00
2	9-B	349	TRP	CA-CB-CG	5.28	123.73	113.70
2	1-B	231	TYR	CB-CG-CD1	-5.28	117.83	121.00
2	4-B	523	SER	CB-CA-C	-5.28	100.07	110.10
1	5-A	286	TRP	CH2-CZ2-CE2	5.28	122.68	117.40
1	7-A	797	SER	N-CA-CB	5.28	118.42	110.50
2	1-B	400	TYR	CD1-CG-CD2	5.28	123.70	117.90
1	3-A	62	ASP	CB-CG-OD2	-5.28	113.55	118.30
3	6-D	30	ALA	N-CA-CB	5.28	117.49	110.10
3	9-D	194	LEU	CB-CG-CD1	5.28	119.97	111.00
1	10-A	346	LYS	N-CA-CB	5.28	120.10	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2-B	349	TRP	CE3-CZ3-CH2	5.28	127.00	121.20
3	2-D	272	PHE	N-CA-C	-5.28	96.76	111.00
3	4-C	109	TYR	CD1-CE1-CZ	5.28	124.55	119.80
3	7-D	362	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	8-A	162	PHE	N-CA-CB	5.28	120.09	110.60
2	6-B	776	TYR	CZ-CE2-CD2	5.27	124.55	119.80
1	8-A	180	THR	N-CA-CB	5.27	120.32	110.30
3	8-D	243	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	2-A	70	LEU	N-CA-CB	5.27	120.94	110.40
1	2-A	555	SER	O-C-N	-5.27	114.26	122.70
1	4-A	126	TRP	CE2-CD2-CE3	5.27	125.03	118.70
3	4-C	347	TRP	CB-CG-CD1	5.27	133.85	127.00
2	7-B	488	PHE	CG-CD2-CE2	5.27	126.60	120.80
3	7-C	133	PHE	CG-CD1-CE1	-5.27	115.00	120.80
3	7-C	197	ASP	OD1-CG-OD2	5.27	133.32	123.30
3	9-D	6	ILE	N-CA-C	-5.27	96.76	111.00
2	10-B	342	TYR	CD1-CE1-CZ	-5.27	115.05	119.80
3	6-C	366	GLN	CB-CA-C	-5.27	99.86	110.40
3	3-D	397	VAL	CA-CB-CG1	-5.27	103.00	110.90
1	4-A	413	TYR	CD1-CE1-CZ	5.27	124.54	119.80
2	4-B	731	PHE	CB-CG-CD1	5.27	124.49	120.80
3	5-D	32	GLY	CA-C-O	5.27	130.09	120.60
1	1-A	584	ILE	CA-CB-CG1	5.27	121.01	111.00
1	2-A	800	ASP	CB-CG-OD1	5.27	123.04	118.30
3	3-C	332	SER	CA-C-O	5.27	131.16	120.10
2	7-B	576	ARG	N-CA-C	-5.27	96.78	111.00
3	7-C	275	PHE	CB-CG-CD2	-5.27	117.11	120.80
2	6-B	729	ASN	CA-CB-CG	-5.27	101.81	113.40
3	7-D	162	TYR	CG-CD2-CE2	5.27	125.51	121.30
1	10-A	112	TYR	CG-CD2-CE2	-5.27	117.09	121.30
1	1-A	663	TYR	CB-CG-CD2	5.26	124.16	121.00
1	7-A	631	VAL	N-CA-CB	5.26	123.08	111.50
3	7-D	48	ASP	CB-CG-OD2	5.26	123.04	118.30
2	8-B	445	PHE	CB-CG-CD1	5.26	124.48	120.80
1	9-A	588	TYR	CG-CD2-CE2	-5.26	117.09	121.30
2	1-B	566	PRO	CA-C-N	5.26	131.84	117.10
3	10-C	28	GLU	OE1-CD-OE2	5.26	129.62	123.30
3	10-D	445	TYR	CG-CD2-CE2	5.26	125.51	121.30
3	1-C	353	HIS	N-CA-C	-5.26	96.79	111.00
3	2-D	224	LEU	N-CA-CB	5.26	120.92	110.40
3	2-D	278	ASP	CB-CG-OD1	-5.26	113.56	118.30
2	4-B	591	TRP	CB-CG-CD1	5.26	133.84	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-A	126	TRP	CD1-CG-CD2	-5.26	102.09	106.30
1	2-A	325	PHE	CB-CG-CD2	-5.26	117.12	120.80
1	8-A	77	TYR	CA-CB-CG	5.26	123.39	113.40
1	4-A	800	ASP	N-CA-CB	5.26	120.06	110.60
3	5-C	170	TYR	CD1-CG-CD2	5.26	123.68	117.90
1	10-A	341	LYS	N-CA-CB	5.26	120.06	110.60
3	10-C	423	PHE	CB-CG-CD1	-5.26	117.12	120.80
3	3-C	379	ASN	N-CA-CB	5.26	120.06	110.60
3	6-D	131	ASP	N-CA-CB	5.26	120.06	110.60
3	6-D	146	THR	CA-CB-CG2	-5.26	105.04	112.40
1	2-A	127	SER	N-CA-C	-5.25	96.81	111.00
3	4-D	252	MET	CG-SD-CE	-5.25	91.79	100.20
3	9-D	295	MET	CG-SD-CE	-5.25	91.79	100.20
2	2-B	558	PHE	CD1-CE1-CZ	-5.25	113.80	120.10
1	4-A	458	TYR	CB-CG-CD2	-5.25	117.85	121.00
3	4-C	59	ARG	N-CA-CB	5.25	120.06	110.60
3	7-D	302	SER	CB-CA-C	-5.25	100.12	110.10
2	9-B	187	TYR	CB-CG-CD1	-5.25	117.85	121.00
2	10-B	805	PHE	CB-CG-CD2	-5.25	117.12	120.80
3	10-C	73	PRO	N-CA-CB	5.25	109.60	103.30
3	10-D	140	HIS	N-CA-CB	5.25	120.06	110.60
1	1-A	302	TYR	CB-CG-CD2	-5.25	117.85	121.00
2	3-B	184	ILE	CB-CA-C	-5.25	101.10	111.60
2	3-B	343	TYR	CD1-CG-CD2	-5.25	112.12	117.90
2	6-B	278	VAL	CG1-CB-CG2	-5.25	102.50	110.90
3	6-D	205	ASP	CB-CG-OD1	5.25	123.03	118.30
3	7-D	434	MET	O-C-N	5.25	131.10	122.70
3	9-D	114	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	10-A	245	GLY	O-C-N	-5.25	114.30	122.70
1	6-A	296	TYR	CD1-CE1-CZ	5.25	124.53	119.80
3	6-D	398	PHE	CB-CG-CD2	5.25	124.47	120.80
1	10-A	638	HIS	CA-CB-CG	5.25	122.53	113.60
2	4-B	576	ARG	NE-CZ-NH2	-5.25	117.68	120.30
3	4-D	62	PHE	N-CA-CB	5.25	120.05	110.60
1	8-A	77	TYR	CB-CG-CD2	-5.25	117.85	121.00
3	8-D	218	ARG	CB-CG-CD	5.25	125.25	111.60
3	9-C	445	TYR	N-CA-CB	5.25	120.05	110.60
2	2-B	464	LEU	CB-CA-C	-5.25	100.23	110.20
3	7-D	298	LEU	CB-CA-C	5.25	120.17	110.20
3	3-C	136	PHE	CB-CA-C	-5.25	99.91	110.40
3	4-C	204	PHE	CB-CG-CD1	-5.25	117.13	120.80
1	6-A	608	LYS	N-CA-CB	5.25	120.04	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	336	ASP	N-CA-CB	5.24	120.04	110.60
2	1-B	545	VAL	CA-CB-CG1	-5.24	103.03	110.90
2	4-B	635	SER	N-CA-CB	5.24	118.37	110.50
2	5-B	816	TYR	CG-CD1-CE1	-5.24	117.11	121.30
2	10-B	661	PHE	CB-CG-CD2	5.24	124.47	120.80
1	3-A	381	PHE	CB-CG-CD1	5.24	124.47	120.80
2	7-B	213	ILE	N-CA-C	-5.24	96.85	111.00
2	10-B	824	TYR	N-CA-CB	5.24	120.04	110.60
1	8-A	193	TYR	CZ-CE2-CD2	-5.24	115.08	119.80
2	9-B	665	THR	CA-CB-CG2	-5.24	105.06	112.40
3	9-D	353	HIS	CA-CB-CG	-5.24	104.69	113.60
1	4-A	333	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	5-B	343	TYR	CB-CG-CD1	-5.24	117.86	121.00
3	7-D	191	LEU	CB-CG-CD2	-5.24	102.09	111.00
1	9-A	193	TYR	CG-CD1-CE1	-5.24	117.11	121.30
3	9-D	202	VAL	CA-CB-CG1	-5.24	103.04	110.90
3	1-D	53	PHE	CB-CA-C	-5.24	99.93	110.40
3	1-D	170	TYR	N-CA-C	-5.24	96.86	111.00
1	10-A	382	ALA	N-CA-CB	5.24	117.43	110.10
3	2-D	344	PHE	CD1-CG-CD2	5.24	125.11	118.30
1	4-A	368	SER	CB-CA-C	-5.24	100.15	110.10
1	6-A	284	TYR	CG-CD2-CE2	-5.24	117.11	121.30
3	6-C	256	TYR	CG-CD2-CE2	5.23	125.49	121.30
2	9-B	504	SER	N-CA-CB	5.23	118.35	110.50
2	1-B	445	PHE	CB-CG-CD2	-5.23	117.14	120.80
3	2-C	390	ALA	N-CA-CB	5.23	117.43	110.10
1	4-A	155	VAL	CA-CB-CG1	-5.23	103.05	110.90
3	4-C	325	ASN	CA-CB-CG	-5.23	101.89	113.40
3	6-C	437	TYR	N-CA-CB	5.23	120.02	110.60
1	8-A	712	SER	N-CA-CB	5.23	118.35	110.50
3	9-D	292	TYR	CB-CG-CD1	-5.23	117.86	121.00
3	10-C	252	MET	CG-SD-CE	5.23	108.57	100.20
2	2-B	356	ARG	NE-CZ-NH1	-5.23	117.69	120.30
3	3-C	365	LEU	CB-CA-C	-5.23	100.26	110.20
3	7-D	341	ARG	N-CA-CB	5.23	120.01	110.60
2	9-B	290	ASN	CA-CB-CG	-5.23	101.89	113.40
3	9-C	432	SER	CB-CA-C	-5.23	100.16	110.10
3	2-D	66	ALA	CB-CA-C	-5.23	102.26	110.10
1	3-A	126	TRP	N-CA-CB	5.23	120.01	110.60
3	6-D	443	ASP	N-CA-C	-5.23	96.88	111.00
2	7-B	578	PHE	CB-CG-CD2	-5.23	117.14	120.80
3	2-D	310	MET	O-C-N	5.23	131.06	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3-B	824	TYR	CG-CD1-CE1	-5.23	117.12	121.30
1	4-A	792	ASP	CB-CG-OD1	-5.23	113.60	118.30
2	4-B	202	PHE	CG-CD1-CE1	-5.23	115.05	120.80
1	10-A	782	PHE	CG-CD1-CE1	5.23	126.55	120.80
2	9-B	562	TYR	CZ-CE2-CD2	-5.23	115.10	119.80
3	9-C	416	MET	N-CA-CB	5.23	120.01	110.60
3	9-D	244	PHE	CB-CG-CD1	5.23	124.46	120.80
3	3-D	170	TYR	N-CA-C	-5.22	96.89	111.00
2	8-B	476	ALA	N-CA-CB	5.22	117.41	110.10
3	8-C	170	TYR	CD1-CG-CD2	5.22	123.65	117.90
2	10-B	343	TYR	N-CA-CB	5.22	120.00	110.60
1	1-A	165	VAL	CA-CB-CG2	-5.22	103.07	110.90
3	1-D	300	ASP	CB-CG-OD1	5.22	123.00	118.30
3	2-C	409	VAL	CA-CB-CG1	-5.22	103.07	110.90
3	7-C	256	TYR	CG-CD1-CE1	5.22	125.48	121.30
3	1-D	65	ARG	CG-CD-NE	-5.22	100.83	111.80
1	8-A	116	TYR	CZ-CE2-CD2	-5.22	115.10	119.80
2	9-B	363	PHE	CB-CG-CD2	-5.22	117.14	120.80
3	2-C	162	TYR	CZ-CE2-CD2	5.22	124.50	119.80
3	3-D	90	ARG	NH1-CZ-NH2	5.22	125.14	119.40
2	6-B	187	TYR	CB-CG-CD1	5.22	124.13	121.00
2	7-B	409	TYR	CB-CG-CD2	-5.22	117.87	121.00
2	10-B	583	TYR	CZ-CE2-CD2	-5.22	115.10	119.80
2	3-B	562	TYR	CD1-CG-CD2	5.22	123.64	117.90
1	8-A	121	ARG	NE-CZ-NH2	-5.22	117.69	120.30
2	1-B	324	ASP	N-CA-CB	5.21	119.98	110.60
2	3-B	278	VAL	CA-CB-CG2	-5.21	103.08	110.90
1	7-A	700	PHE	CA-CB-CG	5.21	126.41	113.90
3	9-D	267	PHE	CB-CG-CD2	5.21	124.45	120.80
2	1-B	409	TYR	CB-CG-CD1	-5.21	117.87	121.00
2	3-B	441	ILE	CA-CB-CG1	5.21	120.90	111.00
1	9-A	450	TYR	CG-CD1-CE1	5.21	125.47	121.30
1	10-A	442	ASN	N-CA-CB	5.21	119.98	110.60
2	2-B	564	LEU	CB-CG-CD2	5.21	119.86	111.00
3	10-C	114	ARG	CG-CD-NE	-5.21	100.86	111.80
1	2-A	126	TRP	CB-CA-C	-5.21	99.98	110.40
2	3-B	429	TYR	CB-CG-CD1	-5.21	117.87	121.00
3	7-D	275	PHE	CB-CG-CD1	-5.21	117.15	120.80
3	1-D	57	ASN	N-CA-CB	5.21	119.98	110.60
1	3-A	469	ARG	CG-CD-NE	-5.21	100.86	111.80
2	3-B	488	PHE	CB-CG-CD2	-5.21	117.15	120.80
3	3-D	217	PHE	CB-CG-CD1	5.21	124.44	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4-D	157	ALA	CB-CA-C	-5.21	102.29	110.10
1	5-A	203	ARG	NE-CZ-NH1	5.21	122.90	120.30
2	8-B	547	ASP	CB-CG-OD1	5.21	122.99	118.30
2	9-B	631	LEU	CB-CG-CD1	5.21	119.85	111.00
3	10-C	333	ARG	NE-CZ-NH2	-5.21	117.70	120.30
2	2-B	315	GLU	CB-CG-CD	-5.21	100.14	114.20
3	2-C	439	ALA	N-CA-CB	-5.21	102.81	110.10
3	3-C	157	ALA	CB-CA-C	-5.21	102.29	110.10
2	5-B	571	VAL	CA-CB-CG1	-5.21	103.09	110.90
1	8-A	478	MET	CG-SD-CE	-5.21	91.87	100.20
3	9-D	296	LEU	CB-CA-C	-5.21	100.31	110.20
3	2-D	115	ASN	CB-CA-C	-5.21	99.99	110.40
1	3-A	370	SER	N-CA-CB	5.20	118.31	110.50
2	3-B	310	ASP	CB-CA-C	-5.20	99.99	110.40
1	7-A	150	TYR	CZ-CE2-CD2	5.20	124.48	119.80
1	8-A	474	PRO	N-CD-CG	5.20	111.00	103.20
1	10-A	140	TYR	CZ-CE2-CD2	-5.20	115.12	119.80
1	2-A	677	GLU	OE1-CD-OE2	5.20	129.54	123.30
3	7-D	377	LEU	CB-CG-CD2	5.20	119.84	111.00
2	4-B	461	ASN	CB-CG-OD1	-5.20	111.20	121.60
3	4-D	205	ASP	CB-CG-OD1	-5.20	113.62	118.30
2	5-B	438	TYR	CB-CG-CD2	-5.20	117.88	121.00
2	6-B	730	THR	CA-CB-CG2	-5.20	105.12	112.40
2	8-B	819	PHE	CB-CG-CD2	5.20	124.44	120.80
1	2-A	664	ARG	NE-CZ-NH1	5.20	122.90	120.30
3	2-D	118	ASP	CB-CG-OD2	-5.20	113.62	118.30
3	3-D	69	MET	N-CA-C	-5.20	96.96	111.00
1	6-A	576	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	2-B	293	ARG	NE-CZ-NH2	-5.20	117.70	120.30
3	2-D	341	ARG	CD-NE-CZ	5.20	130.88	123.60
2	4-B	540	GLY	C-N-CA	5.20	134.69	121.70
3	5-C	286	HIS	N-CA-CB	5.20	119.95	110.60
1	7-A	680	LEU	CB-CA-C	-5.20	100.33	110.20
2	2-B	286	GLU	OE1-CD-OE2	-5.20	117.07	123.30
1	3-A	657	TYR	CB-CA-C	-5.20	100.01	110.40
2	4-B	346	LEU	CB-CG-CD1	5.20	119.83	111.00
2	4-B	421	TRP	CG-CD2-CE3	-5.20	129.22	133.90
3	9-C	79	VAL	CA-CB-CG2	-5.20	103.11	110.90
2	10-B	285	ARG	NE-CZ-NH2	5.20	122.90	120.30
2	1-B	660	ASN	CA-CB-CG	-5.19	101.97	113.40
1	1-A	455	ASN	CB-CG-OD1	-5.19	111.22	121.60
3	2-C	413	PHE	CB-CG-CD2	-5.19	117.17	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-A	582	TYR	CZ-CE2-CD2	5.19	124.47	119.80
1	5-A	403	GLU	CA-CB-CG	5.19	124.82	113.40
2	8-B	819	PHE	CG-CD2-CE2	5.19	126.51	120.80
3	2-C	182	VAL	CA-CB-CG2	-5.19	103.11	110.90
2	7-B	343	TYR	CG-CD1-CE1	-5.19	117.15	121.30
2	7-B	512	LEU	N-CA-CB	5.19	120.78	110.40
1	4-A	302	TYR	CZ-CE2-CD2	5.19	124.47	119.80
2	6-B	587	PHE	CB-CG-CD1	5.19	124.43	120.80
3	6-C	409	VAL	CG1-CB-CG2	5.19	119.20	110.90
3	8-C	117	ASP	CB-CA-C	-5.19	100.02	110.40
1	1-A	165	VAL	N-CA-CB	5.19	122.91	111.50
1	1-A	769	SER	CB-CA-C	-5.19	100.24	110.10
2	1-B	314	ILE	CA-CB-CG2	-5.19	100.52	110.90
1	5-A	597	ARG	NE-CZ-NH1	5.19	122.89	120.30
3	6-C	316	PHE	CB-CA-C	-5.19	100.03	110.40
3	1-C	375	MET	CG-SD-CE	-5.19	91.90	100.20
1	5-A	162	PHE	CB-CG-CD1	5.19	124.43	120.80
1	1-A	638	HIS	CB-CA-C	-5.18	100.03	110.40
3	1-C	344	PHE	CB-CG-CD2	-5.18	117.17	120.80
2	2-B	818	ASN	CA-CB-CG	-5.18	102.00	113.40
3	3-D	1	MET	CG-SD-CE	-5.18	91.91	100.20
1	4-A	587	ARG	NH1-CZ-NH2	5.18	125.10	119.40
2	10-B	439	ARG	N-CA-CB	5.18	119.93	110.60
3	1-C	49	ASP	CB-CG-OD1	5.18	122.97	118.30
3	1-C	249	TYR	CG-CD2-CE2	5.18	125.45	121.30
1	3-A	656	VAL	CA-CB-CG2	5.18	118.67	110.90
1	4-A	757	ALA	N-CA-CB	5.18	117.36	110.10
3	6-C	402	ALA	N-CA-CB	5.18	117.36	110.10
2	10-B	612	ARG	NE-CZ-NH1	-5.18	117.71	120.30
3	2-C	256	TYR	CB-CG-CD1	5.18	124.11	121.00
2	3-B	445	PHE	CB-CG-CD1	5.18	124.43	120.80
3	4-C	182	VAL	CA-CB-CG2	5.18	118.67	110.90
3	7-D	136	PHE	CG-CD2-CE2	-5.18	115.10	120.80
3	4-D	60	ASN	N-CA-CB	5.18	119.92	110.60
3	6-D	241	SER	CB-CA-C	-5.18	100.26	110.10
2	7-B	200	PHE	CZ-CE2-CD2	-5.18	113.89	120.10
3	10-C	247	TYR	CG-CD1-CE1	-5.18	117.16	121.30
3	10-D	341	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	1-B	449	ILE	CA-CB-CG2	5.18	121.26	110.90
1	2-A	574	ILE	CA-CB-CG1	-5.18	101.16	111.00
3	4-C	70	ASP	N-CA-C	-5.18	97.03	111.00
3	4-D	52	PRO	N-CD-CG	5.18	110.97	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6-C	93	TRP	CG-CD2-CE3	-5.18	129.24	133.90
3	10-D	204	PHE	CB-CG-CD1	5.18	124.42	120.80
1	1-A	791	PHE	CD1-CE1-CZ	5.17	126.31	120.10
2	1-B	639	THR	N-CA-CB	5.17	120.13	110.30
1	4-A	631	VAL	CA-CB-CG2	-5.17	103.14	110.90
3	7-D	296	LEU	N-CA-CB	5.17	120.75	110.40
1	10-A	392	LEU	CB-CG-CD2	5.17	119.80	111.00
2	1-B	400	TYR	CD1-CE1-CZ	5.17	124.45	119.80
3	3-C	333	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	4-A	479	ARG	NE-CZ-NH1	-5.17	117.71	120.30
1	8-A	193	TYR	CG-CD1-CE1	-5.17	117.16	121.30
3	4-C	185	TYR	CB-CG-CD1	5.17	124.10	121.00
1	5-A	341	LYS	CB-CA-C	-5.17	100.06	110.40
1	6-A	800	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	10-A	294	ASP	CB-CA-C	-5.17	100.06	110.40
1	10-A	380	ASP	O-C-N	5.17	130.97	122.70
1	3-A	712	SER	O-C-N	5.17	130.97	122.70
1	6-A	588	TYR	CA-CB-CG	5.17	123.22	113.40
1	8-A	397	CYS	CA-CB-SG	-5.17	104.69	114.00
2	9-B	743	THR	CA-CB-CG2	-5.17	105.16	112.40
3	2-D	443	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	4-A	91	GLU	N-CA-CB	5.17	119.90	110.60
2	4-B	421	TRP	CB-CG-CD2	-5.17	119.88	126.60
1	5-A	370	SER	N-CA-CB	5.17	118.25	110.50
3	6-D	341	ARG	NE-CZ-NH1	5.17	122.88	120.30
2	7-B	670	ARG	NE-CZ-NH1	5.17	122.88	120.30
3	7-C	56	GLU	N-CA-CB	5.17	119.90	110.60
3	7-D	63	THR	N-CA-C	-5.17	97.05	111.00
1	8-A	570	LEU	CB-CG-CD2	5.17	119.79	111.00
1	9-A	358	ARG	NE-CZ-NH1	-5.17	117.72	120.30
3	9-D	384	VAL	CG1-CB-CG2	5.17	119.17	110.90
2	2-B	267	PHE	CB-CG-CD1	5.17	124.42	120.80
3	3-C	124	ASP	CB-CG-OD2	-5.17	113.65	118.30
3	3-C	351	ALA	N-CA-C	-5.17	97.05	111.00
3	8-C	93	TRP	CE2-CD2-CE3	5.17	124.90	118.70
3	5-C	292	TYR	N-CA-CB	-5.17	101.30	110.60
1	1-A	278	ASP	CB-CG-OD1	5.16	122.95	118.30
2	2-B	825	ILE	CA-CB-CG1	5.16	120.81	111.00
1	3-A	400	ARG	NH1-CZ-NH2	5.16	125.08	119.40
2	3-B	253	LEU	CB-CG-CD1	5.16	119.78	111.00
3	8-D	72	GLU	CB-CA-C	-5.16	100.07	110.40
3	1-C	19	LYS	N-CA-CB	5.16	119.89	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-A	675	GLU	CB-CA-C	-5.16	100.08	110.40
3	4-D	423	PHE	CG-CD2-CE2	-5.16	115.12	120.80
2	2-B	244	LEU	CB-CG-CD2	5.16	119.77	111.00
3	5-D	344	PHE	CG-CD2-CE2	-5.16	115.13	120.80
2	6-B	758	TYR	CB-CG-CD1	-5.16	117.91	121.00
2	10-B	355	LEU	CB-CG-CD1	5.16	119.77	111.00
2	5-B	284	TYR	CD1-CG-CD2	5.16	123.57	117.90
3	7-D	109	TYR	CG-CD1-CE1	-5.16	117.17	121.30
1	2-A	429	TYR	CB-CG-CD1	5.16	124.09	121.00
3	4-C	445	TYR	CZ-CE2-CD2	-5.16	115.16	119.80
3	5-D	294	VAL	CB-CA-C	5.16	121.20	111.40
1	7-A	178	ASN	CB-CA-C	-5.16	100.09	110.40
2	10-B	415	TYR	CB-CG-CD1	-5.16	117.91	121.00
2	8-B	589	PHE	N-CA-CB	5.15	119.88	110.60
3	10-D	38	GLN	C-N-CA	5.15	134.58	121.70
2	3-B	558	PHE	CB-CG-CD1	-5.15	117.19	120.80
1	5-A	94	ILE	CA-CB-CG1	5.15	120.79	111.00
1	6-A	659	LEU	CB-CG-CD1	5.15	119.76	111.00
3	6-D	63	THR	CA-CB-CG2	-5.15	105.19	112.40
2	9-B	356	ARG	NE-CZ-NH2	-5.15	117.72	120.30
3	9-C	70	ASP	CB-CG-OD2	-5.15	113.66	118.30
3	3-C	310	MET	CG-SD-CE	-5.15	91.96	100.20
2	5-B	363	PHE	CB-CG-CD1	-5.15	117.19	120.80
2	6-B	356	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	10-A	325	PHE	N-CA-C	-5.15	97.10	111.00
3	9-C	247	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	3-A	450	TYR	CB-CG-CD2	5.15	124.09	121.00
3	3-C	362	TYR	CB-CG-CD1	5.15	124.09	121.00
1	4-A	433	HIS	CA-CB-CG	-5.15	104.85	113.60
3	4-C	204	PHE	CZ-CE2-CD2	5.15	126.28	120.10
3	5-C	285	ALA	C-N-CA	5.15	134.57	121.70
2	9-B	504	SER	CB-CA-C	-5.15	100.32	110.10
3	9-C	205	ASP	CB-CG-OD2	-5.15	113.67	118.30
3	3-C	275	PHE	CB-CG-CD2	-5.15	117.20	120.80
2	1-B	356	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	3-A	756	ALA	CB-CA-C	-5.14	102.38	110.10
3	3-D	352	MET	CG-SD-CE	-5.14	91.97	100.20
1	4-A	646	TYR	CB-CG-CD2	-5.14	117.91	121.00
3	7-D	134	GLU	CG-CD-OE1	-5.14	108.01	118.30
2	10-B	345	TYR	CG-CD1-CE1	-5.14	117.18	121.30
2	10-B	399	ALA	CB-CA-C	-5.14	102.38	110.10
3	10-C	93	TRP	CG-CD2-CE3	-5.14	129.27	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	10-C	201	THR	CA-CB-OG1	5.14	119.81	109.00
3	10-D	96	SER	N-CA-CB	5.14	118.22	110.50
2	1-B	824	TYR	CG-CD1-CE1	-5.14	117.19	121.30
3	1-D	176	ARG	CA-CB-CG	5.14	124.71	113.40
2	2-B	412	LEU	CB-CG-CD2	5.14	119.74	111.00
1	5-A	762	GLN	CB-CA-C	-5.14	100.11	110.40
2	6-B	758	TYR	CG-CD1-CE1	-5.14	117.19	121.30
1	7-A	433	HIS	N-CA-CB	5.14	119.86	110.60
3	8-D	178	SER	N-CA-CB	5.14	118.21	110.50
1	2-A	162	PHE	CZ-CE2-CD2	-5.14	113.93	120.10
1	2-A	286	TRP	CB-CG-CD1	5.14	133.68	127.00
3	2-D	395	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	3-A	597	ARG	CD-NE-CZ	-5.14	116.40	123.60
3	3-D	265	LEU	CB-CG-CD2	5.14	119.74	111.00
2	5-B	656	ILE	CA-CB-CG1	5.14	120.76	111.00
3	7-C	278	ASP	CB-CG-OD2	-5.14	113.67	118.30
2	8-B	328	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	9-A	57	ALA	N-CA-CB	5.14	117.30	110.10
2	3-B	236	TYR	CA-CB-CG	5.14	123.16	113.40
2	7-B	343	TYR	CZ-CE2-CD2	-5.14	115.18	119.80
3	7-D	192	ARG	NE-CZ-NH1	-5.14	117.73	120.30
3	8-D	366	GLN	N-CA-C	-5.14	97.13	111.00
3	1-C	226	HIS	N-CA-CB	5.14	119.85	110.60
3	10-D	57	ASN	CB-CG-OD1	-5.14	111.33	121.60
3	10-D	292	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	9-A	248	LEU	CB-CG-CD2	5.13	119.73	111.00
1	9-A	676	LEU	CB-CG-CD2	5.13	119.73	111.00
1	3-A	463	GLN	N-CA-CB	5.13	119.84	110.60
3	3-D	445	TYR	CG-CD1-CE1	5.13	125.41	121.30
1	6-A	119	LEU	CA-CB-CG	5.13	127.10	115.30
2	6-B	216	PHE	CG-CD1-CE1	-5.13	115.16	120.80
1	2-A	393	TYR	CG-CD2-CE2	-5.13	117.20	121.30
2	2-B	741	PHE	CB-CG-CD2	5.13	124.39	120.80
1	6-A	469	ARG	N-CA-C	-5.13	97.15	111.00
2	6-B	399	ALA	CB-CA-C	5.13	117.79	110.10
2	3-B	489	MET	CG-SD-CE	-5.13	92.00	100.20
3	3-D	326	VAL	CG1-CB-CG2	5.13	119.10	110.90
3	8-C	42	SER	N-CA-C	-5.13	97.16	111.00
1	10-A	582	TYR	CG-CD2-CE2	-5.13	117.20	121.30
2	8-B	846	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	1-A	692	LEU	CB-CG-CD2	5.12	119.71	111.00
3	1-C	247	TYR	CG-CD2-CE2	5.12	125.40	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2-C	435	GLU	OE1-CD-OE2	-5.12	117.15	123.30
3	2-D	88	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	3-A	197	PHE	CG-CD2-CE2	-5.12	115.17	120.80
1	6-A	706	PHE	CG-CD1-CE1	-5.12	115.17	120.80
1	10-A	450	TYR	CG-CD1-CE1	5.12	125.40	121.30
2	10-B	502	THR	N-CA-C	-5.12	97.17	111.00
1	2-A	686	ASN	C-N-CA	5.12	134.50	121.70
2	4-B	267	PHE	CG-CD2-CE2	-5.12	115.17	120.80
3	6-D	124	ASP	CB-CG-OD1	5.12	122.91	118.30
1	7-A	587	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	8-A	703	VAL	CA-CB-CG2	-5.12	103.22	110.90
3	8-C	192	ARG	CD-NE-CZ	5.12	130.77	123.60
3	8-C	243	ARG	NE-CZ-NH2	5.12	122.86	120.30
3	8-C	297	ASP	CB-CG-OD2	5.12	122.91	118.30
2	10-B	758	TYR	CG-CD1-CE1	5.12	125.40	121.30
1	2-A	792	ASP	N-CA-CB	5.12	119.82	110.60
3	2-C	96	SER	N-CA-CB	5.12	118.18	110.50
2	5-B	264	TYR	CZ-CE2-CD2	-5.12	115.19	119.80
2	6-B	236	TYR	CG-CD1-CE1	-5.12	117.20	121.30
3	8-D	351	ALA	N-CA-CB	5.12	117.27	110.10
2	10-B	457	VAL	CG1-CB-CG2	5.12	119.09	110.90
3	10-D	284	ILE	CA-CB-CG1	5.12	120.72	111.00
1	5-A	398	TYR	CB-CG-CD2	-5.12	117.93	121.00
3	1-C	215	LYS	O-C-N	-5.12	114.52	122.70
3	2-D	205	ASP	CB-CG-OD1	5.12	122.90	118.30
3	8-C	291	SER	CB-CA-C	-5.12	100.38	110.10
1	1-A	266	MET	CB-CG-SD	5.11	127.74	112.40
3	3-C	90	ARG	NE-CZ-NH1	5.11	122.86	120.30
3	4-D	77	ALA	CB-CA-C	-5.11	102.43	110.10
3	6-C	185	TYR	CB-CG-CD1	-5.11	117.93	121.00
3	6-D	443	ASP	CB-CG-OD1	5.11	122.90	118.30
1	7-A	445	GLU	OE1-CD-OE2	5.11	129.44	123.30
3	8-D	362	TYR	CB-CG-CD1	5.11	124.07	121.00
3	9-C	368	ASN	CA-CB-CG	-5.11	102.15	113.40
3	10-D	87	PHE	CB-CA-C	-5.11	100.17	110.40
3	6-D	365	LEU	CB-CG-CD2	5.11	119.69	111.00
1	7-A	357	VAL	CB-CA-C	-5.11	101.69	111.40
3	7-D	345	PRO	N-CD-CG	5.11	110.87	103.20
3	1-C	310	MET	CG-SD-CE	-5.11	92.02	100.20
3	1-D	109	TYR	CB-CA-C	5.11	120.62	110.40
2	2-B	453	TYR	CB-CG-CD1	5.11	124.07	121.00
1	3-A	393	TYR	CG-CD1-CE1	-5.11	117.21	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-D	437	TYR	CD1-CG-CD2	5.11	123.52	117.90
2	6-B	498	ASP	CB-CG-OD1	5.11	122.90	118.30
2	1-B	299	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	2-A	689	LEU	CB-CG-CD1	5.11	119.68	111.00
2	2-B	379	TYR	CB-CG-CD1	-5.11	117.94	121.00
2	2-B	823	LEU	CB-CG-CD1	5.11	119.68	111.00
3	8-C	324	GLY	CA-C-O	5.11	129.79	120.60
3	9-C	155	LEU	CB-CG-CD2	5.11	119.68	111.00
3	9-C	355	ASN	N-CA-CB	5.11	119.80	110.60
1	1-A	407	LYS	N-CA-CB	5.11	119.79	110.60
1	3-A	558	TYR	CB-CG-CD1	5.11	124.06	121.00
3	4-C	79	VAL	CA-CB-CG2	-5.11	103.24	110.90
1	3-A	587	ARG	NE-CZ-NH2	-5.10	117.75	120.30
2	5-B	451	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	8-A	695	LEU	C-N-CA	5.10	134.45	121.70
1	1-A	160	ARG	CB-CG-CD	5.10	124.86	111.60
3	1-C	62	PHE	CB-CG-CD2	5.10	124.37	120.80
3	1-D	374	GLY	N-CA-C	-5.10	100.35	113.10
3	3-D	376	MET	CB-CA-C	-5.10	100.20	110.40
2	1-B	510	TYR	CB-CG-CD1	5.10	124.06	121.00
2	2-B	551	GLY	C-N-CA	5.10	134.45	121.70
3	2-C	65	ARG	NH1-CZ-NH2	5.10	125.01	119.40
1	3-A	413	TYR	CB-CG-CD1	5.10	124.06	121.00
2	3-B	216	PHE	CB-CG-CD2	-5.10	117.23	120.80
2	5-B	593	PHE	CB-CG-CD1	5.10	124.37	120.80
3	5-C	304	SER	N-CA-CB	5.10	118.15	110.50
1	6-A	582	TYR	CG-CD2-CE2	-5.10	117.22	121.30
3	6-D	319	TYR	O-C-N	5.10	130.86	122.70
1	7-A	74	TYR	CB-CG-CD1	-5.10	117.94	121.00
2	7-B	496	ALA	CB-CA-C	-5.10	102.45	110.10
2	8-B	294	LEU	CB-CG-CD2	-5.10	102.33	111.00
3	9-D	61	LYS	N-CA-CB	5.10	119.78	110.60
2	1-B	824	TYR	CD1-CE1-CZ	5.10	124.39	119.80
1	2-A	168	PHE	CD1-CE1-CZ	5.10	126.22	120.10
3	4-C	13	CYS	CA-CB-SG	-5.10	104.82	114.00
3	8-C	295	MET	CA-CB-CG	5.10	121.97	113.30
2	10-B	299	ARG	NE-CZ-NH1	-5.10	117.75	120.30
3	10-C	131	ASP	CB-CG-OD1	-5.10	113.71	118.30
3	2-C	160	ASP	CB-CG-OD1	5.09	122.89	118.30
2	5-B	758	TYR	CB-CG-CD1	-5.09	117.94	121.00
1	7-A	442	ASN	N-CA-CB	5.09	119.77	110.60
1	7-A	458	TYR	CB-CG-CD1	5.09	124.06	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-C	205	ASP	CB-CG-OD1	5.09	122.88	118.30
3	1-C	407	TYR	CZ-CE2-CD2	5.09	124.38	119.80
1	2-A	565	ASN	N-CA-CB	5.09	119.77	110.60
1	2-A	779	LEU	CB-CG-CD1	5.09	119.65	111.00
3	2-C	265	LEU	N-CA-C	-5.09	97.25	111.00
1	3-A	693	ILE	CA-C-N	5.09	131.36	117.10
3	3-D	205	ASP	CA-CB-CG	-5.09	102.20	113.40
2	6-B	225	PHE	CG-CD1-CE1	5.09	126.40	120.80
1	7-A	76	ARG	NE-CZ-NH2	5.09	122.85	120.30
3	8-C	89	PRO	N-CA-CB	5.09	109.41	103.30
1	10-A	626	VAL	CA-CB-CG1	5.09	118.54	110.90
1	1-A	401	ALA	N-CA-CB	5.09	117.22	110.10
2	7-B	365	ALA	N-CA-CB	5.09	117.22	110.10
2	10-B	495	LYS	C-N-CA	5.09	134.42	121.70
3	2-C	40	PRO	N-CA-CB	5.09	109.41	103.30
2	6-B	557	VAL	C-N-CA	5.09	134.42	121.70
3	10-D	346	SER	N-CA-CB	5.09	118.13	110.50
2	7-B	638	ARG	O-C-N	-5.09	114.56	122.70
1	9-A	75	ILE	N-CA-C	-5.09	97.27	111.00
2	9-B	542	ASP	O-C-N	-5.09	114.56	122.70
3	9-C	128	ASP	CB-CG-OD2	5.09	122.88	118.30
3	1-C	144	GLY	CA-C-N	-5.08	106.03	116.20
3	3-D	347	TRP	CG-CD1-NE1	5.08	115.19	110.10
1	8-A	294	ASP	N-CA-CB	5.08	119.75	110.60
1	2-A	558	TYR	CG-CD2-CE2	-5.08	117.23	121.30
1	2-A	794	TYR	CA-CB-CG	5.08	123.06	113.40
2	4-B	363	PHE	CB-CG-CD2	5.08	124.36	120.80
1	6-A	438	PHE	CB-CG-CD2	-5.08	117.24	120.80
3	7-C	82	THR	CA-CB-CG2	-5.08	105.28	112.40
3	9-C	54	PHE	CB-CG-CD1	-5.08	117.24	120.80
3	9-D	403	PHE	N-CA-CB	5.08	119.75	110.60
2	1-B	464	LEU	CB-CG-CD1	5.08	119.64	111.00
3	1-D	181	VAL	CA-CB-CG1	-5.08	103.28	110.90
1	5-A	353	LEU	CB-CG-CD1	5.08	119.64	111.00
2	5-B	650	SER	N-CA-CB	5.08	118.12	110.50
3	5-C	133	PHE	CB-CG-CD2	5.08	124.36	120.80
1	7-A	455	ASN	CB-CA-C	-5.08	100.24	110.40
3	8-D	352	MET	CG-SD-CE	-5.08	92.07	100.20
1	4-A	438	PHE	CB-CG-CD2	-5.08	117.24	120.80
3	4-C	200	ALA	CB-CA-C	-5.08	102.48	110.10
3	9-C	244	PHE	CB-CG-CD1	-5.08	117.24	120.80
3	3-C	366	GLN	N-CA-CB	5.08	119.74	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	190	TYR	CG-CD2-CE2	5.08	125.36	121.30
2	2-B	758	TYR	CB-CG-CD1	-5.08	117.95	121.00
3	4-D	93	TRP	NE1-CE2-CZ2	5.08	135.99	130.40
3	6-D	394	PHE	CD1-CE1-CZ	5.08	126.19	120.10
3	7-D	133	PHE	CD1-CE1-CZ	-5.08	114.01	120.10
1	9-A	556	ALA	CA-C-O	5.08	130.76	120.10
1	1-A	189	LEU	N-CA-CB	-5.08	100.25	110.40
2	4-B	345	TYR	CG-CD2-CE2	-5.08	117.24	121.30
1	6-A	148	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	8-A	406	LEU	CB-CG-CD1	5.08	119.63	111.00
3	8-C	36	LEU	CB-CG-CD1	5.08	119.63	111.00
1	9-A	123	TYR	CG-CD2-CE2	-5.08	117.24	121.30
3	10-D	88	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	2-A	191	ASN	CB-CA-C	-5.07	100.25	110.40
1	2-A	554	LYS	C-N-CA	5.07	134.38	121.70
3	3-C	216	VAL	CB-CA-C	-5.07	101.76	111.40
2	4-B	562	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	5-A	460	LYS	O-C-N	5.07	130.82	122.70
3	5-C	117	ASP	CB-CG-OD2	5.07	122.87	118.30
1	7-A	687	ARG	NH1-CZ-NH2	5.07	124.98	119.40
2	7-B	341	LEU	C-N-CA	5.07	134.38	121.70
2	8-B	561	ASP	CB-CG-OD1	5.07	122.87	118.30
3	1-C	314	THR	C-N-CA	5.07	134.38	121.70
2	4-B	719	LEU	CB-CA-C	5.07	119.84	110.20
3	6-C	319	TYR	CZ-CE2-CD2	-5.07	115.23	119.80
2	10-B	346	LEU	O-C-N	-5.07	114.58	122.70
3	10-D	209	LEU	CB-CA-C	-5.07	100.56	110.20
2	2-B	400	TYR	CD1-CE1-CZ	5.07	124.36	119.80
3	2-C	395	ASP	CB-CG-OD1	-5.07	113.74	118.30
1	3-A	398	TYR	CG-CD2-CE2	-5.07	117.24	121.30
2	6-B	670	ARG	NE-CZ-NH1	5.07	122.83	120.30
3	9-D	314	THR	CA-CB-CG2	5.07	119.50	112.40
1	10-A	623	ARG	CD-NE-CZ	-5.07	116.50	123.60
2	10-B	213	ILE	N-CA-C	-5.07	97.31	111.00
2	4-B	218	SER	N-CA-CB	5.07	118.10	110.50
1	6-A	198	ARG	N-CA-CB	5.07	119.72	110.60
3	7-D	114	ARG	CD-NE-CZ	5.07	130.70	123.60
1	2-A	90	ILE	C-N-CA	5.07	134.37	121.70
1	2-A	451	ARG	NE-CZ-NH2	-5.07	117.77	120.30
3	2-D	133	PHE	CB-CG-CD1	5.07	124.35	120.80
3	3-C	413	PHE	CB-CG-CD2	-5.07	117.25	120.80
3	4-D	120	LEU	CB-CG-CD2	5.07	119.61	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	8-B	203	ASP	N-CA-C	-5.07	97.32	111.00
2	8-B	342	TYR	N-CA-CB	5.07	119.72	110.60
1	9-A	116	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	2-A	203	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	6-A	450	TYR	CG-CD1-CE1	-5.07	117.25	121.30
1	6-A	794	TYR	CB-CG-CD2	-5.07	117.96	121.00
3	7-D	436	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	8-A	155	VAL	N-CA-CB	5.07	122.64	111.50
2	8-B	666	ARG	NH1-CZ-NH2	5.07	124.97	119.40
2	9-B	482	LEU	C-N-CA	5.07	134.36	121.70
1	10-A	588	TYR	CB-CA-C	-5.07	100.27	110.40
3	10-C	54	PHE	CB-CG-CD1	-5.07	117.25	120.80
3	10-C	248	MET	CB-CA-C	-5.07	100.27	110.40
1	4-A	170	ILE	C-N-CA	5.06	134.36	121.70
1	4-A	755	ASP	CB-CG-OD2	-5.06	113.74	118.30
3	7-C	223	ASP	N-CA-C	-5.06	97.33	111.00
2	8-B	385	PHE	CB-CG-CD2	-5.06	117.25	120.80
1	1-A	62	ASP	CB-CG-OD2	5.06	122.86	118.30
2	3-B	580	ARG	NE-CZ-NH1	-5.06	117.77	120.30
3	3-C	38	GLN	CG-CD-OE1	-5.06	111.48	121.60
3	5-C	128	ASP	CB-CG-OD1	-5.06	113.74	118.30
1	7-A	598	LEU	CB-CG-CD2	5.06	119.61	111.00
3	7-D	325	ASN	N-CA-CB	5.06	119.71	110.60
1	9-A	129	THR	CA-CB-CG2	-5.06	105.31	112.40
3	1-D	348	SER	N-CA-CB	-5.06	102.91	110.50
3	3-D	93	TRP	O-C-N	5.06	130.79	122.70
2	7-B	459	HIS	CB-CA-C	-5.06	100.28	110.40
3	6-D	134	GLU	CB-CA-C	-5.06	100.28	110.40
1	7-A	137	ARG	NE-CZ-NH1	5.06	122.83	120.30
2	7-B	264	TYR	CD1-CG-CD2	-5.06	112.34	117.90
2	7-B	319	PHE	CZ-CE2-CD2	-5.06	114.03	120.10
3	8-C	193	ARG	CD-NE-CZ	-5.06	116.52	123.60
1	9-A	320	TRP	CD1-CG-CD2	-5.06	102.25	106.30
2	3-B	293	ARG	NE-CZ-NH2	5.06	122.83	120.30
2	8-B	362	PHE	N-CA-C	-5.06	97.35	111.00
3	2-D	425	GLU	CB-CA-C	-5.05	100.29	110.40
2	3-B	532	PRO	N-CD-CG	5.05	110.78	103.20
1	9-A	160	ARG	NE-CZ-NH1	-5.05	117.77	120.30
3	1-D	53	PHE	CB-CG-CD1	5.05	124.34	120.80
1	4-A	279	TYR	CG-CD1-CE1	-5.05	117.26	121.30
3	4-D	225	GLN	CB-CA-C	-5.05	100.30	110.40
1	6-A	418	VAL	CA-CB-CG2	-5.05	103.32	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	10-A	304	ASP	CB-CG-OD1	-5.05	113.75	118.30
2	10-B	243	MET	CG-SD-CE	-5.05	92.12	100.20
1	3-A	664	ARG	CG-CD-NE	-5.05	101.20	111.80
2	3-B	284	TYR	CB-CG-CD2	-5.05	117.97	121.00
3	5-D	171	SER	CB-CA-C	-5.05	100.50	110.10
2	7-B	585	ARG	NE-CZ-NH1	5.05	122.83	120.30
2	8-B	535	SER	N-CA-CB	5.05	118.08	110.50
2	10-B	184	ILE	N-CA-CB	5.05	122.41	110.80
3	9-C	105	TRP	NE1-CE2-CZ2	5.05	135.95	130.40
1	2-A	692	LEU	C-N-CA	5.05	134.32	121.70
3	2-C	98	GLY	C-N-CA	5.05	134.32	121.70
1	3-A	614	TYR	CG-CD1-CE1	-5.05	117.26	121.30
3	3-C	301	PRO	N-CA-CB	5.05	109.36	103.30
3	3-C	311	ASN	N-CA-CB	5.05	119.68	110.60
1	4-A	105	PHE	CD1-CG-CD2	-5.05	111.74	118.30
2	4-B	303	HIS	CB-CA-C	-5.05	100.31	110.40
3	4-D	154	LEU	CB-CG-CD2	5.05	119.58	111.00
1	6-A	426	PHE	CB-CG-CD2	-5.05	117.27	120.80
2	7-B	476	ALA	CB-CA-C	-5.05	102.53	110.10
3	8-C	291	SER	O-C-N	5.05	130.78	122.70
3	7-C	93	TRP	N-CA-CB	5.04	119.68	110.60
1	10-A	279	TYR	CG-CD2-CE2	5.04	125.34	121.30
3	6-D	376	MET	CA-CB-CG	5.04	121.87	113.30
2	7-B	184	ILE	CA-CB-CG1	5.04	120.58	111.00
3	8-C	86	PHE	CB-CG-CD2	-5.04	117.27	120.80
3	8-C	329	ARG	NE-CZ-NH1	5.04	122.82	120.30
3	9-C	114	ARG	NE-CZ-NH2	-5.04	117.78	120.30
3	9-D	188	ILE	N-CA-CB	5.04	122.40	110.80
2	10-B	290	ASN	CB-CA-C	-5.04	100.31	110.40
3	10-D	46	ARG	NE-CZ-NH2	-5.04	117.78	120.30
3	10-D	207	ALA	O-C-N	5.04	130.77	122.70
2	1-B	758	TYR	CA-C-O	-5.04	109.51	120.10
3	1-C	79	VAL	CA-CB-CG1	5.04	118.46	110.90
1	3-A	642	THR	N-CA-CB	5.04	119.88	110.30
2	5-B	381	ILE	CA-CB-CG2	-5.04	100.82	110.90
3	7-D	249	TYR	CB-CG-CD1	5.04	124.03	121.00
3	7-D	300	ASP	O-C-N	-5.04	111.52	121.10
1	8-A	160	ARG	NE-CZ-NH2	5.04	122.82	120.30
2	9-B	589	PHE	CB-CG-CD1	5.04	124.33	120.80
1	10-A	651	VAL	O-C-N	-5.04	114.63	122.70
1	1-A	794	TYR	CZ-CE2-CD2	-5.04	115.26	119.80
3	5-C	68	MET	CG-SD-CE	5.04	108.27	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-C	55	ARG	NE-CZ-NH1	-5.04	117.78	120.30
3	1-C	46	ARG	NE-CZ-NH2	-5.04	117.78	120.30
3	1-C	48	ASP	CB-CG-OD2	-5.04	113.77	118.30
3	1-C	137	GLN	CG-CD-NE2	-5.04	104.61	116.70
1	2-A	98	MET	CG-SD-CE	-5.04	92.14	100.20
3	6-C	48	ASP	CB-CA-C	-5.04	100.32	110.40
2	4-B	657	ILE	CA-CB-CG1	5.04	120.57	111.00
3	5-C	26	ALA	N-CA-CB	5.04	117.15	110.10
3	5-C	136	PHE	CB-CG-CD2	-5.04	117.27	120.80
3	5-D	321	THR	CA-CB-OG1	5.04	119.58	109.00
2	9-B	461	ASN	CA-CB-CG	-5.04	102.32	113.40
1	1-A	110	VAL	CA-CB-CG1	5.04	118.45	110.90
3	1-D	296	LEU	CB-CG-CD2	5.04	119.56	111.00
1	2-A	167	ASN	N-CA-C	-5.04	97.40	111.00
3	2-C	247	TYR	CB-CA-C	5.04	120.47	110.40
3	3-D	176	ARG	NH1-CZ-NH2	-5.04	113.86	119.40
2	7-B	249	MET	CG-SD-CE	-5.04	92.14	100.20
1	9-A	364	PRO	N-CD-CG	5.04	110.75	103.20
1	9-A	588	TYR	CG-CD1-CE1	-5.04	117.27	121.30
3	10-D	367	PRO	C-N-CA	5.04	134.29	121.70
3	1-C	117	ASP	N-CA-CB	5.03	119.66	110.60
1	4-A	321	ASP	CB-CG-OD2	-5.03	113.77	118.30
2	4-B	359	TYR	CB-CG-CD1	-5.03	117.98	121.00
2	8-B	598	TYR	CD1-CG-CD2	5.03	123.44	117.90
3	9-C	109	TYR	CB-CG-CD2	-5.03	117.98	121.00
2	4-B	555	TRP	CB-CG-CD1	5.03	133.54	127.00
3	4-C	223	ASP	CB-CG-OD1	5.03	122.83	118.30
1	7-A	181	GLU	OE1-CD-OE2	-5.03	117.26	123.30
1	1-A	398	TYR	CG-CD2-CE2	5.03	125.32	121.30
1	6-A	186	MET	CG-SD-CE	-5.03	92.15	100.20
1	10-A	78	PHE	CB-CG-CD2	-5.03	117.28	120.80
1	1-A	639	PHE	CB-CG-CD2	5.03	124.32	120.80
3	2-C	139	LEU	CB-CA-C	-5.03	100.64	110.20
3	2-D	177	SER	N-CA-CB	5.03	118.04	110.50
3	9-C	86	PHE	CB-CG-CD1	-5.03	117.28	120.80
1	1-A	562	PHE	CB-CG-CD2	5.03	124.32	120.80
2	2-B	391	PRO	N-CA-CB	5.03	109.33	103.30
1	5-A	159	GLU	OE1-CD-OE2	5.03	129.33	123.30
2	5-B	552	SER	C-N-CA	5.03	134.27	121.70
1	1-A	612	TRP	C-N-CA	5.03	134.26	121.70
2	6-B	216	PHE	CZ-CE2-CD2	-5.03	114.07	120.10
3	6-D	148	SER	N-CA-CB	5.03	118.04	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	8-B	658	GLU	N-CA-CB	5.03	119.65	110.60
3	10-C	268	LEU	CB-CA-C	-5.03	100.65	110.20
3	2-C	344	PHE	CB-CG-CD2	-5.02	117.28	120.80
3	3-C	433	LEU	CB-CA-C	-5.02	100.66	110.20
1	4-A	182	VAL	CA-CB-CG1	-5.02	103.36	110.90
2	5-B	429	TYR	CA-CB-CG	5.02	122.95	113.40
3	8-D	362	TYR	CA-CB-CG	5.02	122.94	113.40
2	9-B	565	TYR	CA-C-O	-5.02	109.55	120.10
2	1-B	629	ASN	O-C-N	-5.02	114.67	122.70
3	1-D	252	MET	N-CA-CB	-5.02	101.56	110.60
3	4-D	265	LEU	N-CA-C	-5.02	97.44	111.00
1	8-A	436	LEU	CB-CG-CD2	5.02	119.54	111.00
3	1-D	384	VAL	O-C-N	-5.02	114.67	122.70
3	5-C	316	PHE	CB-CG-CD1	5.02	124.31	120.80
1	7-A	325	PHE	CB-CG-CD1	-5.02	117.28	120.80
2	1-B	474	VAL	CA-CB-CG2	-5.02	103.37	110.90
1	2-A	709	PHE	CB-CA-C	-5.02	100.36	110.40
1	2-A	789	GLU	OE1-CD-OE2	5.02	129.32	123.30
3	4-C	225	GLN	N-CA-CB	5.02	119.64	110.60
3	5-C	8	LEU	CB-CG-CD2	5.02	119.53	111.00
3	5-D	203	VAL	O-C-N	-5.02	114.67	122.70
3	7-C	77	ALA	CB-CA-C	-5.02	102.57	110.10
3	7-C	318	VAL	N-CA-CB	5.02	122.54	111.50
2	3-B	522	LEU	CB-CG-CD1	-5.02	102.47	111.00
3	5-C	243	ARG	NE-CZ-NH1	-5.02	117.79	120.30
2	6-B	187	TYR	CB-CG-CD2	-5.02	117.99	121.00
3	7-D	17	VAL	CB-CA-C	-5.02	101.87	111.40
3	9-D	377	LEU	N-CA-CB	5.02	120.44	110.40
3	10-C	86	PHE	CB-CG-CD1	5.02	124.31	120.80
3	1-D	79	VAL	CA-CB-CG2	5.02	118.42	110.90
2	10-B	612	ARG	N-CA-CB	5.02	119.63	110.60
2	6-B	222	HIS	N-CA-CB	5.01	119.63	110.60
2	6-B	470	TYR	CG-CD1-CE1	-5.01	117.29	121.30
3	6-D	416	MET	CG-SD-CE	-5.01	92.18	100.20
2	7-B	722	ASP	CB-CG-OD1	-5.01	113.79	118.30
3	8-D	4	GLU	CB-CA-C	-5.01	100.37	110.40
3	9-C	253	SER	O-C-N	-5.01	114.68	122.70
2	10-B	640	GLN	N-CA-CB	5.01	119.62	110.60
2	10-B	648	MET	C-N-CA	5.01	134.23	121.70
3	10-D	119	ILE	CA-CB-CG2	-5.01	100.87	110.90
3	4-C	445	TYR	CB-CG-CD2	5.01	124.01	121.00
3	4-D	87	PHE	CB-CG-CD2	-5.01	117.29	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7-A	279	TYR	CA-CB-CG	-5.01	103.88	113.40
3	10-D	48	ASP	CB-CG-OD2	-5.01	113.79	118.30
3	4-D	386	VAL	CG1-CB-CG2	-5.01	102.88	110.90
2	6-B	362	PHE	CZ-CE2-CD2	-5.01	114.09	120.10
2	7-B	652	TYR	CB-CA-C	-5.01	100.38	110.40
2	2-B	446	PHE	CB-CG-CD2	-5.01	117.29	120.80
3	4-D	84	ARG	NE-CZ-NH2	-5.01	117.80	120.30
3	7-C	436	ASP	CB-CG-OD1	-5.01	113.79	118.30
3	9-C	425	GLU	CB-CA-C	-5.01	100.38	110.40
3	9-D	161	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	10-A	137	ARG	CD-NE-CZ	-5.01	116.59	123.60
2	10-B	363	PHE	O-C-N	-5.01	114.69	122.70
1	9-A	393	TYR	CG-CD2-CE2	-5.01	117.29	121.30
3	9-C	204	PHE	CG-CD2-CE2	-5.01	115.29	120.80
2	1-B	471	ARG	CD-NE-CZ	5.01	130.61	123.60
3	4-C	319	TYR	CD1-CG-CD2	5.01	123.41	117.90
2	5-B	301	THR	CA-CB-CG2	-5.01	105.39	112.40
3	8-C	300	ASP	CB-CG-OD2	-5.01	113.79	118.30
2	1-B	565	TYR	CZ-CE2-CD2	-5.00	115.30	119.80
1	3-A	383	ASP	N-CA-CB	5.00	119.61	110.60
1	7-A	203	ARG	NH1-CZ-NH2	5.00	124.91	119.40
3	3-D	407	TYR	CB-CG-CD1	-5.00	118.00	121.00
2	8-B	562	TYR	CB-CA-C	-5.00	100.39	110.40
3	9-D	63	THR	CA-CB-OG1	5.00	119.51	109.00
3	9-D	131	ASP	CB-CG-OD1	-5.00	113.80	118.30
1	10-A	704	TYR	CB-CG-CD2	-5.00	118.00	121.00
2	10-B	534	ASN	N-CA-C	-5.00	97.49	111.00
3	10-C	126	GLU	N-CA-CB	5.00	119.61	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	6-D	73	PRO	CA

All (609) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	112	TYR	Sidechain
1	1-A	123	TYR	Sidechain
1	1-A	140	TYR	Sidechain
1	1-A	181	GLU	Peptide
1	1-A	299	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	1-A	333	ARG	Sidechain
1	1-A	400	ARG	Sidechain
1	1-A	405	PHE	Sidechain
1	1-A	429	TYR	Sidechain
1	1-A	438	PHE	Sidechain
1	1-A	469	ARG	Sidechain
1	1-A	486	PHE	Sidechain
1	1-A	582	TYR	Sidechain
1	1-A	587	ARG	Sidechain
1	1-A	614	TYR	Sidechain
1	1-A	627	ARG	Sidechain
1	1-A	706	PHE	Sidechain
1	1-A	74	TYR	Sidechain
1	1-A	767	TYR	Sidechain
2	1-B	187	TYR	Sidechain
2	1-B	190	TYR	Sidechain
2	1-B	222	HIS	Sidechain
2	1-B	264	TYR	Sidechain
2	1-B	293	ARG	Sidechain
2	1-B	297	TYR	Sidechain
2	1-B	299	ARG	Sidechain
2	1-B	342	TYR	Sidechain
2	1-B	343	TYR	Sidechain
2	1-B	356	ARG	Sidechain
2	1-B	379	TYR	Sidechain
2	1-B	415	TYR	Sidechain
2	1-B	425	PHE	Sidechain
2	1-B	433	TYR	Sidechain
2	1-B	439	ARG	Sidechain
2	1-B	488	PHE	Sidechain
2	1-B	526	ARG	Sidechain
2	1-B	562	TYR	Sidechain
2	1-B	576	ARG	Sidechain
2	1-B	598	TYR	Sidechain
2	1-B	599	PHE	Sidechain
2	1-B	612	ARG	Sidechain
2	1-B	652	TYR	Sidechain
2	1-B	772	PHE	Sidechain
2	1-B	776	TYR	Sidechain
3	1-C	109	TYR	Sidechain
3	1-C	185	TYR	Sidechain
3	1-C	20	PHE	Sidechain

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Mol	Chain	Res	Type	Group
3	1-C	249	TYR	Sidechain
3	1-C	256	TYR	Sidechain
3	1-C	279	TYR	Sidechain
3	1-C	281	HIS	Sidechain
3	1-C	292	TYR	Sidechain
3	1-C	319	TYR	Sidechain
3	1-C	362	TYR	Sidechain
3	1-C	394	PHE	Sidechain
3	1-C	407	TYR	Sidechain
3	1-C	437	TYR	Sidechain
3	1-C	445	TYR	Sidechain
3	1-C	86	PHE	Sidechain
3	1-D	109	TYR	Sidechain
3	1-D	136	PHE	Sidechain
3	1-D	170	TYR	Sidechain
3	1-D	249	TYR	Sidechain
3	1-D	279	TYR	Sidechain
3	1-D	333	ARG	Sidechain
3	1-D	362	TYR	Sidechain
3	1-D	387	PHE	Sidechain
3	1-D	437	TYR	Sidechain
1	10-A	143	ARG	Sidechain
1	10-A	150	TYR	Sidechain
1	10-A	171	ARG	Sidechain
1	10-A	190	TYR	Sidechain
1	10-A	198	ARG	Sidechain
1	10-A	333	ARG	Sidechain
1	10-A	381	PHE	Sidechain
1	10-A	413	TYR	Sidechain
1	10-A	449	HIS	Sidechain
1	10-A	450	TYR	Sidechain
1	10-A	479	ARG	Sidechain
1	10-A	558	TYR	Sidechain
1	10-A	594	TYR	Sidechain
1	10-A	623	ARG	Sidechain
1	10-A	630	ARG	Sidechain
1	10-A	663	TYR	Sidechain
1	10-A	664	ARG	Sidechain
1	10-A	706	PHE	Sidechain
1	10-A	76	ARG	Sidechain
1	10-A	791	PHE	Sidechain
2	10-B	190	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	10-B	231	TYR	Sidechain
2	10-B	242	ARG	Sidechain
2	10-B	288	TYR	Sidechain
2	10-B	297	TYR	Sidechain
2	10-B	342	TYR	Sidechain
2	10-B	343	TYR	Sidechain
2	10-B	356	ARG	Sidechain
2	10-B	411	PHE	Sidechain
2	10-B	429	TYR	Sidechain
2	10-B	438	TYR	Sidechain
2	10-B	446	PHE	Sidechain
2	10-B	453	TYR	Sidechain
2	10-B	470	TYR	Sidechain
2	10-B	471	ARG	Sidechain
2	10-B	562	TYR	Sidechain
2	10-B	592	ARG	Sidechain
2	10-B	598	TYR	Sidechain
2	10-B	652	TYR	Sidechain
2	10-B	670	ARG	Sidechain
2	10-B	731	PHE	Sidechain
2	10-B	741	PHE	Sidechain
2	10-B	772	PHE	Sidechain
2	10-B	805	PHE	Sidechain
2	10-B	824	TYR	Sidechain
3	10-C	109	TYR	Sidechain
3	10-C	192	ARG	Sidechain
3	10-C	247	TYR	Sidechain
3	10-C	272	PHE	Sidechain
3	10-C	333	ARG	Sidechain
3	10-C	341	ARG	Sidechain
3	10-C	358	ARG	Sidechain
3	10-C	398	PHE	Sidechain
3	10-C	407	TYR	Sidechain
3	10-C	437	TYR	Sidechain
3	10-C	90	ARG	Sidechain
3	10-D	16	HIS	Sidechain
3	10-D	161	ARG	Sidechain
3	10-D	170	TYR	Sidechain
3	10-D	173	PHE	Sidechain
3	10-D	218	ARG	Sidechain
3	10-D	247	TYR	Sidechain
3	10-D	249	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	10-D	256	TYR	Sidechain
3	10-D	319	TYR	Sidechain
3	10-D	407	TYR	Sidechain
3	10-D	413	PHE	Sidechain
3	10-D	423	PHE	Sidechain
3	10-D	427	ARG	Sidechain
3	10-D	46	ARG	Sidechain
3	10-D	55	ARG	Sidechain
3	10-D	65	ARG	Sidechain
3	10-D	86	PHE	Sidechain
1	2-A	123	TYR	Sidechain
1	2-A	140	TYR	Sidechain
1	2-A	193	TYR	Sidechain
1	2-A	198	ARG	Sidechain
1	2-A	279	TYR	Sidechain
1	2-A	296	TYR	Sidechain
1	2-A	345	PHE	Sidechain
1	2-A	381	PHE	Sidechain
1	2-A	393	TYR	Sidechain
1	2-A	413	TYR	Sidechain
1	2-A	450	TYR	Sidechain
1	2-A	582	TYR	Sidechain
1	2-A	594	TYR	Sidechain
1	2-A	638	HIS	Sidechain
1	2-A	77	TYR	Sidechain
1	2-A	794	TYR	Sidechain
2	2-B	200	PHE	Sidechain
2	2-B	264	TYR	Sidechain
2	2-B	284	TYR	Sidechain
2	2-B	319	PHE	Sidechain
2	2-B	328	ARG	Sidechain
2	2-B	345	TYR	Sidechain
2	2-B	400	TYR	Sidechain
2	2-B	411	PHE	Sidechain
2	2-B	415	TYR	Sidechain
2	2-B	429	TYR	Sidechain
2	2-B	439	ARG	Sidechain
2	2-B	470	TYR	Sidechain
2	2-B	558	PHE	Sidechain
2	2-B	578	PHE	Sidechain
2	2-B	612	ARG	Sidechain
2	2-B	641	PHE	Sidechain

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Mol	Chain	Res	Type	Group
2	2-B	742	ALA	Peptide
2	2-B	822	ARG	Sidechain
3	2-C	185	TYR	Sidechain
3	2-C	247	TYR	Sidechain
3	2-C	249	TYR	Sidechain
3	2-C	279	TYR	Sidechain
3	2-C	292	TYR	Sidechain
3	2-C	333	ARG	Sidechain
3	2-C	407	TYR	Sidechain
3	2-C	445	TYR	Sidechain
3	2-C	65	ARG	Sidechain
3	2-D	176	ARG	Sidechain
3	2-D	218	ARG	Sidechain
3	2-D	329	ARG	Sidechain
3	2-D	359	ARG	Sidechain
3	2-D	55	ARG	Sidechain
3	2-D	84	ARG	Sidechain
1	3-A	171	ARG	Sidechain
1	3-A	183	ASN	Mainchain
1	3-A	197	PHE	Sidechain
1	3-A	324	TYR	Sidechain
1	3-A	410	PHE	Sidechain
1	3-A	429	TYR	Sidechain
1	3-A	568	TYR	Sidechain
1	3-A	588	TYR	Sidechain
1	3-A	594	TYR	Sidechain
1	3-A	633	HIS	Sidechain
1	3-A	663	TYR	Sidechain
1	3-A	664	ARG	Sidechain
1	3-A	704	TYR	Sidechain
1	3-A	782	PHE	Sidechain
1	3-A	794	TYR	Sidechain
2	3-B	264	TYR	Sidechain
2	3-B	288	TYR	Sidechain
2	3-B	297	TYR	Sidechain
2	3-B	345	TYR	Sidechain
2	3-B	356	ARG	Sidechain
2	3-B	359	TYR	Sidechain
2	3-B	389	ARG	Sidechain
2	3-B	445	PHE	Sidechain
2	3-B	471	ARG	Sidechain
2	3-B	488	PHE	Sidechain

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Mol	Chain	Res	Type	Group
2	3-B	598	TYR	Sidechain
2	3-B	641	PHE	Sidechain
2	3-B	651	TYR	Sidechain
2	3-B	652	TYR	Sidechain
2	3-B	770	TYR	Sidechain
2	3-B	816	TYR	Sidechain
2	3-B	827	ARG	Sidechain
3	3-C	114	ARG	Sidechain
3	3-C	133	PHE	Sidechain
3	3-C	185	TYR	Sidechain
3	3-C	249	TYR	Sidechain
3	3-C	267	PHE	Sidechain
3	3-C	292	TYR	Sidechain
3	3-C	319	TYR	Sidechain
3	3-C	329	ARG	Sidechain
3	3-C	362	TYR	Sidechain
3	3-C	394	PHE	Sidechain
3	3-C	445	TYR	Sidechain
3	3-C	46	ARG	Sidechain
3	3-C	55	ARG	Sidechain
3	3-C	59	ARG	Sidechain
3	3-C	83	PHE	Sidechain
3	3-C	87	PHE	Sidechain
3	3-D	109	TYR	Sidechain
3	3-D	204	PHE	Sidechain
3	3-D	247	TYR	Sidechain
3	3-D	275	PHE	Sidechain
3	3-D	279	TYR	Sidechain
3	3-D	292	TYR	Sidechain
3	3-D	315	TYR	Sidechain
3	3-D	319	TYR	Sidechain
3	3-D	362	TYR	Sidechain
3	3-D	407	TYR	Sidechain
3	3-D	413	PHE	Sidechain
3	3-D	59	ARG	Sidechain
1	4-A	193	TYR	Sidechain
1	4-A	204	ARG	Sidechain
1	4-A	296	TYR	Sidechain
1	4-A	324	TYR	Sidechain
1	4-A	393	TYR	Sidechain
1	4-A	398	TYR	Sidechain
1	4-A	400	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	4-A	405	PHE	Sidechain
1	4-A	450	TYR	Sidechain
1	4-A	469	ARG	Sidechain
1	4-A	479	ARG	Sidechain,Peptide
1	4-A	633	HIS	Sidechain
1	4-A	639	PHE	Sidechain
1	4-A	74	TYR	Sidechain
1	4-A	767	TYR	Sidechain
2	4-B	222	HIS	Sidechain
2	4-B	264	TYR	Sidechain
2	4-B	285	ARG	Sidechain
2	4-B	288	TYR	Sidechain
2	4-B	328	ARG	Sidechain
2	4-B	342	TYR	Sidechain
2	4-B	379	TYR	Sidechain
2	4-B	400	TYR	Sidechain
2	4-B	411	PHE	Sidechain
2	4-B	438	TYR	Sidechain
2	4-B	470	TYR	Sidechain
2	4-B	471	ARG	Sidechain
2	4-B	488	PHE	Sidechain
2	4-B	583	TYR	Sidechain
2	4-B	592	ARG	Sidechain
2	4-B	593	PHE	Sidechain
2	4-B	598	TYR	Sidechain
2	4-B	644	PHE	Sidechain
2	4-B	805	PHE	Sidechain
2	4-B	816	TYR	Sidechain
2	4-B	827	ARG	Sidechain
3	4-C	162	TYR	Sidechain
3	4-C	217	PHE	Sidechain
3	4-C	247	TYR	Sidechain
3	4-C	256	TYR	Sidechain
3	4-C	272	PHE	Sidechain
3	4-C	292	TYR	Sidechain
3	4-C	319	TYR	Sidechain
3	4-C	341	ARG	Sidechain
3	4-C	358	ARG	Sidechain
3	4-C	359	ARG	Sidechain
3	4-C	445	TYR	Sidechain
3	4-C	46	ARG	Sidechain
3	4-C	90	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	4-D	114	ARG	Sidechain
3	4-D	176	ARG	Sidechain
3	4-D	243	ARG	Sidechain
3	4-D	247	TYR	Sidechain
3	4-D	256	TYR	Sidechain
3	4-D	315	TYR	Sidechain
3	4-D	329	ARG	Sidechain
3	4-D	344	PHE	Sidechain
3	4-D	362	TYR	Sidechain
3	4-D	407	TYR	Sidechain
3	4-D	423	PHE	Sidechain
3	4-D	62	PHE	Sidechain
3	4-D	86	PHE	Sidechain
1	5-A	111	ARG	Sidechain
1	5-A	121	ARG	Sidechain
1	5-A	138	PHE	Sidechain
1	5-A	140	TYR	Sidechain
1	5-A	144	ARG	Sidechain
1	5-A	203	ARG	Sidechain
1	5-A	279	TYR	Sidechain
1	5-A	296	TYR	Sidechain
1	5-A	302	TYR	Sidechain
1	5-A	327	ARG	Sidechain
1	5-A	349	ARG	Sidechain
1	5-A	393	TYR	Sidechain
1	5-A	409	PHE	Sidechain
1	5-A	559	HIS	Sidechain
1	5-A	623	ARG	Sidechain
1	5-A	627	ARG	Sidechain
1	5-A	767	TYR	Sidechain
1	5-A	92	PHE	Sidechain
2	5-B	190	TYR	Sidechain
2	5-B	328	ARG	Sidechain
2	5-B	400	TYR	Sidechain
2	5-B	570	LEU	Mainchain
2	5-B	742	ALA	Peptide
2	5-B	770	TYR	Sidechain
2	5-B	776	TYR	Sidechain
3	5-C	114	ARG	Sidechain
3	5-C	162	TYR	Sidechain
3	5-C	170	TYR	Sidechain
3	5-C	176	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	5-C	243	ARG	Sidechain
3	5-C	292	TYR	Sidechain
3	5-C	445	TYR	Sidechain
3	5-C	84	ARG	Sidechain
3	5-D	109	TYR	Sidechain
3	5-D	114	ARG	Sidechain
3	5-D	136	PHE	Sidechain
3	5-D	243	ARG	Sidechain
3	5-D	292	TYR	Sidechain
3	5-D	329	ARG	Sidechain
3	5-D	413	PHE	Sidechain
3	5-D	423	PHE	Sidechain
3	5-D	445	TYR	Sidechain
3	5-D	54	PHE	Sidechain
1	6-A	108	ARG	Sidechain
1	6-A	123	TYR	Sidechain
1	6-A	138	PHE	Sidechain
1	6-A	150	TYR	Sidechain
1	6-A	157	ARG	Sidechain
1	6-A	190	TYR	Sidechain
1	6-A	193	TYR	Sidechain
1	6-A	267	PHE	Sidechain
1	6-A	279	TYR	Sidechain
1	6-A	299	PHE	Sidechain
1	6-A	324	TYR	Sidechain
1	6-A	358	ARG	Sidechain
1	6-A	393	TYR	Sidechain
1	6-A	450	TYR	Sidechain
1	6-A	558	TYR	Sidechain
1	6-A	568	TYR	Sidechain
1	6-A	576	ARG	Sidechain
1	6-A	594	TYR	Sidechain
1	6-A	627	ARG	Sidechain
1	6-A	633	HIS	Sidechain
1	6-A	657	TYR	Sidechain
1	6-A	663	TYR	Sidechain
1	6-A	76	ARG	Sidechain
1	6-A	775	PHE	Sidechain
2	6-B	216	PHE	Sidechain
2	6-B	236	TYR	Sidechain
2	6-B	241	PHE	Sidechain
2	6-B	284	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	6-B	293	ARG	Sidechain
2	6-B	295	ARG	Sidechain
2	6-B	297	TYR	Sidechain
2	6-B	299	ARG	Sidechain
2	6-B	322	HIS	Peptide
2	6-B	328	ARG	Sidechain
2	6-B	345	TYR	Sidechain
2	6-B	409	TYR	Sidechain
2	6-B	430	HIS	Sidechain
2	6-B	438	TYR	Sidechain
2	6-B	469	HIS	Sidechain
2	6-B	470	TYR	Sidechain
2	6-B	590	LEU	Mainchain
2	6-B	824	TYR	Sidechain
2	6-B	827	ARG	Sidechain
3	6-C	109	TYR	Sidechain
3	6-C	114	ARG	Sidechain
3	6-C	162	TYR	Sidechain
3	6-C	176	ARG	Sidechain
3	6-C	244	PHE	Sidechain
3	6-C	256	TYR	Sidechain
3	6-C	275	PHE	Sidechain
3	6-C	358	ARG	Sidechain
3	6-C	362	TYR	Sidechain
3	6-C	394	PHE	Sidechain
3	6-C	423	PHE	Sidechain
3	6-C	59	ARG	Sidechain
3	6-D	185	TYR	Sidechain
3	6-D	192	ARG	Sidechain
3	6-D	249	TYR	Sidechain
3	6-D	279	TYR	Sidechain
3	6-D	292	TYR	Sidechain
3	6-D	407	TYR	Sidechain
3	6-D	437	TYR	Sidechain
3	6-D	62	PHE	Sidechain
1	7-A	112	TYR	Sidechain
1	7-A	116	TYR	Sidechain
1	7-A	121	ARG	Sidechain
1	7-A	143	ARG	Sidechain
1	7-A	190	TYR	Sidechain
1	7-A	197	PHE	Sidechain
1	7-A	198	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	7-A	203	ARG	Sidechain
1	7-A	284	TYR	Sidechain
1	7-A	349	ARG	Sidechain
1	7-A	398	TYR	Sidechain
1	7-A	400	ARG	Sidechain
1	7-A	410	PHE	Sidechain
1	7-A	429	TYR	Sidechain
1	7-A	558	TYR	Sidechain
1	7-A	568	TYR	Sidechain
1	7-A	582	TYR	Sidechain
1	7-A	663	TYR	Sidechain
1	7-A	704	TYR	Sidechain
2	7-B	190	TYR	Sidechain
2	7-B	285	ARG	Sidechain
2	7-B	297	TYR	Sidechain
2	7-B	312	PHE	Sidechain
2	7-B	356	ARG	Sidechain
2	7-B	359	TYR	Sidechain
2	7-B	389	ARG	Sidechain
2	7-B	400	TYR	Sidechain
2	7-B	403	PHE	Sidechain
2	7-B	429	TYR	Sidechain
2	7-B	562	TYR	Sidechain
2	7-B	565	TYR	Sidechain
2	7-B	583	TYR	Sidechain
2	7-B	585	ARG	Sidechain
2	7-B	592	ARG	Sidechain
2	7-B	598	TYR	Sidechain
2	7-B	600	TYR	Sidechain
2	7-B	641	PHE	Sidechain
2	7-B	670	ARG	Sidechain
2	7-B	758	TYR	Sidechain
2	7-B	770	TYR	Sidechain
2	7-B	776	TYR	Sidechain
2	7-B	827	ARG	Sidechain
3	7-C	193	ARG	Sidechain
3	7-C	20	PHE	Sidechain
3	7-C	247	TYR	Sidechain
3	7-C	249	TYR	Sidechain
3	7-C	329	ARG	Sidechain
3	7-C	407	TYR	Sidechain
3	7-C	413	PHE	Sidechain

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Mol	Chain	Res	Type	Group
3	7-C	46	ARG	Sidechain
3	7-C	65	ARG	Sidechain
3	7-D	114	ARG	Sidechain
3	7-D	217	PHE	Sidechain
3	7-D	218	ARG	Sidechain
3	7-D	267	PHE	Sidechain
3	7-D	292	TYR	Sidechain
3	7-D	315	TYR	Sidechain
3	7-D	407	TYR	Sidechain
3	7-D	437	TYR	Sidechain
3	7-D	46	ARG	Sidechain
3	7-D	65	ARG	Sidechain
3	7-D	90	ARG	Sidechain
1	8-A	105	PHE	Sidechain
1	8-A	116	TYR	Sidechain
1	8-A	123	TYR	Sidechain
1	8-A	140	TYR	Sidechain
1	8-A	145	PHE	Sidechain
1	8-A	190	TYR	Sidechain
1	8-A	198	ARG	Sidechain
1	8-A	203	ARG	Sidechain
1	8-A	302	TYR	Sidechain
1	8-A	349	ARG	Sidechain
1	8-A	393	TYR	Sidechain
1	8-A	458	TYR	Sidechain
1	8-A	465	PHE	Sidechain
1	8-A	469	ARG	Sidechain
1	8-A	486	PHE	Sidechain
1	8-A	568	TYR	Sidechain
1	8-A	588	TYR	Sidechain
1	8-A	627	ARG	Sidechain
1	8-A	647	PHE	Sidechain
1	8-A	767	TYR	Sidechain
1	8-A	77	TYR	Sidechain
2	8-B	231	TYR	Sidechain
2	8-B	242	ARG	Sidechain
2	8-B	264	TYR	Sidechain
2	8-B	288	TYR	Sidechain
2	8-B	293	ARG	Sidechain
2	8-B	297	TYR	Sidechain
2	8-B	299	ARG	Sidechain
2	8-B	342	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	8-B	359	TYR	Sidechain
2	8-B	429	TYR	Sidechain
2	8-B	430	HIS	Sidechain
2	8-B	433	TYR	Sidechain
2	8-B	438	TYR	Sidechain
2	8-B	453	TYR	Sidechain
2	8-B	470	TYR	Sidechain
2	8-B	475	PHE	Sidechain
2	8-B	510	TYR	Sidechain
2	8-B	514	ARG	Sidechain
2	8-B	544	ARG	Sidechain
2	8-B	558	PHE	Sidechain
2	8-B	583	TYR	Sidechain
2	8-B	585	ARG	Sidechain
2	8-B	592	ARG	Sidechain
2	8-B	644	PHE	Sidechain
2	8-B	670	ARG	Sidechain
2	8-B	758	TYR	Sidechain
2	8-B	805	PHE	Sidechain
2	8-B	816	TYR	Sidechain
3	8-C	217	PHE	Sidechain
3	8-C	247	TYR	Sidechain
3	8-C	256	TYR	Sidechain
3	8-C	319	TYR	Sidechain
3	8-C	344	PHE	Sidechain
3	8-C	387	PHE	Sidechain
3	8-C	394	PHE	Sidechain
3	8-C	407	TYR	Sidechain
3	8-C	55	ARG	Sidechain
3	8-D	109	TYR	Sidechain
3	8-D	176	ARG	Sidechain
3	8-D	243	ARG	Sidechain
3	8-D	247	TYR	Sidechain
3	8-D	272	PHE	Sidechain
3	8-D	315	TYR	Sidechain
3	8-D	316	PHE	Sidechain
3	8-D	329	ARG	Sidechain
3	8-D	333	ARG	Sidechain
3	8-D	359	ARG	Sidechain
3	8-D	362	TYR	Sidechain
3	8-D	427	ARG	Sidechain
3	8-D	445	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	8-D	90	ARG	Sidechain
1	9-A	123	TYR	Sidechain
1	9-A	129	THR	Peptide
1	9-A	190	TYR	Sidechain
1	9-A	203	ARG	Sidechain
1	9-A	279	TYR	Sidechain
1	9-A	302	TYR	Sidechain
1	9-A	405	PHE	Sidechain
1	9-A	451	ARG	Sidechain
1	9-A	458	TYR	Sidechain
1	9-A	568	TYR	Sidechain
1	9-A	588	TYR	Sidechain
1	9-A	594	TYR	Sidechain
1	9-A	597	ARG	Sidechain
1	9-A	624	ARG	Sidechain
1	9-A	646	TYR	Sidechain
1	9-A	657	TYR	Sidechain
1	9-A	664	ARG	Sidechain
1	9-A	77	TYR	Sidechain
1	9-A	791	PHE	Sidechain
2	9-B	187	TYR	Sidechain
2	9-B	264	TYR	Sidechain
2	9-B	328	ARG	Sidechain
2	9-B	342	TYR	Sidechain
2	9-B	345	TYR	Sidechain
2	9-B	359	TYR	Sidechain
2	9-B	385	PHE	Sidechain
2	9-B	438	TYR	Sidechain
2	9-B	544	ARG	Sidechain
2	9-B	562	TYR	Sidechain
2	9-B	600	TYR	Sidechain
2	9-B	651	TYR	Sidechain
2	9-B	776	TYR	Sidechain
2	9-B	816	TYR	Sidechain
2	9-B	826	PHE	Sidechain
3	9-C	173	PHE	Sidechain
3	9-C	217	PHE	Sidechain
3	9-C	315	TYR	Sidechain
3	9-C	319	TYR	Sidechain
3	9-C	407	TYR	Sidechain
3	9-C	445	TYR	Sidechain
3	9-C	87	PHE	Sidechain

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Mol	Chain	Res	Type	Group
3	9-C	90	ARG	Sidechain
3	9-D	162	TYR	Sidechain
3	9-D	170	TYR	Sidechain
3	9-D	176	ARG	Sidechain
3	9-D	249	TYR	Sidechain
3	9-D	315	TYR	Sidechain
3	9-D	319	TYR	Sidechain
3	9-D	353	HIS	Sidechain
3	9-D	387	PHE	Sidechain
3	9-D	394	PHE	Sidechain
3	9-D	407	TYR	Sidechain
3	9-D	445	TYR	Sidechain
3	9-D	59	ARG	Sidechain
3	9-D	62	PHE	Sidechain
3	9-D	90	ARG	Sidechain

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	1-A	4831	0	4863	190	0
1	2-A	4831	0	4863	139	0
1	3-A	4831	0	4863	114	0
1	4-A	4831	0	4862	119	0
1	5-A	4831	0	4863	124	0
1	6-A	4831	0	4862	112	0
1	7-A	4831	0	4863	112	0
1	8-A	4831	0	4862	142	0
1	9-A	4831	0	4863	146	0
1	10-A	4831	0	4863	153	0
2	1-B	4701	0	4727	182	0
2	2-B	4701	0	4731	142	0
2	3-B	4701	0	4731	119	0
2	4-B	4701	0	4729	135	0
2	5-B	4701	0	4729	144	0
2	6-B	4701	0	4729	177	0
2	7-B	4701	0	4729	124	0
2	8-B	4701	0	4731	179	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	9-B	4701	0	4727	123	0
2	10-B	4701	0	4729	134	0
3	1-C	3483	0	3340	46	0
3	1-D	3483	0	3340	37	0
3	2-C	3483	0	3340	40	0
3	2-D	3483	0	3340	48	0
3	3-C	3483	0	3340	50	0
3	3-D	3483	0	3340	40	0
3	4-C	3483	0	3340	53	0
3	4-D	3483	0	3340	42	0
3	5-C	3483	0	3340	32	0
3	5-D	3483	0	3340	50	0
3	6-C	3483	0	3340	26	0
3	6-D	3483	0	3340	62	0
3	7-C	3483	0	3340	31	0
3	7-D	3483	0	3340	46	0
3	8-C	3483	0	3340	23	0
3	8-D	3483	0	3340	44	0
3	9-C	3483	0	3340	28	0
3	9-D	3483	0	3340	40	0
3	10-C	3483	0	3340	44	0
3	10-D	3483	0	3340	27	0
4	1-E	220	0	46	0	0
4	1-F	220	0	46	1	0
4	2-E	220	0	46	0	0
4	2-F	220	0	46	0	0
4	3-E	220	0	46	0	0
4	3-F	220	0	46	1	0
4	4-E	220	0	46	0	0
4	4-F	220	0	46	0	0
4	5-E	220	0	46	0	0
4	5-F	220	0	46	0	0
4	6-E	220	0	46	0	0
4	6-F	220	0	46	0	0
4	7-E	220	0	46	0	0
4	7-F	220	0	46	0	0
4	8-E	220	0	46	0	0
4	8-F	220	0	46	0	0
4	9-E	220	0	46	0	0
4	9-F	220	0	46	0	0
4	10-E	220	0	46	2	0
4	10-F	220	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	169380	0	163639	2991	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 9.

All (2991) 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:68:ILE:HD13	2:B:216:PHE:CG	1.27	1.67
2:B:405:ILE:CG2	2:B:456:ILE:HD12	1.28	1.57
1:A:68:ILE:CD1	2:B:216:PHE:HB3	1.21	1.55
1:A:131:PHE:CE2	2:B:322:HIS:NE2	1.71	1.54
1:A:68:ILE:HD13	2:B:216:PHE:CB	1.30	1.53
1:A:151:LEU:CD2	2:B:285:ARG:HE	1.25	1.50
1:A:68:ILE:CD1	2:B:216:PHE:CB	1.76	1.49
1:A:296:TYR:OH	2:B:322:HIS:CD2	1.70	1.45
2:B:257:ILE:HD12	2:B:297:TYR:CD1	1.51	1.45
1:A:151:LEU:CG	2:B:285:ARG:HD3	1.49	1.41
1:A:151:LEU:HD23	2:B:285:ARG:NH2	1.25	1.40
1:A:65:ASN:HD21	2:B:215:ASN:CB	1.35	1.40
1:A:131:PHE:HE2	2:B:322:HIS:NE2	0.92	1.39
1:A:151:LEU:HD22	2:B:285:ARG:NE	1.33	1.39
2:B:257:ILE:HD12	2:B:297:TYR:CE1	1.59	1.38
2:B:288:TYR:CE2	2:B:292:ILE:HD11	1.57	1.37
2:B:296:ILE:CD1	2:B:327:ILE:HG12	1.52	1.37
2:B:405:ILE:HA	2:B:456:ILE:CD1	1.54	1.36
1:A:152:LYS:HD3	2:B:285:ARG:NH1	1.08	1.36
1:A:158:LEU:HD23	2:B:281:LYS:NZ	1.37	1.36
1:A:566:ILE:CD1	1:A:574:ILE:HD12	1.55	1.36
1:A:151:LEU:HG	2:B:285:ARG:CD	1.53	1.36
1:A:425:ILE:HD11	1:A:482:LEU:CD2	1.51	1.35
1:A:588:TYR:CD1	1:A:693:ILE:HD11	1.61	1.35
1:A:68:ILE:CD1	2:B:281:LYS:HD2	1.54	1.35
1:A:65:ASN:ND2	2:B:215:ASN:CB	1.90	1.34
1:A:365:THR:HG23	1:A:404:ILE:CD1	1.55	1.33
1:A:152:LYS:CD	2:B:285:ARG:NH1	1.91	1.33
1:A:426:PHE:CZ	1:A:564:ILE:HD11	1.62	1.33
2:B:628:ILE:HD12	2:B:780:ASN:ND2	1.38	1.33
2:B:264:TYR:CZ	2:B:287:ILE:HD11	1.61	1.32
1:A:68:ILE:CD1	2:B:216:PHE:CG	2.02	1.32
2:B:634:ILE:HD11	2:B:772:PHE:CE1	1.61	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:HH21	2:B:328:ARG:CZ	1.43	1.31
2:B:586:ILE:CG2	2:B:735:ILE:CD1	2.08	1.31
3:C:199:ASP:O	3:C:260:ILE:HD13	1.23	1.31
1:A:140:TYR:OH	2:B:296:ILE:HD11	1.31	1.31
2:B:335:PHE:CZ	2:B:339:ILE:HD11	1.65	1.31
1:A:140:TYR:OH	2:B:292:ILE:HG22	1.27	1.30
2:B:610:ILE:CD1	3:D:196:GLU:O	1.78	1.30
2:B:586:ILE:HD12	2:B:732:LEU:CD2	1.59	1.30
2:B:349:TRP:HE1	2:B:364:ILE:CD1	1.43	1.30
1:A:152:LYS:HG2	2:B:285:ARG:NH1	1.41	1.30
2:B:412:LEU:CD2	2:B:463:ILE:HD12	1.58	1.30
2:B:335:PHE:CE1	2:B:339:ILE:HD11	1.67	1.30
1:A:65:ASN:ND2	2:B:215:ASN:HB3	1.43	1.29
3:D:256:TYR:CZ	3:D:260:ILE:HD11	1.65	1.29
2:B:405:ILE:CG2	2:B:456:ILE:CD1	2.09	1.28
1:A:70:LEU:O	2:B:216:PHE:CE2	1.86	1.28
3:D:256:TYR:CE1	3:D:260:ILE:HD12	1.68	1.28
3:D:188:ILE:HD12	3:D:394:PHE:CG	1.65	1.28
1:A:140:TYR:OH	2:B:292:ILE:CG2	1.81	1.27
2:B:405:ILE:HG23	2:B:456:ILE:CD1	1.63	1.27
3:D:188:ILE:HD12	3:D:394:PHE:CB	1.63	1.27
1:A:151:LEU:CD2	2:B:285:ARG:HG3	1.64	1.26
2:B:349:TRP:CD1	2:B:364:ILE:HD11	1.70	1.26
1:A:62:ASP:OD1	1:A:94:ILE:HD11	1.27	1.26
1:A:151:LEU:HB3	2:B:285:ARG:NE	1.48	1.25
3:D:119:ILE:CD1	3:D:154:LEU:HD22	1.66	1.25
2:B:209:ILE:HD12	2:B:222:HIS:NE2	1.50	1.25
2:B:184:ILE:HD12	2:B:217:GLU:OE1	1.37	1.25
1:A:136:GLN:NE2	2:B:327:ILE:CD1	1.99	1.25
1:A:147:GLU:OE1	2:B:292:ILE:CD1	1.86	1.24
1:A:74:TYR:CD2	2:B:216:PHE:HZ	1.55	1.24
1:A:570:LEU:CD2	1:A:573:ILE:HD12	1.67	1.24
2:B:586:ILE:HG22	2:B:735:ILE:CD1	1.68	1.24
2:B:349:TRP:CE2	2:B:364:ILE:HD13	1.72	1.24
2:B:412:LEU:HD22	2:B:463:ILE:CD1	1.68	1.24
1:A:70:LEU:HG	2:B:216:PHE:CE1	1.72	1.24
3:D:188:ILE:CD1	3:D:394:PHE:CB	2.16	1.23
2:B:405:ILE:CD1	2:B:453:TYR:HA	1.67	1.23
2:B:610:ILE:HD12	3:D:196:GLU:O	1.35	1.23
1:A:133:MET:CE	2:B:328:ARG:NH2	2.00	1.23
2:B:339:ILE:CD1	2:B:440:GLY:HA3	1.69	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ASN:OD1	2:B:216:PHE:CE1	1.91	1.22
1:A:356:VAL:HG21	1:A:572:ILE:CD1	1.70	1.22
1:A:70:LEU:O	2:B:216:PHE:CD2	1.92	1.22
1:A:458:TYR:CD1	1:A:484:ILE:CD1	2.22	1.22
2:B:586:ILE:HG23	2:B:735:ILE:CD1	1.70	1.22
2:B:586:ILE:HG23	2:B:735:ILE:CD1	1.70	1.21
2:B:349:TRP:NE1	2:B:364:ILE:HD12	1.55	1.21
2:B:493:ILE:CD1	2:B:598:TYR:HB3	1.69	1.21
1:A:138:PHE:CZ	1:A:275:ILE:CD1	2.24	1.21
1:A:138:PHE:CZ	1:A:275:ILE:HD11	1.75	1.21
2:B:297:TYR:CZ	2:B:330:ILE:HD12	1.76	1.21
2:B:825:ILE:HD11	2:B:841:LEU:CD1	1.70	1.20
2:B:241:PHE:CB	2:B:254:ILE:HD13	1.70	1.20
1:A:566:ILE:HD11	1:A:574:ILE:CD1	1.68	1.20
1:A:140:TYR:CZ	2:B:292:ILE:HG21	1.75	1.20
1:A:137:ARG:HE	2:B:325:LEU:CD1	1.54	1.20
1:A:151:LEU:HD23	2:B:285:ARG:CZ	1.72	1.20
1:A:151:LEU:CB	2:B:285:ARG:NE	2.02	1.20
3:C:125:LYS:HG2	3:D:283:ASP:OD1	1.37	1.20
1:A:152:LYS:CG	2:B:285:ARG:HH11	1.55	1.20
3:C:125:LYS:HG3	3:D:283:ASP:OD2	1.37	1.20
1:A:625:ILE:CD1	1:A:764:LEU:HB3	1.71	1.20
1:A:356:VAL:HG21	1:A:572:ILE:HD11	1.24	1.19
2:B:586:ILE:CG2	2:B:735:ILE:CD1	2.21	1.19
2:B:349:TRP:CD1	2:B:364:ILE:CD1	2.26	1.19
2:B:529:MET:CE	2:B:538:ILE:HD11	1.72	1.19
2:B:349:TRP:CD1	2:B:364:ILE:HD11	1.78	1.19
1:A:68:ILE:CD1	1:A:158:LEU:HD21	1.73	1.18
1:A:151:LEU:CD2	2:B:285:ARG:NE	1.92	1.18
3:C:200:ALA:HB2	3:C:260:ILE:HD11	1.21	1.18
3:D:256:TYR:CZ	3:D:260:ILE:CD1	2.27	1.18
1:A:573:ILE:CD1	1:A:673:GLN:HB3	1.72	1.18
1:A:68:ILE:C	2:B:281:LYS:HZ2	1.46	1.18
3:C:188:ILE:CD1	3:C:394:PHE:CG	2.26	1.18
1:A:426:PHE:CE2	1:A:564:ILE:HD13	1.78	1.18
1:A:151:LEU:CD2	2:B:285:ARG:HD2	1.73	1.18
1:A:566:ILE:HD13	1:A:574:ILE:CD1	1.72	1.17
1:A:595:HIS:ND1	1:A:640:ILE:HD13	1.59	1.17
2:B:586:ILE:HD12	2:B:732:LEU:HD22	1.20	1.17
1:A:114:LYS:CE	1:A:118:ILE:HD11	1.73	1.17
2:B:412:LEU:CD2	2:B:463:ILE:CD1	2.22	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:HD21	2:B:285:ARG:CG	1.75	1.17
1:A:154:LEU:HD21	1:A:177:ILE:HD12	1.17	1.17
2:B:586:ILE:HG23	2:B:735:ILE:HD11	1.27	1.17
1:A:151:LEU:CB	2:B:285:ARG:CD	2.22	1.16
2:B:264:TYR:CZ	2:B:287:ILE:CD1	2.28	1.16
1:A:629:THR:HG21	1:A:710:ILE:HD11	1.21	1.16
3:C:212:ILE:HD13	3:C:275:PHE:CZ	1.81	1.16
1:A:138:PHE:CE2	1:A:275:ILE:CD1	2.29	1.16
1:A:147:GLU:OE1	2:B:292:ILE:HD11	1.01	1.16
2:B:398:LEU:CD2	2:B:449:ILE:HD12	1.75	1.16
2:B:586:ILE:HD12	2:B:735:ILE:HD11	1.26	1.15
1:A:558:TYR:HB2	1:A:693:ILE:HD11	1.15	1.15
1:A:137:ARG:NH2	2:B:325:LEU:HD21	1.59	1.15
1:A:136:GLN:NE2	2:B:323:GLY:HA2	1.58	1.15
1:A:73:THR:HG22	2:B:215:ASN:HA	1.29	1.15
3:C:188:ILE:HD12	3:C:394:PHE:CG	1.80	1.15
2:B:188:VAL:HG13	2:B:224:ILE:HD13	1.27	1.15
1:A:70:LEU:CD1	2:B:281:LYS:NZ	2.11	1.14
1:A:70:LEU:HG	2:B:281:LYS:HZ1	1.05	1.14
1:A:573:ILE:HD12	1:A:673:GLN:CB	1.77	1.14
1:A:255:ILE:HD11	1:A:272:LEU:HD22	1.16	1.14
3:D:188:ILE:CD1	3:D:394:PHE:HB3	1.77	1.14
2:B:570:LEU:CD2	2:B:721:ILE:CD1	2.25	1.14
1:A:70:LEU:HD12	2:B:281:LYS:CE	1.77	1.14
3:D:199:ASP:O	3:D:260:ILE:HD13	1.46	1.14
1:A:70:LEU:HD11	2:B:220:LEU:HD11	1.21	1.14
1:A:151:LEU:CB	2:B:285:ARG:HD3	1.76	1.14
2:B:493:ILE:HD13	2:B:598:TYR:HB3	1.20	1.14
2:B:200:PHE:CZ	2:B:207:ILE:HD11	1.81	1.14
1:A:151:LEU:HD12	2:B:285:ARG:HG3	1.27	1.13
1:A:137:ARG:NE	2:B:325:LEU:HD11	1.63	1.13
1:A:138:PHE:CD2	1:A:275:ILE:HD11	1.82	1.13
3:C:200:ALA:HB2	3:C:260:ILE:HD11	1.22	1.13
1:A:70:LEU:CG	2:B:216:PHE:CE1	2.31	1.13
1:A:66:VAL:HB	1:A:94:ILE:HD12	1.30	1.13
1:A:142:ILE:HD12	1:A:189:LEU:HG	1.17	1.13
1:A:438:PHE:CZ	1:A:484:ILE:HD12	1.83	1.13
2:B:412:LEU:CD1	2:B:463:ILE:HD12	1.77	1.13
3:D:210:LEU:HD22	3:D:222:ILE:CD1	1.77	1.13
1:A:426:PHE:CZ	1:A:564:ILE:CD1	2.30	1.13
1:A:131:PHE:CE2	2:B:322:HIS:CD2	2.35	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:571:VAL:CG2	2:B:721:ILE:HD11	1.77	1.13
3:D:210:LEU:CD2	3:D:222:ILE:HD11	1.77	1.12
1:A:137:ARG:HE	2:B:325:LEU:HD11	1.08	1.12
2:B:209:ILE:HD11	2:B:218:SER:HB3	1.15	1.12
1:A:137:ARG:HH21	2:B:328:ARG:NH2	1.47	1.12
2:B:339:ILE:HD13	2:B:440:GLY:HA3	1.22	1.12
1:A:195:GLU:HG3	1:A:250:ILE:HD13	1.25	1.12
2:B:405:ILE:CD1	2:B:456:ILE:HD12	1.79	1.12
1:A:367:PRO:HB3	1:A:404:ILE:HD13	1.19	1.12
2:B:418:GLU:OE2	2:B:463:ILE:HD11	1.50	1.12
1:A:570:LEU:HD22	1:A:573:ILE:HD12	1.25	1.12
2:B:241:PHE:HB3	2:B:254:ILE:CD1	1.80	1.11
3:D:210:LEU:HD11	3:D:222:ILE:HD11	1.31	1.11
2:B:570:LEU:CD2	2:B:721:ILE:HD12	1.78	1.11
1:A:70:LEU:HG	2:B:281:LYS:NZ	1.64	1.11
2:B:480:ILE:HD11	2:B:537:VAL:CG2	1.80	1.11
1:A:438:PHE:CE2	1:A:484:ILE:HD12	1.84	1.11
2:B:412:LEU:HD22	2:B:463:ILE:HD13	1.32	1.11
2:B:570:LEU:HD23	2:B:721:ILE:HD12	1.21	1.11
3:D:256:TYR:CE1	3:D:260:ILE:HD12	1.85	1.11
1:A:151:LEU:HD22	2:B:285:ARG:CD	1.80	1.11
1:A:640:ILE:HD13	1:A:696:GLN:NE2	1.65	1.11
2:B:586:ILE:HD12	2:B:735:ILE:CD1	1.80	1.11
1:A:128:ASP:HA	2:B:322:HIS:CE1	1.85	1.11
2:B:482:LEU:HD22	2:B:735:ILE:CD1	1.79	1.11
2:B:383:ILE:HD12	2:B:410:ILE:CD1	1.79	1.10
1:A:63:LEU:HB3	1:A:170:ILE:CD1	1.81	1.10
2:B:257:ILE:CD1	2:B:297:TYR:CD1	2.32	1.10
1:A:70:LEU:HD13	2:B:220:LEU:HD22	1.27	1.10
1:A:66:VAL:HG22	2:B:216:PHE:HE1	1.15	1.10
1:A:425:ILE:CD1	1:A:482:LEU:HD22	1.80	1.10
2:B:342:TYR:HE2	2:B:394:ILE:HD11	1.06	1.10
1:A:70:LEU:HD12	2:B:281:LYS:HE2	1.32	1.10
1:A:133:MET:HE1	2:B:328:ARG:NH2	1.64	1.10
3:D:356:ILE:HD13	3:D:358:ARG:HH12	1.12	1.10
2:B:405:ILE:HG23	2:B:456:ILE:CD1	1.80	1.10
3:D:188:ILE:HD12	3:D:394:PHE:CD1	1.86	1.10
1:A:585:ILE:HD11	1:A:683:ILE:HG12	1.14	1.10
3:C:121:ASN:ND2	3:D:218:ARG:HH12	1.49	1.10
2:B:241:PHE:HB3	2:B:254:ILE:HD13	1.24	1.09
1:A:130:SER:OG	2:B:322:HIS:ND1	1.85	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:ILE:CD1	2:B:297:TYR:CE2	2.33	1.09
1:A:70:LEU:HG	2:B:216:PHE:CZ	1.88	1.09
2:B:296:ILE:HD12	2:B:327:ILE:HG12	1.14	1.09
1:A:570:LEU:HD23	1:A:573:ILE:HD12	1.30	1.09
2:B:209:ILE:CD1	2:B:218:SER:HB3	1.82	1.09
1:A:133:MET:HE1	2:B:328:ARG:HH22	0.93	1.09
2:B:586:ILE:CG2	2:B:735:ILE:HD13	1.80	1.09
3:C:195:ILE:HD13	3:C:423:PHE:HE1	1.08	1.09
3:D:188:ILE:HD12	3:D:394:PHE:CG	1.86	1.09
1:A:573:ILE:HD12	1:A:673:GLN:HB3	1.14	1.09
1:A:255:ILE:HD11	1:A:272:LEU:CD2	1.83	1.09
2:B:586:ILE:CG2	2:B:735:ILE:HD13	1.80	1.09
2:B:402:ILE:HD11	2:B:449:ILE:HD11	1.11	1.08
1:A:65:ASN:HB3	2:B:216:PHE:CE1	1.87	1.08
3:D:204:PHE:HE2	3:D:234:ILE:HD12	1.15	1.08
3:D:210:LEU:HD22	3:D:222:ILE:HD11	1.24	1.08
2:B:209:ILE:HD11	2:B:218:SER:HB3	1.29	1.08
3:D:200:ALA:HB2	3:D:260:ILE:HD11	1.32	1.08
1:A:599:LEU:HD22	1:A:640:ILE:HD12	1.33	1.08
1:A:438:PHE:CZ	1:A:484:ILE:HD13	1.86	1.08
2:B:209:ILE:HD13	2:B:222:HIS:CD2	1.88	1.08
1:A:566:ILE:HD12	1:A:574:ILE:HG23	1.36	1.08
1:A:151:LEU:CD2	2:B:285:ARG:NH2	2.16	1.08
2:B:209:ILE:HD11	2:B:218:SER:CB	1.84	1.08
1:A:426:PHE:CE2	1:A:564:ILE:CD1	2.37	1.08
1:A:640:ILE:HD13	1:A:696:GLN:HE22	0.97	1.08
3:D:119:ILE:CD1	3:D:154:LEU:CD2	2.31	1.08
1:A:151:LEU:HD12	2:B:285:ARG:CG	1.68	1.08
1:A:151:LEU:CD2	2:B:285:ARG:CZ	2.31	1.08
1:A:566:ILE:HD13	1:A:571:ASN:HB3	1.30	1.08
2:B:610:ILE:HD11	3:D:196:GLU:O	1.52	1.08
2:B:405:ILE:HG23	2:B:456:ILE:HD12	1.17	1.08
2:B:257:ILE:HD11	2:B:297:TYR:CE2	1.86	1.08
1:A:138:PHE:CZ	1:A:275:ILE:HD12	1.89	1.08
1:A:625:ILE:HD11	1:A:764:LEU:HB3	1.16	1.08
2:B:335:PHE:CE2	2:B:339:ILE:HD11	1.87	1.08
1:A:152:LYS:CD	2:B:285:ARG:HH12	1.58	1.07
1:A:584:ILE:HD12	1:A:687:ARG:HD2	1.29	1.07
2:B:402:ILE:HD11	2:B:449:ILE:HD11	1.34	1.07
1:A:74:TYR:HD2	2:B:216:PHE:CZ	1.70	1.07
1:A:70:LEU:HD12	2:B:220:LEU:CD1	1.83	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:212:ILE:HD13	3:C:275:PHE:CZ	1.89	1.07
1:A:68:ILE:HD11	2:B:216:PHE:CD1	1.90	1.07
1:A:363:ILE:HD13	1:A:413:TYR:HB2	1.36	1.07
3:D:188:ILE:HD11	3:D:394:PHE:HB2	1.14	1.07
1:A:137:ARG:NH2	2:B:328:ARG:CZ	2.18	1.07
3:D:97:ASP:O	3:D:111:ILE:HD12	1.52	1.07
1:A:584:ILE:HD12	1:A:687:ARG:HG3	1.34	1.07
2:B:405:ILE:HD12	2:B:453:TYR:HA	1.13	1.06
1:A:425:ILE:CD1	1:A:482:LEU:CD2	2.32	1.06
1:A:458:TYR:CD1	1:A:484:ILE:HD11	1.90	1.06
2:B:527:HIS:CE1	2:B:538:ILE:CD1	2.38	1.06
3:D:188:ILE:CD1	3:D:394:PHE:CG	2.36	1.06
3:D:258:THR:HG23	3:D:356:ILE:CD1	1.84	1.06
1:A:70:LEU:HD11	2:B:220:LEU:CD1	1.84	1.06
1:A:438:PHE:CE2	1:A:484:ILE:CD1	2.37	1.06
2:B:480:ILE:HD11	2:B:537:VAL:HG21	1.36	1.06
2:B:493:ILE:HD12	2:B:598:TYR:CD2	1.89	1.06
1:A:136:GLN:HE22	2:B:327:ILE:HD13	1.14	1.06
2:B:405:ILE:HD13	2:B:452:GLN:HB3	1.38	1.06
2:B:636:ILE:HD11	3:D:437:TYR:CZ	1.89	1.06
2:B:628:ILE:CD1	2:B:780:ASN:ND2	2.17	1.06
3:D:188:ILE:HD12	3:D:394:PHE:HB2	1.37	1.06
1:A:151:LEU:HD21	2:B:285:ARG:HG3	1.10	1.06
1:A:138:PHE:CZ	1:A:275:ILE:CD1	2.39	1.05
2:B:656:ILE:HD13	2:B:738:HIS:NE2	1.71	1.05
2:B:739:LYS:O	2:B:743:THR:O	1.75	1.05
1:A:367:PRO:CB	1:A:404:ILE:HD13	1.85	1.05
1:A:133:MET:HE3	2:B:328:ARG:NH2	1.65	1.05
1:A:136:GLN:NE2	2:B:327:ILE:HD13	1.66	1.05
2:B:355:LEU:CD2	2:B:364:ILE:HD12	1.85	1.05
2:B:349:TRP:HE1	2:B:364:ILE:HD12	0.89	1.05
2:B:355:LEU:O	2:B:364:ILE:HD12	1.57	1.05
1:A:138:PHE:CE1	1:A:275:ILE:HD12	1.91	1.05
3:D:204:PHE:CE2	3:D:234:ILE:HD12	1.91	1.05
3:D:200:ALA:HB2	3:D:260:ILE:HD11	1.36	1.05
1:A:68:ILE:HD12	2:B:281:LYS:HD2	1.34	1.05
3:D:200:ALA:HB2	3:D:260:ILE:HD11	1.31	1.05
2:B:394:ILE:HD13	2:B:445:PHE:CE2	1.92	1.04
2:B:402:ILE:CD1	2:B:449:ILE:HD11	1.85	1.04
2:B:586:ILE:HG23	2:B:735:ILE:HD13	1.06	1.04
2:B:349:TRP:NE1	2:B:364:ILE:CD1	2.21	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:HB2	2:B:285:ARG:CD	1.86	1.04
3:D:256:TYR:CE1	3:D:260:ILE:HD11	1.91	1.04
2:B:586:ILE:CG2	2:B:735:ILE:HD11	1.86	1.04
3:C:195:ILE:HD13	3:C:423:PHE:CE1	1.91	1.04
1:A:65:ASN:HD21	2:B:215:ASN:CG	1.59	1.04
2:B:405:ILE:HG22	2:B:456:ILE:CD1	1.84	1.04
1:A:128:ASP:HA	2:B:322:HIS:NE2	1.72	1.04
1:A:144:ARG:CZ	2:B:289:GLU:OE2	2.06	1.04
3:D:210:LEU:CD2	3:D:222:ILE:HD11	1.87	1.04
1:A:151:LEU:HB3	2:B:285:ARG:HE	0.88	1.03
1:A:566:ILE:HD11	1:A:574:ILE:HD12	1.04	1.03
1:A:363:ILE:CD1	1:A:413:TYR:HB2	1.88	1.03
2:B:412:LEU:HD23	2:B:463:ILE:HD12	1.36	1.03
3:C:256:TYR:CE2	3:C:260:ILE:HD12	1.93	1.03
2:B:264:TYR:CE1	2:B:287:ILE:HD11	1.93	1.03
2:B:482:LEU:HD22	2:B:735:ILE:HD11	1.36	1.03
1:A:114:LYS:HE3	1:A:118:ILE:CD1	1.88	1.03
1:A:68:ILE:CD1	2:B:216:PHE:CD1	2.40	1.03
2:B:570:LEU:HD23	2:B:721:ILE:CD1	1.84	1.03
1:A:130:SER:OG	2:B:322:HIS:CE1	2.12	1.03
2:B:586:ILE:CD1	2:B:732:LEU:CD2	2.36	1.03
1:A:625:ILE:CD1	1:A:764:LEU:CB	2.36	1.03
2:B:412:LEU:HD21	2:B:463:ILE:HD12	1.40	1.03
2:B:402:ILE:HG13	2:B:449:ILE:HD13	1.35	1.03
1:A:558:TYR:CB	1:A:693:ILE:HD11	1.89	1.03
1:A:641:LYS:HD2	3:C:356:ILE:CD1	1.89	1.02
2:B:493:ILE:CD1	2:B:598:TYR:CB	2.36	1.02
1:A:195:GLU:CD	1:A:250:ILE:CD1	2.27	1.02
1:A:68:ILE:HD11	2:B:281:LYS:HD2	1.37	1.02
2:B:586:ILE:CD1	2:B:735:ILE:HD11	1.87	1.02
2:B:335:PHE:HE1	2:B:339:ILE:HD11	1.03	1.02
1:A:567:PRO:HD2	1:A:574:ILE:HD13	1.39	1.02
2:B:405:ILE:HA	2:B:456:ILE:HD12	1.42	1.02
2:B:480:ILE:HD13	2:B:541:LEU:HD11	1.39	1.02
1:A:61:LYS:HE3	2:B:216:PHE:HE1	1.17	1.02
1:A:595:HIS:ND1	1:A:640:ILE:CD1	2.23	1.02
1:A:199:GLU:CD	1:A:250:ILE:HD12	1.80	1.02
1:A:70:LEU:CD1	2:B:281:LYS:HZ3	1.72	1.02
2:B:656:ILE:CD1	2:B:738:HIS:CE1	2.43	1.02
1:A:158:LEU:CD2	2:B:281:LYS:NZ	2.21	1.02
2:B:335:PHE:CE2	2:B:339:ILE:HD11	1.95	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:THR:CG2	2:B:207:ILE:HD13	1.89	1.02
3:D:188:ILE:CD1	3:D:394:PHE:CG	2.43	1.02
2:B:527:HIS:CE1	2:B:538:ILE:HD12	1.93	1.02
3:C:188:ILE:HD12	3:C:394:PHE:CG	1.94	1.01
2:B:412:LEU:CD1	2:B:463:ILE:CD1	2.37	1.01
1:A:155:VAL:HG11	2:B:285:ARG:HH11	1.25	1.01
2:B:405:ILE:HD11	2:B:456:ILE:CD1	1.89	1.01
3:C:121:ASN:HD21	3:D:218:ARG:NH1	1.57	1.01
2:B:234:LEU:HD22	2:B:257:ILE:HD11	1.43	1.01
2:B:349:TRP:CD2	2:B:364:ILE:HD13	1.96	1.01
2:B:586:ILE:HD12	2:B:732:LEU:HD23	1.41	1.01
1:A:68:ILE:O	2:B:281:LYS:NZ	1.94	1.01
1:A:142:ILE:HD12	1:A:189:LEU:CG	1.89	1.01
2:B:570:LEU:HD22	2:B:721:ILE:CD1	1.91	1.01
2:B:739:LYS:O	2:B:743:THR:O	1.79	1.01
2:B:257:ILE:CD1	2:B:297:TYR:CE1	2.44	1.01
1:A:595:HIS:CE1	1:A:640:ILE:HD13	1.95	1.01
3:C:121:ASN:ND2	3:D:218:ARG:NH1	2.09	1.01
1:A:65:ASN:HD21	2:B:215:ASN:HB3	0.97	1.00
1:A:356:VAL:CG2	1:A:572:ILE:HD11	1.90	1.00
1:A:154:LEU:HD23	2:B:281:LYS:NZ	1.75	1.00
3:D:256:TYR:CE1	3:D:260:ILE:HD12	1.96	1.00
3:C:258:THR:CG2	3:C:356:ILE:CD1	2.39	1.00
3:D:95:ALA:HB1	3:D:111:ILE:HD11	1.42	1.00
2:B:264:TYR:CE2	2:B:287:ILE:HD11	1.96	1.00
2:B:527:HIS:HE1	2:B:538:ILE:HD11	1.25	1.00
2:B:191:THR:HG23	2:B:207:ILE:HD13	1.43	1.00
1:A:570:LEU:CD2	1:A:573:ILE:HD12	1.90	1.00
2:B:656:ILE:HD13	2:B:738:HIS:CE1	1.96	1.00
1:A:66:VAL:HG21	1:A:94:ILE:HD13	1.39	1.00
1:A:74:TYR:CD2	2:B:216:PHE:CZ	2.46	1.00
2:B:349:TRP:CD2	2:B:364:ILE:HD13	1.97	1.00
1:A:625:ILE:HD11	1:A:764:LEU:CB	1.92	0.99
3:C:200:ALA:HB2	3:C:260:ILE:HD11	1.43	0.99
3:C:188:ILE:CD1	3:C:394:PHE:CD2	2.44	0.99
1:A:123:TYR:HE1	2:B:295:ARG:NH2	1.58	0.99
1:A:138:PHE:CD2	1:A:192:ILE:CD1	2.45	0.99
3:D:200:ALA:HA	3:D:260:ILE:HD11	1.38	0.99
2:B:184:ILE:CD1	2:B:217:GLU:OE1	2.10	0.99
1:A:426:PHE:CE1	1:A:564:ILE:HD11	1.96	0.99
2:B:383:ILE:HD12	2:B:410:ILE:HD13	1.42	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:355:LEU:HD21	2:B:364:ILE:CD1	1.92	0.99
3:C:5:ILE:HD11	3:C:252:MET:HG3	1.44	0.99
2:B:586:ILE:HG21	2:B:735:ILE:CD1	1.87	0.99
3:C:200:ALA:HB2	3:C:260:ILE:CD1	1.92	0.99
3:C:256:TYR:CE1	3:C:260:ILE:HD12	1.97	0.99
1:A:356:VAL:CG2	1:A:572:ILE:HD11	1.92	0.99
1:A:640:ILE:HD11	1:A:699:ILE:CD1	1.93	0.99
2:B:349:TRP:CE2	2:B:364:ILE:HD13	1.98	0.99
1:A:623:ARG:CZ	1:A:761:ILE:HD11	1.93	0.99
1:A:138:PHE:CE2	1:A:275:ILE:HD13	1.98	0.99
3:C:342:ILE:HD13	3:C:344:PHE:CZ	1.98	0.99
1:A:138:PHE:CE1	1:A:275:ILE:HD11	1.97	0.99
1:A:144:ARG:NH2	2:B:288:TYR:CD2	2.31	0.99
1:A:109:ILE:HD11	1:A:174:GLU:OE1	1.61	0.99
3:C:256:TYR:CE1	3:C:260:ILE:CD1	2.46	0.98
1:A:66:VAL:CG2	2:B:216:PHE:HE1	1.76	0.98
2:B:586:ILE:HG23	2:B:735:ILE:CD1	1.93	0.98
3:D:200:ALA:HB2	3:D:260:ILE:HD11	1.43	0.98
1:A:70:LEU:CD1	2:B:216:PHE:CZ	2.46	0.98
3:C:255:ILE:HD13	3:C:358:ARG:HD3	1.43	0.98
2:B:586:ILE:HG23	2:B:735:ILE:HD13	1.01	0.98
1:A:65:ASN:CB	2:B:216:PHE:CE1	2.46	0.98
2:B:349:TRP:NE1	2:B:364:ILE:HD11	1.78	0.98
1:A:70:LEU:HB3	2:B:219:GLY:HA3	1.43	0.98
2:B:288:TYR:CE2	2:B:292:ILE:CD1	2.46	0.98
2:B:398:LEU:HD23	2:B:449:ILE:HD12	1.45	0.98
3:C:256:TYR:CD2	3:C:260:ILE:HD12	1.99	0.98
3:D:256:TYR:CE1	3:D:260:ILE:CD1	2.46	0.98
2:B:296:ILE:CD1	2:B:327:ILE:CG1	2.41	0.98
2:B:405:ILE:CA	2:B:456:ILE:CD1	2.41	0.98
1:A:641:LYS:CD	3:C:356:ILE:CD1	2.41	0.98
3:C:188:ILE:HD11	3:C:394:PHE:CB	1.92	0.98
3:C:258:THR:HG21	3:C:356:ILE:HD13	1.44	0.98
1:A:70:LEU:CG	2:B:281:LYS:HZ1	1.77	0.98
3:D:210:LEU:HD11	3:D:222:ILE:CD1	1.94	0.98
1:A:425:ILE:HD13	1:A:478:MET:HA	1.45	0.98
2:B:571:VAL:HG23	2:B:721:ILE:HD11	1.46	0.97
1:A:629:THR:OG1	1:A:710:ILE:HD12	1.64	0.97
3:C:121:ASN:HD21	3:D:218:ARG:HH12	1.09	0.97
1:A:70:LEU:HB2	2:B:216:PHE:HE1	1.26	0.97
2:B:342:TYR:CE2	2:B:394:ILE:HD11	1.97	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:ILE:CD1	2:B:222:HIS:NE2	2.26	0.97
2:B:402:ILE:HD11	2:B:449:ILE:CD1	1.94	0.97
1:A:133:MET:CE	2:B:328:ARG:HH22	1.63	0.97
1:A:73:THR:H	2:B:215:ASN:HB3	1.27	0.97
1:A:68:ILE:O	2:B:216:PHE:CE2	2.18	0.97
2:B:586:ILE:HD13	2:B:732:LEU:HD23	1.45	0.97
1:A:70:LEU:CG	2:B:281:LYS:NZ	2.27	0.97
1:A:70:LEU:HD11	2:B:281:LYS:HZ3	1.27	0.97
1:A:425:ILE:CD1	1:A:482:LEU:CD1	2.41	0.97
3:C:212:ILE:HD13	3:C:275:PHE:CE1	1.98	0.97
1:A:151:LEU:HG	2:B:285:ARG:CG	1.94	0.97
1:A:66:VAL:HG22	2:B:216:PHE:CE1	2.00	0.97
2:B:568:LEU:HA	2:B:721:ILE:HD12	1.47	0.97
1:A:147:GLU:CD	2:B:292:ILE:HD11	1.85	0.97
1:A:199:GLU:OE1	1:A:250:ILE:HD12	1.64	0.97
2:B:288:TYR:HE2	2:B:292:ILE:HD11	1.26	0.97
2:B:296:ILE:HD11	2:B:327:ILE:HG12	1.45	0.97
1:A:137:ARG:NE	2:B:325:LEU:CD1	2.25	0.97
2:B:634:ILE:HD11	2:B:772:PHE:CZ	1.99	0.97
2:B:772:PHE:CE1	2:B:812:ILE:HD12	2.00	0.97
2:B:412:LEU:HD12	2:B:463:ILE:HD12	1.42	0.97
2:B:296:ILE:HD11	2:B:327:ILE:HG23	1.44	0.96
3:C:125:LYS:CG	3:D:283:ASP:OD2	2.12	0.96
1:A:68:ILE:HD12	2:B:216:PHE:CB	1.61	0.96
2:B:412:LEU:CD2	2:B:463:ILE:CD1	2.42	0.96
3:D:188:ILE:CD1	3:D:394:PHE:HB2	1.95	0.96
1:A:135:LEU:CD2	1:A:247:ILE:CD1	2.43	0.96
1:A:65:ASN:OD1	2:B:216:PHE:CD1	2.18	0.96
1:A:640:ILE:CD1	1:A:696:GLN:HE22	1.78	0.96
2:B:586:ILE:HG22	2:B:735:ILE:HD12	1.45	0.96
3:C:275:PHE:H	3:C:284:ILE:CD1	1.78	0.96
1:A:73:THR:CG2	2:B:215:ASN:HD22	1.78	0.96
2:B:586:ILE:CG2	2:B:735:ILE:CD1	2.42	0.96
1:A:365:THR:HG23	1:A:404:ILE:HD13	1.44	0.96
1:A:140:TYR:CZ	2:B:292:ILE:CG2	2.44	0.96
1:A:599:LEU:CD1	1:A:640:ILE:HD11	1.95	0.96
1:A:566:ILE:CD1	1:A:574:ILE:HD12	1.96	0.96
3:D:210:LEU:HD12	3:D:222:ILE:HD11	1.47	0.96
2:B:257:ILE:HD13	2:B:297:TYR:CZ	2.01	0.96
2:B:241:PHE:HB3	2:B:254:ILE:CD1	1.96	0.96
1:A:570:LEU:HD23	1:A:573:ILE:HD12	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:LEU:HD23	1:A:573:ILE:HD12	1.47	0.96
2:B:529:MET:HE1	2:B:538:ILE:HD11	1.45	0.96
2:B:656:ILE:CD1	2:B:738:HIS:NE2	2.27	0.96
2:B:209:ILE:HD11	2:B:222:HIS:NE2	1.79	0.96
2:B:394:ILE:CD1	2:B:445:PHE:CE2	2.49	0.95
1:A:566:ILE:CD1	1:A:574:ILE:HG23	1.95	0.95
2:B:825:ILE:HD11	2:B:841:LEU:HD12	1.44	0.95
1:A:195:GLU:HG3	1:A:250:ILE:CD1	1.94	0.95
2:B:402:ILE:CG1	2:B:449:ILE:HD13	1.96	0.95
2:B:527:HIS:HE1	2:B:538:ILE:CD1	1.73	0.95
2:B:241:PHE:CB	2:B:254:ILE:CD1	2.42	0.95
1:A:438:PHE:HZ	1:A:484:ILE:HD13	1.21	0.95
1:A:138:PHE:CD2	1:A:275:ILE:CD1	2.46	0.95
2:B:405:ILE:HG22	2:B:456:ILE:HD12	1.44	0.95
1:A:62:ASP:OD1	1:A:94:ILE:CD1	2.13	0.95
2:B:634:ILE:HD12	2:B:809:LEU:CD2	1.97	0.95
1:A:151:LEU:CD2	2:B:285:ARG:HH21	1.74	0.95
3:D:199:ASP:O	3:D:260:ILE:HD13	1.67	0.95
2:B:188:VAL:HG13	2:B:224:ILE:HD13	1.45	0.95
2:B:412:LEU:CD2	2:B:463:ILE:HD13	1.90	0.95
3:D:212:ILE:HD11	3:D:302:SER:O	1.67	0.95
1:A:66:VAL:CG2	2:B:216:PHE:CE1	2.50	0.94
2:B:586:ILE:CD1	2:B:732:LEU:HD23	1.96	0.94
1:A:70:LEU:CB	2:B:216:PHE:CE1	2.50	0.94
2:B:209:ILE:HD12	2:B:222:HIS:CE1	2.02	0.94
3:D:119:ILE:HD12	3:D:154:LEU:HD22	1.49	0.94
1:A:70:LEU:CD1	2:B:281:LYS:CE	2.44	0.94
3:D:188:ILE:HD12	3:D:394:PHE:HB2	1.48	0.94
1:A:564:ILE:HD12	1:A:582:TYR:CD2	2.01	0.94
2:B:586:ILE:CD1	2:B:732:LEU:HD23	1.95	0.94
3:D:127:ILE:HD13	3:D:162:TYR:CZ	2.02	0.94
3:D:188:ILE:CD1	3:D:394:PHE:CG	2.50	0.94
3:D:127:ILE:CD1	3:D:161:ARG:HH12	1.81	0.94
3:C:255:ILE:CD1	3:C:358:ARG:CZ	2.44	0.94
1:A:366:ILE:N	1:A:404:ILE:HD11	1.80	0.94
1:A:774:ILE:HD12	1:A:796:SER:CB	1.97	0.94
1:A:70:LEU:HD12	2:B:220:LEU:HD11	1.49	0.94
1:A:696:GLN:HE21	1:A:699:ILE:HD12	1.33	0.94
1:A:696:GLN:NE2	1:A:699:ILE:HD12	1.82	0.94
1:A:458:TYR:CD1	1:A:484:ILE:HD13	2.02	0.94
1:A:137:ARG:CZ	2:B:325:LEU:HD11	1.98	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:ILE:HD12	2:B:327:ILE:CD1	1.97	0.94
1:A:131:PHE:CD2	2:B:322:HIS:NE2	2.36	0.94
1:A:137:ARG:NH2	2:B:325:LEU:HD11	1.83	0.94
1:A:643:ILE:HD13	1:A:692:LEU:HD23	1.50	0.94
1:A:365:THR:HG23	1:A:404:ILE:HD12	1.47	0.94
1:A:588:TYR:CD1	1:A:693:ILE:CD1	2.51	0.94
1:A:135:LEU:HD21	1:A:247:ILE:HD11	1.48	0.93
3:D:188:ILE:HD13	3:D:394:PHE:CD2	2.02	0.93
1:A:581:LYS:HB3	1:A:683:ILE:HD12	1.50	0.93
2:B:241:PHE:HB3	2:B:254:ILE:HD11	1.49	0.93
2:B:349:TRP:CD1	2:B:364:ILE:CD1	2.50	0.93
2:B:570:LEU:HD22	2:B:721:ILE:HD13	1.50	0.93
3:D:210:LEU:HD22	3:D:222:ILE:HD11	1.49	0.93
2:B:586:ILE:CG2	2:B:735:ILE:HD13	1.96	0.93
1:A:362:GLN:NE2	2:B:447:GLU:CG	2.31	0.93
1:A:585:ILE:HD11	1:A:683:ILE:CG1	1.99	0.93
1:A:425:ILE:HD13	1:A:482:LEU:HD11	1.51	0.93
1:A:65:ASN:HB3	2:B:216:PHE:CZ	2.03	0.93
1:A:367:PRO:HG3	1:A:404:ILE:HD12	1.50	0.93
1:A:151:LEU:HG	2:B:285:ARG:HD3	0.94	0.93
2:B:349:TRP:CE2	2:B:364:ILE:CD1	2.52	0.93
1:A:70:LEU:CD1	2:B:220:LEU:CD2	2.46	0.93
2:B:586:ILE:HG21	2:B:735:ILE:CD1	1.97	0.93
3:D:210:LEU:CD1	3:D:222:ILE:HD11	1.99	0.92
2:B:349:TRP:CG	2:B:364:ILE:CD1	2.51	0.92
1:A:70:LEU:HD13	2:B:220:LEU:CD2	1.97	0.92
2:B:586:ILE:HG21	2:B:735:ILE:HD12	1.52	0.92
2:B:405:ILE:HD11	2:B:456:ILE:HD12	0.96	0.92
1:A:356:VAL:HG21	1:A:572:ILE:HD11	0.96	0.92
1:A:73:THR:HG22	2:B:215:ASN:CA	1.95	0.92
1:A:65:ASN:OD1	2:B:216:PHE:HE1	1.40	0.92
2:B:480:ILE:CD1	2:B:537:VAL:HG22	1.99	0.92
1:A:158:LEU:HD23	2:B:281:LYS:HZ1	0.94	0.92
1:A:123:TYR:CE1	2:B:295:ARG:NH2	2.36	0.92
1:A:367:PRO:CB	1:A:404:ILE:CD1	2.47	0.92
2:B:636:ILE:HD13	3:D:442:GLN:OE1	1.69	0.92
2:B:482:LEU:CD2	2:B:735:ILE:CD1	2.47	0.92
2:B:257:ILE:HD11	2:B:297:TYR:CZ	2.04	0.92
1:A:68:ILE:HG13	2:B:281:LYS:NZ	1.85	0.92
1:A:202:GLU:O	1:A:205:THR:O	1.88	0.92
1:A:70:LEU:CD1	2:B:281:LYS:HE2	2.00	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:405:ILE:HG23	2:B:456:ILE:HD12	1.49	0.92
1:A:438:PHE:CZ	1:A:484:ILE:CD1	2.52	0.92
2:B:586:ILE:HG12	2:B:735:ILE:HD12	1.47	0.92
1:A:458:TYR:CE1	1:A:484:ILE:CD1	2.52	0.92
1:A:195:GLU:CG	1:A:250:ILE:HD13	1.99	0.92
2:B:586:ILE:CG2	2:B:735:ILE:HD12	1.99	0.92
1:A:73:THR:HG23	2:B:215:ASN:HD22	1.34	0.92
3:D:188:ILE:CD1	3:D:394:PHE:CG	2.52	0.92
2:B:570:LEU:HD22	2:B:721:ILE:CD1	1.99	0.92
1:A:70:LEU:CD1	2:B:216:PHE:HZ	1.83	0.92
1:A:367:PRO:HB3	1:A:404:ILE:CD1	1.99	0.92
1:A:566:ILE:CD1	1:A:574:ILE:CD1	2.47	0.92
1:A:699:ILE:HD11	1:A:782:PHE:HE2	1.35	0.91
2:B:405:ILE:HG23	2:B:456:ILE:HD12	0.92	0.91
3:C:212:ILE:CD1	3:C:275:PHE:CZ	2.54	0.91
1:A:135:LEU:HD21	1:A:247:ILE:CD1	2.00	0.91
3:D:188:ILE:CD1	3:D:394:PHE:HB3	1.97	0.91
3:D:200:ALA:CA	3:D:260:ILE:HD11	1.99	0.91
2:B:296:ILE:CD1	2:B:327:ILE:HG12	1.98	0.91
3:C:6:ILE:HD12	3:C:127:ILE:HG12	1.52	0.91
3:D:210:LEU:CD1	3:D:222:ILE:HD11	2.00	0.91
1:A:131:PHE:CE2	2:B:322:HIS:CE1	2.57	0.91
2:B:241:PHE:HB3	2:B:254:ILE:CD1	1.99	0.91
1:A:425:ILE:HD11	1:A:482:LEU:HD22	0.92	0.91
1:A:131:PHE:CD2	2:B:322:HIS:CE1	2.58	0.91
1:A:425:ILE:HD13	1:A:482:LEU:CD1	1.98	0.91
1:A:66:VAL:CB	1:A:94:ILE:HD12	2.01	0.91
2:B:427:LYS:HE2	2:B:456:ILE:HD11	1.49	0.91
2:B:241:PHE:CB	2:B:254:ILE:HD13	1.99	0.91
2:B:241:PHE:HB2	2:B:254:ILE:HD13	1.51	0.91
1:A:425:ILE:CD1	1:A:482:LEU:HD13	2.00	0.91
2:B:634:ILE:HD13	2:B:776:TYR:HE1	1.35	0.91
3:D:256:TYR:CD1	3:D:260:ILE:HD12	2.06	0.91
2:B:533:ARG:O	2:B:538:ILE:HD12	1.71	0.91
1:A:70:LEU:HD12	2:B:220:LEU:HD13	1.51	0.91
1:A:158:LEU:CD2	2:B:281:LYS:HZ1	1.81	0.91
1:A:643:ILE:CD1	1:A:692:LEU:HD23	2.01	0.90
2:B:355:LEU:HD21	2:B:364:ILE:HD13	1.51	0.90
3:C:188:ILE:HD13	3:C:394:PHE:CD1	2.05	0.90
1:A:140:TYR:HH	2:B:292:ILE:HG22	1.34	0.90
2:B:586:ILE:CG2	2:B:735:ILE:CD1	2.48	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LYS:HE3	2:B:216:PHE:CE1	2.06	0.90
2:B:586:ILE:CD1	2:B:732:LEU:HD22	1.99	0.90
3:D:188:ILE:CD1	3:D:394:PHE:CB	2.49	0.90
2:B:296:ILE:CD1	2:B:327:ILE:CD1	2.50	0.90
1:A:406:LEU:HD21	1:A:672:ILE:HD11	1.52	0.90
2:B:405:ILE:HA	2:B:456:ILE:HD13	1.52	0.90
1:A:114:LYS:HE3	1:A:118:ILE:HD11	0.94	0.90
3:C:188:ILE:CD1	3:C:394:PHE:CB	2.45	0.90
1:A:70:LEU:CD1	2:B:220:LEU:HD22	2.01	0.90
3:D:119:ILE:HD11	3:D:154:LEU:HD22	1.52	0.90
1:A:151:LEU:CD2	2:B:285:ARG:CG	2.42	0.90
3:C:212:ILE:HD13	3:C:275:PHE:CE2	2.05	0.90
1:A:70:LEU:CB	2:B:216:PHE:HE1	1.85	0.90
1:A:70:LEU:CG	2:B:216:PHE:CZ	2.51	0.90
1:A:641:LYS:HD3	3:C:356:ILE:HD11	1.52	0.90
1:A:303:ASP:O	1:A:304:ASP:O	1.88	0.90
1:A:65:ASN:HD21	2:B:215:ASN:ND2	1.70	0.90
1:A:425:ILE:HD11	1:A:478:MET:HG3	1.54	0.90
1:A:599:LEU:HD12	1:A:640:ILE:HD11	1.54	0.90
1:A:70:LEU:HD11	2:B:220:LEU:CD1	2.01	0.90
1:A:130:SER:OG	2:B:322:HIS:CG	2.24	0.90
1:A:68:ILE:HD11	1:A:158:LEU:HD21	1.53	0.90
2:B:398:LEU:HD11	2:B:449:ILE:HD12	1.54	0.90
1:A:63:LEU:HB3	1:A:170:ILE:HD13	1.54	0.90
3:D:217:PHE:CD1	3:D:280:ILE:HD13	2.07	0.90
1:A:706:PHE:HE2	1:A:768:ILE:CD1	1.85	0.90
1:A:126:TRP:CH2	1:A:196:ILE:HD12	2.07	0.89
3:D:188:ILE:HD11	3:D:394:PHE:CB	1.99	0.89
2:B:293:ARG:HB3	2:B:330:ILE:HD11	1.54	0.89
2:B:355:LEU:CD2	2:B:364:ILE:CD1	2.46	0.89
1:A:425:ILE:HD11	1:A:482:LEU:HB2	1.52	0.89
1:A:641:LYS:HG3	3:C:356:ILE:CD1	2.02	0.89
3:D:258:THR:HG23	3:D:356:ILE:HD13	1.54	0.89
1:A:71:GLU:HA	2:B:216:PHE:CE2	2.06	0.89
3:C:188:ILE:HD11	3:C:394:PHE:HB3	1.54	0.89
1:A:70:LEU:HB3	2:B:216:PHE:HB3	1.52	0.89
2:B:412:LEU:HD11	2:B:463:ILE:CD1	2.01	0.89
1:A:138:PHE:CZ	1:A:275:ILE:HD13	2.05	0.89
3:C:188:ILE:HD13	3:C:394:PHE:CD2	2.08	0.89
1:A:584:ILE:CD1	1:A:687:ARG:HD2	2.02	0.89
2:B:634:ILE:HD11	2:B:772:PHE:HE1	1.13	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:342:TYR:HE2	2:B:394:ILE:CD1	1.85	0.89
1:A:774:ILE:HD12	1:A:796:SER:HB2	1.54	0.89
1:A:65:ASN:ND2	2:B:215:ASN:CG	2.23	0.89
2:B:412:LEU:CD2	2:B:463:ILE:HD11	2.02	0.89
3:D:188:ILE:CD1	3:D:394:PHE:HB2	1.93	0.89
2:B:402:ILE:CG1	2:B:449:ILE:HD13	2.03	0.89
3:C:125:LYS:HG2	3:D:283:ASP:CG	1.93	0.89
2:B:772:PHE:HE1	2:B:812:ILE:HD12	1.33	0.88
1:A:367:PRO:HA	1:A:404:ILE:HD11	1.53	0.88
2:B:241:PHE:HB3	2:B:254:ILE:HD13	1.41	0.88
2:B:296:ILE:HD12	2:B:327:ILE:HD12	1.55	0.88
2:B:335:PHE:CE2	2:B:339:ILE:CD1	2.55	0.88
3:C:125:LYS:CG	3:D:283:ASP:CG	2.41	0.88
2:B:412:LEU:CD2	2:B:463:ILE:HD12	1.95	0.88
1:A:140:TYR:HH	2:B:296:ILE:HD11	1.36	0.88
1:A:71:GLU:O	2:B:208:GLN:NE2	2.06	0.88
1:A:425:ILE:HD12	1:A:482:LEU:HD13	1.54	0.88
1:A:357:VAL:HB	1:A:363:ILE:HD12	1.55	0.88
1:A:151:LEU:HD22	2:B:285:ARG:HB2	1.55	0.88
1:A:365:THR:CG2	1:A:404:ILE:CD1	2.49	0.88
3:C:200:ALA:HB2	3:C:260:ILE:HD11	1.54	0.88
2:B:628:ILE:HD12	2:B:780:ASN:HD21	1.31	0.88
2:B:825:ILE:CD1	2:B:841:LEU:CD1	2.51	0.88
1:A:70:LEU:O	2:B:216:PHE:HE2	1.51	0.88
1:A:625:ILE:HD13	1:A:764:LEU:CB	2.03	0.88
1:A:114:LYS:HE3	1:A:118:ILE:CD1	2.03	0.88
1:A:641:LYS:HB3	3:C:356:ILE:CD1	2.04	0.88
3:D:188:ILE:CD1	3:D:394:PHE:CD2	2.57	0.88
1:A:151:LEU:CG	2:B:285:ARG:CD	2.25	0.88
1:A:699:ILE:HD11	1:A:782:PHE:CE2	2.08	0.88
1:A:195:GLU:CG	1:A:250:ILE:CD1	2.50	0.88
1:A:136:GLN:HE22	2:B:296:ILE:HD11	1.39	0.88
3:C:255:ILE:HD13	3:C:358:ARG:CZ	2.03	0.88
3:C:238:VAL:HG23	3:C:322:ILE:HD12	1.56	0.88
1:A:425:ILE:HD11	1:A:482:LEU:CB	2.04	0.87
1:A:68:ILE:CD1	2:B:281:LYS:CD	2.48	0.87
1:A:356:VAL:HG21	1:A:572:ILE:HD13	1.54	0.87
1:A:425:ILE:HD12	1:A:478:MET:HB3	1.54	0.87
2:B:656:ILE:HD12	2:B:738:HIS:CD2	2.10	0.87
3:D:258:THR:HG23	3:D:356:ILE:HD12	1.55	0.87
2:B:296:ILE:CD1	2:B:327:ILE:HD12	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:ILE:HD11	2:B:449:ILE:HD11	1.56	0.87
1:A:73:THR:N	2:B:215:ASN:HB3	1.88	0.87
1:A:458:TYR:CE1	1:A:484:ILE:HD13	2.09	0.87
1:A:136:GLN:HE22	2:B:322:HIS:HB3	1.38	0.87
1:A:557:ILE:HD12	1:A:594:TYR:CE2	2.10	0.87
2:B:192:LEU:HD21	2:B:287:ILE:HD12	1.56	0.87
1:A:71:GLU:O	2:B:208:GLN:CD	2.12	0.87
2:B:297:TYR:CE2	2:B:330:ILE:HD12	2.10	0.87
1:A:366:ILE:C	1:A:404:ILE:HD12	1.95	0.87
3:D:188:ILE:HD12	3:D:394:PHE:CB	2.03	0.87
3:D:199:ASP:O	3:D:260:ILE:HD13	1.74	0.87
1:A:70:LEU:HD12	2:B:216:PHE:CZ	2.08	0.87
3:D:127:ILE:HD11	3:D:161:ARG:HH12	1.37	0.87
3:C:6:ILE:CD1	3:C:127:ILE:HG12	2.03	0.87
3:C:200:ALA:CB	3:C:260:ILE:HD11	2.03	0.87
3:D:5:ILE:HD11	3:D:252:MET:CE	2.05	0.87
1:A:629:THR:HG21	1:A:710:ILE:CD1	2.04	0.87
2:B:586:ILE:HG23	2:B:735:ILE:HD13	1.55	0.87
3:C:238:VAL:CG2	3:C:322:ILE:CD1	2.52	0.87
1:A:566:ILE:HD12	1:A:574:ILE:HG21	1.57	0.86
3:C:255:ILE:HD13	3:C:358:ARG:NH2	1.90	0.86
2:B:586:ILE:HG12	2:B:735:ILE:CD1	2.04	0.86
3:C:195:ILE:HD12	3:C:430:VAL:HG11	1.57	0.86
2:B:405:ILE:HD12	2:B:453:TYR:CA	2.04	0.86
2:B:224:ILE:HD13	2:B:280:LEU:HD11	1.55	0.86
2:B:405:ILE:HG23	2:B:456:ILE:CD1	1.87	0.86
1:A:133:MET:HE3	2:B:328:ARG:HH21	1.36	0.86
2:B:493:ILE:CD1	2:B:598:TYR:CG	2.59	0.86
1:A:70:LEU:HD11	2:B:220:LEU:HD11	1.58	0.86
1:A:142:ILE:CD1	1:A:189:LEU:HG	2.02	0.86
1:A:68:ILE:HD12	2:B:281:LYS:CD	2.05	0.86
2:B:405:ILE:HD13	2:B:452:GLN:CB	2.04	0.86
2:B:402:ILE:HG13	2:B:449:ILE:HD13	1.58	0.86
1:A:154:LEU:HD23	2:B:281:LYS:CE	2.05	0.86
2:B:532:PRO:HB2	2:B:538:ILE:HD13	1.58	0.86
3:C:188:ILE:CD1	3:C:394:PHE:CD2	2.57	0.86
3:C:200:ALA:HB2	3:C:260:ILE:HD11	1.56	0.86
2:B:349:TRP:CD2	2:B:364:ILE:HD13	2.10	0.86
1:A:567:PRO:HD2	1:A:574:ILE:CD1	2.05	0.86
2:B:296:ILE:HD11	2:B:327:ILE:HG23	1.57	0.86
1:A:151:LEU:CB	2:B:285:ARG:HE	1.72	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:GLN:HE21	2:B:447:GLU:CG	1.89	0.86
1:A:366:ILE:N	1:A:404:ILE:CD1	2.38	0.86
1:A:65:ASN:CG	2:B:216:PHE:CE1	2.49	0.86
2:B:339:ILE:HD13	2:B:440:GLY:CA	2.05	0.86
3:D:199:ASP:O	3:D:260:ILE:HD13	1.76	0.86
1:A:137:ARG:HH21	2:B:325:LEU:HD11	1.40	0.86
2:B:527:HIS:HA	2:B:538:ILE:CD1	2.06	0.85
1:A:362:GLN:HE21	2:B:447:GLU:HG2	1.41	0.85
3:C:258:THR:OG1	3:C:356:ILE:HD11	1.76	0.85
3:D:5:ILE:HD12	3:D:53:PHE:CZ	2.11	0.85
1:A:72:GLY:HA3	2:B:222:HIS:CE1	2.10	0.85
1:A:70:LEU:HB2	2:B:216:PHE:CE1	2.09	0.85
1:A:151:LEU:HD23	2:B:285:ARG:HH21	0.85	0.85
1:A:641:LYS:CD	3:C:356:ILE:HD11	2.04	0.85
2:B:383:ILE:HD11	2:B:410:ILE:HD13	1.55	0.85
1:A:68:ILE:HD13	2:B:216:PHE:HB2	1.57	0.85
2:B:191:THR:CG2	2:B:207:ILE:CD1	2.54	0.85
1:A:136:GLN:NE2	2:B:296:ILE:HD11	1.92	0.85
1:A:362:GLN:HB3	2:B:446:PHE:CE2	2.12	0.85
3:D:356:ILE:CD1	3:D:358:ARG:HH12	1.88	0.85
3:D:188:ILE:HD11	3:D:394:PHE:CB	2.06	0.85
2:B:402:ILE:HD11	2:B:449:ILE:CD1	2.06	0.85
3:D:95:ALA:HB1	3:D:111:ILE:CD1	2.05	0.85
3:C:188:ILE:HD11	3:C:394:PHE:CD2	2.12	0.85
1:A:588:TYR:CE1	1:A:693:ILE:HD11	2.11	0.85
1:A:152:LYS:HD3	2:B:285:ARG:HH11	1.03	0.85
1:A:70:LEU:HD11	2:B:220:LEU:HD13	1.58	0.85
2:B:184:ILE:CD1	2:B:217:GLU:OE1	2.24	0.85
2:B:192:LEU:CD2	2:B:287:ILE:HD12	2.05	0.85
2:B:349:TRP:CE2	2:B:364:ILE:CD1	2.58	0.85
2:B:586:ILE:CG2	2:B:735:ILE:HD11	2.07	0.85
3:C:188:ILE:HD13	3:C:394:PHE:HD1	1.39	0.85
2:B:570:LEU:HD12	2:B:721:ILE:HD13	1.55	0.85
2:B:257:ILE:HD13	2:B:297:TYR:CE2	2.10	0.85
1:A:564:ILE:HD12	1:A:582:TYR:HD2	1.37	0.85
2:B:412:LEU:HD11	2:B:463:ILE:HD11	1.57	0.85
3:C:188:ILE:CD1	3:C:394:PHE:CG	2.60	0.84
3:D:256:TYR:CE1	3:D:260:ILE:HD12	2.11	0.84
2:B:349:TRP:CD2	2:B:364:ILE:CD1	2.59	0.84
3:D:188:ILE:HD11	3:D:394:PHE:HB3	1.60	0.84
1:A:566:ILE:CD1	1:A:574:ILE:HB	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ASN:OD1	2:B:215:ASN:CG	2.14	0.84
2:B:412:LEU:HD21	2:B:463:ILE:HD12	1.59	0.84
1:A:584:ILE:CD1	1:A:687:ARG:HG3	2.07	0.84
2:B:402:ILE:CG1	2:B:449:ILE:HD13	2.07	0.84
2:B:412:LEU:HD23	2:B:463:ILE:CD1	2.07	0.84
3:D:188:ILE:HD12	3:D:394:PHE:HB3	1.55	0.84
1:A:140:TYR:OH	2:B:296:ILE:CD1	2.22	0.84
3:D:199:ASP:O	3:D:260:ILE:CD1	2.26	0.84
2:B:383:ILE:CD1	2:B:410:ILE:CD1	2.55	0.84
3:D:127:ILE:CD1	3:D:161:ARG:NH1	2.39	0.84
2:B:398:LEU:CD1	2:B:449:ILE:HD12	2.08	0.84
2:B:412:LEU:HD23	2:B:463:ILE:HD11	1.58	0.84
3:D:200:ALA:CB	3:D:260:ILE:HD11	2.08	0.84
2:B:349:TRP:CG	2:B:364:ILE:CD1	2.61	0.84
1:A:151:LEU:HD22	2:B:285:ARG:HD2	0.87	0.84
3:C:212:ILE:HD13	3:C:275:PHE:CZ	2.13	0.84
1:A:425:ILE:HD11	1:A:482:LEU:HD21	1.60	0.83
1:A:599:LEU:HD22	1:A:640:ILE:HD11	1.60	0.83
2:B:349:TRP:CE2	2:B:364:ILE:HD13	2.13	0.83
1:A:137:ARG:NH2	2:B:325:LEU:CD2	2.41	0.83
1:A:74:TYR:HB3	2:B:215:ASN:OD1	1.77	0.83
2:B:349:TRP:NE1	2:B:364:ILE:HD11	1.93	0.83
2:B:634:ILE:CD1	2:B:772:PHE:CE1	2.55	0.83
1:A:195:GLU:CD	1:A:250:ILE:HD12	1.98	0.83
1:A:135:LEU:HD22	1:A:247:ILE:HD12	1.60	0.83
1:A:584:ILE:HD12	1:A:687:ARG:CG	2.08	0.83
1:A:70:LEU:O	2:B:216:PHE:HD2	1.54	0.83
1:A:291:ILE:HD11	1:A:358:ARG:HH11	1.41	0.83
2:B:209:ILE:HD12	2:B:222:HIS:HE1	1.40	0.83
2:B:480:ILE:CD1	2:B:537:VAL:CG2	2.55	0.83
2:B:493:ILE:CD1	2:B:598:TYR:CD2	2.60	0.83
1:A:136:GLN:NE2	2:B:327:ILE:HD11	1.93	0.83
1:A:154:LEU:CD2	2:B:281:LYS:HE2	2.09	0.83
1:A:136:GLN:HE21	2:B:327:ILE:HD11	1.43	0.83
3:D:200:ALA:CB	3:D:260:ILE:HD11	2.07	0.83
2:B:349:TRP:NE1	2:B:364:ILE:CD1	2.26	0.83
2:B:808:ASN:ND2	2:B:812:ILE:HD12	1.92	0.83
3:C:200:ALA:HB2	3:C:260:ILE:CD1	2.07	0.83
1:A:155:VAL:HG11	2:B:285:ARG:NH1	1.92	0.83
1:A:625:ILE:HD12	1:A:758:LEU:HD21	1.61	0.83
3:C:125:LYS:CG	3:D:283:ASP:OD1	2.24	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:LYS:HB3	3:C:356:ILE:HD12	1.59	0.83
1:A:151:LEU:HD22	2:B:285:ARG:HE	0.67	0.83
1:A:102:PHE:HB3	1:A:170:ILE:HD12	1.61	0.82
1:A:70:LEU:CD1	2:B:220:LEU:CD1	2.57	0.82
3:C:258:THR:HG23	3:C:356:ILE:CD1	2.08	0.82
1:A:629:THR:OG1	1:A:710:ILE:HD11	1.79	0.82
3:D:127:ILE:HD13	3:D:162:TYR:OH	1.77	0.82
3:D:210:LEU:HD12	3:D:222:ILE:CD1	2.09	0.82
1:A:141:GLU:OE2	2:B:324:ASP:OD2	1.97	0.82
1:A:588:TYR:CD1	1:A:693:ILE:CD1	2.62	0.82
1:A:114:LYS:HE3	1:A:118:ILE:HD11	1.60	0.82
2:B:634:ILE:HD11	2:B:772:PHE:HE1	1.45	0.82
3:D:255:ILE:HD12	3:D:358:ARG:CZ	2.09	0.82
1:A:143:ARG:NH1	2:B:292:ILE:HD13	1.92	0.82
2:B:636:ILE:CD1	3:D:442:GLN:OE1	2.27	0.82
1:A:70:LEU:CD1	2:B:220:LEU:HD11	2.08	0.82
1:A:73:THR:HG22	2:B:215:ASN:HA	1.60	0.82
3:C:212:ILE:CD1	3:C:275:PHE:CZ	2.62	0.82
2:B:634:ILE:CD1	2:B:772:PHE:HE1	1.91	0.82
1:A:584:ILE:CD1	1:A:687:ARG:CD	2.57	0.82
2:B:264:TYR:CE1	2:B:287:ILE:CD1	2.57	0.82
2:B:405:ILE:HG23	2:B:456:ILE:HD13	1.61	0.82
1:A:65:ASN:ND2	2:B:215:ASN:ND2	2.27	0.82
1:A:199:GLU:CD	1:A:250:ILE:CD1	2.48	0.82
1:A:142:ILE:HD11	1:A:186:MET:HG2	1.62	0.82
1:A:143:ARG:HD2	2:B:292:ILE:HD11	1.62	0.82
1:A:365:THR:HG23	1:A:404:ILE:HD13	1.62	0.82
1:A:291:ILE:HD11	1:A:358:ARG:NH1	1.95	0.82
2:B:656:ILE:HD12	2:B:738:HIS:CG	2.15	0.82
1:A:363:ILE:HD11	1:A:413:TYR:CD1	2.14	0.82
1:A:138:PHE:CD2	1:A:192:ILE:HD12	2.14	0.82
1:A:702:ILE:HD11	1:A:767:TYR:CE2	2.14	0.82
2:B:493:ILE:HD12	2:B:598:TYR:CG	2.14	0.82
1:A:640:ILE:HD11	1:A:699:ILE:HD13	1.62	0.81
1:A:367:PRO:CA	1:A:404:ILE:HD11	2.09	0.81
1:A:599:LEU:CD1	1:A:640:ILE:HD12	2.10	0.81
2:B:241:PHE:HB3	2:B:254:ILE:HD11	1.58	0.81
1:A:128:ASP:CA	2:B:322:HIS:CE1	2.64	0.81
2:B:570:LEU:CD2	2:B:721:ILE:HD13	2.09	0.81
3:D:212:ILE:HD12	3:D:303:ASN:OD1	1.80	0.81
1:A:425:ILE:HD13	1:A:482:LEU:HD22	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:349:TRP:NE1	2:B:364:ILE:HD12	1.95	0.81
2:B:480:ILE:HD12	2:B:541:LEU:HD21	1.59	0.81
1:A:641:LYS:HG3	3:C:356:ILE:HD13	1.62	0.81
3:C:238:VAL:HG22	3:C:322:ILE:CD1	2.10	0.81
1:A:70:LEU:HA	1:A:75:ILE:HD13	1.61	0.81
1:A:68:ILE:O	2:B:281:LYS:HD2	1.80	0.81
3:D:119:ILE:HD11	3:D:154:LEU:CD2	2.07	0.81
1:A:154:LEU:HD23	2:B:281:LYS:HZ3	1.41	0.81
2:B:296:ILE:HD13	2:B:327:ILE:HD13	1.62	0.81
1:A:629:THR:OG1	1:A:768:ILE:HD11	1.81	0.81
1:A:588:TYR:CD1	1:A:693:ILE:HD12	2.16	0.81
1:A:774:ILE:CD1	1:A:796:SER:HB3	2.10	0.81
2:B:586:ILE:HG22	2:B:735:ILE:HD11	1.48	0.81
2:B:493:ILE:HD12	2:B:598:TYR:HB2	1.60	0.81
1:A:152:LYS:HD3	2:B:285:ARG:HH12	1.07	0.81
1:A:629:THR:CG2	1:A:710:ILE:HD11	2.09	0.81
1:A:136:GLN:HE21	2:B:327:ILE:CD1	1.90	0.81
1:A:133:MET:HG3	2:B:328:ARG:HH21	1.43	0.81
1:A:137:ARG:HH21	2:B:325:LEU:HD21	1.46	0.81
2:B:257:ILE:HD13	2:B:297:TYR:CE2	2.15	0.81
2:B:349:TRP:CD2	2:B:364:ILE:HD11	2.16	0.81
1:A:137:ARG:HE	2:B:325:LEU:HD12	1.45	0.81
2:B:335:PHE:CE1	2:B:339:ILE:CD1	2.59	0.81
3:D:188:ILE:HD11	3:D:394:PHE:CB	2.09	0.81
2:B:402:ILE:HG12	2:B:449:ILE:HD13	1.63	0.81
3:D:188:ILE:CD1	3:D:394:PHE:CE2	2.64	0.81
1:A:70:LEU:CD1	2:B:220:LEU:HD13	2.10	0.81
2:B:297:TYR:CE2	2:B:330:ILE:CD1	2.63	0.81
3:C:6:ILE:CD1	3:C:127:ILE:HG22	2.10	0.81
3:C:129:SER:OG	3:D:284:ILE:HG13	1.81	0.81
3:C:195:ILE:CD1	3:C:430:VAL:HG11	2.11	0.81
3:C:200:ALA:CB	3:C:260:ILE:HD11	2.11	0.81
1:A:567:PRO:CD	1:A:574:ILE:HD13	2.11	0.81
1:A:135:LEU:CD2	1:A:247:ILE:HD12	2.10	0.80
2:B:480:ILE:CD1	2:B:541:LEU:HD11	2.11	0.80
1:A:573:ILE:HD12	1:A:673:GLN:CG	2.11	0.80
2:B:568:LEU:CA	2:B:721:ILE:HD12	2.11	0.80
2:B:636:ILE:HD13	3:D:351:ALA:HB2	1.63	0.80
3:D:188:ILE:HD13	3:D:394:PHE:CG	2.15	0.80
2:B:586:ILE:HG21	2:B:735:ILE:HD13	1.56	0.80
3:C:200:ALA:CB	3:C:260:ILE:HD11	2.08	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:188:ILE:HD13	3:C:394:PHE:CG	2.17	0.80
2:B:188:VAL:CG1	2:B:224:ILE:HD13	2.10	0.80
3:D:255:ILE:CD1	3:D:358:ARG:CZ	2.59	0.80
2:B:257:ILE:CD1	2:B:297:TYR:CZ	2.64	0.80
1:A:136:GLN:NE2	2:B:296:ILE:CD1	2.44	0.80
2:B:335:PHE:HE1	2:B:339:ILE:CD1	1.92	0.80
2:B:349:TRP:CE2	2:B:364:ILE:HD11	2.17	0.80
2:B:739:LYS:O	2:B:743:THR:O	2.00	0.80
3:C:258:THR:CG2	3:C:356:ILE:HD13	2.08	0.80
1:A:71:GLU:OE1	2:B:222:HIS:NE2	2.14	0.80
1:A:582:TYR:HD1	1:A:683:ILE:HD11	1.45	0.80
2:B:533:ARG:HA	2:B:538:ILE:HD12	1.64	0.80
1:A:570:LEU:CD2	1:A:573:ILE:CD1	2.57	0.80
1:A:584:ILE:HD12	1:A:687:ARG:CD	2.09	0.80
1:A:606:LEU:HD13	1:A:710:ILE:HD11	1.64	0.80
1:A:588:TYR:CE1	1:A:693:ILE:CD1	2.64	0.80
1:A:570:LEU:HD22	1:A:573:ILE:CD1	2.07	0.80
2:B:480:ILE:HD12	2:B:562:TYR:OH	1.82	0.80
2:B:808:ASN:HD21	2:B:812:ILE:CD1	1.95	0.79
2:B:643:GLN:CD	3:D:356:ILE:HD11	2.02	0.79
1:A:699:ILE:HD11	1:A:775:PHE:CZ	2.16	0.79
2:B:241:PHE:HB3	2:B:254:ILE:HD12	1.63	0.79
1:A:62:ASP:CG	1:A:94:ILE:HD11	2.03	0.79
2:B:296:ILE:HD11	2:B:327:ILE:CG1	2.10	0.79
2:B:242:ARG:HA	2:B:254:ILE:HD11	1.64	0.79
2:B:493:ILE:HD11	2:B:598:TYR:HB3	1.64	0.79
1:A:133:MET:CG	2:B:328:ARG:NH2	2.45	0.79
3:D:199:ASP:O	3:D:260:ILE:HD13	1.82	0.79
1:A:566:ILE:HD13	1:A:574:ILE:HD12	0.83	0.79
1:A:140:TYR:HE2	2:B:327:ILE:HD11	1.47	0.79
1:A:136:GLN:OE1	2:B:323:GLY:HA2	1.83	0.79
1:A:66:VAL:HG21	1:A:170:ILE:HD12	1.65	0.79
3:D:127:ILE:HD11	3:D:161:ARG:NH1	1.96	0.79
1:A:128:ASP:OD1	2:B:296:ILE:HD11	1.83	0.79
1:A:158:LEU:HD23	2:B:281:LYS:HZ3	1.48	0.79
1:A:356:VAL:HG21	1:A:572:ILE:CD1	2.09	0.79
1:A:780:ILE:CD1	1:A:789:GLU:CD	2.51	0.79
1:A:365:THR:CG2	1:A:404:ILE:HD13	2.12	0.79
3:C:255:ILE:HD13	3:C:358:ARG:CD	2.13	0.79
3:D:127:ILE:HD12	3:D:161:ARG:HH22	1.48	0.79
1:A:137:ARG:NH2	2:B:324:ASP:OD1	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:TRP:HH2	1:A:196:ILE:HD12	1.44	0.79
2:B:402:ILE:CG1	2:B:449:ILE:CD1	2.60	0.79
1:A:68:ILE:C	2:B:281:LYS:NZ	2.32	0.79
2:B:586:ILE:HG21	2:B:735:ILE:CD1	2.13	0.79
1:A:155:VAL:CG1	2:B:285:ARG:NH1	2.46	0.79
3:D:5:ILE:HD11	3:D:252:MET:HE2	1.65	0.79
1:A:136:GLN:CD	2:B:323:GLY:HA2	2.03	0.79
2:B:402:ILE:HD11	2:B:449:ILE:CD1	2.13	0.79
2:B:493:ILE:HD11	2:B:598:TYR:CB	2.12	0.79
1:A:68:ILE:HD13	1:A:158:LEU:HD21	1.64	0.79
3:D:188:ILE:HD12	3:D:394:PHE:CD1	2.18	0.79
3:C:188:ILE:HD12	3:C:394:PHE:CG	2.18	0.79
2:B:405:ILE:HA	2:B:456:ILE:HD11	1.64	0.79
1:A:365:THR:C	1:A:404:ILE:HD11	2.02	0.78
1:A:74:TYR:HB3	2:B:215:ASN:CG	2.02	0.78
2:B:296:ILE:CD1	2:B:327:ILE:HG23	2.13	0.78
1:A:557:ILE:HD12	1:A:594:TYR:HE2	1.45	0.78
2:B:405:ILE:CG2	2:B:456:ILE:HD12	2.09	0.78
2:B:296:ILE:CD1	2:B:327:ILE:CG1	2.61	0.78
3:C:258:THR:HG23	3:C:356:ILE:HD12	1.65	0.78
2:B:412:LEU:HD13	2:B:463:ILE:HD12	1.66	0.78
3:D:188:ILE:HD13	3:D:394:PHE:CD2	2.17	0.78
2:B:825:ILE:HD11	2:B:841:LEU:HD11	1.64	0.78
1:A:606:LEU:HD22	1:A:710:ILE:CD1	2.13	0.78
2:B:570:LEU:CD1	2:B:721:ILE:HD13	2.13	0.78
2:B:529:MET:SD	2:B:538:ILE:CD1	2.72	0.78
1:A:137:ARG:NH2	2:B:328:ARG:NH2	2.28	0.78
3:D:200:ALA:HA	3:D:260:ILE:CD1	2.12	0.78
2:B:405:ILE:CD1	2:B:453:TYR:CA	2.59	0.78
1:A:614:TYR:O	1:A:623:ARG:HB2	1.83	0.78
2:B:570:LEU:HD22	2:B:721:ILE:HD11	1.65	0.78
3:C:256:TYR:CE2	3:C:260:ILE:CD1	2.67	0.78
1:A:154:LEU:HD23	2:B:281:LYS:HE2	1.66	0.78
2:B:339:ILE:HD12	2:B:439:ARG:HD2	1.66	0.78
1:A:606:LEU:HD21	1:A:710:ILE:HD12	1.64	0.78
1:A:144:ARG:NE	2:B:289:GLU:OE2	2.17	0.78
1:A:641:LYS:HD2	3:C:356:ILE:HD12	1.64	0.78
1:A:138:PHE:CG	1:A:192:ILE:HD12	2.19	0.78
1:A:570:LEU:HD22	1:A:573:ILE:HD12	1.64	0.77
1:A:158:LEU:HD23	2:B:281:LYS:CE	2.12	0.77
3:D:188:ILE:HD11	3:D:394:PHE:CE1	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:HD22	1:A:247:ILE:CD1	2.12	0.77
1:A:702:ILE:CD1	1:A:767:TYR:CD2	2.68	0.77
1:A:158:LEU:CD2	2:B:281:LYS:HZ3	1.98	0.77
1:A:66:VAL:HB	1:A:94:ILE:CD1	2.13	0.77
1:A:68:ILE:HG13	2:B:281:LYS:CE	2.14	0.77
3:D:188:ILE:HD12	3:D:394:PHE:CB	2.13	0.77
2:B:571:VAL:HG21	2:B:721:ILE:HD11	1.67	0.77
1:A:425:ILE:HD13	1:A:482:LEU:HD13	1.66	0.77
1:A:151:LEU:CD1	2:B:285:ARG:HG3	2.15	0.77
1:A:367:PRO:CB	1:A:404:ILE:HD11	2.14	0.77
1:A:623:ARG:NE	1:A:761:ILE:HD11	1.98	0.77
3:D:188:ILE:CD1	3:D:394:PHE:HB2	2.14	0.77
2:B:355:LEU:HD22	2:B:364:ILE:HD12	1.67	0.77
3:D:256:TYR:CD1	3:D:260:ILE:HD12	2.20	0.77
1:A:63:LEU:CB	1:A:170:ILE:CD1	2.60	0.77
3:D:188:ILE:CD1	3:D:394:PHE:CB	2.60	0.77
1:A:138:PHE:CG	1:A:275:ILE:HD11	2.19	0.77
1:A:405:PHE:CZ	1:A:573:ILE:HD11	2.20	0.77
1:A:109:ILE:CD1	1:A:170:ILE:HD11	2.15	0.77
1:A:599:LEU:HD21	1:A:640:ILE:HD12	1.65	0.77
1:A:641:LYS:HD2	3:C:356:ILE:CD1	2.14	0.77
3:C:212:ILE:CD1	3:C:275:PHE:CZ	2.68	0.77
3:D:119:ILE:HD13	3:D:154:LEU:CD2	2.15	0.77
3:C:123:ILE:HD13	3:C:161:ARG:HH22	1.50	0.77
1:A:74:TYR:HD2	2:B:216:PHE:HZ	0.87	0.77
1:A:155:VAL:HG11	2:B:285:ARG:HH22	1.50	0.76
2:B:825:ILE:CD1	2:B:841:LEU:HD12	2.13	0.76
1:A:425:ILE:HD12	1:A:478:MET:CB	2.15	0.76
2:B:571:VAL:HG23	2:B:721:ILE:CD1	2.14	0.76
1:A:144:ARG:NH1	2:B:289:GLU:OE2	2.18	0.76
1:A:589:GLN:NE2	1:A:652:ILE:HD13	2.01	0.76
1:A:255:ILE:HD13	1:A:269:LYS:HG2	1.65	0.76
1:A:66:VAL:CG2	1:A:94:ILE:HD13	2.16	0.76
2:B:634:ILE:CD1	2:B:809:LEU:HG	2.15	0.76
1:A:599:LEU:CD2	1:A:640:ILE:HD12	2.12	0.76
1:A:641:LYS:HD3	3:C:356:ILE:CD1	2.16	0.76
3:C:67:ILE:HD12	3:C:123:ILE:CG2	2.15	0.76
2:B:349:TRP:HE1	2:B:364:ILE:HD13	1.48	0.76
2:B:586:ILE:HG21	2:B:735:ILE:HD11	1.56	0.76
3:D:188:ILE:CD1	3:D:394:PHE:CB	2.62	0.76
1:A:157:ARG:HD3	1:A:176:ILE:HD13	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:ILE:HD11	2:B:218:SER:CB	2.12	0.76
2:B:570:LEU:HD12	2:B:721:ILE:CD1	2.13	0.76
2:B:808:ASN:ND2	2:B:812:ILE:CD1	2.48	0.76
1:A:114:LYS:CE	1:A:118:ILE:CD1	2.58	0.76
2:B:207:ILE:CD1	2:B:221:LEU:HD23	2.16	0.76
2:B:349:TRP:NE1	2:B:364:ILE:CD1	2.48	0.76
1:A:151:LEU:HB2	2:B:285:ARG:HD3	1.52	0.76
1:A:296:TYR:HH	2:B:322:HIS:CD2	1.72	0.76
1:A:68:ILE:HG21	2:B:216:PHE:HB2	1.66	0.76
1:A:68:ILE:HD11	2:B:216:PHE:HD1	1.51	0.76
1:A:63:LEU:HB3	1:A:170:ILE:HD11	1.66	0.76
2:B:405:ILE:HD11	2:B:453:TYR:HA	1.64	0.76
2:B:293:ARG:HB3	2:B:330:ILE:CD1	2.16	0.76
1:A:133:MET:HG3	2:B:328:ARG:NH2	2.01	0.76
1:A:425:ILE:HD12	1:A:564:ILE:HD12	1.68	0.76
3:C:188:ILE:HD12	3:C:394:PHE:CD2	2.21	0.76
3:D:255:ILE:CD1	3:D:358:ARG:NE	2.48	0.76
2:B:529:MET:SD	2:B:538:ILE:HD11	2.25	0.76
2:B:188:VAL:HG11	2:B:224:ILE:CD1	2.16	0.76
2:B:200:PHE:HZ	2:B:207:ILE:HD11	1.49	0.76
1:A:66:VAL:HG23	2:B:216:PHE:CE1	2.20	0.75
3:D:356:ILE:HD13	3:D:358:ARG:NH1	1.96	0.75
1:A:66:VAL:CB	1:A:94:ILE:CD1	2.63	0.75
1:A:131:PHE:CD2	2:B:322:HIS:CD2	2.74	0.75
3:D:188:ILE:HD12	3:D:394:PHE:CG	2.22	0.75
1:A:202:GLU:O	1:A:205:THR:O	2.04	0.75
1:A:65:ASN:OD1	2:B:216:PHE:HE1	1.69	0.75
1:A:425:ILE:CD1	1:A:482:LEU:HB2	2.16	0.75
1:A:141:GLU:OE1	2:B:324:ASP:OD2	2.04	0.75
1:A:706:PHE:CE2	1:A:768:ILE:CD1	2.69	0.75
2:B:628:ILE:HD12	2:B:780:ASN:HD22	1.50	0.75
1:A:68:ILE:HG21	2:B:215:ASN:HD22	1.50	0.75
1:A:131:PHE:HD2	2:B:322:HIS:CE1	2.04	0.75
1:A:138:PHE:CD2	1:A:192:ILE:HD13	2.19	0.75
2:B:743:THR:O	2:B:756:GLN:NE2	2.18	0.75
3:C:238:VAL:HG23	3:C:322:ILE:CD1	2.15	0.75
3:D:210:LEU:HD23	3:D:222:ILE:HD11	1.65	0.75
1:A:625:ILE:HD13	1:A:764:LEU:HB2	1.67	0.75
2:B:570:LEU:CD2	2:B:721:ILE:CD1	2.65	0.75
1:A:774:ILE:HD12	1:A:796:SER:HB3	1.66	0.75
2:B:398:LEU:HD21	2:B:449:ILE:HD12	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:ILE:HD12	1:A:758:LEU:CD2	2.15	0.75
3:D:210:LEU:HD22	3:D:222:ILE:HD13	1.66	0.75
1:A:361:LEU:HD11	2:B:443:THR:HG22	1.69	0.75
2:B:184:ILE:HD12	2:B:217:GLU:OE1	1.85	0.75
1:A:126:TRP:CZ2	1:A:196:ILE:CD1	2.70	0.75
2:B:634:ILE:HD13	2:B:805:PHE:CZ	2.22	0.75
1:A:66:VAL:HA	2:B:216:PHE:CD1	2.22	0.75
3:C:128:ASP:OD2	3:D:281:HIS:CG	2.40	0.75
3:C:188:ILE:CD1	3:C:394:PHE:CG	2.70	0.75
2:B:349:TRP:CG	2:B:364:ILE:CD1	2.70	0.75
2:B:241:PHE:HB3	2:B:254:ILE:HD13	1.69	0.74
2:B:636:ILE:HD11	3:D:437:TYR:CE1	2.22	0.74
2:B:568:LEU:HA	2:B:721:ILE:CD1	2.16	0.74
2:B:412:LEU:HD22	2:B:463:ILE:HD12	1.68	0.74
1:A:133:MET:SD	2:B:328:ARG:NH2	2.60	0.74
3:D:139:LEU:CD2	3:D:235:ILE:HD13	2.16	0.74
2:B:643:GLN:CG	3:D:356:ILE:HD11	2.18	0.74
1:A:109:ILE:HD13	1:A:173:LEU:HD13	1.68	0.74
1:A:70:LEU:HD12	2:B:216:PHE:HZ	1.46	0.74
2:B:402:ILE:HG13	2:B:449:ILE:HD13	1.69	0.74
3:C:200:ALA:HB2	3:C:260:ILE:CD1	2.17	0.74
3:D:256:TYR:CE2	3:D:260:ILE:HD12	2.22	0.74
3:D:188:ILE:HD13	3:D:394:PHE:CG	2.23	0.74
2:B:296:ILE:HD13	2:B:327:ILE:CD1	2.16	0.74
2:B:480:ILE:HD12	2:B:537:VAL:HG22	1.68	0.74
2:B:335:PHE:CE1	2:B:339:ILE:HD11	2.22	0.74
1:A:143:ARG:HD2	2:B:292:ILE:CD1	2.18	0.74
2:B:586:ILE:CG1	2:B:735:ILE:HD12	2.18	0.74
3:C:6:ILE:HD12	3:C:127:ILE:HG22	1.70	0.74
2:B:480:ILE:HD11	2:B:537:VAL:HG22	1.69	0.74
1:A:582:TYR:CD1	1:A:683:ILE:HD11	2.22	0.74
1:A:140:TYR:CE1	2:B:292:ILE:HD13	2.23	0.73
1:A:780:ILE:HD11	1:A:789:GLU:OE1	1.88	0.73
3:C:212:ILE:HD13	3:C:275:PHE:CE1	2.23	0.73
1:A:62:ASP:CG	1:A:94:ILE:CD1	2.55	0.73
3:D:188:ILE:CD1	3:D:394:PHE:CG	2.72	0.73
2:B:643:GLN:HG2	3:D:356:ILE:CD1	2.18	0.73
2:B:586:ILE:CD1	2:B:732:LEU:CD2	2.65	0.73
3:C:123:ILE:CD1	3:C:161:ARG:HH22	2.01	0.73
2:B:349:TRP:NE1	2:B:364:ILE:HD13	1.88	0.73
1:A:155:VAL:CG1	2:B:285:ARG:HH11	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:ILE:CD1	2:B:218:SER:HB3	2.16	0.73
1:A:566:ILE:CD1	1:A:574:ILE:HD13	2.17	0.73
1:A:566:ILE:CD1	1:A:574:ILE:CG2	2.66	0.73
1:A:581:LYS:HB3	1:A:683:ILE:HD12	1.70	0.73
2:B:427:LYS:HE2	2:B:456:ILE:CD1	2.18	0.73
1:A:566:ILE:HD11	1:A:574:ILE:HB	1.69	0.73
3:D:139:LEU:HD21	3:D:235:ILE:HD13	1.69	0.73
3:D:212:ILE:CD1	3:D:303:ASN:OD1	2.36	0.73
3:C:275:PHE:H	3:C:284:ILE:HD12	1.53	0.73
2:B:527:HIS:HA	2:B:538:ILE:HD11	1.71	0.73
2:B:532:PRO:O	2:B:538:ILE:HD12	1.88	0.73
1:A:138:PHE:HZ	1:A:275:ILE:CD1	1.98	0.73
1:A:155:VAL:HG12	2:B:281:LYS:HD3	1.71	0.73
2:B:407:LYS:NZ	2:B:721:ILE:HD12	2.03	0.73
2:B:493:ILE:CD1	2:B:598:TYR:HB2	2.19	0.73
1:A:706:PHE:CE2	1:A:768:ILE:HD12	2.22	0.73
3:C:129:SER:OG	3:D:284:ILE:CG1	2.36	0.73
1:A:566:ILE:CD1	1:A:574:ILE:HD13	2.18	0.73
3:D:258:THR:CG2	3:D:356:ILE:HD12	2.18	0.73
1:A:566:ILE:CD1	1:A:571:ASN:HA	2.19	0.73
2:B:242:ARG:HG3	2:B:254:ILE:CD1	2.19	0.73
2:B:628:ILE:CD1	2:B:780:ASN:HD22	2.01	0.73
1:A:375:ILE:HD11	1:A:400:ARG:NH2	2.04	0.73
3:C:255:ILE:CD1	3:C:358:ARG:NH1	2.51	0.73
3:D:188:ILE:HD11	3:D:394:PHE:HB2	1.71	0.73
1:A:425:ILE:HD12	1:A:478:MET:CB	2.18	0.73
3:C:275:PHE:N	3:C:284:ILE:CD1	2.52	0.73
2:B:656:ILE:CD1	2:B:738:HIS:CD2	2.72	0.73
1:A:458:TYR:CG	1:A:484:ILE:HD11	2.24	0.73
2:B:349:TRP:CD1	2:B:364:ILE:HD11	2.24	0.72
3:C:275:PHE:N	3:C:284:ILE:HD12	2.04	0.72
3:C:255:ILE:HD11	3:C:358:ARG:NH1	2.04	0.72
1:A:367:PRO:CB	1:A:404:ILE:CD1	2.67	0.72
3:C:256:TYR:CE1	3:C:260:ILE:HD11	2.22	0.72
3:C:199:ASP:O	3:C:260:ILE:CD1	2.19	0.72
2:B:405:ILE:CA	2:B:456:ILE:HD13	2.15	0.72
1:A:566:ILE:HD13	1:A:571:ASN:CB	2.15	0.72
1:A:114:LYS:HE2	1:A:118:ILE:HD11	1.70	0.72
1:A:152:LYS:HD2	2:B:285:ARG:HH12	1.53	0.72
2:B:224:ILE:HD11	2:B:283:LEU:HD23	1.71	0.72
1:A:72:GLY:HA3	2:B:215:ASN:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:127:ILE:HD12	3:D:161:ARG:NH2	2.04	0.72
1:A:144:ARG:NH2	2:B:288:TYR:HD2	1.86	0.72
3:D:188:ILE:CD1	3:D:394:PHE:CD1	2.73	0.72
1:A:780:ILE:HD12	1:A:789:GLU:HB2	1.70	0.72
2:B:296:ILE:HD11	2:B:327:ILE:CG2	2.18	0.72
2:B:493:ILE:HD13	2:B:598:TYR:CB	2.08	0.72
1:A:141:GLU:CD	2:B:324:ASP:OD2	2.28	0.72
2:B:405:ILE:HG21	2:B:456:ILE:HD12	1.61	0.72
2:B:634:ILE:HD13	2:B:805:PHE:HZ	1.55	0.72
2:B:355:LEU:O	2:B:364:ILE:CD1	2.37	0.72
1:A:109:ILE:HD12	1:A:170:ILE:HD11	1.70	0.72
2:B:412:LEU:CG	2:B:463:ILE:CD1	2.67	0.72
1:A:71:GLU:HB2	2:B:208:GLN:OE1	1.90	0.72
1:A:566:ILE:HD12	1:A:574:ILE:CG2	2.16	0.72
1:A:151:LEU:HB2	2:B:285:ARG:NE	1.92	0.72
2:B:342:TYR:CE2	2:B:394:ILE:CD1	2.66	0.72
3:C:255:ILE:CD1	3:C:358:ARG:HD3	2.17	0.72
1:A:102:PHE:CE1	1:A:170:ILE:HD11	2.25	0.72
3:C:188:ILE:CD1	3:C:394:PHE:CG	2.72	0.72
2:B:394:ILE:HD11	2:B:445:PHE:CZ	2.25	0.71
2:B:480:ILE:HD12	2:B:537:VAL:HG21	1.69	0.71
1:A:73:THR:HG22	2:B:215:ASN:CA	2.16	0.71
1:A:151:LEU:CG	2:B:285:ARG:HG3	2.20	0.71
3:D:188:ILE:CD1	3:D:394:PHE:CZ	2.72	0.71
1:A:130:SER:CB	2:B:322:HIS:CE1	2.73	0.71
3:D:212:ILE:HD11	3:D:302:SER:O	1.89	0.71
2:B:209:ILE:CD1	2:B:222:HIS:NE2	2.44	0.71
1:A:291:ILE:CD1	1:A:358:ARG:NH1	2.54	0.71
1:A:152:LYS:HG2	2:B:285:ARG:HH11	0.64	0.71
3:D:255:ILE:HD12	3:D:358:ARG:NE	2.05	0.71
2:B:405:ILE:HG23	2:B:456:ILE:HD11	1.69	0.71
2:B:349:TRP:CD2	2:B:364:ILE:CD1	2.73	0.71
1:A:71:GLU:CB	2:B:215:ASN:CG	2.38	0.71
1:A:367:PRO:CG	1:A:404:ILE:HD12	2.18	0.71
1:A:138:PHE:CE1	1:A:142:ILE:HD11	2.25	0.71
3:D:210:LEU:CD2	3:D:222:ILE:CD1	2.67	0.71
2:B:339:ILE:CD1	2:B:440:GLY:N	2.53	0.71
1:A:367:PRO:HB3	1:A:404:ILE:CD1	2.20	0.71
3:D:256:TYR:CE1	3:D:260:ILE:CD1	2.71	0.71
1:A:564:ILE:CD1	1:A:582:TYR:CD2	2.74	0.71
1:A:151:LEU:HD11	2:B:285:ARG:HG3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:188:ILE:CD1	3:C:394:PHE:CD2	2.74	0.71
1:A:126:TRP:CH2	1:A:196:ILE:CD1	2.74	0.71
2:B:402:ILE:HD11	2:B:449:ILE:HD11	1.72	0.71
3:C:188:ILE:CD1	3:C:394:PHE:HD1	2.03	0.71
1:A:130:SER:CB	2:B:322:HIS:ND1	2.53	0.71
3:D:234:ILE:HD13	3:D:270:PRO:HB2	1.72	0.71
3:C:275:PHE:HB2	3:C:284:ILE:HD11	1.73	0.71
3:D:188:ILE:CD1	3:D:394:PHE:HB2	2.20	0.71
3:D:188:ILE:CD1	3:D:394:PHE:CD2	2.74	0.71
1:A:352:ILE:HG22	1:A:572:ILE:HD13	1.72	0.71
1:A:363:ILE:HD11	1:A:413:TYR:CG	2.25	0.71
1:A:566:ILE:HD13	1:A:571:ASN:HA	1.73	0.70
2:B:188:VAL:HG13	2:B:224:ILE:CD1	2.15	0.70
1:A:425:ILE:HD13	1:A:482:LEU:HD13	1.73	0.70
2:B:342:TYR:OH	2:B:394:ILE:HD12	1.90	0.70
1:A:70:LEU:HD22	2:B:216:PHE:O	1.92	0.70
1:A:154:LEU:HD23	2:B:281:LYS:HE3	1.71	0.70
1:A:585:ILE:HD11	1:A:683:ILE:HD11	1.71	0.70
2:B:586:ILE:HD12	2:B:735:ILE:HD12	1.70	0.70
2:B:257:ILE:CD1	2:B:297:TYR:OH	2.39	0.70
1:A:365:THR:HG23	1:A:404:ILE:HD11	1.69	0.70
3:C:67:ILE:CD1	3:C:123:ILE:HG23	2.21	0.70
1:A:68:ILE:HD13	2:B:216:PHE:CD2	2.18	0.70
1:A:142:ILE:HD11	1:A:188:LEU:HD12	1.73	0.70
1:A:155:VAL:HG23	2:B:281:LYS:HD3	1.73	0.70
2:B:570:LEU:CD1	2:B:721:ILE:CD1	2.70	0.70
2:B:634:ILE:HD13	2:B:776:TYR:CE1	2.23	0.70
1:A:159:GLU:OE1	2:B:277:VAL:HG11	1.92	0.70
1:A:625:ILE:CD1	1:A:764:LEU:HB2	2.22	0.70
1:A:155:VAL:HG11	2:B:281:LYS:HG2	1.73	0.70
1:A:255:ILE:CD1	1:A:272:LEU:HD22	2.10	0.70
1:A:71:GLU:H	2:B:216:PHE:HB3	1.56	0.70
3:D:256:TYR:CD1	3:D:260:ILE:HD12	2.27	0.70
2:B:380:HIS:CE1	2:B:573:ASN:HA	2.27	0.70
1:A:114:LYS:CE	1:A:118:ILE:HD11	2.21	0.70
1:A:425:ILE:CD1	1:A:478:MET:HG3	2.21	0.70
2:B:636:ILE:CD1	3:D:437:TYR:CZ	2.72	0.70
3:C:67:ILE:CD1	3:C:123:ILE:HG23	2.20	0.70
3:D:139:LEU:HD22	3:D:235:ILE:CD1	2.21	0.70
1:A:362:GLN:NE2	2:B:447:GLU:OE2	2.25	0.70
1:A:595:HIS:ND1	1:A:640:ILE:CD1	2.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:610:ILE:HD13	3:D:196:GLU:O	1.86	0.70
1:A:425:ILE:HD11	1:A:482:LEU:HD22	1.73	0.70
2:B:412:LEU:CD2	2:B:463:ILE:CD1	2.69	0.70
1:A:570:LEU:CD2	1:A:573:ILE:HD12	2.17	0.70
1:A:74:TYR:HB2	2:B:215:ASN:ND2	2.07	0.69
3:D:188:ILE:HD13	3:D:394:PHE:CD2	2.27	0.69
1:A:296:TYR:OH	2:B:322:HIS:NE2	1.92	0.69
1:A:140:TYR:HD2	2:B:324:ASP:OD1	1.58	0.69
1:A:142:ILE:HD12	1:A:193:TYR:OH	1.92	0.69
2:B:209:ILE:HD11	2:B:222:HIS:HE2	1.57	0.69
2:B:434:GLN:HE21	2:B:448:ILE:HD12	1.56	0.69
2:B:296:ILE:CD1	2:B:327:ILE:CD1	2.69	0.69
1:A:625:ILE:HD11	1:A:764:LEU:C	2.11	0.69
3:C:292:TYR:OH	3:C:323:ILE:HD13	1.92	0.69
1:A:72:GLY:HA2	2:B:215:ASN:O	1.92	0.69
1:A:296:TYR:OH	2:B:322:HIS:CG	2.43	0.69
1:A:150:TYR:CD1	1:A:177:ILE:CD1	2.75	0.69
2:B:188:VAL:HG11	2:B:224:ILE:HD13	1.74	0.69
1:A:70:LEU:CD1	2:B:216:PHE:CE1	2.73	0.69
2:B:349:TRP:CH2	2:B:383:ILE:CD1	2.75	0.69
2:B:430:HIS:HB3	2:B:448:ILE:HD12	1.72	0.69
2:B:493:ILE:HD11	2:B:598:TYR:HB2	1.75	0.69
1:A:365:THR:CG2	1:A:404:ILE:HD12	2.18	0.69
2:B:636:ILE:CD1	3:D:351:ALA:HB2	2.23	0.69
1:A:68:ILE:O	2:B:216:PHE:CD2	2.46	0.69
2:B:586:ILE:HD13	2:B:732:LEU:CD2	2.22	0.69
1:A:367:PRO:HB3	1:A:404:ILE:HD11	1.73	0.69
2:B:656:ILE:HD13	2:B:738:HIS:HB2	1.74	0.69
1:A:66:VAL:HG21	1:A:94:ILE:CD1	2.19	0.69
3:D:200:ALA:CB	3:D:260:ILE:HD11	2.19	0.69
1:A:629:THR:HG21	1:A:710:ILE:CD1	2.22	0.69
2:B:293:ARG:HD3	2:B:330:ILE:HD12	1.74	0.69
3:C:195:ILE:CD1	3:C:430:VAL:CG1	2.70	0.69
3:D:188:ILE:HD11	3:D:394:PHE:HB3	1.68	0.69
2:B:402:ILE:CD1	2:B:449:ILE:CD1	2.60	0.69
2:B:533:ARG:O	2:B:538:ILE:CD1	2.41	0.69
3:C:199:ASP:C	3:C:260:ILE:HD13	2.11	0.69
3:D:234:ILE:HD13	3:D:270:PRO:CB	2.23	0.69
2:B:412:LEU:HG	2:B:463:ILE:CD1	2.23	0.69
3:D:289:HIS:HE1	3:D:323:ILE:HD13	1.58	0.69
2:B:634:ILE:HD12	2:B:809:LEU:CG	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:VAL:CG2	1:A:363:ILE:HD12	2.23	0.69
3:C:21:LEU:HD22	3:C:235:ILE:HD11	1.75	0.69
1:A:595:HIS:ND1	1:A:640:ILE:HD11	2.08	0.69
1:A:73:THR:HG23	2:B:215:ASN:ND2	2.05	0.69
1:A:584:ILE:CD1	1:A:687:ARG:NE	2.55	0.69
1:A:602:THR:HG23	1:A:710:ILE:HD12	1.74	0.69
2:B:264:TYR:CZ	2:B:287:ILE:HD13	2.27	0.69
2:B:402:ILE:CD1	2:B:449:ILE:CD1	2.71	0.69
2:B:398:LEU:HD11	2:B:449:ILE:HD12	1.74	0.69
1:A:599:LEU:HD11	1:A:640:ILE:HD12	1.75	0.69
2:B:364:ILE:HD13	2:B:403:PHE:HD1	1.57	0.69
1:A:109:ILE:HG22	1:A:177:ILE:HD11	1.75	0.68
3:C:256:TYR:CE1	3:C:260:ILE:HD12	2.28	0.68
3:D:127:ILE:CD1	3:D:162:TYR:OH	2.41	0.68
2:B:188:VAL:CG1	2:B:224:ILE:HD13	2.22	0.68
2:B:296:ILE:HD12	2:B:327:ILE:HG12	1.72	0.68
2:B:296:ILE:HG21	2:B:327:ILE:HD13	1.74	0.68
3:D:5:ILE:HD12	3:D:53:PHE:CE1	2.28	0.68
3:D:188:ILE:CD1	3:D:394:PHE:CD2	2.75	0.68
1:A:154:LEU:CD2	2:B:281:LYS:HE3	2.24	0.68
1:A:194:GLU:HB3	1:A:250:ILE:CD1	2.23	0.68
1:A:640:ILE:CD1	1:A:696:GLN:NE2	2.47	0.68
2:B:296:ILE:HD13	2:B:327:ILE:HD11	1.74	0.68
3:D:188:ILE:HD11	3:D:394:PHE:CG	2.29	0.68
2:B:646:SER:OG	3:D:356:ILE:HD12	1.93	0.68
3:D:188:ILE:HD12	3:D:394:PHE:CG	2.29	0.68
2:B:284:TYR:CE1	2:B:291:ILE:HD13	2.28	0.68
2:B:480:ILE:CD1	2:B:541:LEU:HD21	2.23	0.68
2:B:567:PRO:HG2	2:B:721:ILE:HD13	1.76	0.68
3:C:210:LEU:HG	3:C:222:ILE:HD11	1.74	0.68
3:D:256:TYR:CZ	3:D:260:ILE:HD12	2.22	0.68
2:B:402:ILE:CG1	2:B:449:ILE:HD13	2.24	0.68
2:B:257:ILE:HD13	2:B:297:TYR:CD2	2.29	0.68
2:B:586:ILE:CG1	2:B:735:ILE:CD1	2.72	0.68
1:A:699:ILE:HD12	1:A:782:PHE:HZ	1.58	0.68
2:B:412:LEU:CD1	2:B:463:ILE:HD12	2.24	0.68
1:A:68:ILE:CD1	1:A:158:LEU:CD2	2.63	0.68
2:B:209:ILE:CD1	2:B:222:HIS:CD2	2.65	0.68
1:A:566:ILE:CG1	1:A:574:ILE:HD12	2.21	0.68
2:B:349:TRP:CH2	2:B:383:ILE:HD11	2.29	0.68
3:C:193:ARG:HH12	3:C:419:VAL:HG13	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:ILE:HD13	2:B:327:ILE:HA	1.74	0.68
2:B:634:ILE:HD12	2:B:809:LEU:HG	1.76	0.68
1:A:599:LEU:HD11	1:A:640:ILE:HD11	1.75	0.67
3:C:200:ALA:HB2	3:C:260:ILE:CD1	2.14	0.67
1:A:585:ILE:HD13	1:A:683:ILE:HG12	1.76	0.67
1:A:641:LYS:HD2	3:C:356:ILE:HD12	1.75	0.67
3:C:195:ILE:HD12	3:C:430:VAL:CG1	2.25	0.67
1:A:136:GLN:HB3	2:B:324:ASP:OD2	1.95	0.67
2:B:412:LEU:CG	2:B:463:ILE:HD12	2.24	0.67
3:C:6:ILE:CD1	3:C:127:ILE:CG1	2.72	0.67
2:B:405:ILE:HG12	2:B:456:ILE:HD12	1.77	0.67
1:A:65:ASN:CG	2:B:216:PHE:CD1	2.66	0.67
1:A:68:ILE:HD12	2:B:216:PHE:HB3	0.67	0.67
2:B:339:ILE:CD1	2:B:440:GLY:CA	2.63	0.67
1:A:570:LEU:HD12	1:A:573:ILE:HD11	1.74	0.67
1:A:109:ILE:CG2	1:A:177:ILE:HD11	2.25	0.67
3:D:127:ILE:CD1	3:D:162:TYR:CZ	2.77	0.67
2:B:209:ILE:HD13	2:B:222:HIS:NE2	1.99	0.67
2:B:296:ILE:CD1	2:B:327:ILE:HD13	2.25	0.67
2:B:296:ILE:HD12	2:B:327:ILE:HD11	1.75	0.67
1:A:780:ILE:HD11	1:A:789:GLU:CD	2.14	0.67
3:D:127:ILE:HD12	3:D:161:ARG:HH12	1.59	0.67
3:C:67:ILE:CD1	3:C:123:ILE:CG2	2.73	0.67
2:B:777:CYS:O	2:B:780:ASN:O	2.13	0.67
3:C:188:ILE:HD12	3:C:394:PHE:CD2	2.24	0.67
2:B:412:LEU:HG	2:B:463:ILE:HD13	1.77	0.67
3:C:199:ASP:O	3:C:260:ILE:HD13	1.94	0.67
1:A:640:ILE:CD1	1:A:699:ILE:CD1	2.73	0.67
2:B:394:ILE:HD11	2:B:445:PHE:CE2	2.28	0.67
2:B:380:HIS:HE1	2:B:573:ASN:HA	1.60	0.67
3:D:210:LEU:HD21	3:D:222:ILE:HD11	1.73	0.67
1:A:73:THR:HG22	2:B:215:ASN:HD22	1.58	0.67
1:A:75:ILE:HD12	2:B:216:PHE:CE1	2.29	0.67
1:A:65:ASN:CG	2:B:215:ASN:CG	2.53	0.67
3:C:212:ILE:HD11	3:C:301:PRO:HA	1.75	0.67
1:A:363:ILE:CD1	1:A:413:TYR:CB	2.69	0.67
1:A:70:LEU:N	2:B:216:PHE:CD1	2.62	0.67
2:B:405:ILE:HG23	2:B:456:ILE:CD1	2.24	0.67
1:A:143:ARG:NH1	2:B:292:ILE:CD1	2.57	0.67
2:B:586:ILE:HD11	2:B:732:LEU:HD23	1.77	0.67
1:A:143:ARG:CZ	2:B:292:ILE:HD13	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:ILE:HD13	2:B:403:PHE:HA	1.76	0.67
2:B:402:ILE:HD11	2:B:449:ILE:HD11	1.75	0.67
2:B:335:PHE:CZ	2:B:339:ILE:CD1	2.59	0.67
2:B:241:PHE:CB	2:B:254:ILE:HD11	2.24	0.66
3:C:125:LYS:HG3	3:D:283:ASP:CG	2.07	0.66
1:A:65:ASN:ND2	2:B:215:ASN:HB2	2.04	0.66
2:B:480:ILE:HD11	2:B:520:VAL:HG13	1.77	0.66
2:B:402:ILE:CG1	2:B:449:ILE:HD13	2.26	0.66
2:B:296:ILE:HD13	2:B:327:ILE:CD1	2.24	0.66
1:A:566:ILE:HD11	1:A:571:ASN:HB3	1.77	0.66
2:B:610:ILE:HD11	3:D:196:GLU:O	1.95	0.66
2:B:634:ILE:HD11	2:B:772:PHE:CE1	2.28	0.66
3:C:188:ILE:CD1	3:C:394:PHE:CD2	2.78	0.66
3:D:127:ILE:HD12	3:D:162:TYR:OH	1.94	0.66
1:A:641:LYS:HD3	3:C:356:ILE:HD12	1.75	0.66
1:A:607:ASN:HA	1:A:630:ARG:HH22	1.60	0.66
1:A:641:LYS:HB3	3:C:356:ILE:HD11	1.76	0.66
3:D:36:LEU:HD22	3:D:36:LEU:H	1.61	0.66
2:B:364:ILE:CD1	2:B:403:PHE:HA	2.25	0.66
1:A:142:ILE:HD12	1:A:193:TYR:CZ	2.30	0.66
2:B:207:ILE:HD13	2:B:221:LEU:HD23	1.78	0.66
3:D:5:ILE:HD12	3:D:53:PHE:CE1	2.30	0.66
2:B:184:ILE:HD13	2:B:217:GLU:CD	2.14	0.66
2:B:264:TYR:CE1	2:B:287:ILE:HD11	2.30	0.66
3:D:210:LEU:HD21	3:D:222:ILE:CD1	2.26	0.66
2:B:349:TRP:CD1	2:B:364:ILE:HD12	2.29	0.66
1:A:136:GLN:CD	2:B:323:GLY:HA2	2.16	0.66
2:B:209:ILE:HD12	2:B:222:HIS:CE1	2.28	0.66
1:A:154:LEU:HD21	1:A:177:ILE:CD1	2.10	0.66
1:A:70:LEU:HD12	2:B:216:PHE:CE1	2.30	0.66
2:B:412:LEU:HD22	2:B:463:ILE:HD11	1.76	0.66
1:A:135:LEU:CD1	1:A:247:ILE:HD11	2.26	0.66
2:B:412:LEU:CD2	2:B:463:ILE:HD12	2.25	0.66
2:B:512:LEU:HD23	2:B:558:PHE:CD2	2.31	0.66
3:C:127:ILE:HD13	3:C:162:TYR:OH	1.96	0.66
2:B:349:TRP:CD2	2:B:364:ILE:CD1	2.78	0.66
2:B:739:LYS:HD2	2:B:743:THR:O	1.95	0.66
3:C:188:ILE:HD11	3:C:394:PHE:HA	1.76	0.66
3:C:5:ILE:CD1	3:C:252:MET:HG3	2.25	0.66
1:A:566:ILE:CD1	1:A:574:ILE:CD1	2.50	0.66
2:B:296:ILE:HD11	2:B:327:ILE:HG12	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:586:ILE:HD13	2:B:736:LEU:HD13	1.75	0.66
3:D:284:ILE:HD11	3:D:287:LYS:HA	1.78	0.66
2:B:636:ILE:CD1	3:D:437:TYR:CE1	2.79	0.66
3:C:229:GLN:OE1	3:C:280:ILE:HD11	1.96	0.66
3:D:139:LEU:HD21	3:D:235:ILE:HD13	1.77	0.66
2:B:482:LEU:CD2	2:B:735:ILE:HD12	2.24	0.65
1:A:148:ASP:OD1	2:B:285:ARG:NH2	2.29	0.65
2:B:586:ILE:HD11	2:B:732:LEU:CD2	2.26	0.65
3:D:200:ALA:CB	3:D:260:ILE:CD1	2.75	0.65
1:A:702:ILE:HD11	1:A:767:TYR:CD2	2.31	0.65
3:D:258:THR:CG2	3:D:356:ILE:CD1	2.70	0.65
1:A:599:LEU:HD11	1:A:640:ILE:HD12	1.78	0.65
1:A:68:ILE:HG13	2:B:281:LYS:HZ3	1.62	0.65
1:A:706:PHE:HE2	1:A:768:ILE:HD11	1.61	0.65
1:A:641:LYS:CG	3:C:356:ILE:HD13	2.26	0.65
1:A:625:ILE:HD11	1:A:765:ILE:HD11	1.79	0.65
1:A:72:GLY:HA3	2:B:222:HIS:HE1	1.58	0.65
2:B:823:LEU:C	2:B:823:LEU:HD13	2.16	0.65
3:C:131:ASP:OD1	3:D:284:ILE:HD12	1.96	0.65
3:C:188:ILE:HD12	3:C:394:PHE:CD1	2.31	0.65
3:D:188:ILE:HD11	3:D:394:PHE:CD2	2.31	0.65
2:B:206:GLN:HE21	2:B:209:ILE:CD1	2.09	0.65
2:B:402:ILE:CG1	2:B:449:ILE:CD1	2.72	0.65
2:B:405:ILE:CG2	2:B:456:ILE:CD1	2.59	0.65
2:B:527:HIS:HA	2:B:538:ILE:HD13	1.77	0.65
3:C:188:ILE:HD12	3:C:394:PHE:CD1	2.31	0.65
1:A:129:THR:N	2:B:322:HIS:CE1	2.65	0.65
2:B:825:ILE:CD1	2:B:841:LEU:HD11	2.22	0.65
1:A:71:GLU:CA	2:B:216:PHE:CE2	2.79	0.65
1:A:129:THR:N	2:B:322:HIS:HE1	1.94	0.65
1:A:780:ILE:HD13	1:A:789:GLU:CD	2.16	0.65
1:A:136:GLN:HE21	2:B:296:ILE:CD1	2.10	0.65
3:D:5:ILE:HD12	3:D:53:PHE:CZ	2.32	0.65
3:D:256:TYR:CE1	3:D:260:ILE:CD1	2.79	0.65
3:C:125:LYS:HD3	3:D:283:ASP:CG	2.17	0.65
1:A:151:LEU:HD21	2:B:285:ARG:HG2	1.77	0.65
1:A:70:LEU:CD1	2:B:220:LEU:HD13	2.27	0.65
3:D:123:ILE:HG22	3:D:127:ILE:HD12	1.78	0.65
1:A:68:ILE:CG1	2:B:281:LYS:HD2	2.27	0.65
1:A:137:ARG:HH21	2:B:325:LEU:CD1	2.08	0.65
3:C:328:PRO:HD2	3:C:331:ILE:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ILE:CD1	1:A:272:LEU:CD2	2.67	0.65
1:A:585:ILE:CD1	1:A:683:ILE:HG12	2.09	0.65
1:A:68:ILE:HD12	2:B:216:PHE:CG	2.31	0.65
2:B:339:ILE:HD13	2:B:439:ARG:HG3	1.79	0.65
1:A:137:ARG:NH2	2:B:325:LEU:CD1	2.58	0.65
1:A:155:VAL:HG11	2:B:285:ARG:NH2	2.12	0.65
1:A:65:ASN:OD1	2:B:215:ASN:ND2	2.30	0.65
3:C:67:ILE:HD12	3:C:123:ILE:HG23	1.79	0.65
1:A:584:ILE:CD1	1:A:687:ARG:CG	2.72	0.65
2:B:412:LEU:HD13	2:B:463:ILE:CD1	2.26	0.65
3:C:188:ILE:HD11	3:C:394:PHE:HB3	1.79	0.65
1:A:641:LYS:HG2	3:C:356:ILE:HD11	1.79	0.65
1:A:154:LEU:CD2	2:B:281:LYS:NZ	2.55	0.65
1:A:102:PHE:HB3	1:A:170:ILE:CD1	2.26	0.64
3:C:188:ILE:HD12	3:C:394:PHE:CB	2.19	0.64
2:B:405:ILE:HG12	2:B:456:ILE:CD1	2.27	0.64
1:A:68:ILE:O	2:B:281:LYS:CE	2.44	0.64
2:B:656:ILE:HD11	2:B:738:HIS:CE1	2.30	0.64
1:A:606:LEU:HG	1:A:710:ILE:CD1	2.27	0.64
1:A:127:SER:HB3	2:B:299:ARG:HH12	1.62	0.64
2:B:586:ILE:HD13	2:B:735:ILE:HD12	1.79	0.64
1:A:699:ILE:HD12	1:A:782:PHE:CZ	2.32	0.64
3:D:210:LEU:CD1	3:D:222:ILE:CD1	2.75	0.64
1:A:632:LEU:CD2	1:A:768:ILE:HD12	2.27	0.64
3:D:256:TYR:CD1	3:D:260:ILE:CD1	2.80	0.64
3:D:188:ILE:HD12	3:D:394:PHE:CG	2.32	0.64
3:C:127:ILE:HD13	3:C:162:TYR:HE2	1.62	0.64
3:D:200:ALA:HB2	3:D:260:ILE:CD1	2.27	0.64
1:A:425:ILE:CD1	1:A:482:LEU:CB	2.74	0.64
1:A:64:LEU:HG	2:B:216:PHE:HE2	1.63	0.64
2:B:398:LEU:CD1	2:B:449:ILE:HD12	2.27	0.64
3:D:188:ILE:HD12	3:D:394:PHE:CD1	2.32	0.64
2:B:634:ILE:HD12	2:B:809:LEU:HD23	1.77	0.64
1:A:573:ILE:CD1	1:A:673:GLN:CB	2.51	0.64
2:B:402:ILE:HG12	2:B:449:ILE:CD1	2.25	0.64
1:A:151:LEU:HD13	2:B:285:ARG:HG3	1.80	0.64
1:A:623:ARG:NH2	1:A:761:ILE:HD11	2.11	0.64
1:A:152:LYS:HD2	2:B:285:ARG:NH1	2.06	0.64
2:B:188:VAL:HB	2:B:224:ILE:HD12	1.79	0.64
2:B:398:LEU:HD11	2:B:449:ILE:HD12	1.77	0.64
2:B:257:ILE:HD13	2:B:297:TYR:OH	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:306:VAL:HG23	3:D:382:THR:HG21	1.78	0.64
2:B:209:ILE:HD13	2:B:222:HIS:CE1	2.33	0.64
2:B:405:ILE:CB	2:B:456:ILE:HD13	2.28	0.64
1:A:66:VAL:HG11	1:A:94:ILE:CD1	2.28	0.64
1:A:152:LYS:CG	2:B:285:ARG:NH1	2.32	0.64
3:C:21:LEU:HD11	3:C:235:ILE:HD13	1.80	0.64
1:A:558:TYR:CD1	1:A:693:ILE:CD1	2.80	0.64
1:A:606:LEU:HD22	1:A:710:ILE:HD11	1.79	0.63
1:A:66:VAL:HG23	1:A:94:ILE:HD13	1.80	0.63
1:A:425:ILE:HD12	1:A:482:LEU:HB2	1.79	0.63
2:B:418:GLU:OE2	2:B:463:ILE:CD1	2.39	0.63
2:B:184:ILE:HD13	2:B:217:GLU:OE1	1.98	0.63
1:A:570:LEU:HD23	1:A:573:ILE:CD1	2.26	0.63
2:B:349:TRP:CD1	2:B:364:ILE:CD1	2.80	0.63
2:B:412:LEU:HD22	2:B:463:ILE:HD12	1.72	0.63
1:A:63:LEU:CD2	1:A:170:ILE:HD12	2.29	0.63
1:A:151:LEU:HD11	2:B:285:ARG:NE	2.13	0.63
1:A:136:GLN:CD	2:B:323:GLY:CA	2.66	0.63
1:A:152:LYS:CG	2:B:285:ARG:HD2	2.28	0.63
1:A:63:LEU:CD2	1:A:170:ILE:HD12	2.29	0.63
1:A:706:PHE:HE2	1:A:768:ILE:HD12	1.57	0.63
2:B:209:ILE:HD13	2:B:213:ILE:CD1	2.29	0.63
3:D:256:TYR:CE2	3:D:260:ILE:CD1	2.81	0.63
1:A:599:LEU:HD22	1:A:640:ILE:CD1	2.18	0.63
3:D:188:ILE:CD1	3:D:394:PHE:CE1	2.81	0.63
3:C:128:ASP:OD2	3:D:281:HIS:ND1	2.31	0.63
2:B:257:ILE:HD12	2:B:301:THR:OG1	1.98	0.63
1:A:148:ASP:CG	2:B:285:ARG:HH21	2.02	0.63
3:C:137:GLN:NE2	3:C:235:ILE:HD11	2.13	0.63
3:D:188:ILE:CD1	3:D:394:PHE:CB	2.76	0.63
2:B:412:LEU:HD22	2:B:463:ILE:CD1	2.28	0.63
3:C:129:SER:OG	3:D:283:ASP:CG	2.37	0.63
1:A:606:LEU:HD21	1:A:710:ILE:CD1	2.28	0.63
2:B:402:ILE:HD11	2:B:449:ILE:CD1	2.29	0.63
1:A:62:ASP:CG	1:A:94:ILE:HD13	2.19	0.63
1:A:155:VAL:HG12	2:B:281:LYS:CD	2.28	0.63
1:A:136:GLN:HB3	2:B:323:GLY:HA2	1.79	0.63
1:A:362:GLN:NE2	2:B:447:GLU:HG3	2.12	0.63
1:A:425:ILE:CD1	1:A:482:LEU:HD22	2.27	0.63
1:A:150:TYR:HD1	1:A:177:ILE:CD1	2.12	0.63
3:C:67:ILE:HD12	3:C:123:ILE:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:LYS:O	1:A:683:ILE:HD13	1.99	0.63
2:B:349:TRP:CG	2:B:364:ILE:HD13	2.33	0.63
2:B:634:ILE:CD1	2:B:809:LEU:CD2	2.76	0.63
1:A:135:LEU:CD1	1:A:247:ILE:HD13	2.29	0.62
1:A:366:ILE:H	1:A:404:ILE:CD1	2.11	0.62
2:B:418:GLU:HB3	2:B:463:ILE:HD13	1.81	0.62
1:A:140:TYR:CB	2:B:324:ASP:OD1	2.47	0.62
2:B:296:ILE:HD11	2:B:327:ILE:CB	2.29	0.62
1:A:74:TYR:CB	2:B:215:ASN:ND2	2.62	0.62
1:A:426:PHE:CD2	1:A:564:ILE:CD1	2.82	0.62
3:D:255:ILE:HD12	3:D:358:ARG:CD	2.29	0.62
3:C:200:ALA:CB	3:C:260:ILE:HD11	2.29	0.62
3:C:238:VAL:CG2	3:C:322:ILE:HD12	2.23	0.62
3:C:255:ILE:HD11	3:C:358:ARG:CZ	2.29	0.62
1:A:151:LEU:HD22	2:B:285:ARG:CB	2.28	0.62
2:B:394:ILE:HD13	2:B:445:PHE:CD2	2.34	0.62
1:A:133:MET:SD	2:B:328:ARG:NH2	2.72	0.62
1:A:137:ARG:HA	2:B:324:ASP:OD1	1.99	0.62
3:D:139:LEU:HD22	3:D:235:ILE:HD11	1.80	0.62
1:A:126:TRP:CZ2	1:A:196:ILE:HD11	2.35	0.62
1:A:137:ARG:NH2	2:B:328:ARG:NE	2.47	0.62
2:B:407:LYS:HZ1	2:B:721:ILE:HD12	1.63	0.62
2:B:412:LEU:HD22	2:B:463:ILE:CD1	2.29	0.62
1:A:585:ILE:CD1	1:A:683:ILE:HD11	2.29	0.62
1:A:74:TYR:CE2	2:B:216:PHE:HZ	2.14	0.62
1:A:416:ILE:HD11	1:A:664:ARG:HG2	1.82	0.62
1:A:157:ARG:CD	1:A:176:ILE:HD13	2.29	0.62
1:A:66:VAL:HA	1:A:75:ILE:HD11	1.82	0.62
2:B:335:PHE:CE2	2:B:339:ILE:CD1	2.74	0.62
1:A:363:ILE:HD11	1:A:404:ILE:CG2	2.29	0.62
2:B:568:LEU:HD22	2:B:568:LEU:H	1.63	0.62
3:D:188:ILE:HD12	3:D:394:PHE:HB2	1.78	0.62
3:D:127:ILE:HD12	3:D:161:ARG:NH1	2.12	0.62
1:A:66:VAL:CG2	1:A:94:ILE:CD1	2.77	0.62
1:A:68:ILE:O	2:B:281:LYS:CD	2.47	0.62
2:B:184:ILE:HD13	2:B:213:ILE:CD1	2.30	0.62
2:B:402:ILE:HD11	2:B:449:ILE:CD1	2.30	0.62
1:A:628:ALA:HB1	1:A:765:ILE:HD13	1.82	0.62
1:A:126:TRP:HZ2	1:A:196:ILE:HD11	1.64	0.62
3:D:188:ILE:HD12	3:D:394:PHE:CE2	2.35	0.62
3:D:188:ILE:HD11	3:D:394:PHE:CZ	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:THR:HG22	2:B:207:ILE:CD1	2.30	0.62
1:A:137:ARG:HH22	2:B:325:LEU:HD21	1.61	0.62
1:A:362:GLN:NE2	2:B:447:GLU:CD	2.52	0.61
2:B:192:LEU:HD21	2:B:287:ILE:CD1	2.29	0.61
2:B:772:PHE:HD1	2:B:812:ILE:HD12	1.65	0.61
2:B:739:LYS:O	2:B:743:THR:O	2.19	0.61
3:C:175:ALA:HB3	3:C:178:SER:HB3	1.82	0.61
1:A:699:ILE:CD1	1:A:782:PHE:CE2	2.81	0.61
1:A:699:ILE:CD1	1:A:782:PHE:CZ	2.83	0.61
3:D:255:ILE:HD12	3:D:358:ARG:HD3	1.83	0.61
3:D:188:ILE:HD13	3:D:394:PHE:CG	2.35	0.61
1:A:78:PHE:CE1	4:F:21:UNK:CB	2.83	0.61
2:B:210:PRO:HG2	2:B:213:ILE:HD13	1.81	0.61
1:A:65:ASN:O	2:B:216:PHE:CE2	2.53	0.61
2:B:355:LEU:H	2:B:355:LEU:HD23	1.65	0.61
3:D:188:ILE:HD12	3:D:394:PHE:CD1	2.35	0.61
3:D:111:ILE:HG12	3:D:114:ARG:HH21	1.65	0.61
1:A:425:ILE:HD12	1:A:478:MET:HB3	1.81	0.61
1:A:70:LEU:CD1	2:B:220:LEU:CD1	2.70	0.61
1:A:296:TYR:OH	2:B:322:HIS:CE1	2.53	0.61
2:B:412:LEU:HD13	2:B:463:ILE:HD13	1.82	0.61
1:A:365:THR:HA	1:A:404:ILE:HD11	1.81	0.61
2:B:383:ILE:CD1	2:B:410:ILE:HG21	2.31	0.61
1:A:68:ILE:HD11	2:B:216:PHE:HD1	1.64	0.61
1:A:624:ARG:H	1:A:624:ARG:HE	1.48	0.61
3:C:6:ILE:CD1	3:C:126:GLU:HG3	2.30	0.61
1:A:599:LEU:HD11	1:A:640:ILE:CD1	2.31	0.61
2:B:284:TYR:CE1	2:B:291:ILE:HD13	2.36	0.61
1:A:588:TYR:HD1	1:A:693:ILE:CD1	2.14	0.61
1:A:128:ASP:OD2	2:B:295:ARG:HG2	2.00	0.61
3:D:200:ALA:HB2	3:D:260:ILE:CD1	2.23	0.61
1:A:558:TYR:CD1	1:A:693:ILE:HD13	2.35	0.61
2:B:241:PHE:CG	2:B:254:ILE:HD13	2.33	0.61
2:B:772:PHE:HB2	2:B:812:ILE:HD13	1.82	0.61
3:D:127:ILE:CD1	3:D:162:TYR:OH	2.49	0.61
1:A:73:THR:HB	2:B:215:ASN:HA	1.82	0.61
3:D:166:ILE:HD12	3:D:256:TYR:CD2	2.36	0.61
1:A:570:LEU:CD2	1:A:573:ILE:CD1	2.73	0.60
1:A:375:ILE:HD13	1:A:396:LYS:HD2	1.83	0.60
1:A:362:GLN:HB3	2:B:446:PHE:HE2	1.66	0.60
1:A:137:ARG:NH2	2:B:325:LEU:HD22	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ASP:OD1	2:B:285:ARG:NE	2.34	0.60
1:A:138:PHE:CG	1:A:192:ILE:CD1	2.80	0.60
1:A:151:LEU:HG	2:B:285:ARG:HG2	1.82	0.60
2:B:296:ILE:HD11	2:B:327:ILE:CD1	2.31	0.60
2:B:634:ILE:HD13	2:B:772:PHE:CZ	2.36	0.60
2:B:402:ILE:HD11	2:B:449:ILE:HD11	1.83	0.60
2:B:742:ALA:HB1	2:B:743:THR:HG23	1.82	0.60
1:A:353:LEU:HD13	1:A:572:ILE:HD13	1.81	0.60
3:D:195:ILE:HD12	3:D:423:PHE:HE1	1.66	0.60
1:A:567:PRO:CD	1:A:574:ILE:CD1	2.77	0.60
2:B:366:GLU:OE1	2:B:381:ILE:HD13	2.00	0.60
1:A:641:LYS:HD2	3:C:356:ILE:HD13	1.82	0.60
3:D:139:LEU:CD2	3:D:235:ILE:HD13	2.31	0.60
2:B:346:LEU:HD13	2:B:402:ILE:HD13	1.82	0.60
2:B:383:ILE:CD1	2:B:410:ILE:HD11	2.31	0.60
2:B:209:ILE:CD1	2:B:222:HIS:CE1	2.84	0.60
1:A:641:LYS:CG	3:C:356:ILE:CD1	2.78	0.60
1:A:426:PHE:CD2	1:A:564:ILE:HD13	2.35	0.60
1:A:66:VAL:HG11	1:A:94:ILE:HD11	1.83	0.60
1:A:147:GLU:HB2	2:B:285:ARG:HD3	1.83	0.60
2:B:482:LEU:HD22	2:B:657:ILE:HG21	1.83	0.60
1:A:142:ILE:CD1	1:A:189:LEU:HD21	2.31	0.60
2:B:242:ARG:N	2:B:254:ILE:CD1	2.64	0.60
2:B:480:ILE:CD1	2:B:537:VAL:HG21	2.31	0.60
1:A:366:ILE:HG12	1:A:368:SER:H	1.67	0.60
3:C:6:ILE:CD1	3:C:127:ILE:CG2	2.80	0.60
1:A:137:ARG:HH21	2:B:328:ARG:NE	1.95	0.60
1:A:68:ILE:HG12	2:B:281:LYS:HD2	1.84	0.60
2:B:772:PHE:HD1	2:B:812:ILE:CD1	2.15	0.60
2:B:728:HIS:CE1	2:B:732:LEU:HD11	2.35	0.60
1:A:138:PHE:CE2	1:A:275:ILE:HD13	2.36	0.60
2:B:668:LEU:O	2:B:671:THR:O	2.19	0.60
2:B:634:ILE:HG21	2:B:809:LEU:HD21	1.84	0.60
2:B:224:ILE:HD13	2:B:280:LEU:CD1	2.30	0.60
1:A:606:LEU:HD22	1:A:710:ILE:HD12	1.82	0.60
2:B:296:ILE:HD13	2:B:327:ILE:HD12	1.84	0.60
3:C:255:ILE:HD11	3:C:358:ARG:CZ	2.31	0.60
3:D:255:ILE:HD13	3:D:358:ARG:CZ	2.32	0.60
1:A:74:TYR:HB2	2:B:215:ASN:HD21	1.66	0.59
2:B:349:TRP:CG	2:B:364:ILE:HD12	2.37	0.59
3:C:188:ILE:CD1	3:C:394:PHE:HB2	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LYS:HA	2:B:285:ARG:CZ	2.31	0.59
1:A:129:THR:H	2:B:322:HIS:HE1	1.48	0.59
3:C:188:ILE:CD1	3:C:394:PHE:CD2	2.85	0.59
2:B:590:LEU:HD22	2:B:657:ILE:HD13	1.83	0.59
3:D:139:LEU:HD22	3:D:235:ILE:HD11	1.82	0.59
1:A:599:LEU:HD11	1:A:640:ILE:CD1	2.32	0.59
1:A:774:ILE:HD13	1:A:796:SER:HB3	1.81	0.59
1:A:558:TYR:CB	1:A:693:ILE:CD1	2.75	0.59
1:A:137:ARG:HH22	2:B:328:ARG:CZ	2.15	0.59
1:A:140:TYR:CE1	2:B:292:ILE:HG21	2.35	0.59
2:B:296:ILE:HD13	2:B:327:ILE:HD13	1.84	0.59
2:B:418:GLU:HG3	2:B:463:ILE:HD12	1.83	0.59
1:A:357:VAL:CB	1:A:363:ILE:HD12	2.29	0.59
1:A:599:LEU:CD2	1:A:640:ILE:HD12	2.32	0.59
1:A:65:ASN:HB2	1:A:94:ILE:HD11	1.84	0.59
2:B:349:TRP:CH2	2:B:383:ILE:HD13	2.37	0.59
2:B:398:LEU:CD1	2:B:449:ILE:HD12	2.27	0.59
3:C:188:ILE:HD13	3:C:394:PHE:CB	2.32	0.59
3:D:200:ALA:HB2	3:D:260:ILE:HD12	1.84	0.59
1:A:138:PHE:CE1	1:A:275:ILE:CD1	2.73	0.59
1:A:71:GLU:HA	2:B:216:PHE:CZ	2.37	0.59
3:D:188:ILE:HD12	3:D:394:PHE:HB2	1.83	0.59
2:B:386:ASN:HD21	2:B:389:ARG:H	1.51	0.59
1:A:641:LYS:CB	3:C:356:ILE:HD12	2.31	0.59
1:A:195:GLU:CD	1:A:250:ILE:HD11	2.21	0.59
1:A:151:LEU:HD11	2:B:285:ARG:CD	2.32	0.59
1:A:109:ILE:HD11	1:A:170:ILE:HD11	1.83	0.59
2:B:493:ILE:CD1	2:B:598:TYR:CB	2.81	0.59
1:A:566:ILE:HD12	1:A:574:ILE:HB	1.83	0.59
3:D:210:LEU:HD11	3:D:222:ILE:HD11	1.83	0.59
1:A:143:ARG:NH2	2:B:288:TYR:OH	2.36	0.59
2:B:808:ASN:HD21	2:B:812:ILE:HD11	1.65	0.59
2:B:398:LEU:HD23	2:B:449:ILE:CD1	2.29	0.59
2:B:257:ILE:HD12	2:B:297:TYR:CG	2.29	0.59
1:A:147:GLU:CG	2:B:285:ARG:CD	2.66	0.59
2:B:743:THR:O	2:B:756:GLN:N	2.36	0.59
1:A:152:LYS:HG2	2:B:285:ARG:CZ	2.29	0.59
3:C:274:PRO:HB2	3:C:284:ILE:HD12	1.84	0.59
2:B:480:ILE:HD13	2:B:541:LEU:CD1	2.26	0.59
2:B:405:ILE:HG23	2:B:456:ILE:HD12	1.85	0.59
2:B:631:LEU:O	2:B:634:ILE:HG12	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:739:LYS:O	2:B:743:THR:O	2.20	0.59
1:A:134:VAL:HG12	1:A:275:ILE:HG23	1.85	0.58
2:B:405:ILE:CG1	2:B:456:ILE:HD12	2.32	0.58
1:A:65:ASN:ND2	2:B:215:ASN:HD22	2.01	0.58
2:B:643:GLN:CG	3:D:356:ILE:CD1	2.80	0.58
2:B:643:GLN:HG2	3:D:356:ILE:HD13	1.84	0.58
1:A:154:LEU:CD2	2:B:281:LYS:CE	2.74	0.58
2:B:242:ARG:CA	2:B:254:ILE:HD11	2.32	0.58
3:C:188:ILE:CD1	3:C:394:PHE:CD1	2.83	0.58
2:B:634:ILE:HD11	2:B:809:LEU:HG	1.84	0.58
1:A:588:TYR:CE1	1:A:693:ILE:HD12	2.37	0.58
2:B:207:ILE:HD11	2:B:221:LEU:HD23	1.84	0.58
1:A:144:ARG:CD	2:B:289:GLU:OE2	2.51	0.58
3:D:200:ALA:CA	3:D:260:ILE:CD1	2.74	0.58
1:A:74:TYR:CB	2:B:215:ASN:CG	2.71	0.58
2:B:184:ILE:HD13	2:B:217:GLU:OE2	2.02	0.58
1:A:63:LEU:CB	1:A:170:ILE:HD11	2.29	0.58
3:C:258:THR:HG21	3:C:356:ILE:CD1	2.09	0.58
1:A:151:LEU:CD1	2:B:285:ARG:HE	2.16	0.58
2:B:383:ILE:HD11	2:B:410:ILE:CD1	2.31	0.58
3:C:255:ILE:CD1	3:C:358:ARG:NH2	2.63	0.58
2:B:284:TYR:HE1	2:B:291:ILE:HD13	1.68	0.58
2:B:656:ILE:CD1	2:B:738:HIS:CG	2.86	0.58
2:B:634:ILE:CD1	2:B:772:PHE:CZ	2.81	0.58
3:D:139:LEU:HD22	3:D:235:ILE:CD1	2.32	0.58
2:B:288:TYR:HE2	2:B:292:ILE:CD1	1.97	0.58
1:A:425:ILE:HD11	1:A:478:MET:CG	2.30	0.58
2:B:405:ILE:HG22	2:B:456:ILE:HD13	1.83	0.58
1:A:375:ILE:CD1	1:A:396:LYS:HD2	2.33	0.58
3:D:188:ILE:CD1	3:D:394:PHE:CG	2.86	0.58
3:C:195:ILE:CD1	3:C:423:PHE:CE1	2.79	0.58
2:B:739:LYS:O	2:B:743:THR:O	2.20	0.58
3:D:166:ILE:HD12	3:D:256:TYR:CE2	2.39	0.58
1:A:606:LEU:CD1	1:A:710:ILE:HD11	2.34	0.58
3:D:188:ILE:HD13	3:D:394:PHE:CD1	2.38	0.58
2:B:405:ILE:CD1	2:B:452:GLN:CB	2.80	0.58
1:A:625:ILE:HD13	1:A:765:ILE:HG13	1.85	0.58
1:A:255:ILE:CD1	1:A:269:LYS:HG2	2.34	0.58
2:B:529:MET:HE2	2:B:538:ILE:HD11	1.77	0.58
2:B:493:ILE:HD12	2:B:598:TYR:CB	2.34	0.58
1:A:68:ILE:HD11	2:B:216:PHE:CD1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:284:ILE:HD11	3:D:371:GLU:HG2	1.86	0.58
3:C:255:ILE:HD13	3:C:358:ARG:NH2	2.17	0.58
2:B:768:SER:HB3	2:B:812:ILE:HD13	1.86	0.57
1:A:136:GLN:HE21	2:B:296:ILE:HD12	1.69	0.57
3:C:200:ALA:CB	3:C:260:ILE:CD1	2.71	0.57
2:B:634:ILE:HD12	2:B:809:LEU:HD21	1.85	0.57
2:B:207:ILE:HD13	2:B:221:LEU:CD2	2.34	0.57
1:A:140:TYR:HB3	2:B:324:ASP:OD1	2.04	0.57
1:A:570:LEU:HD22	1:A:573:ILE:CD1	2.34	0.57
3:D:200:ALA:HB2	3:D:260:ILE:CD1	2.27	0.57
1:A:142:ILE:HD12	1:A:189:LEU:CD2	2.35	0.57
3:C:242:ILE:HD11	3:C:252:MET:SD	2.45	0.57
2:B:567:PRO:O	2:B:570:LEU:HD12	2.04	0.57
1:A:599:LEU:CD1	1:A:640:ILE:CD1	2.82	0.57
2:B:571:VAL:HG23	2:B:721:ILE:HD11	1.86	0.57
2:B:634:ILE:HD11	2:B:776:TYR:CD2	2.38	0.57
1:A:352:ILE:CG2	1:A:572:ILE:HD13	2.35	0.57
1:A:258:ASN:HD22	1:A:260:GLY:H	1.53	0.57
3:C:258:THR:OG1	3:C:356:ILE:CD1	2.51	0.57
1:A:643:ILE:HD12	1:A:692:LEU:HD23	1.85	0.57
3:C:72:GLU:H	3:C:73:PRO:CD	2.17	0.57
1:A:65:ASN:HD21	2:B:215:ASN:HD22	1.49	0.57
3:D:238:VAL:HG22	3:D:375:MET:SD	2.45	0.57
1:A:487:ASP:H	1:A:559:HIS:HB3	1.68	0.57
1:A:134:VAL:HG13	1:A:275:ILE:HB	1.86	0.57
2:B:194:ALA:HA	2:B:232:GLN:HG2	1.85	0.57
2:B:383:ILE:HD12	2:B:410:ILE:HG21	1.87	0.57
1:A:150:TYR:CD1	1:A:177:ILE:HD11	2.38	0.57
3:D:5:ILE:HD12	3:D:53:PHE:CZ	2.39	0.57
1:A:348:LEU:HD21	1:A:352:ILE:HD11	1.86	0.57
1:A:135:LEU:CD1	1:A:247:ILE:CD1	2.82	0.57
2:B:241:PHE:CG	2:B:254:ILE:CD1	2.87	0.57
1:A:70:LEU:CG	2:B:281:LYS:HZ3	2.05	0.57
2:B:260:GLU:OE2	2:B:330:ILE:CD1	2.53	0.57
2:B:772:PHE:CE1	2:B:812:ILE:CD1	2.84	0.57
1:A:365:THR:HG23	1:A:404:ILE:CD1	2.34	0.57
1:A:458:TYR:CE1	1:A:484:ILE:HD12	2.36	0.57
3:D:188:ILE:HD12	3:D:394:PHE:CD1	2.32	0.57
1:A:75:ILE:HD12	2:B:216:PHE:HE1	1.67	0.57
3:D:199:ASP:O	3:D:260:ILE:CD1	2.49	0.57
1:A:80:ASP:O	1:A:90:ILE:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:335:PHE:CD1	2:B:339:ILE:HD11	2.35	0.56
3:D:234:ILE:HD11	3:D:303:ASN:ND2	2.20	0.56
1:A:137:ARG:NH2	2:B:328:ARG:CZ	2.68	0.56
1:A:66:VAL:CG2	1:A:94:ILE:HD13	2.35	0.56
3:D:234:ILE:HD13	3:D:303:ASN:ND2	2.19	0.56
1:A:375:ILE:HD11	1:A:396:LYS:CB	2.34	0.56
2:B:222:HIS:HA	2:B:225:PHE:CE2	2.40	0.56
1:A:136:GLN:HG3	2:B:323:GLY:O	2.04	0.56
3:D:210:LEU:HD11	3:D:222:ILE:HD13	1.87	0.56
1:A:72:GLY:CA	2:B:215:ASN:O	2.53	0.56
3:D:200:ALA:CB	3:D:260:ILE:HD11	2.22	0.56
1:A:66:VAL:CG1	1:A:94:ILE:CD1	2.83	0.56
3:C:127:ILE:CD1	3:C:162:TYR:CE2	2.88	0.56
1:A:137:ARG:CZ	2:B:325:LEU:CD1	2.74	0.56
1:A:73:THR:CG2	2:B:215:ASN:HA	2.33	0.56
2:B:571:VAL:CG2	2:B:721:ILE:CD1	2.66	0.56
3:C:125:LYS:HE3	3:D:282:ASP:O	2.05	0.56
1:A:194:GLU:HB3	1:A:250:ILE:HD11	1.86	0.56
3:C:383:VAL:HG12	3:C:387:PHE:CZ	2.41	0.56
3:D:127:ILE:HD12	3:D:161:ARG:CZ	2.36	0.56
1:A:410:PHE:HA	1:A:415:LEU:H	1.70	0.56
2:B:241:PHE:CB	2:B:254:ILE:HD13	2.34	0.56
3:D:175:ALA:HB2	3:D:206:ASN:HB3	1.88	0.56
1:A:625:ILE:CD1	1:A:758:LEU:CD2	2.84	0.56
2:B:563:ILE:HG12	2:B:564:LEU:HD23	1.86	0.56
1:A:641:LYS:CD	3:C:356:ILE:CD1	2.83	0.56
1:A:628:ALA:CB	1:A:765:ILE:HD13	2.36	0.56
1:A:135:LEU:HD11	1:A:247:ILE:CD1	2.35	0.56
2:B:209:ILE:CD1	2:B:213:ILE:CD1	2.83	0.56
3:C:212:ILE:CD1	3:C:275:PHE:CE2	2.86	0.56
1:A:363:ILE:HD13	1:A:413:TYR:CB	2.25	0.56
1:A:68:ILE:HG13	2:B:281:LYS:HE3	1.87	0.56
1:A:128:ASP:HB3	2:B:299:ARG:HD3	1.87	0.56
1:A:296:TYR:CE2	2:B:322:HIS:HD2	2.23	0.56
2:B:570:LEU:CD2	2:B:721:ILE:HD13	2.30	0.56
1:A:151:LEU:CD2	2:B:285:ARG:CB	2.84	0.56
3:C:188:ILE:HD11	3:C:394:PHE:CB	2.36	0.56
1:A:641:LYS:HG2	3:C:356:ILE:CD1	2.35	0.56
3:D:188:ILE:CD1	3:D:394:PHE:CD1	2.89	0.56
2:B:209:ILE:CD1	2:B:222:HIS:CE1	2.89	0.56
1:A:425:ILE:CD1	1:A:482:LEU:HB2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLY:H	1:A:75:ILE:HB	1.71	0.56
3:D:210:LEU:HD11	3:D:222:ILE:CD1	2.35	0.56
1:A:140:TYR:CG	2:B:324:ASP:OD1	2.58	0.56
2:B:412:LEU:CG	2:B:463:ILE:HD12	2.36	0.56
1:A:68:ILE:HD12	2:B:216:PHE:CB	2.36	0.56
1:A:352:ILE:HG22	1:A:572:ILE:CD1	2.36	0.56
1:A:296:TYR:OH	2:B:322:HIS:HB2	2.05	0.56
1:A:155:VAL:CG1	2:B:285:ARG:HH22	2.17	0.56
3:C:256:TYR:CD1	3:C:260:ILE:CD1	2.88	0.56
1:A:151:LEU:HD11	2:B:285:ARG:CG	2.36	0.55
2:B:532:PRO:O	2:B:538:ILE:HD11	2.06	0.55
2:B:349:TRP:CG	2:B:364:ILE:HD12	2.41	0.55
1:A:65:ASN:CG	2:B:215:ASN:ND2	2.60	0.55
2:B:608:ASN:HB3	3:D:260:ILE:HD13	1.87	0.55
1:A:406:LEU:HD21	1:A:672:ILE:CD1	2.30	0.55
2:B:634:ILE:CD1	2:B:809:LEU:CG	2.82	0.55
1:A:365:THR:CA	1:A:404:ILE:HD11	2.36	0.55
3:D:356:ILE:HD11	3:D:358:ARG:HH22	1.71	0.55
3:C:75:VAL:HG21	3:C:94:VAL:HG22	1.88	0.55
3:C:72:GLU:HA	3:C:75:VAL:HG12	1.87	0.55
2:B:297:TYR:OH	2:B:330:ILE:HD12	2.04	0.55
2:B:482:LEU:HD22	2:B:657:ILE:CG2	2.37	0.55
2:B:339:ILE:HD12	2:B:440:GLY:H	1.71	0.55
1:A:595:HIS:ND1	1:A:640:ILE:HD12	2.15	0.55
1:A:68:ILE:CD1	2:B:216:PHE:HB2	2.14	0.55
3:C:70:ASP:CG	3:C:71:SER:H	2.09	0.55
2:B:200:PHE:CZ	2:B:207:ILE:CD1	2.74	0.55
2:B:586:ILE:CG2	2:B:735:ILE:HD13	2.26	0.55
1:A:61:LYS:CE	2:B:216:PHE:CE1	2.86	0.55
1:A:630:ARG:HA	1:A:633:HIS:CD2	2.42	0.55
1:A:65:ASN:CG	2:B:215:ASN:CB	2.70	0.55
1:A:780:ILE:HD13	1:A:789:GLU:OE2	2.06	0.55
1:A:367:PRO:CG	1:A:404:ILE:HD13	2.35	0.55
1:A:632:LEU:HD22	1:A:768:ILE:HD12	1.88	0.55
3:C:342:ILE:CD1	3:C:344:PHE:CZ	2.83	0.55
1:A:641:LYS:CD	3:C:356:ILE:HD12	2.30	0.55
1:A:606:LEU:HG	1:A:710:ILE:HD11	1.87	0.55
1:A:133:MET:HG3	2:B:322:HIS:HA	1.87	0.55
3:C:256:TYR:CD1	3:C:260:ILE:HD12	2.40	0.55
2:B:779:LEU:HD21	2:B:805:PHE:HB3	1.88	0.55
3:C:131:ASP:CG	3:D:284:ILE:HD12	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:HH21	2:B:325:LEU:CD2	2.15	0.55
1:A:68:ILE:O	2:B:220:LEU:HD11	2.07	0.55
1:A:138:PHE:CD1	1:A:275:ILE:HD12	2.39	0.55
2:B:296:ILE:HD13	2:B:327:ILE:CG2	2.37	0.55
1:A:375:ILE:CD1	1:A:396:LYS:CB	2.84	0.55
1:A:140:TYR:HE2	2:B:327:ILE:HD11	1.72	0.55
2:B:289:GLU:CD	2:B:289:GLU:H	2.10	0.55
1:A:203:ARG:HH22	1:A:243:LYS:HD3	1.71	0.55
2:B:209:ILE:HD11	2:B:222:HIS:CE1	2.41	0.55
2:B:271:LEU:CD1	2:B:287:ILE:HD11	2.37	0.55
1:A:126:TRP:HZ2	1:A:196:ILE:CD1	2.17	0.55
2:B:636:ILE:HD13	3:D:437:TYR:CD1	2.42	0.55
1:A:714:ARG:O	1:A:760:LEU:HD22	2.07	0.55
3:C:5:ILE:HD11	3:C:137:GLN:HB2	1.88	0.55
3:D:5:ILE:CD1	3:D:252:MET:CE	2.84	0.55
1:A:702:ILE:HG23	1:A:768:ILE:CD1	2.37	0.55
3:D:309:ALA:H	3:D:385:ASN:HD21	1.55	0.55
2:B:656:ILE:CD1	2:B:738:HIS:HE1	2.18	0.54
1:A:102:PHE:CB	1:A:170:ILE:HD12	2.34	0.54
2:B:610:ILE:HD11	3:D:196:GLU:O	1.96	0.54
1:A:150:TYR:HD1	1:A:177:ILE:HD12	1.72	0.54
2:B:206:GLN:NE2	2:B:209:ILE:CD1	2.71	0.54
1:A:133:MET:HG3	2:B:322:HIS:HA	1.89	0.54
1:A:137:ARG:HH12	2:B:325:LEU:HD13	1.73	0.54
1:A:595:HIS:ND1	1:A:640:ILE:CD1	2.70	0.54
3:C:127:ILE:HD13	3:C:162:TYR:CE2	2.42	0.54
1:A:137:ARG:NE	2:B:325:LEU:HB2	2.21	0.54
3:D:139:LEU:CD2	3:D:235:ILE:CD1	2.80	0.54
3:C:255:ILE:CD1	3:C:358:ARG:CZ	2.85	0.54
3:C:277:SER:HB3	3:C:279:TYR:H	1.71	0.54
1:A:425:ILE:HD13	1:A:482:LEU:CD2	2.34	0.54
1:A:366:ILE:O	1:A:404:ILE:HD12	2.07	0.54
2:B:271:LEU:HD11	2:B:287:ILE:HD11	1.87	0.54
2:B:405:ILE:CG2	2:B:456:ILE:HD12	2.28	0.54
1:A:109:ILE:HD11	1:A:170:ILE:HD11	1.89	0.54
3:C:189:LEU:HD21	3:C:420:GLN:HG2	1.89	0.54
2:B:402:ILE:HG13	2:B:449:ILE:HD13	1.87	0.54
3:D:139:LEU:CD2	3:D:235:ILE:CD1	2.86	0.54
1:A:62:ASP:OD1	1:A:94:ILE:CD1	2.56	0.54
3:C:212:ILE:HD13	3:C:275:PHE:CE1	2.42	0.54
1:A:150:TYR:CD1	1:A:177:ILE:HD12	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PHE:CG	1:A:275:ILE:CD1	2.85	0.54
1:A:422:LEU:HD13	1:A:564:ILE:CD1	2.38	0.54
1:A:367:PRO:CB	1:A:404:ILE:HD12	2.37	0.54
2:B:453:TYR:O	2:B:457:VAL:HG22	2.07	0.54
3:C:129:SER:OG	3:D:284:ILE:O	2.22	0.54
1:A:109:ILE:HG22	1:A:177:ILE:CD1	2.37	0.54
3:D:217:PHE:CG	3:D:280:ILE:HD13	2.42	0.54
3:D:393:THR:O	3:D:397:VAL:HG23	2.06	0.54
1:A:638:HIS:CE1	3:C:340:GLN:HE22	2.25	0.54
3:C:128:ASP:OD2	3:D:281:HIS:CE1	2.61	0.54
3:C:200:ALA:HB2	3:C:260:ILE:CD1	2.28	0.54
1:A:365:THR:HA	1:A:404:ILE:HD11	1.89	0.54
2:B:405:ILE:HG23	2:B:456:ILE:HD13	1.90	0.54
2:B:455:GLU:O	2:B:459:HIS:CD2	2.61	0.54
3:D:188:ILE:HD12	3:D:394:PHE:CE1	2.40	0.54
1:A:63:LEU:HD23	1:A:109:ILE:HD11	1.90	0.54
1:A:433:HIS:CD2	3:C:2:GLY:HA3	2.41	0.54
3:D:255:ILE:CD1	3:D:320:ASN:HD21	2.20	0.54
1:A:142:ILE:HD12	1:A:193:TYR:OH	2.08	0.54
1:A:71:GLU:OE1	2:B:216:PHE:CD1	2.61	0.54
1:A:140:TYR:CD2	2:B:324:ASP:HB3	2.43	0.54
2:B:407:LYS:HZ3	2:B:721:ILE:HD12	1.73	0.54
1:A:613:LYS:HG3	1:A:714:ARG:O	2.07	0.54
3:C:67:ILE:CD1	3:C:123:ILE:CG2	2.86	0.54
2:B:335:PHE:CZ	2:B:339:ILE:HD12	2.43	0.54
3:C:315:TYR:HA	3:C:346:SER:HB2	1.89	0.54
3:C:139:LEU:CD2	3:C:235:ILE:HD13	2.38	0.54
1:A:70:LEU:CD1	2:B:220:LEU:HD21	2.34	0.53
2:B:296:ILE:CD1	2:B:327:ILE:HD13	2.38	0.53
1:A:71:GLU:CD	2:B:222:HIS:NE2	2.62	0.53
2:B:296:ILE:CD1	2:B:327:ILE:HA	2.38	0.53
1:A:142:ILE:HD11	1:A:186:MET:CG	2.37	0.53
1:A:135:LEU:HD13	1:A:247:ILE:HD13	1.90	0.53
1:A:641:LYS:HD2	3:C:356:ILE:HD13	1.86	0.53
3:C:200:ALA:HB2	3:C:260:ILE:HD13	1.85	0.53
2:B:493:ILE:HD12	2:B:598:TYR:HB2	1.90	0.53
1:A:367:PRO:HG3	1:A:404:ILE:CD1	2.30	0.53
3:D:268:LEU:HD23	3:D:379:ASN:HD22	1.74	0.53
2:B:284:TYR:CE1	2:B:291:ILE:CD1	2.91	0.53
2:B:349:TRP:HE1	2:B:364:ILE:CD1	2.19	0.53
2:B:284:TYR:CE1	2:B:291:ILE:HD13	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:CD1	2:B:285:ARG:NE	2.71	0.53
1:A:66:VAL:CG2	1:A:170:ILE:HD12	2.36	0.53
1:A:147:GLU:CG	2:B:285:ARG:HD3	2.38	0.53
3:C:238:VAL:HG22	3:C:322:ILE:HD13	1.91	0.53
1:A:405:PHE:HZ	1:A:573:ILE:HD11	1.69	0.53
3:C:6:ILE:HD13	3:C:126:GLU:HG3	1.91	0.53
1:A:62:ASP:OD1	1:A:94:ILE:HD11	2.08	0.53
1:A:143:ARG:HH11	2:B:292:ILE:CD1	2.20	0.53
1:A:70:LEU:CD1	2:B:220:LEU:CD1	2.77	0.53
2:B:568:LEU:N	2:B:721:ILE:HD12	2.23	0.53
2:B:656:ILE:HD12	2:B:738:HIS:NE2	2.19	0.53
1:A:567:PRO:CG	1:A:574:ILE:HD13	2.38	0.53
1:A:62:ASP:OD2	1:A:94:ILE:HD13	2.09	0.53
3:C:238:VAL:HG22	3:C:322:ILE:HD11	1.90	0.53
2:B:586:ILE:CB	2:B:735:ILE:HD13	2.38	0.53
1:A:358:ARG:NH2	2:B:443:THR:CG2	2.71	0.53
2:B:586:ILE:HD11	2:B:732:LEU:HB3	1.90	0.53
3:C:32:GLY:H	3:C:36:LEU:H	1.57	0.53
2:B:192:LEU:CD2	2:B:287:ILE:CD1	2.81	0.53
2:B:583:TYR:CE1	2:B:732:LEU:HD13	2.43	0.53
1:A:142:ILE:CD1	1:A:189:LEU:CD2	2.87	0.53
2:B:529:MET:SD	2:B:538:ILE:HD13	2.49	0.53
1:A:151:LEU:HD13	2:B:285:ARG:HE	1.74	0.53
1:A:326:ILE:HD12	1:A:332:LEU:HD22	1.91	0.53
1:A:625:ILE:HA	1:A:761:ILE:HD11	1.90	0.53
1:A:425:ILE:CD1	1:A:482:LEU:CG	2.85	0.53
3:D:13:CYS:O	3:D:17:VAL:HG23	2.09	0.53
3:C:188:ILE:HD11	3:C:394:PHE:CG	2.43	0.53
3:D:13:CYS:SG	3:D:224:LEU:HD11	2.49	0.53
1:A:566:ILE:HD13	1:A:574:ILE:O	2.09	0.53
3:D:29:HIS:HA	3:D:46:ARG:HH12	1.74	0.53
1:A:570:LEU:HD23	1:A:573:ILE:CD1	2.29	0.53
1:A:136:GLN:C	2:B:324:ASP:OD1	2.48	0.53
2:B:568:LEU:HG	2:B:721:ILE:HD12	1.91	0.53
2:B:646:SER:CB	3:D:356:ILE:HD12	2.38	0.53
2:B:339:ILE:HD13	2:B:439:ARG:CG	2.38	0.53
1:A:143:ARG:NH1	2:B:292:ILE:HD13	2.23	0.53
1:A:348:LEU:O	1:A:348:LEU:HD23	2.09	0.53
3:C:13:CYS:HA	3:C:228:ASN:HD21	1.74	0.53
2:B:586:ILE:CD1	2:B:735:ILE:CD1	2.64	0.53
1:A:684:MET:HA	1:A:687:ARG:HE	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:ARG:NH2	1:A:761:ILE:HD12	2.23	0.53
1:A:55:GLN:HE22	1:A:97:LYS:HD2	1.74	0.53
1:A:155:VAL:HG11	2:B:282:SER:OG	2.08	0.52
2:B:209:ILE:HD13	2:B:213:ILE:HD11	1.91	0.52
1:A:151:LEU:CD2	2:B:285:ARG:HB2	2.33	0.52
1:A:137:ARG:HH22	2:B:325:LEU:HD23	1.73	0.52
1:A:587:ARG:O	1:A:591:VAL:HG23	2.10	0.52
1:A:136:GLN:NE2	2:B:323:GLY:CA	2.51	0.52
2:B:820:LYS:HA	2:B:823:LEU:HD12	1.91	0.52
1:A:64:LEU:CD2	1:A:68:ILE:HD12	2.39	0.52
3:C:188:ILE:HD11	3:C:394:PHE:CB	2.39	0.52
1:A:112:TYR:OH	1:A:177:ILE:HD11	2.08	0.52
2:B:480:ILE:CD1	2:B:541:LEU:HD11	2.39	0.52
1:A:137:ARG:NH2	2:B:325:LEU:CG	2.72	0.52
3:C:4:GLU:HA	3:C:52:PRO:HA	1.92	0.52
3:D:256:TYR:OH	3:D:260:ILE:CD1	2.56	0.52
3:D:75:VAL:HG21	3:D:94:VAL:CG1	2.39	0.52
3:D:276:THR:HG21	3:D:284:ILE:HD12	1.91	0.52
1:A:367:PRO:CB	1:A:404:ILE:HD11	2.35	0.52
2:B:206:GLN:HE21	2:B:209:ILE:HD11	1.75	0.52
2:B:405:ILE:CA	2:B:456:ILE:HD11	2.30	0.52
1:A:581:LYS:CB	1:A:683:ILE:HD12	2.33	0.52
1:A:696:GLN:HE21	1:A:699:ILE:CD1	2.14	0.52
1:A:365:THR:HG22	1:A:404:ILE:HD13	1.90	0.52
1:A:62:ASP:CG	1:A:94:ILE:HD13	2.27	0.52
1:A:138:PHE:CZ	1:A:275:ILE:HD13	2.26	0.52
1:A:357:VAL:CG2	1:A:363:ILE:CD1	2.88	0.52
1:A:108:ARG:HG3	1:A:177:ILE:HD11	1.90	0.52
2:B:296:ILE:HD13	2:B:327:ILE:CD1	2.32	0.52
1:A:640:ILE:HD11	1:A:699:ILE:HD11	1.86	0.52
3:C:55:ARG:HH11	3:D:284:ILE:HD13	1.74	0.52
1:A:70:LEU:HD11	2:B:281:LYS:NZ	1.96	0.52
1:A:366:ILE:C	1:A:404:ILE:CD1	2.72	0.52
1:A:632:LEU:HD23	1:A:768:ILE:HD12	1.91	0.52
2:B:264:TYR:CZ	2:B:287:ILE:HD11	2.44	0.52
1:A:585:ILE:CD1	1:A:683:ILE:CD1	2.87	0.52
3:C:170:TYR:CE2	3:C:235:ILE:HD12	2.45	0.52
1:A:65:ASN:OD1	2:B:216:PHE:CE1	2.58	0.52
2:B:296:ILE:HD12	2:B:327:ILE:HD13	1.90	0.52
2:B:207:ILE:CD1	2:B:221:LEU:CD2	2.86	0.52
2:B:206:GLN:NE2	2:B:209:ILE:HD12	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:LYS:CB	1:A:683:ILE:HD12	2.39	0.52
3:D:212:ILE:HD13	3:D:275:PHE:CZ	2.45	0.52
1:A:66:VAL:HA	2:B:216:PHE:CE1	2.45	0.52
1:A:72:GLY:O	2:B:222:HIS:HE1	1.92	0.52
1:A:72:GLY:HA3	2:B:222:HIS:ND1	2.23	0.52
1:A:143:ARG:HH22	2:B:296:ILE:HD11	1.74	0.52
2:B:191:THR:CG2	2:B:207:ILE:HD13	2.39	0.52
1:A:64:LEU:HD21	1:A:68:ILE:HD12	1.91	0.52
3:C:6:ILE:HD12	3:C:127:ILE:CG2	2.40	0.52
1:A:630:ARG:HA	1:A:633:HIS:CD2	2.44	0.52
3:D:188:ILE:CD1	3:D:394:PHE:CD1	2.93	0.52
3:D:256:TYR:CD1	3:D:260:ILE:HD12	2.45	0.52
2:B:398:LEU:HD13	2:B:449:ILE:HD12	1.88	0.52
1:A:696:GLN:NE2	1:A:699:ILE:CD1	2.67	0.52
3:D:119:ILE:HD13	3:D:154:LEU:HD21	1.90	0.52
1:A:367:PRO:CG	1:A:404:ILE:CD1	2.88	0.52
2:B:634:ILE:CD1	2:B:809:LEU:HD21	2.40	0.52
1:A:128:ASP:OD1	2:B:295:ARG:HD3	2.10	0.52
3:C:6:ILE:HD13	3:C:126:GLU:CG	2.40	0.52
2:B:218:SER:O	2:B:222:HIS:CD2	2.63	0.52
1:A:361:LEU:HD21	2:B:443:THR:HG23	1.90	0.52
1:A:567:PRO:CG	1:A:574:ILE:CD1	2.87	0.52
2:B:386:ASN:ND2	2:B:389:ARG:H	2.07	0.52
2:B:527:HIS:CE1	2:B:538:ILE:HD11	2.14	0.52
2:B:241:PHE:C	2:B:254:ILE:CD1	2.78	0.52
2:B:296:ILE:HD11	2:B:327:ILE:CG1	2.38	0.52
3:D:289:HIS:CE1	3:D:323:ILE:HD13	2.44	0.52
1:A:595:HIS:O	1:A:599:LEU:HD13	2.09	0.52
3:D:234:ILE:HD11	3:D:303:ASN:CG	2.31	0.51
2:B:349:TRP:CD2	2:B:364:ILE:HD11	2.45	0.51
3:D:5:ILE:HD12	3:D:53:PHE:HZ	1.72	0.51
1:A:405:PHE:CZ	1:A:573:ILE:HD11	2.45	0.51
3:D:217:PHE:CD1	3:D:280:ILE:CD1	2.90	0.51
1:A:68:ILE:HD13	2:B:216:PHE:N	2.24	0.51
1:A:706:PHE:CE2	1:A:768:ILE:HD11	2.40	0.51
3:D:204:PHE:HE1	3:D:234:ILE:HD12	1.74	0.51
1:A:614:TYR:O	1:A:714:ARG:NH2	2.44	0.51
2:B:662:LYS:HD3	3:D:329:ARG:HH12	1.75	0.51
2:B:412:LEU:HD22	2:B:463:ILE:CD1	2.40	0.51
1:A:114:LYS:HE3	1:A:118:ILE:HD12	1.87	0.51
2:B:405:ILE:HG23	2:B:456:ILE:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:586:ILE:CB	2:B:735:ILE:CD1	2.87	0.51
3:C:173:PHE:CD1	3:C:203:VAL:HG13	2.46	0.51
1:A:595:HIS:ND1	1:A:640:ILE:HD13	2.24	0.51
3:D:123:ILE:CD1	3:D:154:LEU:HD11	2.40	0.51
1:A:93:LYS:HD3	4:F:28:UNK:CB	2.40	0.51
1:A:126:TRP:CH2	1:A:196:ILE:HD11	2.46	0.51
1:A:70:LEU:CD1	2:B:220:LEU:HD11	2.33	0.51
2:B:430:HIS:CB	2:B:448:ILE:HD12	2.40	0.51
3:D:188:ILE:HD11	3:D:394:PHE:HB3	1.92	0.51
1:A:707:CYS:O	1:A:711:LYS:HG3	2.10	0.51
3:D:5:ILE:CD1	3:D:252:MET:HE1	2.40	0.51
3:D:12:GLN:H	3:D:12:GLN:CD	2.13	0.51
1:A:68:ILE:CG1	2:B:281:LYS:HE3	2.40	0.51
1:A:584:ILE:CD1	1:A:687:ARG:HB2	2.41	0.51
3:D:299:LEU:H	3:D:299:LEU:HD22	1.75	0.51
3:D:256:TYR:HE1	3:D:260:ILE:CD1	2.16	0.51
1:A:70:LEU:CG	2:B:216:PHE:HE1	2.01	0.51
1:A:409:PHE:HB3	1:A:415:LEU:HB2	1.93	0.51
1:A:599:LEU:HD22	1:A:640:ILE:HD13	1.91	0.51
3:D:328:PRO:HG2	3:D:331:ILE:HG22	1.93	0.51
3:C:281:HIS:CD2	3:C:282:ASP:H	2.29	0.51
2:B:405:ILE:HD13	2:B:453:TYR:HA	1.93	0.51
1:A:367:PRO:HB2	1:A:404:ILE:HD11	1.93	0.51
3:D:342:ILE:HD13	3:D:344:PHE:CZ	2.46	0.51
1:A:155:VAL:CG1	2:B:281:LYS:HG2	2.40	0.51
2:B:346:LEU:HD13	2:B:402:ILE:HD13	1.91	0.51
1:A:296:TYR:OH	2:B:322:HIS:NE2	2.43	0.51
2:B:242:ARG:HG3	2:B:254:ILE:HD13	1.93	0.51
2:B:297:TYR:CZ	2:B:330:ILE:CD1	2.67	0.51
1:A:135:LEU:HD13	1:A:247:ILE:HD11	1.92	0.51
1:A:625:ILE:HD12	1:A:761:ILE:HG23	1.92	0.51
1:A:138:PHE:CE1	1:A:192:ILE:HD13	2.45	0.51
1:A:102:PHE:CE1	1:A:170:ILE:CD1	2.94	0.51
2:B:590:LEU:CD2	2:B:657:ILE:HD13	2.40	0.51
1:A:135:LEU:CD2	1:A:247:ILE:HD11	2.19	0.51
1:A:641:LYS:HD3	3:C:356:ILE:CD1	2.19	0.51
1:A:282:MET:HB3	1:A:292:LEU:HD11	1.93	0.51
1:A:195:GLU:OE1	1:A:250:ILE:HD12	2.10	0.51
3:C:308:THR:HG22	3:C:310:MET:H	1.76	0.51
1:A:135:LEU:HD11	1:A:247:ILE:HD11	1.94	0.50
2:B:765:LEU:O	2:B:769:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:LEU:HD13	1:A:484:ILE:HG13	1.93	0.50
1:A:422:LEU:CD1	1:A:564:ILE:HD12	2.41	0.50
2:B:408:SER:HA	2:B:411:PHE:CE2	2.46	0.50
2:B:264:TYR:OH	2:B:287:ILE:HD13	2.11	0.50
3:D:284:ILE:HD12	3:D:369:GLU:OE1	2.11	0.50
1:A:357:VAL:HG23	1:A:363:ILE:HD12	1.93	0.50
3:D:232:SER:HA	3:D:235:ILE:HG22	1.93	0.50
3:D:188:ILE:HD13	3:D:394:PHE:CG	2.45	0.50
1:A:142:ILE:HD11	1:A:188:LEU:CD1	2.40	0.50
3:D:242:ILE:HD13	3:D:252:MET:SD	2.50	0.50
1:A:135:LEU:HD13	1:A:247:ILE:CD1	2.41	0.50
1:A:757:ALA:O	1:A:761:ILE:HG13	2.12	0.50
3:D:210:LEU:HD11	3:D:222:ILE:HD13	1.88	0.50
1:A:137:ARG:NE	2:B:324:ASP:HA	2.26	0.50
2:B:586:ILE:HG21	2:B:735:ILE:HD11	1.92	0.50
1:A:296:TYR:OH	2:B:322:HIS:CE1	2.63	0.50
2:B:184:ILE:O	2:B:188:VAL:HG23	2.12	0.50
1:A:136:GLN:CD	2:B:323:GLY:N	2.65	0.50
1:A:332:LEU:HB3	1:A:334:ASP:H	1.76	0.50
2:B:339:ILE:HD11	2:B:440:GLY:HA3	1.83	0.50
2:B:479:ASN:HB3	2:B:485:LYS:HE3	1.92	0.50
1:A:62:ASP:CB	1:A:94:ILE:HD13	2.41	0.50
3:D:189:LEU:HD23	3:D:192:ARG:HH22	1.77	0.50
1:A:247:ILE:HD13	1:A:275:ILE:HG21	1.94	0.50
3:C:205:ASP:H	3:C:303:ASN:HB3	1.75	0.50
1:A:635:LYS:HA	1:A:638:HIS:CD2	2.47	0.50
1:A:606:LEU:HB2	1:A:710:ILE:HD13	1.93	0.50
2:B:296:ILE:CD1	2:B:327:ILE:HG23	2.42	0.50
2:B:312:PHE:CZ	2:B:316:LEU:HD11	2.46	0.50
2:B:775:VAL:HG12	2:B:780:ASN:HD21	1.77	0.50
1:A:189:LEU:O	1:A:192:ILE:HG12	2.12	0.50
3:C:51:LYS:HB3	3:C:52:PRO:HD3	1.94	0.50
3:D:123:ILE:HD11	3:D:154:LEU:HD11	1.93	0.50
1:A:422:LEU:CD1	1:A:564:ILE:CD1	2.90	0.50
1:A:425:ILE:CD1	1:A:482:LEU:HD21	2.27	0.50
1:A:606:LEU:HD13	1:A:710:ILE:HG21	1.93	0.50
1:A:599:LEU:CD2	1:A:640:ILE:CD1	2.83	0.50
2:B:656:ILE:CD1	2:B:738:HIS:HB2	2.40	0.50
1:A:152:LYS:HG2	2:B:285:ARG:HD2	1.94	0.50
1:A:134:VAL:HG11	1:A:247:ILE:HD12	1.93	0.50
1:A:361:LEU:HD11	2:B:443:THR:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLY:N	2:B:216:PHE:CE1	2.80	0.50
2:B:185:LEU:HD11	2:B:272:VAL:HA	1.92	0.50
1:A:638:HIS:CD2	3:C:354:VAL:HG21	2.47	0.50
1:A:609:THR:H	1:A:610:PRO:CD	2.25	0.50
1:A:566:ILE:HD13	1:A:574:ILE:CG1	2.39	0.50
1:A:130:SER:OG	2:B:322:HIS:CD2	2.64	0.50
2:B:643:GLN:HG2	3:D:356:ILE:HD11	1.83	0.50
2:B:319:PHE:HA	2:B:322:HIS:CD2	2.46	0.50
1:A:142:ILE:HD13	1:A:189:LEU:HD21	1.92	0.50
2:B:480:ILE:HD12	2:B:541:LEU:HD11	1.94	0.50
3:D:143:ALA:HA	3:D:183:GLN:HE22	1.76	0.50
1:A:137:ARG:NH1	2:B:325:LEU:HD13	2.27	0.49
1:A:73:THR:H	2:B:215:ASN:HA	1.75	0.49
3:D:28:GLU:O	3:D:365:LEU:HD12	2.12	0.49
3:C:67:ILE:HD12	3:C:123:ILE:CG2	2.42	0.49
1:A:367:PRO:CG	1:A:404:ILE:CD1	2.86	0.49
1:A:612:TRP:HA	1:A:630:ARG:HH22	1.76	0.49
3:C:272:PHE:HB2	3:C:303:ASN:HD21	1.77	0.49
3:D:75:VAL:HG21	3:D:94:VAL:HG13	1.93	0.49
3:C:323:ILE:HD12	3:C:332:SER:HB3	1.94	0.49
1:A:142:ILE:HD13	1:A:189:LEU:CD2	2.42	0.49
1:A:70:LEU:HD11	2:B:223:LEU:HD11	1.94	0.49
3:D:205:ASP:H	3:D:304:SER:HA	1.76	0.49
3:C:276:THR:HG22	3:C:277:SER:H	1.77	0.49
3:C:312:ASN:HD22	3:C:382:THR:HG21	1.78	0.49
1:A:140:TYR:HB2	2:B:324:ASP:OD1	2.11	0.49
1:A:66:VAL:CG1	1:A:94:ILE:HD12	2.42	0.49
1:A:629:THR:HG21	1:A:710:ILE:HD12	1.93	0.49
3:C:326:VAL:HG23	3:C:362:TYR:CD2	2.47	0.49
3:C:327:GLU:HB3	3:C:331:ILE:HD12	1.93	0.49
1:A:63:LEU:HD11	1:A:109:ILE:HD12	1.93	0.49
1:A:584:ILE:HD11	1:A:687:ARG:HB2	1.94	0.49
3:C:32:GLY:H	3:C:36:LEU:N	2.11	0.49
1:A:561:LYS:HG3	1:A:587:ARG:HH11	1.77	0.49
3:D:101:ALA:HB1	3:D:107:ASN:HB2	1.94	0.49
1:A:585:ILE:HD12	1:A:683:ILE:CG1	2.41	0.49
1:A:425:ILE:HD11	1:A:482:LEU:HA	1.93	0.49
1:A:366:ILE:O	1:A:404:ILE:HD12	2.13	0.49
2:B:264:TYR:CE2	2:B:287:ILE:CD1	2.81	0.49
3:C:258:THR:OG1	3:C:356:ILE:CD1	2.61	0.49
1:A:142:ILE:HD12	1:A:193:TYR:CE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ILE:HD11	1:A:482:LEU:HB3	1.92	0.49
2:B:418:GLU:HB3	2:B:463:ILE:CD1	2.43	0.49
2:B:742:ALA:CB	2:B:743:THR:HG23	2.42	0.49
1:A:67:LEU:HD13	1:A:109:ILE:HD13	1.94	0.49
3:D:9:GLN:HE21	3:D:15:ASN:HA	1.77	0.49
1:A:462:LEU:HD13	1:A:484:ILE:HD12	1.93	0.49
1:A:714:ARG:O	1:A:760:LEU:CD2	2.60	0.49
2:B:586:ILE:HG12	2:B:735:ILE:HD13	1.89	0.49
3:C:6:ILE:HD11	3:C:126:GLU:HG3	1.94	0.49
1:A:584:ILE:HD12	1:A:687:ARG:CB	2.43	0.49
1:A:438:PHE:CE1	1:A:484:ILE:CD1	2.95	0.49
3:D:5:ILE:HD11	3:D:252:MET:HE1	1.90	0.49
2:B:363:PHE:CG	2:B:390:VAL:HG12	2.47	0.49
2:B:402:ILE:CG1	2:B:449:ILE:CD1	2.86	0.49
2:B:402:ILE:HG12	2:B:449:ILE:HD13	1.90	0.49
2:B:335:PHE:CZ	2:B:339:ILE:HD11	2.43	0.49
2:B:296:ILE:HD12	2:B:327:ILE:CG1	2.09	0.49
3:C:111:ILE:HG23	3:C:114:ARG:HH21	1.77	0.49
2:B:493:ILE:HD13	2:B:595:LYS:HA	1.95	0.49
3:C:5:ILE:HD12	3:C:53:PHE:CZ	2.48	0.49
1:A:367:PRO:N	1:A:404:ILE:HD12	2.26	0.49
3:C:12:GLN:O	3:C:16:HIS:CD2	2.66	0.49
1:A:72:GLY:CA	2:B:222:HIS:HE1	2.23	0.49
2:B:402:ILE:HG12	2:B:449:ILE:HD13	1.94	0.49
2:B:634:ILE:HD12	2:B:809:LEU:HD21	1.86	0.49
2:B:284:TYR:CE1	2:B:291:ILE:CD1	2.94	0.49
1:A:137:ARG:N	2:B:324:ASP:OD1	2.46	0.49
1:A:641:LYS:CG	3:C:356:ILE:CD1	2.90	0.49
1:A:780:ILE:CD1	1:A:789:GLU:HB2	2.40	0.49
1:A:78:PHE:HB2	1:A:93:LYS:HD2	1.95	0.49
1:A:140:TYR:CD2	2:B:324:ASP:OD2	2.66	0.49
2:B:463:ILE:HG12	2:B:467:LYS:HD2	1.94	0.49
2:B:586:ILE:CB	2:B:735:ILE:HD13	2.43	0.49
3:D:48:ASP:H	3:D:243:ARG:HA	1.78	0.49
1:A:606:LEU:CD2	1:A:710:ILE:HD11	2.43	0.49
2:B:184:ILE:CD1	2:B:213:ILE:HG13	2.43	0.49
2:B:434:GLN:HG3	2:B:448:ILE:HD11	1.95	0.49
1:A:127:SER:HB3	1:A:143:ARG:HH22	1.78	0.49
2:B:402:ILE:CD1	2:B:449:ILE:HD11	2.21	0.49
2:B:568:LEU:N	2:B:721:ILE:CD1	2.76	0.49
3:C:1:MET:HG3	3:C:3:GLY:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:127:ILE:HD12	3:D:161:ARG:NH1	2.27	0.49
1:A:625:ILE:CD1	1:A:758:LEU:HD22	2.43	0.49
3:C:69:MET:SD	3:C:119:ILE:HD13	2.52	0.49
1:A:367:PRO:CA	1:A:404:ILE:CD1	2.87	0.49
2:B:230:LEU:HD22	2:B:295:ARG:HA	1.95	0.49
1:A:422:LEU:CD1	1:A:574:ILE:HD13	2.43	0.49
1:A:640:ILE:CD1	1:A:699:ILE:HD13	2.36	0.49
1:A:641:LYS:CD	3:C:356:ILE:HD12	2.42	0.49
1:A:267:PHE:CE2	1:A:271:LEU:HD11	2.48	0.48
1:A:566:ILE:CD1	1:A:574:ILE:HG21	2.38	0.48
2:B:731:PHE:CE2	2:B:735:ILE:HD11	2.48	0.48
2:B:224:ILE:HG22	2:B:284:TYR:CD1	2.48	0.48
2:B:480:ILE:HD11	2:B:520:VAL:CG1	2.43	0.48
3:D:268:LEU:CD2	3:D:379:ASN:HD22	2.25	0.48
1:A:195:GLU:HG3	1:A:250:ILE:HD13	1.94	0.48
2:B:455:GLU:O	2:B:459:HIS:CG	2.66	0.48
3:C:124:ASP:OD2	3:D:281:HIS:NE2	2.46	0.48
1:A:74:TYR:CE2	2:B:216:PHE:CZ	2.96	0.48
1:A:566:ILE:HD12	1:A:574:ILE:HD13	1.91	0.48
1:A:588:TYR:CD1	1:A:693:ILE:HD11	2.47	0.48
1:A:143:ARG:CD	2:B:292:ILE:HD11	2.40	0.48
3:C:139:LEU:HD23	3:C:170:TYR:HB2	1.95	0.48
1:A:68:ILE:HD13	1:A:158:LEU:CD2	2.37	0.48
2:B:503:PRO:HG2	2:B:550:HIS:CE1	2.48	0.48
1:A:602:THR:HG22	1:A:710:ILE:HD12	1.95	0.48
1:A:438:PHE:CE2	1:A:484:ILE:HD11	2.43	0.48
2:B:296:ILE:HD12	2:B:327:ILE:HG23	1.96	0.48
3:C:384:VAL:HG11	3:C:431:GLN:HG2	1.95	0.48
1:A:112:TYR:HE2	1:A:177:ILE:HD13	1.77	0.48
2:B:402:ILE:CG1	2:B:449:ILE:CD1	2.92	0.48
2:B:313:LEU:HD13	2:B:391:PRO:HA	1.96	0.48
2:B:427:LYS:NZ	2:B:456:ILE:HD13	2.29	0.48
3:C:188:ILE:HD12	3:C:394:PHE:HB2	1.93	0.48
1:A:375:ILE:CD1	1:A:396:LYS:HB2	2.43	0.48
1:A:603:TRP:CZ2	1:A:633:HIS:HB2	2.48	0.48
3:C:188:ILE:HD12	3:C:394:PHE:CD2	2.46	0.48
2:B:362:PHE:CE2	2:B:364:ILE:HD11	2.49	0.48
2:B:257:ILE:CD1	2:B:301:THR:OG1	2.61	0.48
1:A:599:LEU:HD22	1:A:640:ILE:CD1	2.43	0.48
3:C:55:ARG:HB3	3:C:65:ARG:CZ	2.43	0.48
3:D:76:ILE:HA	3:D:79:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ILE:HG23	1:A:367:PRO:HD2	1.96	0.48
2:B:349:TRP:HH2	2:B:383:ILE:HD13	1.78	0.48
2:B:430:HIS:CD2	2:B:448:ILE:HG22	2.48	0.48
3:D:123:ILE:HD13	3:D:158:LEU:HD21	1.95	0.48
1:A:587:ARG:O	1:A:591:VAL:HG23	2.13	0.48
1:A:625:ILE:CD1	1:A:761:ILE:HG23	2.44	0.48
1:A:75:ILE:HD12	2:B:216:PHE:CZ	2.48	0.48
2:B:241:PHE:CB	2:B:254:ILE:HD13	2.44	0.48
1:A:641:LYS:HD3	3:C:356:ILE:HD13	1.95	0.48
3:D:234:ILE:HD11	3:D:303:ASN:CG	2.34	0.48
2:B:349:TRP:CZ3	2:B:383:ILE:CD1	2.96	0.48
1:A:152:LYS:HG3	2:B:285:ARG:HD2	1.94	0.48
2:B:288:TYR:CZ	2:B:292:ILE:HD11	2.34	0.48
3:C:199:ASP:O	3:C:260:ILE:HD13	2.14	0.48
2:B:533:ARG:HA	2:B:538:ILE:CD1	2.40	0.48
3:C:5:ILE:HD12	3:C:53:PHE:CE1	2.49	0.48
3:D:188:ILE:HD11	3:D:394:PHE:HB2	1.81	0.48
2:B:207:ILE:HD13	2:B:221:LEU:HG	1.95	0.48
3:D:204:PHE:CE2	3:D:234:ILE:CD1	2.81	0.48
1:A:588:TYR:CG	1:A:693:ILE:HD11	2.37	0.48
1:A:706:PHE:CE2	1:A:710:ILE:HD11	2.48	0.48
2:B:493:ILE:CD1	2:B:598:TYR:HD2	2.23	0.48
1:A:134:VAL:CG1	1:A:247:ILE:HD12	2.43	0.48
3:D:166:ILE:HD12	3:D:256:TYR:CG	2.48	0.48
3:C:127:ILE:HD11	3:C:162:TYR:HE2	1.77	0.48
1:A:128:ASP:CA	2:B:322:HIS:HE1	2.22	0.48
2:B:322:HIS:HD2	2:B:327:ILE:HD13	1.77	0.48
3:D:326:VAL:HG12	3:D:361:PRO:HB3	1.96	0.48
3:C:12:GLN:O	3:C:16:HIS:CD2	2.66	0.48
3:C:188:ILE:CD1	3:C:394:PHE:CB	2.90	0.48
1:A:557:ILE:CD1	1:A:594:TYR:CD2	2.96	0.48
2:B:284:TYR:CZ	2:B:291:ILE:HD13	2.48	0.48
2:B:779:LEU:HD13	2:B:780:ASN:O	2.14	0.48
1:A:136:GLN:CD	2:B:323:GLY:H	2.16	0.48
1:A:131:PHE:CD2	2:B:322:HIS:CG	3.02	0.48
1:A:136:GLN:NE2	2:B:327:ILE:HD12	2.13	0.48
1:A:63:LEU:HD22	1:A:170:ILE:HD12	1.96	0.48
3:C:199:ASP:O	3:C:260:ILE:HD13	2.14	0.48
1:A:195:GLU:CD	1:A:250:ILE:CD1	2.82	0.48
3:C:152:SER:HB3	3:C:193:ARG:HG3	1.96	0.48
1:A:140:TYR:CE1	2:B:292:ILE:CD1	2.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:567:PRO:C	2:B:721:ILE:CD1	2.82	0.48
3:C:344:PHE:HB3	3:C:345:PRO:HD3	1.95	0.48
1:A:425:ILE:HD13	1:A:482:LEU:CD1	2.43	0.48
3:D:180:VAL:HB	3:D:182:VAL:HG22	1.96	0.48
1:A:702:ILE:CD1	1:A:767:TYR:CE2	2.88	0.48
3:C:138:LEU:HG	3:C:140:HIS:CD2	2.49	0.48
1:A:625:ILE:HD13	1:A:764:LEU:HB3	1.64	0.48
2:B:412:LEU:HD22	2:B:463:ILE:HD13	1.95	0.48
2:B:610:ILE:CD1	3:D:196:GLU:O	2.60	0.48
3:C:205:ASP:O	3:C:209:LEU:HD13	2.14	0.48
1:A:133:MET:HA	2:B:323:GLY:H	1.79	0.48
3:C:67:ILE:CD1	3:C:123:ILE:HG22	2.42	0.48
1:A:425:ILE:HD11	1:A:482:LEU:CA	2.44	0.47
1:A:128:ASP:OD2	2:B:295:ARG:HD3	2.14	0.47
1:A:585:ILE:HD12	1:A:683:ILE:HG12	1.97	0.47
3:D:143:ALA:HB2	3:D:174:PRO:HB3	1.96	0.47
3:D:188:ILE:HD13	3:D:394:PHE:CD2	2.49	0.47
3:D:12:GLN:O	3:D:16:HIS:CD2	2.68	0.47
3:C:322:ILE:HD11	3:C:358:ARG:NH2	2.29	0.47
1:A:195:GLU:OE2	1:A:250:ILE:HD11	2.14	0.47
3:D:280:ILE:HG23	3:D:281:HIS:CD2	2.48	0.47
3:D:316:PHE:HB2	3:D:347:TRP:CZ3	2.49	0.47
1:A:66:VAL:HG13	1:A:75:ILE:HD12	1.96	0.47
3:C:8:LEU:HD13	3:C:154:LEU:HD21	1.97	0.47
3:C:212:ILE:HD13	3:C:275:PHE:CE2	2.49	0.47
2:B:398:LEU:CD2	2:B:449:ILE:CD1	2.69	0.47
2:B:323:GLY:O	2:B:327:ILE:HD12	2.15	0.47
2:B:293:ARG:CD	2:B:330:ILE:HD12	2.44	0.47
3:D:188:ILE:CD1	3:D:394:PHE:CD2	2.94	0.47
3:C:9:GLN:HE21	3:C:15:ASN:HA	1.79	0.47
2:B:563:ILE:HG12	2:B:564:LEU:H	1.79	0.47
3:C:155:LEU:HD11	3:C:194:LEU:HD12	1.96	0.47
1:A:71:GLU:CD	2:B:222:HIS:CD2	2.87	0.47
3:C:13:CYS:O	3:C:17:VAL:HG23	2.15	0.47
2:B:188:VAL:CG1	2:B:224:ILE:CD1	2.86	0.47
2:B:405:ILE:HG12	2:B:456:ILE:HD13	1.94	0.47
3:C:199:ASP:O	3:C:260:ILE:HD13	2.15	0.47
2:B:304:LEU:HD22	2:B:312:PHE:CE1	2.49	0.47
1:A:573:ILE:HD12	1:A:673:GLN:HG2	1.92	0.47
1:A:151:LEU:CD1	2:B:285:ARG:HG3	2.43	0.47
1:A:566:ILE:HD11	1:A:571:ASN:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:VAL:HG21	3:C:231:ILE:HD12	1.96	0.47
1:A:108:ARG:HB3	1:A:177:ILE:HD13	1.97	0.47
3:D:363:LEU:H	3:D:363:LEU:HD22	1.78	0.47
2:B:402:ILE:CD1	2:B:449:ILE:HD13	2.39	0.47
3:C:317:ASN:O	3:C:318:VAL:HG13	2.15	0.47
2:B:634:ILE:HD11	2:B:772:PHE:CD1	2.50	0.47
3:D:5:ILE:HD11	3:D:252:MET:CE	2.45	0.47
2:B:335:PHE:CD2	2:B:339:ILE:HD12	2.50	0.47
3:C:67:ILE:HD11	3:C:123:ILE:HG23	1.96	0.47
1:A:140:TYR:HE1	2:B:292:ILE:CD1	2.28	0.47
1:A:155:VAL:CG1	2:B:285:ARG:NH2	2.77	0.47
2:B:464:LEU:HD22	2:B:470:TYR:CE2	2.49	0.47
2:B:586:ILE:CB	2:B:735:ILE:CD1	2.93	0.47
3:C:127:ILE:HD11	3:C:162:TYR:CE2	2.50	0.47
2:B:405:ILE:HG12	2:B:456:ILE:HD11	1.96	0.47
2:B:405:ILE:HG21	2:B:456:ILE:CD1	2.28	0.47
3:C:129:SER:CB	3:D:284:ILE:HD12	2.45	0.47
2:B:570:LEU:HD23	2:B:721:ILE:HD13	1.85	0.47
2:B:480:ILE:HD11	2:B:537:VAL:HG22	1.97	0.47
2:B:589:PHE:CD2	2:B:739:LYS:HG3	2.50	0.47
3:D:353:HIS:CE1	3:D:355:ASN:H	2.33	0.47
3:C:104:SER:HA	3:C:186:ASN:HD21	1.80	0.47
1:A:62:ASP:CG	1:A:94:ILE:CD1	2.82	0.47
3:C:6:ILE:HD11	3:C:127:ILE:HG22	1.94	0.47
1:A:348:LEU:CD2	1:A:352:ILE:HD11	2.45	0.47
3:D:255:ILE:HD11	3:D:320:ASN:HD21	1.79	0.47
1:A:352:ILE:CD1	1:A:572:ILE:HG21	2.44	0.47
1:A:422:LEU:HD13	1:A:564:ILE:HD11	1.97	0.47
2:B:493:ILE:HD11	2:B:598:TYR:CB	2.43	0.47
1:A:140:TYR:OH	2:B:326:THR:HG23	2.14	0.47
1:A:557:ILE:HD12	1:A:594:TYR:CD2	2.48	0.47
3:C:125:LYS:CE	3:D:282:ASP:O	2.63	0.47
1:A:706:PHE:CZ	1:A:710:ILE:HD11	2.50	0.47
1:A:70:LEU:CD1	2:B:220:LEU:CG	2.93	0.47
3:C:127:ILE:HD13	3:C:162:TYR:CZ	2.50	0.47
3:D:188:ILE:HD11	3:D:427:ARG:NH2	2.30	0.47
1:A:572:ILE:HG12	1:A:572:ILE:O	2.15	0.47
1:A:73:THR:CG2	2:B:215:ASN:ND2	2.62	0.47
1:A:68:ILE:CD1	2:B:216:PHE:CB	2.93	0.47
1:A:638:HIS:HE1	3:C:340:GLN:HE22	1.62	0.47
3:C:127:ILE:CD1	3:C:162:TYR:HE2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:ILE:HD13	2:B:225:PHE:HA	1.97	0.47
1:A:65:ASN:CB	2:B:216:PHE:CD1	2.98	0.46
2:B:383:ILE:HD11	2:B:410:ILE:HD11	1.96	0.46
3:C:119:ILE:HD12	3:C:154:LEU:HD13	1.97	0.46
2:B:339:ILE:CD1	2:B:440:GLY:CA	2.93	0.46
1:A:71:GLU:CB	2:B:208:GLN:OE1	2.61	0.46
1:A:458:TYR:CG	1:A:484:ILE:CD1	2.85	0.46
1:A:142:ILE:HD11	1:A:189:LEU:HD21	1.97	0.46
1:A:78:PHE:HD2	1:A:80:ASP:O	1.98	0.46
2:B:405:ILE:CB	2:B:456:ILE:CD1	2.92	0.46
3:C:188:ILE:HD13	3:C:394:PHE:CD2	2.48	0.46
1:A:609:THR:HA	1:A:612:TRP:CE2	2.50	0.46
2:B:191:THR:HG23	2:B:207:ILE:HD13	1.97	0.46
1:A:154:LEU:HD21	2:B:281:LYS:HE3	1.98	0.46
3:D:258:THR:HG21	3:D:356:ILE:HD13	1.97	0.46
1:A:148:ASP:OD1	2:B:285:ARG:CZ	2.64	0.46
1:A:702:ILE:HG23	1:A:768:ILE:HD13	1.97	0.46
1:A:138:PHE:CE2	1:A:192:ILE:HD13	2.50	0.46
1:A:140:TYR:CD2	2:B:324:ASP:CB	2.98	0.46
1:A:71:GLU:H	2:B:216:PHE:CB	2.27	0.46
1:A:574:ILE:HD11	1:A:579:MET:HG2	1.98	0.46
3:C:125:LYS:NZ	3:D:281:HIS:O	2.45	0.46
1:A:564:ILE:HD13	1:A:574:ILE:HG21	1.96	0.46
2:B:302:GLU:HB2	4:E:1:UNK:H2	1.79	0.46
1:A:662:CYS:O	1:A:666:PRO:HD2	2.15	0.46
2:B:239:GLU:OE1	2:B:239:GLU:HA	2.14	0.46
3:D:195:ILE:HD12	3:D:423:PHE:CE1	2.48	0.46
1:A:91:GLU:HG3	1:A:92:PHE:H	1.80	0.46
1:A:63:LEU:HD21	1:A:170:ILE:CD1	2.46	0.46
3:C:123:ILE:HG21	3:C:161:ARG:HH12	1.81	0.46
1:A:643:ILE:HD12	1:A:692:LEU:CD2	2.45	0.46
2:B:775:VAL:HG11	2:B:805:PHE:HA	1.97	0.46
2:B:284:TYR:CE1	2:B:291:ILE:CD1	2.98	0.46
1:A:799:VAL:HG12	1:A:800:ASP:O	2.15	0.46
3:C:330:GLN:H	3:C:330:GLN:CD	2.18	0.46
2:B:362:PHE:CD2	2:B:364:ILE:CD1	2.98	0.46
1:A:67:LEU:HD22	1:A:154:LEU:HD11	1.98	0.46
2:B:260:GLU:OE2	2:B:330:ILE:HD13	2.14	0.46
2:B:349:TRP:CZ2	2:B:364:ILE:HG21	2.51	0.46
1:A:638:HIS:CE1	1:A:642:THR:HG21	2.51	0.46
3:D:138:LEU:HB3	3:D:169:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:TYR:CE2	2:B:287:ILE:HD11	2.51	0.46
2:B:296:ILE:CD1	2:B:327:ILE:CG2	2.93	0.46
2:B:482:LEU:HD21	2:B:735:ILE:HD12	1.96	0.46
1:A:66:VAL:HG21	1:A:170:ILE:CD1	2.41	0.46
3:C:97:ASP:HB3	3:C:114:ARG:HH11	1.81	0.46
1:A:195:GLU:OE2	1:A:250:ILE:CD1	2.62	0.46
2:B:296:ILE:CD1	2:B:327:ILE:CB	2.91	0.46
2:B:339:ILE:CD1	2:B:439:ARG:NH1	2.79	0.46
2:B:493:ILE:HD13	2:B:595:LYS:HA	1.97	0.46
3:C:292:TYR:CZ	3:C:374:GLY:HA3	2.50	0.46
2:B:731:PHE:CE1	2:B:735:ILE:HD11	2.51	0.46
3:C:46:ARG:HA	3:C:244:PHE:CE2	2.51	0.46
1:A:366:ILE:HG22	1:A:368:SER:H	1.80	0.46
1:A:638:HIS:CE1	3:C:340:GLN:NE2	2.84	0.46
1:A:641:LYS:CD	3:C:356:ILE:HD12	2.45	0.46
1:A:780:ILE:HD12	1:A:789:GLU:CB	2.43	0.46
2:B:339:ILE:HD11	2:B:440:GLY:CA	2.46	0.46
1:A:628:ALA:HB3	1:A:765:ILE:HD13	1.97	0.46
2:B:545:VAL:HB	2:B:550:HIS:CD2	2.50	0.46
1:A:55:GLN:O	1:A:59:VAL:HG23	2.16	0.46
2:B:339:ILE:CD1	2:B:440:GLY:H	2.21	0.46
2:B:405:ILE:CG1	2:B:456:ILE:CD1	2.93	0.46
3:D:192:ARG:C	3:D:192:ARG:HE	2.19	0.46
1:A:375:ILE:CD1	1:A:396:LYS:CD	2.94	0.46
1:A:120:THR:HA	1:A:123:TYR:CD2	2.51	0.46
1:A:367:PRO:HA	1:A:404:ILE:CD1	2.36	0.46
3:D:138:LEU:HB2	3:D:169:THR:HG22	1.98	0.46
2:B:548:LEU:H	2:B:548:LEU:HD12	1.81	0.46
2:B:349:TRP:CE2	2:B:364:ILE:CD1	2.92	0.46
3:D:7:THR:HG23	3:D:137:GLN:HE21	1.80	0.46
1:A:135:LEU:HD11	1:A:247:ILE:HD11	1.97	0.46
1:A:140:TYR:CD1	2:B:324:ASP:OD2	2.69	0.46
2:B:364:ILE:HD11	2:B:403:PHE:CA	2.45	0.46
1:A:66:VAL:CG1	1:A:109:ILE:HD12	2.46	0.46
1:A:142:ILE:CD1	1:A:186:MET:HG2	2.41	0.46
2:B:192:LEU:HD22	2:B:227:ALA:HB3	1.98	0.46
1:A:63:LEU:HD21	1:A:170:ILE:HD12	1.97	0.46
1:A:362:GLN:NE2	2:B:447:GLU:HG2	2.08	0.46
2:B:335:PHE:CD2	2:B:339:ILE:CD1	2.98	0.46
2:B:381:ILE:O	2:B:381:ILE:HG22	2.16	0.46
2:B:349:TRP:CZ3	2:B:383:ILE:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:GLN:CD	1:A:652:ILE:HD13	2.36	0.46
3:D:49:ASP:HA	3:D:52:PRO:HD2	1.99	0.45
3:C:217:PHE:CD1	3:C:281:HIS:CD2	3.04	0.45
2:B:772:PHE:HB2	2:B:812:ILE:HD13	1.98	0.45
3:D:25:LEU:O	3:D:29:HIS:CD2	2.69	0.45
2:B:279:SER:H	2:B:282:SER:HB2	1.81	0.45
1:A:595:HIS:ND1	1:A:640:ILE:HD13	2.31	0.45
3:D:401:GLY:HA2	3:D:404:LEU:HD13	1.99	0.45
1:A:585:ILE:CD1	1:A:683:ILE:CD1	2.94	0.45
3:C:217:PHE:CD2	3:C:280:ILE:HD13	2.50	0.45
3:C:129:SER:HA	3:D:283:ASP:HB3	1.98	0.45
1:A:138:PHE:CE2	1:A:192:ILE:CD1	2.98	0.45
1:A:470:GLN:HE22	1:A:474:PRO:HA	1.81	0.45
2:B:405:ILE:CD1	2:B:452:GLN:HB2	2.45	0.45
3:D:191:LEU:HD13	3:D:427:ARG:CD	2.46	0.45
1:A:352:ILE:HD13	1:A:572:ILE:HG21	1.97	0.45
2:B:184:ILE:O	2:B:188:VAL:HG23	2.16	0.45
2:B:640:GLN:HG2	3:D:354:VAL:HG11	1.98	0.45
2:B:224:ILE:CD1	2:B:283:LEU:HD23	2.43	0.45
2:B:335:PHE:HB3	2:B:439:ARG:HH21	1.81	0.45
1:A:138:PHE:CD1	1:A:275:ILE:CD1	2.97	0.45
1:A:625:ILE:HA	1:A:761:ILE:CD1	2.46	0.45
1:A:142:ILE:CD1	1:A:188:LEU:HD12	2.45	0.45
1:A:72:GLY:HA2	2:B:215:ASN:C	2.37	0.45
1:A:585:ILE:HD13	1:A:683:ILE:CG1	2.45	0.45
1:A:108:ARG:HH12	1:A:112:TYR:HB2	1.80	0.45
1:A:577:THR:HG23	1:A:680:LEU:HD22	1.97	0.45
3:C:193:ARG:NH1	3:C:419:VAL:HG13	2.29	0.45
1:A:414:ASP:O	1:A:418:VAL:HG23	2.16	0.45
2:B:541:LEU:HD12	2:B:541:LEU:H	1.81	0.45
1:A:151:LEU:HD11	2:B:282:SER:HA	1.98	0.45
1:A:595:HIS:CE1	1:A:640:ILE:HG21	2.51	0.45
1:A:65:ASN:O	2:B:216:PHE:CZ	2.70	0.45
3:C:219:ASN:HD21	3:C:280:ILE:HD11	1.81	0.45
3:C:70:ASP:CG	3:C:71:SER:H	2.20	0.45
1:A:109:ILE:HD13	1:A:173:LEU:CD1	2.44	0.45
1:A:68:ILE:HG13	2:B:281:LYS:HZ2	1.78	0.45
3:D:212:ILE:HD13	3:D:275:PHE:CZ	2.51	0.45
1:A:402:ASN:HB3	1:A:669:ALA:H	1.80	0.45
1:A:70:LEU:CD1	2:B:223:LEU:HD11	2.46	0.45
1:A:154:LEU:HA	1:A:154:LEU:HD12	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:LYS:HG3	3:C:356:ILE:HD11	1.96	0.45
2:B:411:PHE:HB2	2:B:570:LEU:HD22	1.98	0.45
3:D:9:GLN:HE21	3:D:15:ASN:HA	1.81	0.45
3:D:284:ILE:HD13	3:D:284:ILE:HG21	1.77	0.45
1:A:72:GLY:CA	2:B:215:ASN:HB3	2.46	0.45
1:A:567:PRO:HG2	1:A:574:ILE:CD1	2.47	0.45
3:C:234:ILE:HD13	3:C:303:ASN:CG	2.37	0.45
2:B:639:THR:HA	2:B:642:GLN:HE21	1.82	0.45
3:D:127:ILE:CD1	3:D:161:ARG:CZ	2.91	0.45
1:A:141:GLU:OE2	2:B:324:ASP:CG	2.54	0.45
2:B:296:ILE:CD1	2:B:327:ILE:CD1	2.90	0.45
1:A:65:ASN:HB3	2:B:216:PHE:CE2	2.52	0.45
3:D:138:LEU:HB3	3:D:169:THR:HG22	1.99	0.45
2:B:245:ASN:HD21	2:B:254:ILE:HD12	1.81	0.45
1:A:774:ILE:CD1	1:A:796:SER:HB2	2.47	0.45
1:A:96:LYS:HE3	1:A:107:ARG:HH12	1.82	0.45
3:C:6:ILE:HD11	3:C:127:ILE:HA	1.98	0.45
1:A:694:PRO:HB2	1:A:794:TYR:CE2	2.52	0.45
3:D:21:LEU:HD23	3:D:22:TRP:CZ3	2.52	0.45
3:D:4:GLU:HA	3:D:52:PRO:HB3	1.97	0.45
3:D:70:ASP:CG	3:D:71:SER:H	2.20	0.45
1:A:611:SER:HB3	1:A:630:ARG:HH11	1.82	0.45
3:D:51:LYS:HB3	3:D:52:PRO:HD3	1.99	0.45
1:A:147:GLU:OE2	2:B:288:TYR:CD2	2.70	0.45
2:B:412:LEU:HD23	2:B:419:VAL:H	1.82	0.45
3:C:384:VAL:HA	3:C:387:PHE:CD2	2.52	0.45
2:B:426:SER:O	2:B:430:HIS:CD2	2.70	0.45
2:B:480:ILE:HD11	2:B:537:VAL:HG13	1.99	0.45
3:D:318:VAL:HG22	3:D:319:TYR:N	2.31	0.45
1:A:629:THR:OG1	1:A:710:ILE:CD1	2.50	0.45
1:A:797:SER:O	1:A:800:ASP:O	2.35	0.45
2:B:780:ASN:O	2:B:801:LEU:HD23	2.17	0.45
1:A:137:ARG:HH12	2:B:325:LEU:CD1	2.30	0.45
2:B:402:ILE:HD11	2:B:449:ILE:CD1	2.45	0.45
2:B:251:LYS:O	2:B:255:ILE:HG13	2.16	0.45
2:B:227:ALA:HB2	2:B:291:ILE:CD1	2.46	0.45
1:A:379:ASN:O	1:A:382:ALA:HB3	2.17	0.45
2:B:646:SER:OG	3:D:356:ILE:HD12	2.17	0.45
1:A:188:LEU:HD13	1:A:268:LEU:HD11	1.98	0.45
2:B:582:GLU:HG2	2:B:585:ARG:HH21	1.81	0.44
3:D:312:ASN:HB3	3:D:385:ASN:HD21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:ILE:HD12	1:A:765:ILE:CG2	2.48	0.44
3:C:188:ILE:HD11	3:C:394:PHE:CD2	2.39	0.44
2:B:339:ILE:CD1	2:B:439:ARG:HD2	2.41	0.44
1:A:194:GLU:HB3	1:A:250:ILE:HD12	1.98	0.44
2:B:184:ILE:HD12	2:B:280:LEU:HG	1.99	0.44
2:B:325:LEU:HD22	2:B:325:LEU:H	1.81	0.44
2:B:405:ILE:CG2	2:B:456:ILE:HD12	2.46	0.44
2:B:362:PHE:CD2	2:B:364:ILE:HD12	2.53	0.44
3:D:366:GLN:HB3	3:D:369:GLU:HG3	1.98	0.44
1:A:573:ILE:HG22	1:A:673:GLN:HE22	1.82	0.44
2:B:528:LEU:HG	2:B:529:MET:H	1.81	0.44
3:D:189:LEU:HG	3:D:420:GLN:HE21	1.81	0.44
1:A:64:LEU:HD13	1:A:168:PHE:HB3	1.99	0.44
2:B:257:ILE:CD1	2:B:297:TYR:HE2	2.17	0.44
2:B:583:TYR:CD1	2:B:732:LEU:HD13	2.52	0.44
1:A:425:ILE:CD1	1:A:478:MET:HB3	2.38	0.44
1:A:363:ILE:CD1	1:A:413:TYR:CG	2.94	0.44
3:C:188:ILE:HG23	3:C:423:PHE:CD2	2.52	0.44
1:A:581:LYS:HD3	1:A:680:LEU:HD22	2.00	0.44
3:C:188:ILE:HD13	3:C:394:PHE:CE2	2.52	0.44
1:A:296:TYR:OH	2:B:318:ILE:HD11	2.17	0.44
2:B:455:GLU:HG2	2:B:459:HIS:CE1	2.52	0.44
1:A:585:ILE:HD11	1:A:683:ILE:CD1	2.47	0.44
1:A:137:ARG:CA	2:B:324:ASP:OD1	2.66	0.44
2:B:634:ILE:HD11	2:B:772:PHE:HD1	1.83	0.44
2:B:808:ASN:ND2	2:B:812:ILE:HD11	2.25	0.44
2:B:646:SER:HB2	3:D:356:ILE:CD1	2.48	0.44
3:D:188:ILE:HD13	3:D:394:PHE:CG	2.51	0.44
2:B:191:THR:CG2	2:B:207:ILE:CD1	2.95	0.44
3:C:235:ILE:O	3:C:238:VAL:HG22	2.17	0.44
3:D:29:HIS:CE1	3:D:363:LEU:HG	2.53	0.44
1:A:348:LEU:CD2	1:A:352:ILE:CD1	2.95	0.44
1:A:192:ILE:HG22	1:A:250:ILE:HG21	1.99	0.44
3:C:71:SER:HA	3:C:95:ALA:H	1.82	0.44
2:B:245:ASN:ND2	2:B:254:ILE:HD12	2.33	0.44
2:B:293:ARG:HD3	2:B:330:ILE:CD1	2.45	0.44
3:C:241:SER:HB3	3:C:322:ILE:HD12	2.00	0.44
1:A:373:ILE:HG21	1:A:373:ILE:HD13	1.84	0.44
3:C:313:PRO:HG2	3:C:382:THR:HA	1.99	0.44
2:B:293:ARG:HE	2:B:326:THR:HB	1.81	0.44
3:C:259:LEU:HA	3:C:318:VAL:HG11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LEU:HG	2:B:216:PHE:CE2	2.49	0.44
2:B:474:VAL:HG21	2:B:668:LEU:HD13	1.98	0.44
3:D:183:GLN:HE21	3:D:187:THR:HG23	1.82	0.44
2:B:421:TRP:HB3	2:B:422:THR:H	1.62	0.44
3:D:166:ILE:HD13	3:D:256:TYR:CD2	2.52	0.44
1:A:365:THR:CG2	1:A:404:ILE:HD13	2.32	0.44
1:A:151:LEU:O	1:A:155:VAL:HG12	2.18	0.44
1:A:356:VAL:CG2	1:A:572:ILE:CD1	2.65	0.44
2:B:206:GLN:HE22	4:E:18:UNK:CB	2.31	0.44
3:C:363:LEU:H	3:C:363:LEU:HD22	1.82	0.44
3:C:29:HIS:CE1	3:C:49:ASP:HB3	2.52	0.44
3:C:265:LEU:HD12	3:C:265:LEU:HA	1.91	0.44
3:D:111:ILE:HG12	3:D:114:ARG:HH21	1.83	0.44
1:A:171:ARG:HD2	1:A:171:ARG:H	1.83	0.44
3:D:70:ASP:CG	3:D:71:SER:H	2.21	0.44
2:B:656:ILE:HD13	2:B:738:HIS:CG	2.52	0.44
1:A:140:TYR:CB	2:B:324:ASP:HB2	2.48	0.44
3:D:217:PHE:CE1	3:D:280:ILE:HD13	2.49	0.44
2:B:636:ILE:HD11	3:D:437:TYR:CD1	2.52	0.44
1:A:567:PRO:HG2	1:A:574:ILE:HD13	2.00	0.44
3:C:9:GLN:HE22	3:C:22:TRP:HE1	1.66	0.44
1:A:384:LEU:HB2	1:A:389:ASN:HD22	1.82	0.44
3:D:6:ILE:HG21	3:D:126:GLU:HB3	2.00	0.44
3:D:199:ASP:O	3:D:260:ILE:HD13	2.18	0.44
3:D:105:TRP:CH2	3:D:109:TYR:CD1	3.05	0.44
3:D:119:ILE:HD11	3:D:154:LEU:HD23	1.98	0.44
2:B:183:ASP:HA	2:B:186:LYS:HE2	1.99	0.44
2:B:604:MET:SD	2:B:769:VAL:HG21	2.58	0.44
3:C:5:ILE:HD13	3:C:137:GLN:NE2	2.32	0.44
1:A:151:LEU:CD1	2:B:285:ARG:CG	2.91	0.44
3:D:344:PHE:HB2	3:D:345:PRO:HD3	2.00	0.44
2:B:570:LEU:HD11	2:B:721:ILE:HD13	1.98	0.44
2:B:505:ASP:HA	2:B:550:HIS:HE1	1.83	0.44
2:B:296:ILE:CD1	2:B:327:ILE:CA	2.95	0.44
3:D:195:ILE:CD1	3:D:423:PHE:HE1	2.30	0.44
1:A:303:ASP:OD1	1:A:304:ASP:O	2.36	0.44
1:A:286:TRP:CE2	1:A:351:GLY:HA3	2.53	0.44
2:B:544:ARG:CZ	2:B:544:ARG:HA	2.47	0.44
2:B:227:ALA:HB2	2:B:291:ILE:HD13	2.00	0.44
1:A:562:PHE:O	1:A:583:GLN:HB3	2.18	0.44
3:D:188:ILE:CD1	3:D:394:PHE:CD1	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:188:ILE:HD13	3:C:394:PHE:CE2	2.50	0.43
1:A:584:ILE:HD11	1:A:687:ARG:NE	2.29	0.43
2:B:188:VAL:CG1	2:B:224:ILE:HD13	2.45	0.43
1:A:327:ARG:HE	1:A:328:LYS:H	1.65	0.43
1:A:155:VAL:CG1	2:B:281:LYS:HE3	2.48	0.43
1:A:195:GLU:CG	1:A:250:ILE:HD11	2.41	0.43
2:B:418:GLU:CB	2:B:463:ILE:CD1	2.96	0.43
1:A:78:PHE:CD2	1:A:80:ASP:O	2.71	0.43
3:C:6:ILE:HD13	3:C:126:GLU:HG3	2.00	0.43
2:B:411:PHE:HB2	2:B:721:ILE:HD11	1.99	0.43
2:B:636:ILE:HD12	3:D:442:GLN:HA	1.99	0.43
2:B:398:LEU:HG	2:B:449:ILE:HD12	2.00	0.43
2:B:483:MET:HG2	2:B:489:MET:SD	2.58	0.43
1:A:599:LEU:HD22	1:A:640:ILE:CD1	2.41	0.43
2:B:489:MET:O	2:B:493:ILE:HG13	2.18	0.43
3:C:289:HIS:H	3:C:289:HIS:CD2	2.36	0.43
3:D:167:LEU:HD22	3:D:167:LEU:N	2.33	0.43
2:B:586:ILE:HA	2:B:735:ILE:HD13	1.99	0.43
3:D:340:GLN:HB3	3:D:353:HIS:ND1	2.33	0.43
3:D:234:ILE:HD13	3:D:303:ASN:OD1	2.18	0.43
1:A:595:HIS:CD2	1:A:696:GLN:HE21	2.36	0.43
2:B:364:ILE:HD11	2:B:403:PHE:HA	1.98	0.43
2:B:465:ASN:HB3	2:B:471:ARG:HE	1.83	0.43
3:C:189:LEU:HD21	3:C:420:GLN:HG2	2.00	0.43
3:C:200:ALA:HB1	3:C:260:ILE:HD11	1.96	0.43
1:A:438:PHE:CZ	1:A:484:ILE:HD11	2.48	0.43
1:A:557:ILE:HD13	1:A:700:PHE:CD2	2.53	0.43
1:A:603:TRP:CZ2	1:A:633:HIS:HB2	2.54	0.43
3:D:173:PHE:CE2	3:D:191:LEU:HD21	2.53	0.43
3:D:5:ILE:HD11	3:D:252:MET:HE1	2.00	0.43
2:B:482:LEU:CD2	2:B:657:ILE:HG22	2.48	0.43
1:A:599:LEU:HD21	1:A:640:ILE:HD12	1.99	0.43
2:B:383:ILE:HD12	2:B:410:ILE:HD12	1.88	0.43
1:A:140:TYR:CE1	2:B:292:ILE:HD13	2.52	0.43
1:A:439:LEU:HD22	1:A:594:TYR:HA	2.00	0.43
3:C:264:GLU:HB2	3:C:433:LEU:HG	2.00	0.43
2:B:323:GLY:CA	2:B:327:ILE:HD12	2.48	0.43
1:A:112:TYR:OH	1:A:177:ILE:CD1	2.67	0.43
2:B:405:ILE:CG2	2:B:456:ILE:HD13	2.47	0.43
1:A:151:LEU:HD22	2:B:285:ARG:CD	2.35	0.43
1:A:128:ASP:CG	2:B:295:ARG:HD3	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:LEU:CD1	2:B:449:ILE:HD12	2.48	0.43
2:B:586:ILE:HD11	2:B:732:LEU:CB	2.49	0.43
2:B:480:ILE:CD1	2:B:520:VAL:HG13	2.47	0.43
1:A:147:GLU:CB	2:B:285:ARG:HD3	2.47	0.43
3:D:328:PRO:HG2	3:D:331:ILE:CD1	2.49	0.43
1:A:150:TYR:CE1	1:A:177:ILE:CD1	3.01	0.43
3:D:111:ILE:HG12	3:D:114:ARG:NH2	2.33	0.43
1:A:138:PHE:O	1:A:142:ILE:HG13	2.18	0.43
2:B:209:ILE:CD1	2:B:213:ILE:HD13	2.48	0.43
2:B:525:LEU:HD13	2:B:525:LEU:O	2.19	0.43
2:B:204:HIS:CG	2:B:204:HIS:O	2.72	0.43
2:B:362:PHE:CE2	2:B:364:ILE:HD12	2.54	0.43
2:B:427:LYS:HE3	2:B:431:VAL:HG13	2.01	0.43
1:A:606:LEU:CG	1:A:710:ILE:HD11	2.48	0.43
2:B:362:PHE:HE2	2:B:364:ILE:HD12	1.84	0.43
2:B:631:LEU:HD12	2:B:780:ASN:HD22	1.83	0.43
3:C:234:ILE:CD1	3:C:303:ASN:CG	2.87	0.43
1:A:152:LYS:HA	2:B:285:ARG:NH2	2.33	0.43
1:A:425:ILE:HD12	1:A:478:MET:CG	2.49	0.43
1:A:557:ILE:CD1	1:A:700:PHE:CE2	3.01	0.43
1:A:78:PHE:HB3	1:A:90:ILE:HD12	2.01	0.43
1:A:363:ILE:HD11	1:A:404:ILE:HG21	1.99	0.43
2:B:608:ASN:HD21	3:D:260:ILE:HB	1.83	0.43
1:A:151:LEU:HD12	2:B:285:ARG:HH21	1.84	0.43
2:B:339:ILE:HG21	2:B:439:ARG:HG2	2.01	0.43
1:A:367:PRO:HB3	1:A:404:ILE:HD12	1.97	0.43
2:B:560:LEU:HB2	2:B:587:PHE:CE2	2.54	0.43
1:A:66:VAL:O	1:A:75:ILE:HD11	2.18	0.43
3:C:275:PHE:CB	3:C:284:ILE:HD11	2.45	0.43
1:A:120:THR:HA	1:A:123:TYR:CE2	2.53	0.43
1:A:296:TYR:CZ	2:B:318:ILE:HD11	2.54	0.43
1:A:135:LEU:HD11	1:A:247:ILE:HD13	1.99	0.43
2:B:743:THR:HG22	2:B:759:PRO:HD3	2.01	0.43
3:C:230:LEU:O	3:C:234:ILE:HG13	2.18	0.43
1:A:595:HIS:CE1	1:A:640:ILE:HD11	2.54	0.43
1:A:366:ILE:HB	1:A:367:PRO:HD3	2.00	0.43
1:A:158:LEU:HD22	2:B:281:LYS:HZ3	1.82	0.43
3:D:51:LYS:H	3:D:52:PRO:CD	2.32	0.43
3:C:5:ILE:HD12	3:C:53:PHE:CZ	2.53	0.43
1:A:425:ILE:HD11	1:A:482:LEU:CD2	2.46	0.43
1:A:140:TYR:CG	2:B:324:ASP:CB	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:822:ARG:HH22	2:B:841:LEU:HD22	1.84	0.43
3:C:212:ILE:HD13	3:C:275:PHE:CE1	2.53	0.43
3:D:127:ILE:CD1	3:D:162:TYR:CE2	3.01	0.43
3:D:188:ILE:HD11	3:D:394:PHE:CG	2.37	0.43
3:C:67:ILE:HD12	3:C:123:ILE:HG23	1.96	0.43
1:A:421:HIS:O	1:A:425:ILE:HG22	2.18	0.43
1:A:425:ILE:CD1	1:A:482:LEU:HD13	2.46	0.43
2:B:430:HIS:HB3	2:B:448:ILE:HG21	2.01	0.43
3:C:393:THR:O	3:C:397:VAL:HG23	2.18	0.43
2:B:602:LYS:HB3	2:B:602:LYS:HE3	1.95	0.43
3:D:259:LEU:HD21	3:D:377:LEU:HB3	2.01	0.43
1:A:641:LYS:CG	3:C:356:ILE:HD12	2.49	0.43
1:A:780:ILE:CD1	1:A:789:GLU:CB	2.96	0.43
3:C:9:GLN:HE22	3:C:22:TRP:HE1	1.67	0.43
1:A:557:ILE:HD11	1:A:594:TYR:HD2	1.83	0.43
1:A:109:ILE:HD11	1:A:174:GLU:CD	2.35	0.43
1:A:632:LEU:HD11	1:A:765:ILE:HA	2.01	0.43
2:B:808:ASN:ND2	2:B:812:ILE:HD11	2.34	0.43
3:D:70:ASP:HA	3:D:146:THR:HG21	2.00	0.42
3:C:292:TYR:CD2	3:C:372:VAL:HG12	2.54	0.42
3:D:412:LEU:HG	3:D:419:VAL:HG11	2.00	0.42
2:B:214:PRO:HB2	2:B:217:GLU:CB	2.49	0.42
2:B:184:ILE:HD11	2:B:213:ILE:HG13	2.01	0.42
2:B:398:LEU:CD1	2:B:449:ILE:CD1	2.90	0.42
2:B:350:LEU:HD22	2:B:405:ILE:HG13	2.00	0.42
3:C:7:THR:O	3:C:66:ALA:HA	2.19	0.42
3:D:133:PHE:CZ	3:D:135:GLY:O	2.72	0.42
2:B:199:LEU:HD23	2:B:200:PHE:CE2	2.53	0.42
2:B:261:LEU:HD12	2:B:293:ARG:HH22	1.84	0.42
3:C:210:LEU:HD22	3:C:222:ILE:CD1	2.49	0.42
1:A:123:TYR:OH	2:B:288:TYR:CZ	2.51	0.42
2:B:216:PHE:O	2:B:216:PHE:CG	2.72	0.42
1:A:425:ILE:HG23	1:A:426:PHE:CD1	2.54	0.42
1:A:62:ASP:HB3	1:A:94:ILE:HD13	2.01	0.42
3:D:255:ILE:CD1	3:D:358:ARG:CD	2.95	0.42
1:A:154:LEU:CD2	2:B:281:LYS:HZ1	2.31	0.42
2:B:636:ILE:HG21	2:B:636:ILE:HD13	1.87	0.42
1:A:68:ILE:HG22	1:A:158:LEU:HD13	2.00	0.42
1:A:372:ASP:OD1	1:A:375:ILE:HD12	2.18	0.42
2:B:209:ILE:CD1	2:B:218:SER:CB	2.66	0.42
2:B:188:VAL:HG21	2:B:280:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:209:LEU:HD21	3:D:231:ILE:HD11	2.01	0.42
3:C:24:GLN:HE22	3:C:233:THR:HA	1.85	0.42
3:D:316:PHE:CD1	3:D:345:PRO:HB3	2.55	0.42
3:D:127:ILE:CD1	3:D:162:TYR:CZ	3.02	0.42
1:A:123:TYR:HA	1:A:126:TRP:CE3	2.54	0.42
2:B:405:ILE:CG2	2:B:456:ILE:CD1	2.74	0.42
3:D:204:PHE:CD2	3:D:231:ILE:HG23	2.54	0.42
1:A:630:ARG:HA	1:A:633:HIS:CD2	2.54	0.42
2:B:527:HIS:O	2:B:527:HIS:CG	2.70	0.42
1:A:779:LEU:HD22	1:A:779:LEU:HA	1.84	0.42
1:A:348:LEU:HD23	1:A:352:ILE:CD1	2.49	0.42
3:C:299:LEU:H	3:C:299:LEU:HD22	1.84	0.42
3:C:266:HIS:H	3:C:266:HIS:CD2	2.38	0.42
2:B:660:ASN:HD22	2:B:735:ILE:HG23	1.85	0.42
2:B:500:LEU:HD21	2:B:558:PHE:HB2	2.00	0.42
2:B:402:ILE:CD1	2:B:449:ILE:CD1	2.96	0.42
3:D:202:VAL:HG22	3:D:268:LEU:HD23	2.00	0.42
2:B:634:ILE:CD1	2:B:776:TYR:HE1	2.16	0.42
2:B:348:ASN:OD1	2:B:355:LEU:HD23	2.20	0.42
1:A:625:ILE:HD13	1:A:765:ILE:CG1	2.49	0.42
1:A:70:LEU:HG	2:B:281:LYS:HZ3	1.67	0.42
1:A:151:LEU:HD12	2:B:282:SER:HA	2.02	0.42
2:B:526:ARG:O	2:B:538:ILE:HD11	2.19	0.42
2:B:463:ILE:HG21	2:B:463:ILE:HD13	1.79	0.42
2:B:427:LYS:HD3	2:B:452:GLN:HE22	1.83	0.42
3:C:188:ILE:HD11	3:C:394:PHE:CG	2.21	0.42
1:A:137:ARG:CZ	2:B:325:LEU:HD22	2.49	0.42
3:D:6:ILE:HD11	3:D:126:GLU:HB3	2.02	0.42
1:A:357:VAL:HG23	1:A:363:ILE:CD1	2.49	0.42
1:A:693:ILE:HG23	1:A:694:PRO:HD3	2.00	0.42
3:D:231:ILE:O	3:D:235:ILE:HG13	2.18	0.42
3:C:188:ILE:HD11	3:C:394:PHE:CG	2.52	0.42
3:D:356:ILE:CD1	3:D:358:ARG:NH1	2.69	0.42
3:D:188:ILE:CD1	3:D:394:PHE:CG	3.02	0.42
1:A:375:ILE:HD11	1:A:396:LYS:CG	2.50	0.42
1:A:375:ILE:HD11	1:A:396:LYS:HB3	2.00	0.42
3:D:72:GLU:O	3:D:76:ILE:HG13	2.19	0.42
3:C:275:PHE:O	3:C:276:THR:HG23	2.20	0.42
2:B:349:TRP:CE2	2:B:364:ILE:CD1	3.03	0.42
1:A:114:LYS:HE3	1:A:118:ILE:HD12	2.00	0.42
1:A:63:LEU:HD23	1:A:170:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:188:VAL:HB	2:B:224:ILE:CD1	2.48	0.42
3:C:29:HIS:CE1	3:C:49:ASP:HA	2.54	0.42
1:A:603:TRP:CD2	1:A:633:HIS:HB2	2.55	0.42
2:B:482:LEU:HD13	2:B:731:PHE:CZ	2.55	0.42
2:B:641:PHE:CD1	2:B:765:LEU:HD21	2.55	0.42
3:C:238:VAL:CG2	3:C:322:ILE:HD13	2.43	0.42
2:B:322:HIS:HD2	2:B:327:ILE:CD1	2.33	0.42
2:B:253:LEU:HD22	2:B:334:LEU:HD23	2.00	0.42
2:B:586:ILE:CG2	2:B:735:ILE:HD12	2.14	0.42
2:B:449:ILE:HG21	2:B:449:ILE:HD13	1.87	0.42
3:D:142:VAL:O	3:D:142:VAL:HG12	2.20	0.42
3:D:69:MET:SD	3:D:119:ILE:HD11	2.59	0.42
3:D:119:ILE:O	3:D:123:ILE:HG13	2.20	0.42
1:A:598:LEU:HA	1:A:598:LEU:HD13	1.89	0.42
3:D:75:VAL:HG11	3:D:94:VAL:HG22	2.02	0.42
1:A:425:ILE:HD12	1:A:478:MET:O	2.20	0.42
1:A:98:MET:H	1:A:98:MET:HE3	1.85	0.42
2:B:349:TRP:CD1	2:B:364:ILE:HD12	2.52	0.42
3:C:272:PHE:O	3:C:275:PHE:CE1	2.73	0.42
3:D:9:GLN:HE21	3:D:15:ASN:HA	1.84	0.42
2:B:405:ILE:CG1	2:B:456:ILE:HD13	2.49	0.42
1:A:405:PHE:HZ	1:A:573:ILE:HD11	1.83	0.42
1:A:73:THR:H	2:B:215:ASN:CA	2.33	0.42
1:A:415:LEU:HD22	1:A:663:TYR:CE1	2.55	0.42
2:B:264:TYR:CD2	2:B:287:ILE:HD11	2.47	0.42
2:B:287:ILE:HG23	2:B:291:ILE:HD11	2.01	0.42
2:B:651:TYR:CE1	3:D:333:ARG:HG2	2.55	0.42
3:C:256:TYR:CZ	3:C:260:ILE:HD12	2.52	0.42
3:D:173:PHE:CD1	3:D:174:PRO:HD2	2.54	0.42
3:C:105:TRP:CH2	3:C:109:TYR:CE2	3.08	0.42
1:A:570:LEU:HB3	1:A:573:ILE:HD12	2.00	0.42
3:C:258:THR:CB	3:C:356:ILE:CD1	2.97	0.42
2:B:311:THR:O	2:B:314:ILE:HG12	2.20	0.42
2:B:480:ILE:CD1	2:B:541:LEU:CD1	2.98	0.42
3:D:289:HIS:H	3:D:289:HIS:CD2	2.37	0.42
1:A:450:TYR:CE1	1:A:559:HIS:CE1	3.08	0.42
2:B:499:ILE:HD13	2:B:511:LYS:CB	2.49	0.42
1:A:650:ASN:HD21	3:C:333:ARG:HD3	1.84	0.42
1:A:259:LEU:HA	1:A:259:LEU:HD22	1.96	0.42
2:B:574:VAL:HG13	2:B:574:VAL:O	2.19	0.42
3:C:299:LEU:CD2	3:C:299:LEU:H	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:ILE:CD1	1:A:683:ILE:HD11	2.49	0.42
1:A:80:ASP:O	1:A:90:ILE:N	2.53	0.42
3:C:5:ILE:HD12	3:C:53:PHE:CE2	2.55	0.42
3:C:320:ASN:HD21	3:C:358:ARG:HG3	1.84	0.42
1:A:136:GLN:HG2	2:B:324:ASP:H	1.85	0.42
3:C:125:LYS:HG3	3:D:283:ASP:CG	2.41	0.42
1:A:375:ILE:HD13	1:A:396:LYS:CD	2.48	0.42
1:A:449:HIS:CG	1:A:450:TYR:H	2.37	0.42
1:A:584:ILE:CD1	1:A:687:ARG:CB	2.98	0.42
2:B:238:VAL:O	2:B:254:ILE:HD12	2.20	0.42
1:A:245:GLY:HA3	1:A:332:LEU:HA	2.02	0.42
2:B:411:PHE:CE1	2:B:570:LEU:HD23	2.55	0.42
1:A:105:PHE:CZ	1:A:177:ILE:HD12	2.55	0.41
2:B:192:LEU:CD2	2:B:227:ALA:HB3	2.50	0.41
1:A:137:ARG:HE	2:B:328:ARG:NH2	2.18	0.41
2:B:485:LYS:HG2	2:B:488:PHE:H	1.85	0.41
2:B:772:PHE:HB2	2:B:812:ILE:CD1	2.46	0.41
1:A:595:HIS:HE2	1:A:699:ILE:HG22	1.85	0.41
1:A:66:VAL:HG23	1:A:94:ILE:CD1	2.47	0.41
2:B:533:ARG:O	2:B:538:ILE:HD12	2.19	0.41
3:D:69:MET:O	3:D:70:ASP:HB2	2.20	0.41
1:A:602:THR:CG2	1:A:710:ILE:HD12	2.48	0.41
1:A:585:ILE:HD12	1:A:683:ILE:HD11	2.01	0.41
3:C:193:ARG:HH12	3:C:419:VAL:CG1	2.32	0.41
3:D:119:ILE:HD12	3:D:154:LEU:HD23	2.01	0.41
2:B:210:PRO:HG2	2:B:213:ILE:CD1	2.47	0.41
1:A:128:ASP:CG	2:B:299:ARG:HD2	2.32	0.41
1:A:56:GLU:O	1:A:60:VAL:HG23	2.20	0.41
1:A:449:HIS:CD2	1:A:450:TYR:H	2.38	0.41
1:A:65:ASN:OD1	2:B:216:PHE:HD1	1.93	0.41
2:B:543:ALA:HB2	2:B:558:PHE:CE2	2.55	0.41
1:A:425:ILE:CD1	1:A:478:MET:HA	2.33	0.41
1:A:140:TYR:CE1	2:B:292:ILE:CD1	3.03	0.41
2:B:192:LEU:HD22	2:B:268:VAL:HG21	2.02	0.41
3:C:256:TYR:CD1	3:C:260:ILE:HD11	2.52	0.41
3:D:333:ARG:HD3	3:D:333:ARG:HH11	1.68	0.41
1:A:363:ILE:HD11	1:A:413:TYR:CB	2.45	0.41
1:A:115:GLN:O	1:A:118:ILE:HG22	2.20	0.41
1:A:714:ARG:HH12	1:A:758:LEU:HD13	1.84	0.41
1:A:119:LEU:HD21	1:A:143:ARG:HA	2.00	0.41
1:A:489:GLU:HG3	1:A:559:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:LEU:CG	1:A:710:ILE:HD11	2.50	0.41
1:A:151:LEU:O	1:A:155:VAL:HG23	2.20	0.41
2:B:349:TRP:CD1	2:B:362:PHE:CE2	3.08	0.41
1:A:416:ILE:CD1	1:A:664:ARG:HG2	2.48	0.41
1:A:795:ASP:O	1:A:799:VAL:HG23	2.20	0.41
3:D:70:ASP:HA	3:D:146:THR:HG21	2.02	0.41
1:A:787:SER:HB2	1:A:790:LYS:HG2	2.01	0.41
1:A:70:LEU:HD22	2:B:219:GLY:HA2	2.01	0.41
3:C:121:ASN:HD22	3:D:218:ARG:HH12	1.50	0.41
2:B:269:ASN:HA	2:B:272:VAL:HG22	2.01	0.41
2:B:342:TYR:CZ	2:B:394:ILE:HD12	2.56	0.41
1:A:557:ILE:HD11	1:A:594:TYR:CD2	2.55	0.41
1:A:71:GLU:OE1	2:B:222:HIS:CE1	2.71	0.41
2:B:323:GLY:O	2:B:327:ILE:HD12	2.20	0.41
2:B:214:PRO:HB2	2:B:217:GLU:HB3	2.02	0.41
3:C:72:GLU:H	3:C:73:PRO:HD2	1.85	0.41
1:A:138:PHE:CZ	1:A:142:ILE:HD11	2.56	0.41
1:A:97:LYS:H	1:A:98:MET:HE3	1.86	0.41
1:A:409:PHE:HB3	1:A:415:LEU:HD22	2.02	0.41
3:D:199:ASP:HB3	3:D:260:ILE:HD11	2.02	0.41
2:B:527:HIS:HB2	2:B:533:ARG:HD2	2.02	0.41
1:A:151:LEU:HD23	2:B:285:ARG:NE	1.82	0.41
2:B:719:LEU:HD23	2:B:719:LEU:HA	1.82	0.41
2:B:405:ILE:HG12	2:B:456:ILE:HD12	2.03	0.41
3:C:292:TYR:CD2	3:C:372:VAL:HB	2.56	0.41
2:B:242:ARG:N	2:B:254:ILE:HD11	2.33	0.41
2:B:823:LEU:HD13	2:B:824:TYR:N	2.35	0.41
1:A:695:LEU:HD22	1:A:793:PHE:CE2	2.55	0.41
1:A:70:LEU:HD13	2:B:220:LEU:CG	2.50	0.41
3:D:381:SER:O	3:D:384:VAL:HG22	2.20	0.41
1:A:140:TYR:CG	2:B:324:ASP:CG	2.94	0.41
1:A:151:LEU:CD2	2:B:285:ARG:HD3	2.39	0.41
2:B:335:PHE:CD1	2:B:339:ILE:CD1	2.99	0.41
3:C:234:ILE:HD11	3:C:303:ASN:ND2	2.35	0.41
1:A:128:ASP:OD2	2:B:295:ARG:CD	2.67	0.41
3:D:188:ILE:HG23	3:D:423:PHE:CD2	2.56	0.41
1:A:296:TYR:HH	2:B:322:HIS:CE1	2.24	0.41
1:A:143:ARG:HD2	2:B:292:ILE:HD13	1.99	0.41
1:A:73:THR:CB	2:B:215:ASN:HA	2.50	0.41
1:A:425:ILE:HD13	1:A:482:LEU:CG	2.51	0.41
2:B:572:LEU:HA	2:B:572:LEU:HD23	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:564:LEU:HD12	2:B:568:LEU:HD23	2.03	0.41
3:D:408:ASN:ND2	3:D:417:GLN:HE21	2.19	0.41
2:B:430:HIS:HB3	2:B:448:ILE:HD13	2.02	0.41
3:C:305:LEU:O	3:C:306:VAL:HG13	2.20	0.41
3:D:222:ILE:HD13	3:D:222:ILE:HG21	1.78	0.41
1:A:606:LEU:CD2	1:A:710:ILE:HD11	2.51	0.41
1:A:68:ILE:HD12	1:A:158:LEU:HD21	1.87	0.41
2:B:296:ILE:HD13	2:B:327:ILE:CA	2.44	0.41
2:B:636:ILE:HD11	3:D:437:TYR:CE2	2.47	0.41
3:C:260:ILE:HD13	3:C:266:HIS:HB2	2.03	0.41
3:D:345:PRO:O	3:D:347:TRP:CE2	2.74	0.41
3:D:95:ALA:HB1	3:D:111:ILE:HD13	1.97	0.41
3:C:67:ILE:HD11	3:C:123:ILE:HA	2.03	0.41
3:D:111:ILE:HA	3:D:114:ARG:HE	1.85	0.41
3:D:136:PHE:CZ	3:D:158:LEU:HD12	2.55	0.41
3:D:347:TRP:HA	3:D:347:TRP:CE3	2.56	0.41
1:A:626:VAL:O	1:A:630:ARG:HG2	2.21	0.41
3:C:142:VAL:HG13	3:C:190:ALA:CB	2.50	0.41
1:A:113:GLY:HA2	1:A:116:TYR:CE2	2.55	0.41
1:A:247:ILE:CG2	1:A:275:ILE:HD13	2.51	0.41
3:C:342:ILE:HD12	3:C:344:PHE:CE1	2.56	0.41
3:C:5:ILE:HD12	3:C:53:PHE:CZ	2.55	0.41
1:A:469:ARG:HH21	1:A:477:LEU:HG	1.84	0.41
1:A:564:ILE:HG21	1:A:564:ILE:HD13	1.91	0.41
1:A:159:GLU:OE1	2:B:277:VAL:HG12	2.21	0.41
3:D:212:ILE:HD13	3:D:275:PHE:CE2	2.55	0.41
3:D:6:ILE:HD13	3:D:126:GLU:HB2	2.03	0.41
2:B:257:ILE:HD13	2:B:257:ILE:HG21	1.93	0.41
2:B:241:PHE:C	2:B:254:ILE:HD13	2.41	0.41
2:B:634:ILE:HG21	2:B:634:ILE:HD13	1.92	0.41
1:A:362:GLN:HB3	2:B:446:PHE:CZ	2.53	0.41
2:B:600:TYR:CE1	2:B:765:LEU:HB3	2.55	0.41
1:A:68:ILE:CD1	2:B:215:ASN:HB3	2.50	0.41
1:A:98:MET:CE	1:A:170:ILE:HD11	2.51	0.41
1:A:247:ILE:CD1	1:A:275:ILE:HD13	2.50	0.41
1:A:248:LEU:HD11	1:A:279:TYR:CG	2.56	0.41
2:B:546:LEU:HB3	2:B:547:ASP:H	1.68	0.41
1:A:195:GLU:CG	1:A:250:ILE:HD13	2.51	0.41
1:A:778:CYS:HA	1:A:781:ASN:HD22	1.86	0.41
2:B:405:ILE:CG2	2:B:456:ILE:CD1	2.96	0.41
2:B:563:ILE:HG12	2:B:564:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LEU:HD23	1:A:352:ILE:HD12	2.03	0.41
1:A:358:ARG:HA	1:A:363:ILE:HB	2.03	0.41
3:C:188:ILE:HD12	3:C:394:PHE:HD2	1.82	0.41
3:D:230:LEU:O	3:D:234:ILE:HG13	2.20	0.41
2:B:346:LEU:CD1	2:B:402:ILE:HD13	2.49	0.41
2:B:507:LEU:HB3	2:B:508:PRO:HD3	2.03	0.41
1:A:630:ARG:HA	1:A:633:HIS:ND1	2.36	0.41
3:D:95:ALA:HB1	3:D:111:ILE:CD1	2.51	0.41
1:A:415:LEU:HD13	1:A:570:LEU:HG	2.03	0.41
1:A:68:ILE:CD1	2:B:216:PHE:HB3	2.51	0.41
2:B:470:TYR:HE2	2:B:724:LEU:HD22	1.86	0.41
2:B:665:THR:O	2:B:669:GLN:HG2	2.21	0.41
3:D:238:VAL:HG13	3:D:322:ILE:HD12	2.02	0.41
1:A:247:ILE:HG21	1:A:275:ILE:HD13	2.03	0.41
2:B:656:ILE:HG21	2:B:738:HIS:CE1	2.56	0.41
1:A:558:TYR:CA	1:A:693:ILE:HD11	2.48	0.41
2:B:516:LEU:HD21	2:B:541:LEU:HB3	2.02	0.41
2:B:349:TRP:CE3	2:B:364:ILE:HD11	2.56	0.40
2:B:822:ARG:NH2	2:B:841:LEU:HD22	2.35	0.40
3:C:188:ILE:HD13	3:C:394:PHE:CD2	2.52	0.40
2:B:765:LEU:O	2:B:769:VAL:HG23	2.20	0.40
3:D:256:TYR:HE1	3:D:260:ILE:CD1	2.23	0.40
1:A:292:LEU:HD21	1:A:299:PHE:CD2	2.56	0.40
1:A:291:ILE:HD12	1:A:358:ARG:NH1	2.33	0.40
2:B:535:SER:H	2:B:538:ILE:HD11	1.86	0.40
3:C:128:ASP:OD2	3:D:281:HIS:CD2	2.74	0.40
3:D:291:SER:O	3:D:295:MET:HG3	2.22	0.40
1:A:188:LEU:HD22	1:A:268:LEU:HD11	2.03	0.40
3:C:315:TYR:CE2	3:C:438:VAL:O	2.74	0.40
3:C:125:LYS:HD3	3:D:283:ASP:OD2	2.20	0.40
3:C:129:SER:HB3	3:D:284:ILE:HB	2.03	0.40
1:A:128:ASP:C	2:B:322:HIS:CE1	2.94	0.40
2:B:499:ILE:HD13	2:B:511:LYS:HB2	2.03	0.40
3:C:328:PRO:HD2	3:C:331:ILE:CD1	2.51	0.40
1:A:774:ILE:HD13	1:A:796:SER:HB2	2.01	0.40
3:C:107:ASN:HD21	3:C:409:VAL:HG23	1.86	0.40
3:D:106:ALA:CB	3:D:407:TYR:HA	2.51	0.40
1:A:143:ARG:CZ	2:B:292:ILE:HG23	2.51	0.40
2:B:346:LEU:CD1	2:B:402:ILE:HD13	2.51	0.40
3:C:120:LEU:HD22	3:C:161:ARG:NH1	2.36	0.40
1:A:434:ASN:CB	1:A:469:ARG:HE	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:591:TRP:CZ2	2:B:595:LYS:HD3	2.56	0.40
2:B:300:PHE:CE2	2:B:319:PHE:CE1	3.09	0.40
3:C:13:CYS:HB2	3:C:141:SER:HB3	2.02	0.40
2:B:493:ILE:HD13	2:B:595:LYS:HA	2.03	0.40
2:B:347:MET:SD	2:B:428:LYS:HA	2.61	0.40
1:A:761:ILE:O	1:A:765:ILE:HG23	2.21	0.40
2:B:735:ILE:HD13	2:B:735:ILE:HG21	1.90	0.40
3:D:8:LEU:HD23	3:D:67:ILE:CG2	2.52	0.40
1:A:335:CYS:HA	1:A:340:ASP:HB3	2.04	0.40
1:A:73:THR:HG21	2:B:213:ILE:O	2.21	0.40
3:C:121:ASN:O	3:C:125:LYS:HG3	2.21	0.40
2:B:339:ILE:CD1	2:B:440:GLY:N	2.85	0.40
3:C:127:ILE:HD13	3:C:162:TYR:CE2	2.48	0.40
1:A:589:GLN:NE2	1:A:652:ILE:HD13	2.36	0.40
1:A:592:LEU:HA	1:A:696:GLN:OE1	2.21	0.40
1:A:70:LEU:HB3	1:A:92:PHE:CE1	2.55	0.40
3:C:2:GLY:HA3	3:C:132:ASN:HD22	1.86	0.40
3:D:306:VAL:HG13	3:D:382:THR:HG21	2.03	0.40
3:D:255:ILE:CD1	3:D:358:ARG:HD3	2.49	0.40
3:C:129:SER:OG	3:D:284:ILE:CB	2.70	0.40
2:B:364:ILE:CD1	2:B:403:PHE:CA	2.98	0.40
2:B:739:LYS:O	2:B:743:THR:O	2.40	0.40
2:B:355:LEU:C	2:B:364:ILE:HD12	2.33	0.40
3:C:182:VAL:HG12	3:C:403:PHE:HB3	2.02	0.40
2:B:253:LEU:HD12	2:B:334:LEU:HG	2.02	0.40
2:B:241:PHE:HB3	2:B:254:ILE:HD13	2.03	0.40
3:D:123:ILE:HD13	3:D:158:LEU:HD21	2.03	0.40
2:B:564:LEU:H	2:B:564:LEU:HD23	1.86	0.40
3:D:261:PRO:HD2	3:D:266:HIS:HA	2.04	0.40
1:A:639:PHE:CE2	1:A:775:PHE:HB3	2.57	0.40
2:B:200:PHE:HB2	2:B:207:ILE:CD1	2.51	0.40
1:A:69:GLY:HA2	2:B:216:PHE:CG	2.56	0.40
3:C:172:VAL:HG22	3:C:231:ILE:HD13	2.04	0.40
2:B:455:GLU:HG2	2:B:459:HIS:NE2	2.36	0.40
1:A:201:GLU:HA	1:A:204:ARG:HH21	1.87	0.40
1:A:566:ILE:H	1:A:566:ILE:HG12	1.64	0.40
2:B:199:LEU:HD13	2:B:199:LEU:O	2.21	0.40
2:B:287:ILE:HD13	2:B:287:ILE:HG21	1.91	0.40
2:B:335:PHE:CD2	2:B:439:ARG:HG2	2.57	0.40
1:A:136:GLN:OE1	2:B:323:GLY:N	2.53	0.40
1:A:776:ARG:HH11	1:A:776:ARG:HD2	1.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:TYR:CE2	2:B:292:ILE:HG21	2.57	0.40
3:D:105:TRP:CZ2	3:D:193:ARG:NH2	2.90	0.40
1:A:482:LEU:HD11	1:A:562:PHE:HB3	2.03	0.40
3:C:404:LEU:HA	3:C:404:LEU:HD12	1.97	0.40
3:C:129:SER:OG	3:D:284:ILE:HB	2.21	0.40
3:D:119:ILE:HG21	3:D:154:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	561/823 (68%)	518 (92%)	20 (4%)	23 (4%)	3	35
1	2-A	561/823 (68%)	534 (95%)	17 (3%)	10 (2%)	11	53
1	3-A	561/823 (68%)	522 (93%)	23 (4%)	16 (3%)	6	43
1	4-A	561/823 (68%)	529 (94%)	20 (4%)	12 (2%)	9	50
1	5-A	561/823 (68%)	525 (94%)	20 (4%)	16 (3%)	6	43
1	6-A	561/823 (68%)	538 (96%)	13 (2%)	10 (2%)	11	53
1	7-A	561/823 (68%)	529 (94%)	23 (4%)	9 (2%)	12	56
1	8-A	561/823 (68%)	523 (93%)	23 (4%)	15 (3%)	6	45
1	9-A	561/823 (68%)	530 (94%)	23 (4%)	8 (1%)	14	58
1	10-A	561/823 (68%)	521 (93%)	29 (5%)	11 (2%)	9	51
2	1-B	553/846 (65%)	519 (94%)	23 (4%)	11 (2%)	9	51
2	2-B	553/846 (65%)	520 (94%)	21 (4%)	12 (2%)	8	49
2	3-B	553/846 (65%)	521 (94%)	20 (4%)	12 (2%)	8	49
2	4-B	553/846 (65%)	515 (93%)	28 (5%)	10 (2%)	11	53
2	5-B	553/846 (65%)	516 (93%)	30 (5%)	7 (1%)	15	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	6-B	553/846 (65%)	513 (93%)	27 (5%)	13 (2%)	7	47
2	7-B	553/846 (65%)	514 (93%)	23 (4%)	16 (3%)	6	43
2	8-B	553/846 (65%)	525 (95%)	19 (3%)	9 (2%)	12	56
2	9-B	553/846 (65%)	521 (94%)	24 (4%)	8 (1%)	14	58
2	10-B	553/846 (65%)	517 (94%)	22 (4%)	14 (2%)	7	46
3	1-C	443/473 (94%)	392 (88%)	32 (7%)	19 (4%)	3	34
3	1-D	443/473 (94%)	404 (91%)	28 (6%)	11 (2%)	7	46
3	2-C	443/473 (94%)	400 (90%)	30 (7%)	13 (3%)	6	43
3	2-D	443/473 (94%)	411 (93%)	22 (5%)	10 (2%)	8	48
3	3-C	443/473 (94%)	384 (87%)	37 (8%)	22 (5%)	3	31
3	3-D	443/473 (94%)	402 (91%)	27 (6%)	14 (3%)	5	41
3	4-C	443/473 (94%)	399 (90%)	35 (8%)	9 (2%)	9	51
3	4-D	443/473 (94%)	392 (88%)	38 (9%)	13 (3%)	6	43
3	5-C	443/473 (94%)	408 (92%)	19 (4%)	16 (4%)	4	38
3	5-D	443/473 (94%)	399 (90%)	36 (8%)	8 (2%)	11	53
3	6-C	443/473 (94%)	396 (89%)	36 (8%)	11 (2%)	7	46
3	6-D	443/473 (94%)	400 (90%)	29 (6%)	14 (3%)	5	41
3	7-C	443/473 (94%)	406 (92%)	26 (6%)	11 (2%)	7	46
3	7-D	443/473 (94%)	393 (89%)	34 (8%)	16 (4%)	4	38
3	8-C	443/473 (94%)	399 (90%)	27 (6%)	17 (4%)	4	37
3	8-D	443/473 (94%)	395 (89%)	32 (7%)	16 (4%)	4	38
3	9-C	443/473 (94%)	396 (89%)	35 (8%)	12 (3%)	6	45
3	9-D	443/473 (94%)	399 (90%)	32 (7%)	12 (3%)	6	45
3	10-C	443/473 (94%)	404 (91%)	27 (6%)	12 (3%)	6	45
3	10-D	443/473 (94%)	390 (88%)	38 (9%)	15 (3%)	5	40
All	All	20000/26150 (76%)	18419 (92%)	1068 (5%)	513 (3%)	11	45

All (513) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	91	GLU
1	1-A	99	ASP
1	1-A	261	ASP

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Mol	Chain	Res	Type
1	1-A	322	THR
1	1-A	364	PRO
1	1-A	571	ASN
2	1-B	212	LYS
3	1-C	51	LYS
3	1-C	275	PHE
3	1-C	280	ILE
3	1-C	315	TYR
3	1-C	416	MET
3	1-D	51	LYS
1	2-A	91	GLU
1	2-A	297	GLN
1	2-A	473	ASN
2	2-B	357	ALA
2	2-B	416	CYS
2	2-B	574	VAL
3	2-C	99	ALA
3	2-D	261	PRO
1	3-A	91	GLU
1	3-A	97	LYS
1	3-A	365	THR
2	3-B	194	ALA
3	3-C	325	ASN
3	3-C	366	GLN
3	3-C	370	ASN
3	3-D	354	VAL
3	3-D	415	SER
1	4-A	91	GLU
2	4-B	611	ILE
3	4-C	59	ARG
3	4-D	60	ASN
1	5-A	91	GLU
1	5-A	609	THR
2	5-B	357	ALA
3	5-C	97	ASP
3	5-C	178	SER
3	5-C	286	HIS
3	5-C	325	ASN
1	6-A	91	GLU
1	6-A	98	MET
2	6-B	210	PRO
2	6-B	417	LYS

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Mol	Chain	Res	Type
3	6-C	59	ARG
3	6-C	132	ASN
3	6-C	248	MET
3	6-C	274	PRO
3	6-C	325	ASN
3	6-D	73	PRO
3	6-D	325	ASN
1	7-A	786	LEU
2	7-B	198	ALA
2	7-B	210	PRO
2	7-B	214	PRO
2	7-B	548	LEU
3	7-C	70	ASP
3	7-C	351	ALA
3	7-D	223	ASP
3	7-D	279	TYR
3	7-D	286	HIS
3	7-D	325	ASN
3	7-D	351	ALA
1	8-A	91	GLU
1	8-A	259	LEU
1	8-A	570	LEU
3	8-C	103	ASN
3	8-C	309	ALA
3	8-C	325	ASN
3	8-C	363	LEU
3	8-D	58	SER
3	8-D	325	ASN
1	9-A	91	GLU
1	9-A	130	SER
2	9-B	206	GLN
3	9-C	325	ASN
3	9-C	352	MET
3	9-C	403	PHE
3	9-D	51	LYS
3	9-D	248	MET
3	9-D	325	ASN
3	9-D	365	LEU
1	10-A	91	GLU
1	10-A	362	GLN
2	10-B	208	GLN
2	10-B	247	SER

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Mol	Chain	Res	Type
2	10-B	547	ASP
2	10-B	610	ILE
3	10-C	310	MET
3	10-D	103	ASN
3	10-D	311	ASN
1	1-A	297	GLN
1	1-A	432	GLY
1	1-A	691	ASP
2	1-B	354	LEU
2	1-B	416	CYS
2	1-B	547	ASP
2	1-B	577	PRO
3	1-C	70	ASP
3	1-C	221	ASN
3	1-C	223	ASP
3	1-C	302	SER
3	1-C	369	GLU
3	1-D	70	ASP
3	1-D	100	SER
3	1-D	278	ASP
3	1-D	326	VAL
1	2-A	128	ASP
1	2-A	333	ARG
1	2-A	361	LEU
2	2-B	204	HIS
2	2-B	382	PRO
2	2-B	537	VAL
3	2-C	265	LEU
3	2-C	277	SER
3	2-C	325	ASN
3	2-D	40	PRO
3	2-D	50	THR
3	2-D	441	GLU
1	3-A	332	LEU
1	3-A	667	THR
1	3-A	786	LEU
2	3-B	279	SER
2	3-B	383	ILE
2	3-B	438	TYR
2	3-B	439	ARG
2	3-B	533	ARG
2	3-B	576	ARG

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Mol	Chain	Res	Type
3	3-C	70	ASP
3	3-C	100	SER
3	3-C	132	ASN
3	3-C	163	PRO
3	3-C	280	ILE
3	3-C	308	THR
3	3-C	354	VAL
3	3-D	41	ASP
3	3-D	70	ASP
3	3-D	287	LYS
3	3-D	307	SER
3	3-D	325	ASN
3	3-D	444	SER
1	4-A	361	LEU
1	4-A	365	THR
1	4-A	432	GLY
1	4-A	608	LYS
2	4-B	356	ARG
2	4-B	392	ALA
3	4-C	70	ASP
3	4-C	261	PRO
3	4-C	351	ALA
3	4-D	30	ALA
3	4-D	70	ASP
3	4-D	104	SER
3	4-D	175	ALA
3	4-D	284	ILE
3	4-D	285	ALA
1	5-A	169	SER
1	5-A	365	THR
1	5-A	432	GLY
1	5-A	471	SER
2	5-B	417	LYS
3	5-C	41	ASP
3	5-C	163	PRO
3	5-C	246	SER
3	5-C	307	SER
3	5-D	42	SER
1	6-A	429	TYR
1	6-A	432	GLY
2	6-B	194	ALA
2	6-B	439	ARG

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Mol	Chain	Res	Type
2	6-B	575	ASN
3	6-C	99	ALA
3	6-D	261	PRO
3	6-D	279	TYR
3	6-D	364	PRO
1	7-A	91	GLU
1	7-A	97	LYS
1	7-A	296	TYR
1	7-A	432	GLY
1	7-A	571	ASN
1	7-A	572	ILE
2	7-B	206	GLN
2	7-B	246	ILE
2	7-B	416	CYS
2	7-B	419	VAL
3	7-C	99	ALA
3	7-D	43	SER
1	8-A	388	SER
1	8-A	489	GLU
2	8-B	358	THR
2	8-B	530	ASN
3	8-C	261	PRO
3	8-C	285	ALA
3	8-D	60	ASN
3	8-D	70	ASP
3	8-D	276	THR
3	8-D	301	PRO
3	8-D	351	ALA
3	8-D	442	GLN
1	9-A	555	SER
2	9-B	246	ILE
2	9-B	570	LEU
3	9-C	70	ASP
3	9-C	261	PRO
3	9-C	277	SER
3	9-D	70	ASP
3	9-D	100	SER
3	9-D	309	ALA
1	10-A	432	GLY
1	10-A	666	PRO
2	10-B	194	ALA
2	10-B	212	LYS

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Mol	Chain	Res	Type
2	10-B	274	SER
2	10-B	524	SER
3	10-C	70	ASP
3	10-C	101	ALA
3	10-C	222	ILE
3	10-C	309	ALA
3	10-C	328	PRO
3	10-C	364	PRO
3	10-D	70	ASP
3	10-D	177	SER
3	10-D	325	ASN
1	1-A	72	GLY
1	1-A	296	TYR
1	1-A	299	PHE
1	1-A	337	SER
1	1-A	570	LEU
2	1-B	204	HIS
2	1-B	243	MET
2	1-B	526	ARG
3	1-C	61	LYS
3	1-C	277	SER
3	1-D	328	PRO
1	2-A	362	GLN
1	2-A	414	ASP
2	2-B	274	SER
2	2-B	532	PRO
2	2-B	533	ARG
2	2-B	577	PRO
3	2-C	70	ASP
3	2-C	416	MET
3	2-D	403	PHE
1	3-A	487	ASP
1	3-A	666	PRO
2	3-B	577	PRO
2	3-B	835	ASP
3	3-C	175	ALA
3	3-C	311	ASN
3	3-C	313	PRO
3	3-D	101	ALA
3	3-D	266	HIS
1	4-A	128	ASP
1	4-A	129	THR

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Mol	Chain	Res	Type
1	4-A	413	TYR
2	4-B	198	ALA
2	4-B	214	PRO
3	4-C	58	SER
3	4-C	313	PRO
3	4-C	325	ASN
1	5-A	128	ASP
2	5-B	382	PRO
3	5-C	70	ASP
3	5-C	143	ALA
3	5-C	361	PRO
3	5-D	45	GLU
3	5-D	70	ASP
3	5-D	218	ARG
3	5-D	277	SER
1	6-A	261	ASP
1	6-A	366	ILE
2	6-B	198	ALA
2	6-B	204	HIS
3	6-C	70	ASP
3	6-C	72	GLU
3	6-C	96	SER
3	6-D	45	GLU
1	7-A	364	PRO
2	7-B	469	HIS
2	7-B	524	SER
2	7-B	551	GLY
3	7-C	274	PRO
3	7-C	276	THR
3	7-C	325	ASN
3	7-D	70	ASP
3	7-D	179	GLU
3	7-D	278	ASP
3	7-D	308	THR
3	7-D	442	GLN
1	8-A	97	LYS
1	8-A	296	TYR
1	8-A	297	GLN
1	8-A	298	GLU
1	8-A	361	LEU
1	8-A	412	GLY
2	8-B	439	ARG

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Mol	Chain	Res	Type
2	8-B	529	MET
2	8-B	550	HIS
3	8-C	70	ASP
3	8-C	96	SER
3	8-C	364	PRO
3	8-D	59	ARG
3	8-D	343	LYS
1	9-A	74	TYR
1	9-A	666	PRO
2	9-B	547	ASP
2	9-B	577	PRO
3	9-C	314	THR
3	9-D	102	GLY
3	9-D	266	HIS
1	10-A	259	LEU
1	10-A	295	PRO
2	10-B	204	HIS
2	10-B	358	THR
2	10-B	416	CYS
2	10-B	720	ASN
3	10-C	38	GLN
3	10-D	45	GLU
3	10-D	246	SER
3	10-D	248	MET
3	10-D	443	ASP
1	1-A	331	LEU
1	1-A	366	ILE
1	1-A	449	HIS
1	1-A	472	GLU
2	1-B	324	ASP
3	1-C	178	SER
3	1-C	219	ASN
3	1-C	328	PRO
3	1-D	246	SER
1	2-A	70	LEU
3	2-C	96	SER
3	2-C	143	ALA
3	2-C	163	PRO
3	2-C	311	ASN
3	2-C	367	PRO
3	2-D	276	THR
1	3-A	300	MET

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Mol	Chain	Res	Type
1	3-A	569	PRO
1	3-A	608	LYS
2	3-B	324	ASP
2	3-B	382	PRO
3	3-C	261	PRO
3	3-C	263	PRO
3	3-C	266	HIS
3	3-C	314	THR
3	3-D	131	ASP
3	3-D	163	PRO
3	3-D	353	HIS
2	4-B	527	HIS
2	4-B	563	ILE
3	4-D	103	ASN
3	4-D	311	ASN
3	4-D	325	ASN
3	4-D	343	LYS
1	5-A	97	LYS
1	5-A	360	SER
1	5-A	786	LEU
2	5-B	416	CYS
3	5-C	45	GLU
3	5-C	442	GLN
1	6-A	259	LEU
2	6-B	203	ASP
2	6-B	419	VAL
2	6-B	483	MET
3	6-C	178	SER
3	6-C	312	ASN
3	6-D	38	GLN
3	6-D	70	ASP
3	6-D	98	GLY
3	6-D	361	PRO
2	7-B	247	SER
2	7-B	417	LYS
3	7-C	163	PRO
3	7-C	353	HIS
3	7-D	364	PRO
3	7-D	415	SER
1	8-A	487	ASP
2	8-B	244	LEU
2	8-B	247	SER

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Mol	Chain	Res	Type
2	8-B	381	ILE
2	8-B	416	CYS
3	8-C	132	ASN
3	8-C	280	ILE
3	8-C	361	PRO
3	8-D	100	SER
3	8-D	102	GLY
3	8-D	307	SER
2	9-B	247	SER
2	9-B	524	SER
3	9-C	163	PRO
3	9-C	364	PRO
3	9-D	286	HIS
1	10-A	296	TYR
1	10-A	610	PRO
2	10-B	324	ASP
2	10-B	381	ILE
3	10-C	42	SER
3	10-C	265	LEU
3	10-C	279	TYR
3	10-D	43	SER
1	1-A	336	ASP
1	1-A	566	ILE
2	1-B	358	THR
3	1-C	248	MET
3	1-C	350	SER
3	1-C	361	PRO
3	1-D	104	SER
3	1-D	416	MET
2	2-B	243	MET
3	2-D	163	PRO
1	3-A	295	PRO
1	3-A	331	LEU
1	3-A	364	PRO
1	3-A	613	LYS
2	3-B	779	LEU
3	3-C	309	ALA
3	3-C	351	ALA
1	4-A	298	GLU
2	4-B	610	ILE
3	4-C	309	ALA
3	4-C	403	PHE

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Mol	Chain	Res	Type
3	4-D	32	GLY
1	5-A	299	PHE
1	5-A	362	GLN
1	5-A	371	SER
1	5-A	785	GLU
2	5-B	534	ASN
3	5-C	279	TYR
1	6-A	169	SER
1	6-A	361	LEU
2	6-B	246	ILE
2	6-B	552	SER
3	6-D	277	SER
3	6-D	281	HIS
3	6-D	417	GLN
3	7-C	30	ALA
3	7-D	361	PRO
3	8-C	100	SER
3	8-C	371	GLU
3	8-D	415	SER
1	9-A	472	GLU
3	9-C	282	ASP
3	9-D	369	GLU
1	10-A	129	THR
1	10-A	489	GLU
1	10-A	609	THR
3	10-C	444	SER
3	10-D	277	SER
3	1-D	277	SER
1	2-A	786	LEU
2	2-B	526	ARG
3	2-C	42	SER
3	2-D	282	ASP
3	3-C	47	ASP
3	3-D	367	PRO
1	4-A	414	ASP
2	4-B	550	HIS
1	5-A	412	GLY
2	5-B	528	LEU
2	5-B	546	LEU
3	5-D	3	GLY
2	7-B	357	ALA
2	7-B	529	MET

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Mol	Chain	Res	Type
2	7-B	546	LEU
3	7-C	44	THR
3	8-D	163	PRO
1	9-A	567	PRO
2	9-B	274	SER
3	9-C	45	GLU
3	9-C	98	GLY
3	9-D	40	PRO
3	10-D	36	LEU
3	10-D	261	PRO
3	10-D	287	LYS
3	10-D	441	GLU
1	1-A	165	VAL
2	1-B	611	ILE
3	1-C	367	PRO
3	1-D	261	PRO
3	3-C	174	PRO
1	4-A	666	PRO
2	4-B	419	VAL
1	5-A	367	PRO
3	8-C	367	PRO
3	2-C	261	PRO
3	2-D	245	PRO
3	5-D	327	GLU
1	6-A	428	GLY
3	7-D	98	GLY
3	8-C	3	GLY
3	8-D	40	PRO
3	4-D	181	VAL
3	5-D	345	PRO
2	6-B	309	GLY
3	7-C	280	ILE
3	7-D	220	PRO
1	8-A	573	ILE
1	1-A	573	ILE
3	2-D	328	PRO
1	3-A	132	GLY
3	5-C	261	PRO
1	7-A	295	PRO
1	8-A	473	ASN
1	8-A	666	PRO
3	8-C	354	VAL

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Mol	Chain	Res	Type
1	9-A	364	PRO
3	3-C	245	PRO
3	5-C	51	LYS
3	6-D	174	PRO
1	1-A	569	PRO
1	4-A	569	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	1-A	542/766 (71%)	513 (95%)	29 (5%)	27	64
1	2-A	542/766 (71%)	509 (94%)	33 (6%)	23	60
1	3-A	542/766 (71%)	520 (96%)	22 (4%)	37	71
1	4-A	542/766 (71%)	518 (96%)	24 (4%)	35	69
1	5-A	542/766 (71%)	519 (96%)	23 (4%)	36	70
1	6-A	542/766 (71%)	511 (94%)	31 (6%)	25	62
1	7-A	542/766 (71%)	514 (95%)	28 (5%)	29	65
1	8-A	542/766 (71%)	510 (94%)	32 (6%)	24	61
1	9-A	542/766 (71%)	520 (96%)	22 (4%)	37	71
1	10-A	542/766 (71%)	513 (95%)	29 (5%)	27	64
2	1-B	528/787 (67%)	511 (97%)	17 (3%)	46	76
2	2-B	528/787 (67%)	508 (96%)	20 (4%)	40	73
2	3-B	528/787 (67%)	508 (96%)	20 (4%)	40	73
2	4-B	528/787 (67%)	501 (95%)	27 (5%)	29	66
2	5-B	528/787 (67%)	504 (96%)	24 (4%)	34	69
2	6-B	528/787 (67%)	504 (96%)	24 (4%)	34	69
2	7-B	528/787 (67%)	500 (95%)	28 (5%)	28	64
2	8-B	528/787 (67%)	519 (98%)	9 (2%)	68	87
2	9-B	528/787 (67%)	507 (96%)	21 (4%)	38	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	10-B	528/787 (67%)	496 (94%)	32 (6%)	23	60
3	1-C	395/420 (94%)	373 (94%)	22 (6%)	26	62
3	1-D	395/420 (94%)	383 (97%)	12 (3%)	48	77
3	2-C	395/420 (94%)	377 (95%)	18 (5%)	33	68
3	2-D	395/420 (94%)	376 (95%)	19 (5%)	31	67
3	3-C	395/420 (94%)	385 (98%)	10 (2%)	55	81
3	3-D	395/420 (94%)	380 (96%)	15 (4%)	40	73
3	4-C	395/420 (94%)	381 (96%)	14 (4%)	43	74
3	4-D	395/420 (94%)	387 (98%)	8 (2%)	63	85
3	5-C	395/420 (94%)	379 (96%)	16 (4%)	37	71
3	5-D	395/420 (94%)	367 (93%)	28 (7%)	18	55
3	6-C	395/420 (94%)	373 (94%)	22 (6%)	26	62
3	6-D	395/420 (94%)	382 (97%)	13 (3%)	45	76
3	7-C	395/420 (94%)	377 (95%)	18 (5%)	33	68
3	7-D	395/420 (94%)	378 (96%)	17 (4%)	35	70
3	8-C	395/420 (94%)	378 (96%)	17 (4%)	35	70
3	8-D	395/420 (94%)	375 (95%)	20 (5%)	29	66
3	9-C	395/420 (94%)	378 (96%)	17 (4%)	35	70
3	9-D	395/420 (94%)	379 (96%)	16 (4%)	37	71
3	10-C	395/420 (94%)	383 (97%)	12 (3%)	48	77
3	10-D	395/420 (94%)	376 (95%)	19 (5%)	31	67
All	All	18600/23930 (78%)	17772 (96%)	828 (4%)	38	69

All (828) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	67	LEU
1	1-A	91	GLU
1	1-A	168	PHE
1	1-A	186	MET
1	1-A	272	LEU
1	1-A	275	ILE
1	1-A	288	THR
1	1-A	300	MET
1	1-A	302	TYR

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Mol	Chain	Res	Type
1	1-A	344	LEU
1	1-A	354	LEU
1	1-A	364	PRO
1	1-A	395	ASP
1	1-A	411	GLN
1	1-A	415	LEU
1	1-A	422	LEU
1	1-A	427	LEU
1	1-A	430	GLN
1	1-A	463	GLN
1	1-A	471	SER
1	1-A	571	ASN
1	1-A	576	ARG
1	1-A	599	LEU
1	1-A	633	HIS
1	1-A	670	VAL
1	1-A	700	PHE
1	1-A	764	LEU
1	1-A	768	ILE
1	1-A	799	VAL
2	1-B	246	ILE
2	1-B	325	LEU
2	1-B	389	ARG
2	1-B	404	MET
2	1-B	445	PHE
2	1-B	471	ARG
2	1-B	502	THR
2	1-B	504	SER
2	1-B	525	LEU
2	1-B	604	MET
2	1-B	725	GLU
2	1-B	757	PRO
2	1-B	772	PHE
2	1-B	774	LYS
2	1-B	805	PHE
2	1-B	837	GLU
2	1-B	838	LEU
3	1-C	15	ASN
3	1-C	72	GLU
3	1-C	115	ASN
3	1-C	140	HIS
3	1-C	209	LEU

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Mol	Chain	Res	Type
3	1-C	216	VAL
3	1-C	230	LEU
3	1-C	266	HIS
3	1-C	292	TYR
3	1-C	306	VAL
3	1-C	314	THR
3	1-C	315	TYR
3	1-C	321	THR
3	1-C	329	ARG
3	1-C	367	PRO
3	1-C	371	GLU
3	1-C	379	ASN
3	1-C	383	VAL
3	1-C	391	CYS
3	1-C	420	GLN
3	1-C	437	TYR
3	1-C	438	VAL
3	1-D	43	SER
3	1-D	45	GLU
3	1-D	140	HIS
3	1-D	146	THR
3	1-D	160	ASP
3	1-D	182	VAL
3	1-D	183	GLN
3	1-D	236	SER
3	1-D	256	TYR
3	1-D	328	PRO
3	1-D	376	MET
3	1-D	422	GLU
1	2-A	64	LEU
1	2-A	91	GLU
1	2-A	97	LYS
1	2-A	108	ARG
1	2-A	123	TYR
1	2-A	140	TYR
1	2-A	161	ASP
1	2-A	165	VAL
1	2-A	167	ASN
1	2-A	171	ARG
1	2-A	193	TYR
1	2-A	248	LEU
1	2-A	249	LYS

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Mol	Chain	Res	Type
1	2-A	258	ASN
1	2-A	274	ASN
1	2-A	333	ARG
1	2-A	354	LEU
1	2-A	400	ARG
1	2-A	458	TYR
1	2-A	461	LEU
1	2-A	576	ARG
1	2-A	595	HIS
1	2-A	610	PRO
1	2-A	624	ARG
1	2-A	633	HIS
1	2-A	655	GLU
1	2-A	663	TYR
1	2-A	684	MET
1	2-A	704	TYR
1	2-A	713	MET
1	2-A	777	LYS
1	2-A	779	LEU
1	2-A	794	TYR
2	2-B	183	ASP
2	2-B	225	PHE
2	2-B	250	LYS
2	2-B	270	ASN
2	2-B	280	LEU
2	2-B	299	ARG
2	2-B	348	ASN
2	2-B	362	PHE
2	2-B	363	PHE
2	2-B	395	PRO
2	2-B	460	THR
2	2-B	471	ARG
2	2-B	481	LEU
2	2-B	512	LEU
2	2-B	541	LEU
2	2-B	588	ASN
2	2-B	604	MET
2	2-B	664	MET
2	2-B	765	LEU
2	2-B	772	PHE
3	2-C	45	GLU
3	2-C	91	ASN

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Mol	Chain	Res	Type
3	2-C	140	HIS
3	2-C	159	CYS
3	2-C	187	THR
3	2-C	192	ARG
3	2-C	211	ASN
3	2-C	224	LEU
3	2-C	273	THR
3	2-C	311	ASN
3	2-C	339	GLN
3	2-C	359	ARG
3	2-C	375	MET
3	2-C	393	THR
3	2-C	409	VAL
3	2-C	413	PHE
3	2-C	423	PHE
3	2-C	438	VAL
3	2-D	12	GLN
3	2-D	21	LEU
3	2-D	57	ASN
3	2-D	97	ASP
3	2-D	122	LYS
3	2-D	129	SER
3	2-D	138	LEU
3	2-D	140	HIS
3	2-D	193	ARG
3	2-D	211	ASN
3	2-D	248	MET
3	2-D	268	LEU
3	2-D	319	TYR
3	2-D	340	GLN
3	2-D	354	VAL
3	2-D	358	ARG
3	2-D	359	ARG
3	2-D	389	ASN
3	2-D	411	ASP
1	3-A	73	THR
1	3-A	74	TYR
1	3-A	76	ARG
1	3-A	141	GLU
1	3-A	157	ARG
1	3-A	251	PHE
1	3-A	273	ASN

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Mol	Chain	Res	Type
1	3-A	300	MET
1	3-A	353	LEU
1	3-A	354	LEU
1	3-A	385	MET
1	3-A	395	ASP
1	3-A	409	PHE
1	3-A	454	ASN
1	3-A	458	TYR
1	3-A	558	TYR
1	3-A	595	HIS
1	3-A	597	ARG
1	3-A	603	TRP
1	3-A	633	HIS
1	3-A	687	ARG
1	3-A	689	LEU
2	3-B	297	TYR
2	3-B	319	PHE
2	3-B	348	ASN
2	3-B	363	PHE
2	3-B	397	GLU
2	3-B	418	GLU
2	3-B	423	ASN
2	3-B	438	TYR
2	3-B	439	ARG
2	3-B	508	PRO
2	3-B	512	LEU
2	3-B	532	PRO
2	3-B	544	ARG
2	3-B	574	VAL
2	3-B	633	ARG
2	3-B	657	ILE
2	3-B	728	HIS
2	3-B	731	PHE
2	3-B	767	ASN
2	3-B	832	ASN
3	3-C	140	HIS
3	3-C	153	ASN
3	3-C	246	SER
3	3-C	248	MET
3	3-C	299	LEU
3	3-C	318	VAL
3	3-C	329	ARG

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Mol	Chain	Res	Type
3	3-C	354	VAL
3	3-C	362	TYR
3	3-C	365	LEU
3	3-D	48	ASP
3	3-D	86	PHE
3	3-D	118	ASP
3	3-D	140	HIS
3	3-D	146	THR
3	3-D	183	GLN
3	3-D	201	THR
3	3-D	206	ASN
3	3-D	209	LEU
3	3-D	265	LEU
3	3-D	292	TYR
3	3-D	302	SER
3	3-D	360	SER
3	3-D	394	PHE
3	3-D	427	ARG
1	4-A	60	VAL
1	4-A	133	MET
1	4-A	138	PHE
1	4-A	160	ARG
1	4-A	173	LEU
1	4-A	197	PHE
1	4-A	262	ARG
1	4-A	268	LEU
1	4-A	334	ASP
1	4-A	361	LEU
1	4-A	364	PRO
1	4-A	380	ASP
1	4-A	398	TYR
1	4-A	413	TYR
1	4-A	477	LEU
1	4-A	570	LEU
1	4-A	603	TRP
1	4-A	633	HIS
1	4-A	645	GLU
1	4-A	674	ASN
1	4-A	680	LEU
1	4-A	699	ILE
1	4-A	714	ARG
1	4-A	794	TYR

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Mol	Chain	Res	Type
2	4-B	200	PHE
2	4-B	236	TYR
2	4-B	238	VAL
2	4-B	268	VAL
2	4-B	270	ASN
2	4-B	308	SER
2	4-B	322	HIS
2	4-B	342	TYR
2	4-B	356	ARG
2	4-B	386	ASN
2	4-B	391	PRO
2	4-B	446	PHE
2	4-B	471	ARG
2	4-B	522	LEU
2	4-B	541	LEU
2	4-B	545	VAL
2	4-B	546	LEU
2	4-B	555	TRP
2	4-B	556	ASP
2	4-B	568	LEU
2	4-B	610	ILE
2	4-B	638	ARG
2	4-B	657	ILE
2	4-B	731	PHE
2	4-B	739	LYS
2	4-B	772	PHE
2	4-B	801	LEU
3	4-C	158	LEU
3	4-C	191	LEU
3	4-C	192	ARG
3	4-C	238	VAL
3	4-C	242	ILE
3	4-C	248	MET
3	4-C	258	THR
3	4-C	282	ASP
3	4-C	315	TYR
3	4-C	352	MET
3	4-C	362	TYR
3	4-C	376	MET
3	4-C	387	PHE
3	4-C	412	LEU
3	4-D	19	LYS

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Mol	Chain	Res	Type
3	4-D	45	GLU
3	4-D	148	SER
3	4-D	192	ARG
3	4-D	213	SER
3	4-D	245	PRO
3	4-D	299	LEU
3	4-D	428	GLU
1	5-A	77	TYR
1	5-A	91	GLU
1	5-A	97	LYS
1	5-A	129	THR
1	5-A	133	MET
1	5-A	165	VAL
1	5-A	171	ARG
1	5-A	181	GLU
1	5-A	279	TYR
1	5-A	288	THR
1	5-A	302	TYR
1	5-A	303	ASP
1	5-A	354	LEU
1	5-A	385	MET
1	5-A	400	ARG
1	5-A	414	ASP
1	5-A	429	TYR
1	5-A	438	PHE
1	5-A	624	ARG
1	5-A	633	HIS
1	5-A	676	LEU
1	5-A	695	LEU
1	5-A	704	TYR
2	5-B	186	LYS
2	5-B	220	LEU
2	5-B	225	PHE
2	5-B	297	TYR
2	5-B	342	TYR
2	5-B	398	LEU
2	5-B	400	TYR
2	5-B	439	ARG
2	5-B	446	PHE
2	5-B	450	ASN
2	5-B	507	LEU
2	5-B	509	ASN

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Mol	Chain	Res	Type
2	5-B	512	LEU
2	5-B	547	ASP
2	5-B	568	LEU
2	5-B	595	LYS
2	5-B	596	ASN
2	5-B	604	MET
2	5-B	644	PHE
2	5-B	722	ASP
2	5-B	731	PHE
2	5-B	772	PHE
2	5-B	779	LEU
2	5-B	843	LYS
3	5-C	73	PRO
3	5-C	94	VAL
3	5-C	138	LEU
3	5-C	156	GLU
3	5-C	161	ARG
3	5-C	176	ARG
3	5-C	187	THR
3	5-C	210	LEU
3	5-C	265	LEU
3	5-C	278	ASP
3	5-C	279	TYR
3	5-C	301	PRO
3	5-C	305	LEU
3	5-C	329	ARG
3	5-C	412	LEU
3	5-C	437	TYR
3	5-D	9	GLN
3	5-D	29	HIS
3	5-D	34	ASP
3	5-D	61	LYS
3	5-D	100	SER
3	5-D	130	THR
3	5-D	140	HIS
3	5-D	158	LEU
3	5-D	177	SER
3	5-D	183	GLN
3	5-D	188	ILE
3	5-D	206	ASN
3	5-D	211	ASN
3	5-D	248	MET

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Mol	Chain	Res	Type
3	5-D	266	HIS
3	5-D	270	PRO
3	5-D	273	THR
3	5-D	289	HIS
3	5-D	301	PRO
3	5-D	312	ASN
3	5-D	315	TYR
3	5-D	318	VAL
3	5-D	319	TYR
3	5-D	329	ARG
3	5-D	333	ARG
3	5-D	376	MET
3	5-D	379	ASN
3	5-D	385	ASN
1	6-A	56	GLU
1	6-A	73	THR
1	6-A	137	ARG
1	6-A	146	LEU
1	6-A	186	MET
1	6-A	188	LEU
1	6-A	259	LEU
1	6-A	284	TYR
1	6-A	338	GLU
1	6-A	406	LEU
1	6-A	420	LYS
1	6-A	442	ASN
1	6-A	450	TYR
1	6-A	454	ASN
1	6-A	455	ASN
1	6-A	458	TYR
1	6-A	476	ASN
1	6-A	588	TYR
1	6-A	590	LEU
1	6-A	603	TRP
1	6-A	605	ASP
1	6-A	633	HIS
1	6-A	637	ASN
1	6-A	650	ASN
1	6-A	659	LEU
1	6-A	674	ASN
1	6-A	692	LEU
1	6-A	764	LEU

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Mol	Chain	Res	Type
1	6-A	765	ILE
1	6-A	782	PHE
1	6-A	793	PHE
2	6-B	199	LEU
2	6-B	212	LYS
2	6-B	225	PHE
2	6-B	230	LEU
2	6-B	326	THR
2	6-B	338	MET
2	6-B	362	PHE
2	6-B	388	GLU
2	6-B	404	MET
2	6-B	442	SER
2	6-B	445	PHE
2	6-B	471	ARG
2	6-B	488	PHE
2	6-B	522	LEU
2	6-B	545	VAL
2	6-B	547	ASP
2	6-B	570	LEU
2	6-B	603	GLU
2	6-B	633	ARG
2	6-B	643	GLN
2	6-B	666	ARG
2	6-B	758	TYR
2	6-B	810	LYS
2	6-B	845	LEU
3	6-C	12	GLN
3	6-C	44	THR
3	6-C	46	ARG
3	6-C	49	ASP
3	6-C	52	PRO
3	6-C	73	PRO
3	6-C	88	ASP
3	6-C	141	SER
3	6-C	150	LEU
3	6-C	176	ARG
3	6-C	180	VAL
3	6-C	192	ARG
3	6-C	210	LEU
3	6-C	242	ILE
3	6-C	254	SER

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Mol	Chain	Res	Type
3	6-C	266	HIS
3	6-C	276	THR
3	6-C	348	SER
3	6-C	353	HIS
3	6-C	377	LEU
3	6-C	394	PHE
3	6-C	444	SER
3	6-D	12	GLN
3	6-D	46	ARG
3	6-D	150	LEU
3	6-D	152	SER
3	6-D	164	LYS
3	6-D	176	ARG
3	6-D	208	SER
3	6-D	253	SER
3	6-D	292	TYR
3	6-D	295	MET
3	6-D	299	LEU
3	6-D	364	PRO
3	6-D	394	PHE
1	7-A	61	LYS
1	7-A	108	ARG
1	7-A	133	MET
1	7-A	140	TYR
1	7-A	162	PHE
1	7-A	165	VAL
1	7-A	168	PHE
1	7-A	189	LEU
1	7-A	191	ASN
1	7-A	203	ARG
1	7-A	271	LEU
1	7-A	278	ASP
1	7-A	279	TYR
1	7-A	294	ASP
1	7-A	296	TYR
1	7-A	300	MET
1	7-A	332	LEU
1	7-A	354	LEU
1	7-A	426	PHE
1	7-A	449	HIS
1	7-A	609	THR
1	7-A	629	THR

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Mol	Chain	Res	Type
1	7-A	637	ASN
1	7-A	638	HIS
1	7-A	653	ASP
1	7-A	659	LEU
1	7-A	708	LYS
1	7-A	794	TYR
2	7-B	185	LEU
2	7-B	196	THR
2	7-B	285	ARG
2	7-B	297	TYR
2	7-B	307	LEU
2	7-B	380	HIS
2	7-B	390	VAL
2	7-B	396	LYS
2	7-B	415	TYR
2	7-B	432	LEU
2	7-B	503	PRO
2	7-B	512	LEU
2	7-B	534	ASN
2	7-B	565	TYR
2	7-B	581	LYS
2	7-B	590	LEU
2	7-B	598	TYR
2	7-B	602	LYS
2	7-B	612	ARG
2	7-B	629	ASN
2	7-B	641	PHE
2	7-B	654	ASN
2	7-B	660	ASN
2	7-B	661	PHE
2	7-B	727	VAL
2	7-B	762	LEU
2	7-B	776	TYR
2	7-B	779	LEU
3	7-C	50	THR
3	7-C	84	ARG
3	7-C	113	THR
3	7-C	140	HIS
3	7-C	180	VAL
3	7-C	181	VAL
3	7-C	187	THR
3	7-C	230	LEU

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Mol	Chain	Res	Type
3	7-C	243	ARG
3	7-C	247	TYR
3	7-C	272	PHE
3	7-C	292	TYR
3	7-C	317	ASN
3	7-C	318	VAL
3	7-C	354	VAL
3	7-C	382	THR
3	7-C	412	LEU
3	7-C	433	LEU
3	7-D	1	MET
3	7-D	43	SER
3	7-D	84	ARG
3	7-D	86	PHE
3	7-D	121	ASN
3	7-D	148	SER
3	7-D	180	VAL
3	7-D	182	VAL
3	7-D	183	GLN
3	7-D	208	SER
3	7-D	230	LEU
3	7-D	329	ARG
3	7-D	362	TYR
3	7-D	363	LEU
3	7-D	394	PHE
3	7-D	416	MET
3	7-D	437	TYR
1	8-A	56	GLU
1	8-A	71	GLU
1	8-A	76	ARG
1	8-A	92	PHE
1	8-A	117	MET
1	8-A	133	MET
1	8-A	135	LEU
1	8-A	140	TYR
1	8-A	167	ASN
1	8-A	185	GLN
1	8-A	248	LEU
1	8-A	249	LYS
1	8-A	272	LEU
1	8-A	300	MET
1	8-A	330	VAL

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Mol	Chain	Res	Type
1	8-A	339	GLU
1	8-A	365	THR
1	8-A	415	LEU
1	8-A	422	LEU
1	8-A	427	LEU
1	8-A	435	VAL
1	8-A	442	ASN
1	8-A	446	LEU
1	8-A	449	HIS
1	8-A	609	THR
1	8-A	633	HIS
1	8-A	637	ASN
1	8-A	647	PHE
1	8-A	676	LEU
1	8-A	691	ASP
1	8-A	767	TYR
1	8-A	784	GLN
2	8-B	199	LEU
2	8-B	214	PRO
2	8-B	411	PHE
2	8-B	472	ASP
2	8-B	530	ASN
2	8-B	557	VAL
2	8-B	564	LEU
2	8-B	604	MET
2	8-B	827	ARG
3	8-C	15	ASN
3	8-C	22	TRP
3	8-C	23	SER
3	8-C	131	ASP
3	8-C	176	ARG
3	8-C	192	ARG
3	8-C	199	ASP
3	8-C	287	LYS
3	8-C	318	VAL
3	8-C	328	PRO
3	8-C	354	VAL
3	8-C	361	PRO
3	8-C	371	GLU
3	8-C	372	VAL
3	8-C	398	PHE
3	8-C	418	ASN

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Mol	Chain	Res	Type
3	8-C	432	SER
3	8-D	16	HIS
3	8-D	113	THR
3	8-D	115	ASN
3	8-D	134	GLU
3	8-D	140	HIS
3	8-D	167	LEU
3	8-D	185	TYR
3	8-D	192	ARG
3	8-D	217	PHE
3	8-D	256	TYR
3	8-D	306	VAL
3	8-D	316	PHE
3	8-D	318	VAL
3	8-D	319	TYR
3	8-D	364	PRO
3	8-D	365	LEU
3	8-D	384	VAL
3	8-D	393	THR
3	8-D	442	GLN
3	8-D	443	ASP
1	9-A	64	LEU
1	9-A	148	ASP
1	9-A	268	LEU
1	9-A	300	MET
1	9-A	361	LEU
1	9-A	395	ASP
1	9-A	458	TYR
1	9-A	560	LEU
1	9-A	576	ARG
1	9-A	587	ARG
1	9-A	590	LEU
1	9-A	597	ARG
1	9-A	598	LEU
1	9-A	603	TRP
1	9-A	609	THR
1	9-A	610	PRO
1	9-A	613	LYS
1	9-A	633	HIS
1	9-A	680	LEU
1	9-A	776	ARG
1	9-A	779	LEU

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Mol	Chain	Res	Type
1	9-A	794	TYR
2	9-B	276	THR
2	9-B	300	PHE
2	9-B	324	ASP
2	9-B	327	ILE
2	9-B	348	ASN
2	9-B	363	PHE
2	9-B	445	PHE
2	9-B	470	TYR
2	9-B	478	LYS
2	9-B	508	PRO
2	9-B	526	ARG
2	9-B	527	HIS
2	9-B	558	PHE
2	9-B	570	LEU
2	9-B	600	TYR
2	9-B	636	ILE
2	9-B	643	GLN
2	9-B	644	PHE
2	9-B	817	LYS
2	9-B	823	LEU
2	9-B	843	LYS
3	9-C	51	LYS
3	9-C	84	ARG
3	9-C	88	ASP
3	9-C	124	ASP
3	9-C	140	HIS
3	9-C	192	ARG
3	9-C	217	PHE
3	9-C	248	MET
3	9-C	259	LEU
3	9-C	270	PRO
3	9-C	333	ARG
3	9-C	337	LYS
3	9-C	338	LEU
3	9-C	386	VAL
3	9-C	394	PHE
3	9-C	433	LEU
3	9-C	434	MET
3	9-D	19	LYS
3	9-D	78	ASP
3	9-D	125	LYS

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Mol	Chain	Res	Type
3	9-D	140	HIS
3	9-D	165	LYS
3	9-D	199	ASP
3	9-D	223	ASP
3	9-D	248	MET
3	9-D	270	PRO
3	9-D	310	MET
3	9-D	319	TYR
3	9-D	329	ARG
3	9-D	333	ARG
3	9-D	341	ARG
3	9-D	359	ARG
3	9-D	365	LEU
1	10-A	76	ARG
1	10-A	78	PHE
1	10-A	98	MET
1	10-A	146	LEU
1	10-A	165	VAL
1	10-A	248	LEU
1	10-A	251	PHE
1	10-A	261	ASP
1	10-A	271	LEU
1	10-A	279	TYR
1	10-A	296	TYR
1	10-A	322	THR
1	10-A	330	VAL
1	10-A	332	LEU
1	10-A	354	LEU
1	10-A	398	TYR
1	10-A	408	LEU
1	10-A	409	PHE
1	10-A	473	ASN
1	10-A	474	PRO
1	10-A	478	MET
1	10-A	562	PHE
1	10-A	567	PRO
1	10-A	568	TYR
1	10-A	609	THR
1	10-A	624	ARG
1	10-A	638	HIS
1	10-A	680	LEU
1	10-A	775	PHE

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Mol	Chain	Res	Type
2	10-B	180	PRO
2	10-B	197	SER
2	10-B	220	LEU
2	10-B	225	PHE
2	10-B	300	PHE
2	10-B	304	LEU
2	10-B	310	ASP
2	10-B	311	THR
2	10-B	329	LYS
2	10-B	427	LYS
2	10-B	445	PHE
2	10-B	481	LEU
2	10-B	483	MET
2	10-B	488	PHE
2	10-B	508	PRO
2	10-B	512	LEU
2	10-B	525	LEU
2	10-B	541	LEU
2	10-B	546	LEU
2	10-B	553	VAL
2	10-B	556	ASP
2	10-B	564	LEU
2	10-B	580	ARG
2	10-B	593	PHE
2	10-B	660	ASN
2	10-B	671	THR
2	10-B	756	GLN
2	10-B	769	VAL
2	10-B	772	PHE
2	10-B	774	LYS
2	10-B	805	PHE
2	10-B	816	TYR
3	10-C	12	GLN
3	10-C	46	ARG
3	10-C	52	PRO
3	10-C	140	HIS
3	10-C	192	ARG
3	10-C	230	LEU
3	10-C	249	TYR
3	10-C	292	TYR
3	10-C	293	ASP
3	10-C	318	VAL

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Mol	Chain	Res	Type
3	10-C	363	LEU
3	10-C	371	GLU
3	10-D	24	GLN
3	10-D	70	ASP
3	10-D	71	SER
3	10-D	179	GLU
3	10-D	217	PHE
3	10-D	248	MET
3	10-D	252	MET
3	10-D	264	GLU
3	10-D	265	LEU
3	10-D	266	HIS
3	10-D	292	TYR
3	10-D	299	LEU
3	10-D	304	SER
3	10-D	319	TYR
3	10-D	337	LYS
3	10-D	344	PHE
3	10-D	345	PRO
3	10-D	362	TYR
3	10-D	375	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (264) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	115	GLN
1	1-A	136	GLN
1	1-A	362	GLN
1	1-A	402	ASN
1	1-A	411	GLN
1	1-A	454	ASN
1	1-A	485	GLN
1	1-A	589	GLN
1	1-A	637	ASN
1	1-A	638	HIS
1	1-A	648	ASN
2	1-B	215	ASN
2	1-B	430	HIS
2	1-B	452	GLN
2	1-B	640	GLN
2	1-B	660	ASN
2	1-B	728	HIS

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Mol	Chain	Res	Type
2	1-B	756	GLN
2	1-B	808	ASN
3	1-C	183	GLN
3	1-C	211	ASN
3	1-C	266	HIS
3	1-C	311	ASN
3	1-C	320	ASN
3	1-C	368	ASN
3	1-D	225	GLN
3	1-D	266	HIS
3	1-D	281	HIS
3	1-D	392	ASN
1	2-A	79	ASN
1	2-A	136	GLN
1	2-A	258	ASN
1	2-A	449	HIS
1	2-A	454	ASN
1	2-A	607	ASN
2	2-B	215	ASN
2	2-B	270	ASN
2	2-B	462	GLN
2	2-B	550	HIS
2	2-B	738	HIS
3	2-C	24	GLN
3	2-C	211	ASN
3	2-C	312	ASN
3	2-C	320	ASN
3	2-C	379	ASN
3	2-C	385	ASN
3	2-D	12	GLN
3	2-D	57	ASN
3	2-D	225	GLN
3	2-D	229	GLN
3	2-D	317	ASN
3	2-D	385	ASN
3	2-D	408	ASN
1	3-A	258	ASN
1	3-A	389	ASN
1	3-A	421	HIS
1	3-A	424	GLN
1	3-A	485	GLN
1	3-A	593	GLN

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Mol	Chain	Res	Type
1	3-A	637	ASN
1	3-A	638	HIS
1	3-A	665	ASN
1	3-A	673	GLN
2	3-B	204	HIS
2	3-B	215	ASN
2	3-B	222	HIS
2	3-B	322	HIS
2	3-B	386	ASN
2	3-B	497	ASN
2	3-B	642	GLN
2	3-B	643	GLN
2	3-B	780	ASN
2	3-B	806	ASN
3	3-C	9	GLN
3	3-C	219	ASN
3	3-C	408	ASN
3	3-D	16	HIS
3	3-D	121	ASN
3	3-D	281	HIS
3	3-D	289	HIS
3	3-D	325	ASN
3	3-D	340	GLN
3	3-D	353	HIS
3	3-D	417	GLN
1	4-A	589	GLN
1	4-A	595	HIS
1	4-A	638	HIS
2	4-B	208	GLN
2	4-B	270	ASN
2	4-B	322	HIS
2	4-B	430	HIS
2	4-B	434	GLN
2	4-B	479	ASN
2	4-B	808	ASN
3	4-C	24	GLN
3	4-C	116	GLN
3	4-C	266	HIS
3	4-D	9	GLN
3	4-D	183	GLN
3	4-D	219	ASN
3	4-D	281	HIS

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Mol	Chain	Res	Type
3	4-D	286	HIS
3	4-D	289	HIS
1	5-A	253	GLN
1	5-A	376	GLN
1	5-A	470	GLN
1	5-A	559	HIS
1	5-A	589	GLN
1	5-A	673	GLN
1	5-A	686	ASN
1	5-A	696	GLN
1	5-A	770	ASN
2	5-B	206	GLN
2	5-B	215	ASN
2	5-B	444	ASN
2	5-B	450	ASN
2	5-B	527	HIS
2	5-B	573	ASN
2	5-B	608	ASN
2	5-B	642	GLN
2	5-B	645	ASN
2	5-B	756	GLN
2	5-B	780	ASN
2	5-B	818	ASN
2	5-B	832	ASN
3	5-C	137	GLN
3	5-C	389	ASN
3	5-C	418	ASN
3	5-C	442	GLN
3	5-D	81	ASN
3	5-D	91	ASN
3	5-D	137	GLN
3	5-D	186	ASN
3	5-D	266	HIS
3	5-D	289	HIS
3	5-D	320	ASN
3	5-D	392	ASN
1	6-A	65	ASN
1	6-A	115	GLN
1	6-A	362	GLN
1	6-A	376	GLN
1	6-A	421	HIS
1	6-A	433	HIS

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Mol	Chain	Res	Type
1	6-A	476	ASN
1	6-A	485	GLN
1	6-A	589	GLN
1	6-A	633	HIS
2	6-B	222	HIS
2	6-B	322	HIS
2	6-B	452	GLN
2	6-B	728	HIS
2	6-B	808	ASN
3	6-C	16	HIS
3	6-C	219	ASN
3	6-C	281	HIS
3	6-C	303	ASN
3	6-C	379	ASN
3	6-C	420	GLN
3	6-D	24	GLN
3	6-D	29	HIS
3	6-D	266	HIS
3	6-D	312	ASN
3	6-D	385	ASN
1	7-A	55	GLN
1	7-A	65	ASN
1	7-A	79	ASN
1	7-A	258	ASN
1	7-A	369	ASN
1	7-A	389	ASN
1	7-A	423	GLN
1	7-A	442	ASN
1	7-A	665	ASN
1	7-A	696	GLN
2	7-B	380	HIS
2	7-B	534	ASN
2	7-B	597	ASN
2	7-B	640	GLN
2	7-B	642	GLN
2	7-B	654	ASN
2	7-B	728	HIS
2	7-B	738	HIS
3	7-C	9	GLN
3	7-C	16	HIS
3	7-C	121	ASN
3	7-C	225	GLN

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Mol	Chain	Res	Type
3	7-C	289	HIS
3	7-C	303	ASN
3	7-D	379	ASN
3	7-D	420	GLN
1	8-A	252	GLN
1	8-A	273	ASN
1	8-A	289	GLN
1	8-A	424	GLN
1	8-A	430	GLN
1	8-A	463	GLN
1	8-A	476	ASN
1	8-A	650	ASN
1	8-A	674	ASN
1	8-A	696	GLN
1	8-A	698	GLN
2	8-B	222	HIS
2	8-B	322	HIS
2	8-B	815	GLN
3	8-C	103	ASN
3	8-C	228	ASN
3	8-C	229	GLN
3	8-C	303	ASN
3	8-D	29	HIS
3	8-D	81	ASN
3	8-D	303	ASN
1	9-A	65	ASN
1	9-A	379	ASN
1	9-A	421	HIS
1	9-A	473	ASN
1	9-A	559	HIS
1	9-A	638	HIS
2	9-B	322	HIS
2	9-B	348	ASN
2	9-B	458	ASN
2	9-B	642	GLN
2	9-B	660	ASN
2	9-B	669	GLN
2	9-B	808	ASN
3	9-C	9	GLN
3	9-C	107	ASN
3	9-C	289	HIS
3	9-C	312	ASN

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Mol	Chain	Res	Type
3	9-C	330	GLN
3	9-D	29	HIS
3	9-D	281	HIS
3	9-D	368	ASN
1	10-A	136	GLN
1	10-A	191	ASN
1	10-A	273	ASN
1	10-A	421	HIS
1	10-A	559	HIS
1	10-A	589	GLN
1	10-A	638	HIS
1	10-A	781	ASN
2	10-B	206	GLN
2	10-B	232	GLN
2	10-B	322	HIS
2	10-B	333	ASN
2	10-B	430	HIS
2	10-B	462	GLN
2	10-B	550	HIS
2	10-B	608	ASN
2	10-B	645	ASN
2	10-B	734	ASN
2	10-B	756	GLN
3	10-C	132	ASN
3	10-C	137	GLN
3	10-C	186	ASN
3	10-C	228	ASN
3	10-C	392	ASN
3	10-C	408	ASN
3	10-C	418	ASN
3	10-C	431	GLN
3	10-D	9	GLN
3	10-D	303	ASN
3	10-D	325	ASN
3	10-D	366	GLN
3	10-D	392	ASN
3	10-D	418	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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.