



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:34 PM UTC

PDB ID : 1HC1 / pdb_00001hc1
Title : CRYSTAL STRUCTURE OF HEXAMERIC HAEMOCYANIN FROM PAN-
ULIRUS INTERRUPTUS REFINED AT 3.2 ANGSTROMS RESOLUTION
Authors : Volbeda, A.; Hol, W.G.J.
Deposited on : 1991-05-15
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

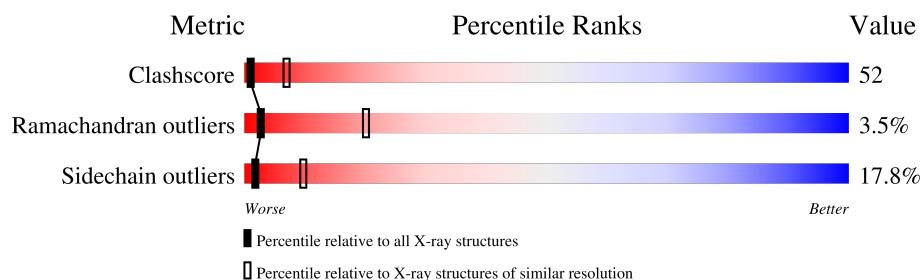
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	657	
1	B	657	
1	C	657	
1	D	657	
1	E	657	
1	F	657	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32166 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ARTHROPODAN HEMOCYANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			
1	B	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			
1	C	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			
1	D	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			
1	E	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			
1	F	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ASP	GLU	conflict	UNP P04254
A	163	PRO	GLN	conflict	UNP P04254
A	458	ASN	LYS	conflict	UNP P04254
A	514	SER	LYS	conflict	UNP P04254
B	32	ASP	GLU	conflict	UNP P04254
B	163	PRO	GLN	conflict	UNP P04254
B	458	ASN	LYS	conflict	UNP P04254
B	514	SER	LYS	conflict	UNP P04254
C	32	ASP	GLU	conflict	UNP P04254
C	163	PRO	GLN	conflict	UNP P04254
C	458	ASN	LYS	conflict	UNP P04254
C	514	SER	LYS	conflict	UNP P04254
D	32	ASP	GLU	conflict	UNP P04254
D	163	PRO	GLN	conflict	UNP P04254
D	458	ASN	LYS	conflict	UNP P04254
D	514	SER	LYS	conflict	UNP P04254
E	32	ASP	GLU	conflict	UNP P04254

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Chain	Residue	Modelled	Actual	Comment	Reference
E	163	PRO	GLN	conflict	UNP P04254
E	458	ASN	LYS	conflict	UNP P04254
E	514	SER	LYS	conflict	UNP P04254
F	32	ASP	GLU	conflict	UNP P04254
F	163	PRO	GLN	conflict	UNP P04254
F	458	ASN	LYS	conflict	UNP P04254
F	514	SER	LYS	conflict	UNP P04254

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cu 2 2	0	0
2	B	2	Total Cu 2 2	0	0
2	C	2	Total Cu 2 2	0	0
2	D	2	Total Cu 2 2	0	0
2	E	2	Total Cu 2 2	0	0
2	F	2	Total Cu 2 2	0	0

- Molecule 3 is water.

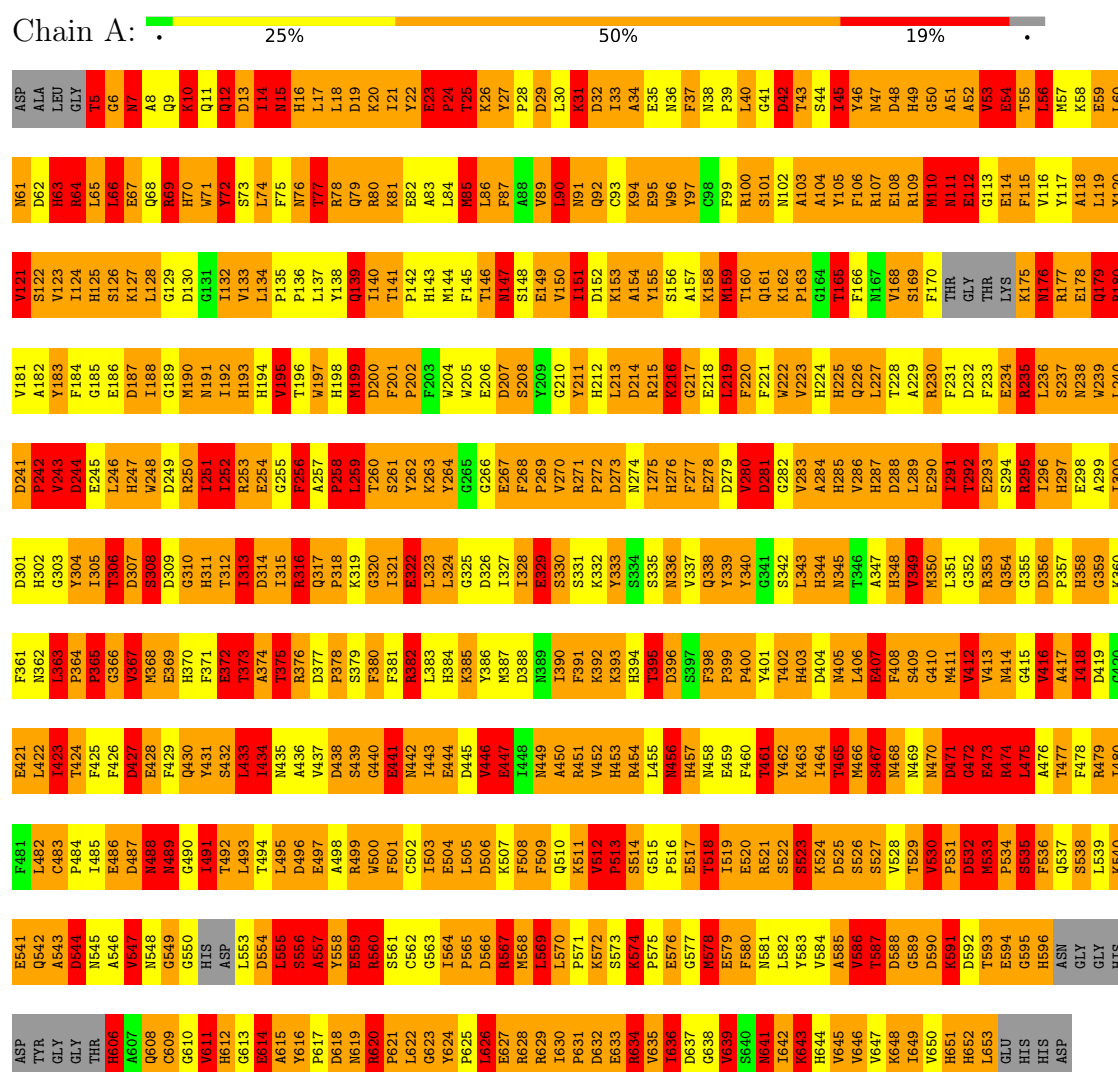
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	186	Total O 186 186	0	0
3	B	186	Total O 186 186	0	0
3	C	186	Total O 186 186	0	0
3	D	186	Total O 186 186	0	0
3	E	186	Total O 186 186	0	0
3	F	186	Total O 186 186	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

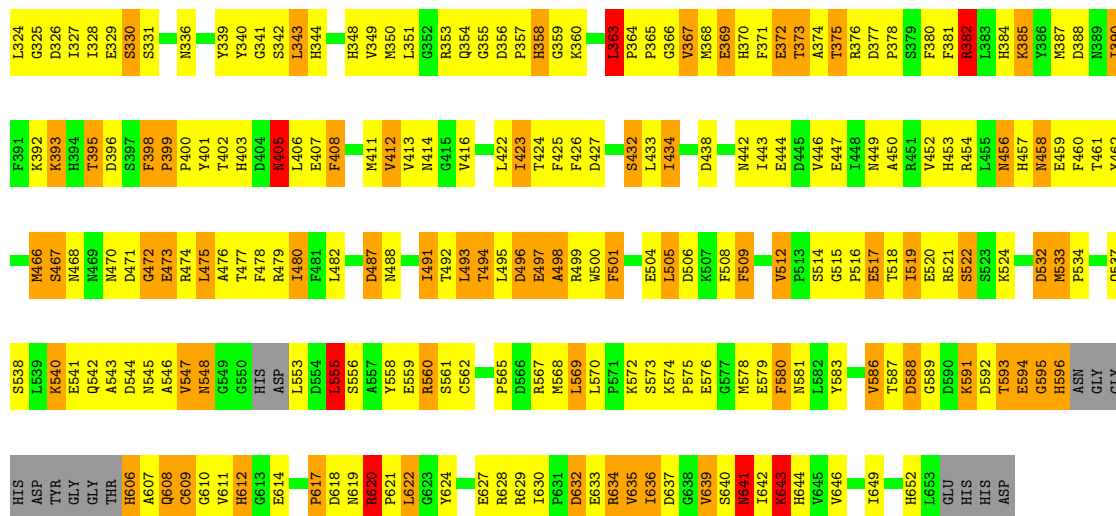
Note EDS was not executed.

• Molecule 1: ARTHROPODAN HEMOCYANIN

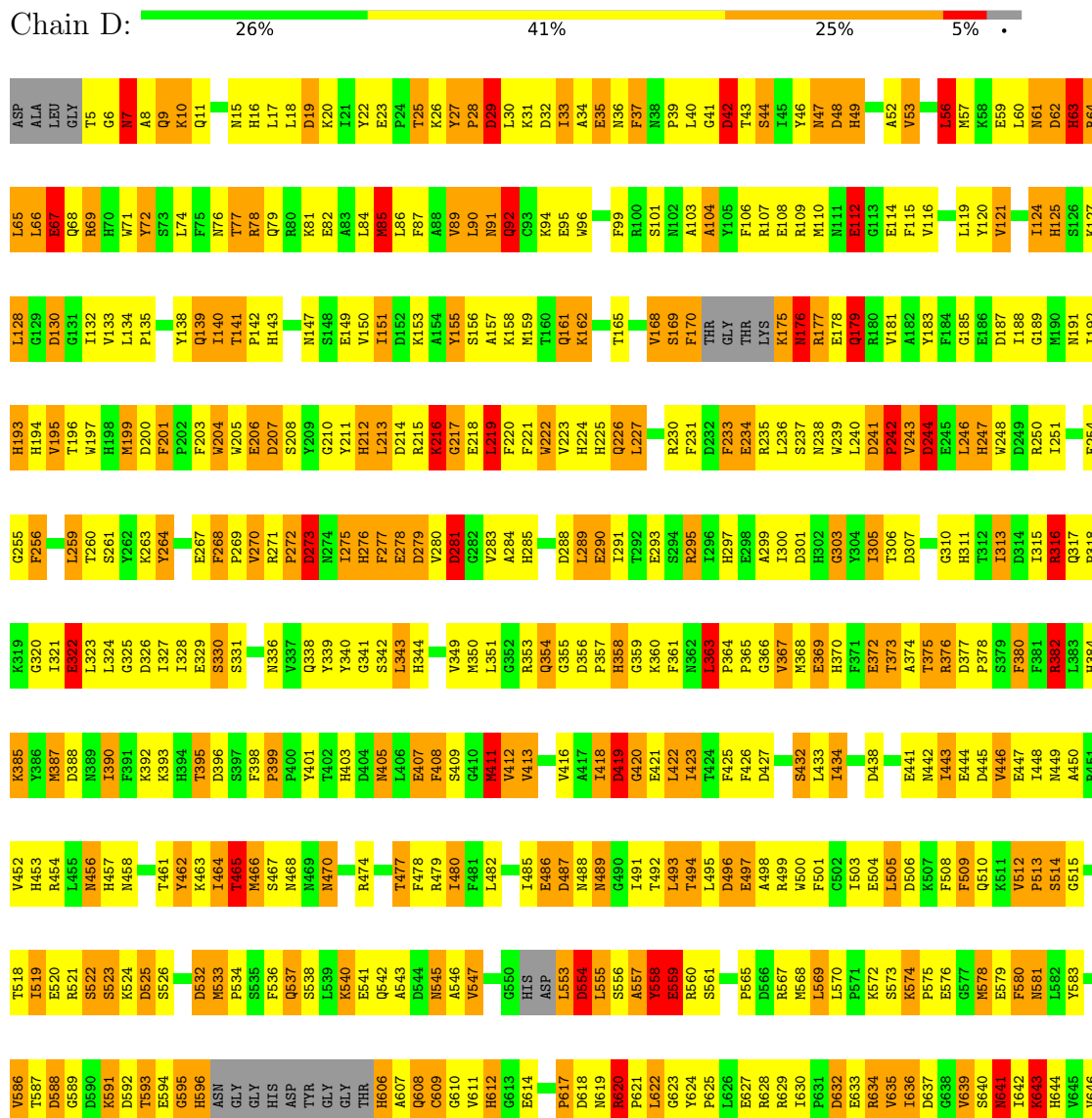


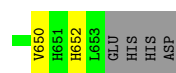
• Molecule 1: ARTHROPODAN HEMOCYANIN





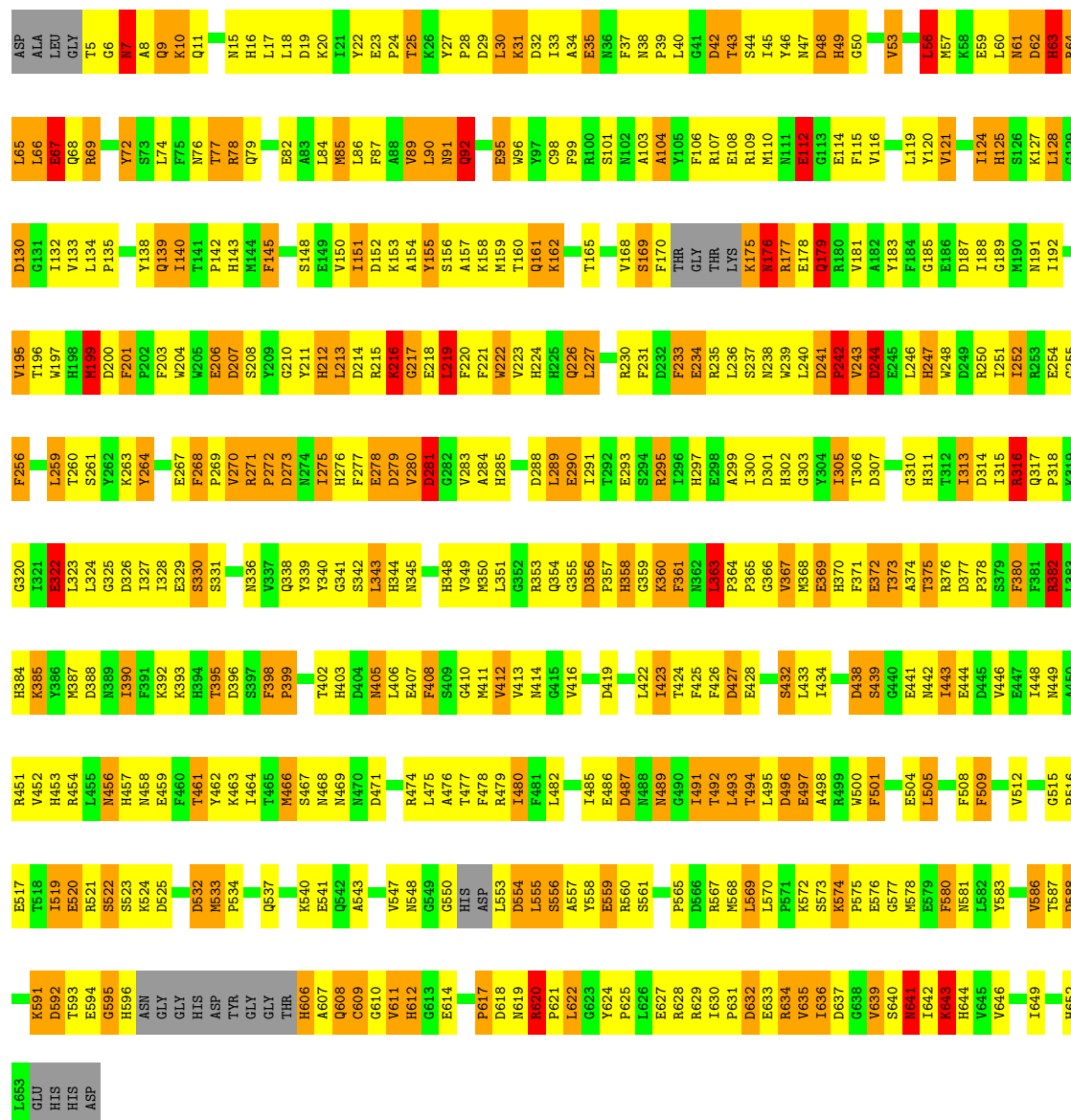
• Molecule 1: ARTHROPODAN HEMOCYANIN





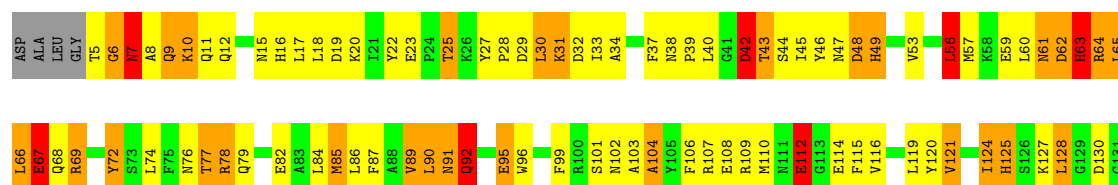
• Molecule 1: ARTHROPODAN HEMOCYANIN

Chain E: 27% 44% 22%



• Molecule 1: ARTHROPODAN HEMOCYANIN

Chain F: 26% 44% 23%



H652	D588	E520	R454	M387	E322	L259	T196
L653	K591	R521	L455	D388	L323	T260	V133
HIS	D592	S522	M456	M389	L324	S261	L134
HIS	E593	S523	M457	I390	G325	Y262	P135
ASP	E594	D532	M458	F391	D326	K263	
	G595	M533	E459	K392	I327	Y264	Y138
	H596	P534	F460	K393	I328		Q139
ASN	GLY	S535	T461	H394	E329	F203	I140
GLY	F536	S536	Y462	T395	S330	W204	T141
GLY	Q537	K463	K463	S397	S331	W205	P142
HIS				F398		E206	H143
ASP				P399	N336	D207	M144
		K540	M466		V337		F145
		E541	S467		Q338	P272	
		Q542	M468	T402	Y339	D273	
		A543	M469	H403	Y340	R274	S148
		D544	M470	D403	I275	I276	E149
		N545	D471	D404	G341	H276	L150
		A546	G472	M405	S342	F277	I151
		F547	E473	L406	L343	E278	D152
		N548	R474	E407	H344	D279	K153
		G549	L475	F408	N345	V280	A154
		G550	A476	S409		G217	
		HIS	T477	Q410	H348	E281	E218
		ASP	F478	M411	V283	L219	F220
			R479	M412	M350	A157	A157
			L480	V413	A284	F221	K158
			F481	M414	L351	W222	M159
			L482	V416	G352	V223	T160
					R353	H224	Q161
					Q354	H225	K162
					G355	Q226	
					D356	L227	T165
					P357		
					H358	R230	V168
					G359	F231	S169
					K360	D232	F170
						F233	THR
						E234	GLY
						R235	THR
						L236	LYS
						S237	K175
						I300	N176
						D301	R177
						H302	W239
						G303	L240
						Y304	E178
						I305	Q179
						T306	R180
						D307	V181
							A182
							E245
							Y183
							F184
							G185
							E186
							D187
							I188
							G189
							I251
							M190
							I252
							R253
							N191
							I192
							H193
							H194
							F256

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.80Å 193.10Å 122.20Å 90.00° 118.10° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.201 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32166	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
CU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.82	57/5316 (1.1%)	4.64	1635/7205 (22.7%)
1	B	1.80	69/5316 (1.3%)	4.48	1555/7205 (21.6%)
1	C	0.88	2/5316 (0.0%)	2.19	254/7205 (3.5%)
1	D	0.89	3/5316 (0.1%)	2.20	273/7205 (3.8%)
1	E	0.88	3/5316 (0.1%)	2.17	234/7205 (3.2%)
1	F	0.87	2/5316 (0.0%)	2.18	262/7205 (3.6%)
All	All	1.27	136/31896 (0.4%)	3.18	4213/43230 (9.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	141	THR	CA-CB	8.51	1.63	1.53
1	A	194	HIS	CG-ND1	8.14	1.47	1.38
1	A	216	LYS	C-O	7.95	1.33	1.24
1	A	491	ILE	C-N	-7.90	1.22	1.33
1	A	494	THR	CA-CB	7.67	1.63	1.53
1	B	348	HIS	CG-CD2	7.63	1.44	1.35
1	B	38	ASN	N-CA	7.37	1.53	1.46
1	A	214	ASP	N-CA	-7.31	1.37	1.46
1	B	437	VAL	N-CA	7.28	1.55	1.46
1	B	494	THR	CA-CB	7.24	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	494	THR	CA-CB	7.16	1.62	1.53
1	A	212	HIS	C-O	7.04	1.31	1.24
1	B	358	HIS	N-CA	7.00	1.55	1.46
1	A	422	LEU	C-O	6.94	1.32	1.24
1	A	491	ILE	CA-C	-6.87	1.43	1.52
1	A	217	GLY	N-CA	6.79	1.55	1.45
1	B	344	HIS	CE1-NE2	6.67	1.39	1.32
1	B	215	ARG	NE-CZ	6.64	1.40	1.33
1	B	89	VAL	C-O	6.63	1.31	1.24
1	A	568	MET	C-O	6.63	1.32	1.24
1	B	132	ILE	C-N	-6.59	1.25	1.33
1	A	582	LEU	N-CA	6.55	1.54	1.46
1	A	574	LYS	N-CA	6.53	1.52	1.45
1	B	196	THR	C-O	6.53	1.31	1.24
1	A	92	GLN	CA-CB	-6.43	1.44	1.53
1	A	264	TYR	N-CA	6.43	1.53	1.46
1	A	141	THR	CA-CB	6.42	1.61	1.53
1	B	582	LEU	N-CA	6.40	1.53	1.46
1	B	352	GLY	C-O	6.36	1.32	1.23
1	A	132	ILE	CA-CB	6.36	1.61	1.54
1	E	550	GLY	C-O	6.32	1.36	1.23
1	B	221	PHE	C-O	6.27	1.31	1.24
1	B	357	PRO	C-O	6.27	1.32	1.24
1	A	213	LEU	N-CA	6.26	1.53	1.46
1	B	70	HIS	C-O	6.23	1.31	1.23
1	A	93	CYS	C-O	6.13	1.31	1.23
1	A	232	ASP	C-O	6.09	1.31	1.24
1	A	100	ARG	N-CA	6.07	1.53	1.46
1	B	72	TYR	N-CA	6.05	1.53	1.46
1	B	135	PRO	C-N	-6.05	1.27	1.33
1	A	515	GLY	N-CA	6.01	1.52	1.44
1	A	623	GLY	N-CA	6.00	1.53	1.45
1	B	217	GLY	N-CA	5.96	1.54	1.45
1	A	584	VAL	C-O	5.96	1.30	1.24
1	B	474	ARG	NE-CZ	5.89	1.39	1.33
1	A	229	ALA	C-O	5.86	1.30	1.24
1	A	222	TRP	C-O	5.86	1.30	1.24
1	B	326	ASP	C-O	-5.84	1.17	1.24
1	A	201	PHE	CA-CB	-5.82	1.45	1.53
1	A	213	LEU	CA-CB	-5.82	1.45	1.53
1	A	69	ARG	CZ-NH2	5.80	1.41	1.33
1	B	365	PRO	C-N	-5.79	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	268	PHE	CA-C	5.77	1.59	1.53
1	B	219	LEU	N-CA	5.76	1.53	1.46
1	B	135	PRO	C-O	-5.75	1.18	1.24
1	A	198	HIS	ND1-CE1	5.73	1.38	1.32
1	B	438	ASP	N-CA	5.72	1.53	1.46
1	A	434	ILE	CA-CB	5.68	1.61	1.54
1	A	647	VAL	C-O	5.67	1.30	1.24
1	B	406	LEU	C-O	5.65	1.30	1.24
1	B	289	LEU	C-N	-5.64	1.25	1.33
1	B	10	LYS	N-CA	5.60	1.52	1.46
1	A	89	VAL	N-CA	5.59	1.53	1.46
1	A	8	ALA	C-O	-5.58	1.17	1.24
1	C	494	THR	CA-CB	5.57	1.62	1.53
1	B	195	VAL	C-N	-5.56	1.26	1.33
1	B	65	LEU	N-CA	5.54	1.52	1.45
1	F	494	THR	CA-CB	5.53	1.62	1.53
1	B	85	MET	N-CA	5.51	1.53	1.46
1	B	283	VAL	C-O	5.51	1.30	1.24
1	B	375	THR	CB-OG1	5.51	1.52	1.43
1	A	358	HIS	C-O	5.47	1.31	1.24
1	A	198	HIS	CG-CD2	5.43	1.41	1.35
1	B	393	LYS	C-N	-5.43	1.26	1.33
1	D	494	THR	CA-CB	5.40	1.62	1.53
1	B	75	PHE	C-O	5.40	1.31	1.24
1	A	291	ILE	C-N	-5.39	1.27	1.33
1	A	340	TYR	C-O	5.39	1.31	1.24
1	B	273	ASP	N-CA	5.39	1.52	1.45
1	A	378	PRO	C-O	5.39	1.30	1.24
1	B	382	ARG	CZ-NH1	5.39	1.40	1.32
1	B	65	LEU	C-O	5.38	1.30	1.23
1	A	282	GLY	C-O	5.38	1.31	1.24
1	B	14	ILE	CA-CB	5.37	1.60	1.54
1	A	431	TYR	C-O	5.36	1.30	1.23
1	A	479	ARG	C-O	5.35	1.30	1.24
1	A	134	LEU	CA-C	-5.35	1.46	1.53
1	B	201	PHE	CA-CB	-5.33	1.45	1.53
1	B	111	ASN	N-CA	5.33	1.52	1.45
1	B	457	HIS	C-N	-5.31	1.26	1.33
1	B	465	THR	CA-CB	5.30	1.60	1.53
1	D	132	ILE	CA-CB	5.30	1.60	1.54
1	A	302	HIS	C-O	5.29	1.30	1.24
1	B	302	HIS	ND1-CE1	5.28	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	485	ILE	C-N	-5.25	1.25	1.33
1	E	132	ILE	CA-CB	5.25	1.60	1.54
1	B	125	HIS	CA-CB	5.24	1.61	1.53
1	B	6	GLY	N-CA	5.23	1.52	1.45
1	B	50	GLY	CA-C	-5.22	1.44	1.51
1	B	16	HIS	CE1-NE2	-5.21	1.27	1.32
1	D	465	THR	CB-OG1	5.21	1.52	1.43
1	B	214	ASP	C-O	5.20	1.30	1.24
1	A	199	MET	CG-SD	5.19	1.93	1.80
1	A	366	GLY	C-O	5.18	1.30	1.23
1	C	132	ILE	CA-CB	5.18	1.60	1.54
1	A	198	HIS	CE1-NE2	5.17	1.37	1.32
1	B	322	GLU	N-CA	5.17	1.52	1.46
1	B	350	MET	N-CA	5.16	1.52	1.46
1	F	132	ILE	CA-CB	5.15	1.60	1.54
1	A	196	THR	CA-CB	5.14	1.61	1.53
1	B	197	TRP	N-CA	5.14	1.52	1.46
1	A	101	SER	C-O	5.14	1.30	1.24
1	A	205	TRP	C-N	-5.14	1.26	1.33
1	B	376	ARG	N-CA	5.13	1.52	1.46
1	B	393	LYS	C-O	-5.13	1.18	1.24
1	B	216	LYS	N-CA	5.12	1.52	1.46
1	A	353	ARG	CZ-NH2	5.12	1.40	1.33
1	B	208	SER	CB-OG	5.11	1.52	1.42
1	B	403	HIS	C-O	-5.11	1.18	1.24
1	A	27	TYR	N-CA	5.10	1.52	1.46
1	A	494	THR	C-O	5.09	1.31	1.23
1	A	433	LEU	C-N	-5.08	1.27	1.33
1	B	475	LEU	C-O	5.08	1.30	1.23
1	B	336	ASN	C-N	-5.06	1.28	1.34
1	B	587	THR	CB-OG1	5.06	1.51	1.43
1	B	5	THR	CB-OG1	5.05	1.51	1.43
1	A	214	ASP	C-O	5.05	1.29	1.24
1	B	506	ASP	C-O	5.05	1.29	1.23
1	B	436	ALA	C-O	5.04	1.30	1.24
1	A	110	MET	CA-C	5.04	1.59	1.52
1	B	183	TYR	C-N	-5.03	1.26	1.33
1	B	215	ARG	CZ-NH2	5.02	1.40	1.33
1	B	462	TYR	CA-CB	5.02	1.60	1.53
1	B	425	PHE	C-O	5.02	1.28	1.24
1	B	595	GLY	C-O	5.02	1.30	1.23
1	A	527	SER	C-O	5.01	1.30	1.24

All (4213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ARG	NE-CZ-NH2	50.81	164.93	119.20
1	A	64	ARG	CD-NE-CZ	37.85	177.39	124.40
1	B	48	ASP	CA-CB-CG	34.83	147.43	112.60
1	B	17	LEU	O-C-N	26.82	149.69	122.07
1	B	17	LEU	CA-C-O	-26.67	92.81	120.82
1	A	64	ARG	NH1-CZ-NH2	-25.66	85.94	119.30
1	B	316	ARG	CD-NE-CZ	25.49	160.08	124.40
1	B	408	PHE	CA-CB-CG	25.38	139.18	113.80
1	A	399	PRO	O-C-N	24.36	132.51	121.31
1	A	435	ASN	OD1-CG-ND2	24.29	146.89	122.60
1	C	7	ASN	CA-CB-CG	23.92	136.52	112.60
1	D	7	ASN	CA-CB-CG	23.91	136.51	112.60
1	F	7	ASN	CA-CB-CG	23.55	136.15	112.60
1	A	458	ASN	CA-CB-CG	23.36	135.96	112.60
1	A	25	THR	O-C-N	23.28	150.33	122.86
1	A	65	LEU	O-C-N	-23.16	95.59	122.68
1	E	7	ASN	CA-CB-CG	23.05	135.65	112.60
1	B	554	ASP	CA-CB-CG	22.88	135.48	112.60
1	B	469	ASN	OD1-CG-ND2	22.12	144.72	122.60
1	B	16	HIS	O-C-N	22.05	145.91	122.09
1	B	434	ILE	CA-C-O	-21.91	97.27	120.71
1	A	534	PRO	CA-C-O	-21.89	96.91	121.43
1	A	567	ARG	CD-NE-CZ	21.70	154.78	124.40
1	A	190	MET	O-C-N	21.68	144.41	122.07
1	B	99	PHE	CA-CB-CG	21.67	135.47	113.80
1	B	560	ARG	CA-C-N	21.49	157.22	120.68
1	B	560	ARG	C-N-CA	21.49	157.22	120.68
1	C	548	ASN	CA-CB-CG	21.46	134.06	112.60
1	A	152	ASP	O-C-N	21.01	146.10	122.15
1	A	180	ARG	O-C-N	20.80	143.98	121.93
1	A	99	PHE	CA-CB-CG	20.45	134.25	113.80
1	B	271	ARG	NE-CZ-NH1	20.42	141.92	121.50
1	A	632	ASP	CA-CB-CG	20.29	132.88	112.60
1	A	486	GLU	O-C-N	-19.76	97.61	123.10
1	A	147	ASN	CA-CB-CG	-19.68	92.92	112.60
1	B	432	SER	CA-C-O	19.16	141.39	120.32
1	B	183	TYR	CA-C-O	-19.13	99.97	120.63
1	A	316	ARG	CD-NE-CZ	19.06	151.08	124.40
1	B	226	GLN	OE1-CD-NE2	18.90	141.50	122.60
1	B	145	PHE	CA-CB-CG	18.86	132.66	113.80
1	A	47	ASN	CA-CB-CG	18.82	131.42	112.60
1	A	643	LYS	CA-CB-CG	18.77	151.64	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	LEU	CA-C-O	-18.68	100.24	121.16
1	B	442	ASN	CA-CB-CG	-18.56	94.04	112.60
1	B	61	ASN	OD1-CG-ND2	18.51	141.11	122.60
1	A	407	GLU	CA-C-O	18.41	141.03	120.96
1	A	231	PHE	O-C-N	18.36	141.12	122.03
1	A	279	ASP	CA-CB-CG	18.25	130.85	112.60
1	A	460	PHE	CA-CB-CG	18.13	131.93	113.80
1	B	53	VAL	CA-C-O	18.11	139.78	120.95
1	A	235	ARG	NE-CZ-NH1	-18.06	103.44	121.50
1	A	17	LEU	O-C-N	17.47	140.06	122.07
1	B	80	ARG	NE-CZ-NH2	-17.33	103.61	119.20
1	D	458	ASN	CA-CB-CG	17.21	129.81	112.60
1	A	152	ASP	CA-C-O	-17.21	102.18	120.42
1	A	207	ASP	CB-CG-OD1	17.16	157.88	118.40
1	A	139	GLN	CA-C-O	-17.07	100.36	119.14
1	B	353	ARG	NE-CZ-NH1	-17.01	104.49	121.50
1	A	48	ASP	CA-CB-CG	16.91	129.51	112.60
1	E	99	PHE	CA-CB-CG	16.90	130.70	113.80
1	A	309	ASP	CA-CB-CG	-16.78	95.82	112.60
1	F	99	PHE	CA-CB-CG	16.75	130.54	113.80
1	A	59	GLU	O-C-N	16.74	140.17	122.09
1	B	528	VAL	CA-C-O	-16.74	103.40	120.14
1	B	70	HIS	CA-C-O	-16.72	103.27	121.33
1	C	99	PHE	CA-CB-CG	16.69	130.49	113.80
1	A	128	LEU	O-C-N	16.60	142.00	122.25
1	A	460	PHE	CA-C-O	-16.50	103.51	121.33
1	D	99	PHE	CA-CB-CG	16.50	130.30	113.80
1	B	75	PHE	CA-C-O	-16.42	100.06	119.27
1	A	548	ASN	CA-CB-CG	16.35	128.95	112.60
1	A	76	ASN	OD1-CG-ND2	16.31	138.91	122.60
1	B	353	ARG	NH1-CZ-NH2	16.27	140.45	119.30
1	B	106	PHE	O-C-N	16.26	139.65	122.09
1	A	456	ASN	CA-C-O	16.23	138.95	121.10
1	B	418	ILE	N-CA-CB	16.23	131.91	111.46
1	B	439	SER	CA-C-O	-16.14	100.43	120.28
1	A	299	ALA	N-CA-C	-16.13	90.43	111.24
1	B	561	SER	N-CA-C	16.08	132.50	112.23
1	A	215	ARG	NE-CZ-NH2	16.06	133.65	119.20
1	A	235	ARG	NH1-CZ-NH2	15.99	140.09	119.30
1	A	25	THR	N-CA-CB	15.96	133.16	110.17
1	B	390	ILE	N-CA-C	-15.93	96.64	111.45
1	A	308	SER	O-C-N	15.92	145.67	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	LYS	CB-CA-C	15.87	130.51	108.76
1	A	543	ALA	CA-C-N	15.84	143.09	120.28
1	A	543	ALA	C-N-CA	15.84	143.09	120.28
1	A	308	SER	CA-C-O	-15.83	98.85	119.11
1	A	491	ILE	CA-C-O	-15.83	98.79	119.53
1	A	519	ILE	CA-C-O	15.83	139.95	121.11
1	B	63	HIS	O-C-N	15.72	143.50	122.59
1	A	494	THR	N-CA-C	15.71	133.77	111.30
1	A	273	ASP	CB-CG-OD1	15.70	154.52	118.40
1	A	7	ASN	OD1-CG-ND2	15.69	138.29	122.60
1	A	212	HIS	CA-C-O	-15.69	102.91	120.32
1	A	31	LYS	O-C-N	15.68	138.34	122.03
1	B	544	ASP	CA-CB-CG	15.67	128.27	112.60
1	B	296	ILE	O-C-N	15.65	137.24	121.91
1	B	449	ASN	CA-CB-CG	15.60	128.20	112.60
1	A	231	PHE	CA-C-O	-15.59	104.63	121.00
1	B	12	GLN	OE1-CD-NE2	-15.50	107.10	122.60
1	B	434	ILE	O-C-N	15.46	142.25	121.84
1	A	70	HIS	CA-C-O	-15.46	104.63	121.33
1	A	370	HIS	CA-CB-CG	15.46	129.26	113.80
1	C	169	SER	N-CA-C	15.46	132.44	113.12
1	D	169	SER	N-CA-C	15.40	132.37	113.12
1	E	169	SER	N-CA-C	15.39	132.36	113.12
1	A	273	ASP	CA-CB-CG	15.37	127.97	112.60
1	F	169	SER	N-CA-C	15.36	132.32	113.12
1	F	32	ASP	CA-CB-CG	15.34	127.94	112.60
1	B	260	THR	CA-CB-OG1	-15.33	86.61	109.60
1	B	432	SER	O-C-N	-15.33	105.18	123.27
1	A	326	ASP	CA-CB-CG	15.32	127.92	112.60
1	A	567	ARG	NE-CZ-NH1	15.32	136.82	121.50
1	A	560	ARG	CD-NE-CZ	-15.31	102.96	124.40
1	A	61	ASN	CA-CB-CG	-15.31	97.29	112.60
1	B	166	PHE	CA-C-O	15.31	136.94	120.71
1	B	273	ASP	CB-CG-OD1	15.31	153.61	118.40
1	B	314	ASP	CA-C-O	-15.31	104.35	121.19
1	B	460	PHE	O-C-N	15.28	140.67	123.25
1	A	25	THR	CA-C-O	-15.28	104.91	121.56
1	B	49	HIS	CA-C-N	15.27	151.34	121.41
1	B	49	HIS	C-N-CA	15.27	151.34	121.41
1	C	32	ASP	CA-CB-CG	15.27	127.87	112.60
1	B	313	ILE	CA-C-O	15.23	135.24	120.31
1	B	132	ILE	CA-C-O	-15.23	105.91	121.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	518	THR	O-C-N	15.23	137.51	123.50
1	A	213	LEU	CA-C-N	15.05	141.71	120.79
1	A	213	LEU	C-N-CA	15.05	141.71	120.79
1	A	471	ASP	CA-CB-CG	15.04	127.64	112.60
1	A	62	ASP	CB-CG-OD2	15.02	152.94	118.40
1	A	432	SER	CA-C-O	14.97	136.87	120.70
1	B	560	ARG	CD-NE-CZ	14.96	145.35	124.40
1	C	316	ARG	CD-NE-CZ	14.90	145.26	124.40
1	F	458	ASN	CA-CB-CG	14.89	127.49	112.60
1	B	458	ASN	CA-CB-CG	14.83	127.43	112.60
1	A	234	GLU	O-C-N	14.79	137.80	122.12
1	E	316	ARG	CD-NE-CZ	14.78	145.09	124.40
1	D	316	ARG	CD-NE-CZ	14.71	144.99	124.40
1	F	316	ARG	CD-NE-CZ	14.70	144.98	124.40
1	A	162	LYS	N-CA-C	-14.70	88.13	110.32
1	A	169	SER	N-CA-C	14.62	133.10	112.04
1	C	458	ASN	CA-CB-CG	14.61	127.21	112.60
1	A	234	GLU	CA-C-O	-14.59	104.88	120.63
1	B	554	ASP	CA-C-O	14.55	137.00	119.98
1	A	80	ARG	CA-C-O	-14.54	105.00	120.55
1	E	32	ASP	CA-CB-CG	14.53	127.13	112.60
1	B	306	THR	CA-C-O	-14.51	105.33	120.71
1	A	177	ARG	CA-C-O	14.49	141.23	120.51
1	B	295	ARG	NE-CZ-NH2	14.49	132.24	119.20
1	A	486	GLU	CA-C-O	14.49	139.09	121.56
1	A	637	ASP	CA-CB-CG	14.47	127.07	112.60
1	A	390	ILE	N-CA-C	-14.46	96.25	111.58
1	B	554	ASP	CA-C-N	14.46	144.25	122.56
1	B	554	ASP	C-N-CA	14.46	144.25	122.56
1	A	111	ASN	CA-C-O	-14.39	106.29	121.55
1	B	242	PRO	O-C-N	-14.39	103.21	122.64
1	B	7	ASN	CA-CB-CG	14.38	126.97	112.60
1	D	32	ASP	CA-CB-CG	14.33	126.93	112.60
1	A	461	THR	CA-C-O	14.32	138.21	121.46
1	B	529	THR	O-C-N	-14.30	104.60	123.19
1	B	147	ASN	OD1-CG-ND2	14.29	136.90	122.60
1	B	63	HIS	N-CA-CB	14.28	134.63	110.49
1	A	317	GLN	OE1-CD-NE2	-14.28	108.32	122.60
1	B	469	ASN	O-C-N	14.25	142.12	122.46
1	B	469	ASN	CA-CB-CG	-14.22	98.38	112.60
1	A	471	ASP	CA-C-N	14.18	149.20	121.41
1	A	471	ASP	C-N-CA	14.18	149.20	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	486	GLU	CA-C-N	14.17	144.81	120.58
1	A	486	GLU	C-N-CA	14.17	144.81	120.58
1	A	629	ARG	NE-CZ-NH2	14.16	131.95	119.20
1	B	117	TYR	CA-C-O	-14.16	106.13	121.00
1	E	494	THR	N-CA-C	14.14	131.53	111.30
1	B	53	VAL	O-C-N	-14.12	108.17	121.87
1	B	25	THR	CA-CB-OG1	-14.11	88.44	109.60
1	B	587	THR	CA-C-N	14.09	145.29	122.32
1	B	587	THR	C-N-CA	14.09	145.29	122.32
1	B	91	ASN	CA-C-O	-14.08	105.49	120.42
1	B	272	PRO	O-C-N	14.07	140.31	123.14
1	A	489	ASN	CA-C-O	14.07	140.63	120.51
1	B	344	HIS	ND1-CG-CD2	14.07	120.17	106.10
1	A	228	THR	CA-CB-OG1	-14.06	88.51	109.60
1	B	25	THR	O-C-N	14.04	138.82	122.96
1	A	560	ARG	NH1-CZ-NH2	14.00	137.50	119.30
1	B	399	PRO	O-C-N	13.99	137.96	121.46
1	A	406	LEU	N-CA-CB	-13.96	88.64	110.28
1	B	522	SER	N-CA-C	13.95	132.14	109.95
1	A	86	LEU	O-C-N	13.93	136.58	122.09
1	B	199	MET	N-CA-C	-13.89	95.93	113.43
1	B	529	THR	CA-C-O	13.86	136.78	121.11
1	B	194	HIS	CA-CB-CG	-13.86	99.94	113.80
1	B	520	GLU	CB-CG-CD	13.82	136.09	112.60
1	A	386	TYR	CA-C-O	-13.79	104.89	121.02
1	B	414	ASN	CA-C-O	-13.78	103.89	120.56
1	B	163	PRO	O-C-N	13.72	139.50	123.04
1	A	423	ILE	O-C-N	13.69	137.86	123.07
1	A	419	ASP	CA-CB-CG	13.68	126.28	112.60
1	A	532	ASP	CA-CB-CG	13.67	126.27	112.60
1	A	303	GLY	O-C-N	13.64	140.44	122.70
1	B	88	ALA	CA-C-O	-13.62	103.02	119.49
1	A	161	GLN	OE1-CD-NE2	13.59	136.19	122.60
1	A	513	PRO	CB-CA-C	13.56	130.82	110.75
1	A	180	ARG	NE-CZ-NH2	-13.50	107.05	119.20
1	B	543	ALA	CA-C-N	13.49	138.75	120.54
1	B	543	ALA	C-N-CA	13.49	138.75	120.54
1	A	458	ASN	CA-C-O	-13.45	105.91	121.11
1	A	632	ASP	O-C-N	13.41	138.96	123.27
1	A	147	ASN	OD1-CG-ND2	13.40	136.00	122.60
1	A	545	ASN	OD1-CG-ND2	13.31	135.91	122.60
1	A	487	ASP	CA-C-O	-13.28	105.50	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42	ASP	CA-CB-CG	13.27	125.87	112.60
1	A	212	HIS	O-C-N	13.25	138.82	123.31
1	A	206	GLU	CG-CD-OE2	13.25	148.87	118.40
1	A	80	ARG	NE-CZ-NH2	-13.22	107.30	119.20
1	A	260	THR	CA-CB-OG1	-13.22	89.77	109.60
1	B	472	GLY	CA-C-N	13.20	146.12	121.69
1	B	472	GLY	C-N-CA	13.20	146.12	121.69
1	B	65	LEU	N-CA-CB	-13.20	89.97	110.56
1	B	140	ILE	CA-C-N	13.16	137.32	122.85
1	B	140	ILE	C-N-CA	13.16	137.32	122.85
1	B	468	ASN	OD1-CG-ND2	13.13	135.73	122.60
1	A	139	GLN	OE1-CD-NE2	13.10	135.70	122.60
1	B	268	PHE	O-C-N	13.10	131.69	121.47
1	B	191	ASN	OD1-CG-ND2	13.04	135.64	122.60
1	A	560	ARG	NE-CZ-NH1	-13.04	108.46	121.50
1	B	456	ASN	CA-CB-CG	-13.02	99.58	112.60
1	B	276	HIS	CA-CB-CG	-13.02	100.78	113.80
1	B	546	ALA	CA-C-N	-13.02	110.21	122.97
1	B	546	ALA	C-N-CA	-13.02	110.21	122.97
1	A	245	GLU	O-C-N	-13.00	108.08	123.16
1	D	632	ASP	CA-CB-CG	12.98	125.58	112.60
1	B	169	SER	N-CA-C	12.98	129.34	113.12
1	A	412	VAL	N-CA-CB	-12.95	92.82	111.99
1	A	422	LEU	CB-CA-C	12.94	136.17	110.42
1	B	462	TYR	O-C-N	12.92	138.15	123.16
1	B	279	ASP	CA-CB-CG	12.91	125.51	112.60
1	B	364	PRO	CA-C-O	-12.89	101.87	120.56
1	A	183	TYR	O-C-N	12.88	139.14	122.39
1	A	331	SER	CA-C-O	-12.86	105.34	121.55
1	A	64	ARG	NE-CZ-NH1	-12.85	108.65	121.50
1	B	326	ASP	CA-CB-CG	12.85	125.45	112.60
1	A	52	ALA	O-C-N	12.84	135.81	122.08
1	A	151	ILE	O-C-N	12.82	134.46	121.89
1	B	332	LYS	O-C-N	12.79	138.74	122.37
1	A	349	VAL	CA-C-O	12.78	134.27	120.47
1	B	461	THR	CA-CB-OG1	-12.77	90.45	109.60
1	A	89	VAL	CB-CA-C	12.74	132.19	111.29
1	C	632	ASP	CA-CB-CG	12.74	125.34	112.60
1	B	469	ASN	CB-CG-ND2	-12.72	97.32	116.40
1	B	439	SER	O-C-N	12.71	138.86	123.36
1	B	287	HIS	O-C-N	12.70	139.34	122.33
1	B	470	ASN	CA-CB-CG	12.67	125.27	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	ARG	NH1-CZ-NH2	-12.65	102.85	119.30
1	F	632	ASP	CA-CB-CG	12.65	125.25	112.60
1	A	529	THR	CA-C-N	12.63	145.50	122.13
1	A	529	THR	C-N-CA	12.63	145.50	122.13
1	A	52	ALA	CA-C-O	-12.63	107.18	121.07
1	A	80	ARG	O-C-N	12.62	137.44	122.17
1	B	46	TYR	CA-C-O	-12.61	106.31	120.69
1	A	145	PHE	CA-CB-CG	12.61	126.41	113.80
1	B	65	LEU	O-C-N	-12.60	108.79	123.03
1	A	247	HIS	CA-C-O	-12.59	106.89	121.11
1	B	86	LEU	CA-C-O	-12.56	107.11	120.42
1	A	59	GLU	CA-C-O	-12.54	107.79	120.70
1	E	632	ASP	CA-CB-CG	12.51	125.11	112.60
1	B	439	SER	N-CA-C	-12.49	86.58	108.69
1	A	208	SER	CA-C-O	-12.47	106.40	120.24
1	B	31	LYS	CA-C-O	-12.47	107.33	120.55
1	A	489	ASN	N-CA-C	-12.44	84.30	110.80
1	B	69	ARG	CB-CG-CD	12.44	139.91	111.30
1	B	518	THR	CA-C-O	-12.43	107.58	120.63
1	B	228	THR	CA-C-O	-12.43	106.06	120.10
1	A	487	ASP	O-C-N	12.38	138.32	122.23
1	A	635	VAL	N-CA-C	12.38	122.01	110.74
1	B	77	THR	CA-C-O	-12.37	104.52	119.49
1	B	399	PRO	CA-C-O	-12.37	102.63	120.56
1	A	246	LEU	CA-C-O	-12.36	106.95	121.05
1	A	633	GLU	CA-C-O	12.36	134.06	120.10
1	B	632	ASP	CA-CB-CG	12.35	124.95	112.60
1	B	423	ILE	CB-CA-C	12.33	129.76	110.28
1	B	30	LEU	CB-CA-C	12.32	130.23	110.88
1	B	61	ASN	CA-CB-CG	-12.31	100.29	112.60
1	A	49	HIS	CA-CB-CG	-12.29	101.51	113.80
1	B	479	ARG	NE-CZ-NH2	12.29	130.26	119.20
1	A	376	ARG	CA-C-N	12.29	137.13	120.67
1	A	376	ARG	C-N-CA	12.29	137.13	120.67
1	A	322	GLU	CA-CB-CG	12.28	138.65	114.10
1	B	132	ILE	O-C-N	12.27	135.70	122.57
1	D	132	ILE	N-CA-C	12.27	125.41	109.58
1	B	289	LEU	CB-CA-C	12.22	131.03	110.86
1	A	501	PHE	CA-C-O	12.21	133.56	119.27
1	A	369	GLU	CA-CB-CG	12.19	138.48	114.10
1	A	415	GLY	O-C-N	12.18	134.74	123.54
1	C	132	ILE	N-CA-C	12.16	125.27	109.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	542	GLN	OE1-CD-NE2	12.15	134.75	122.60
1	B	403	HIS	N-CA-CB	12.15	127.59	109.98
1	B	307	ASP	O-C-N	12.14	137.72	122.43
1	B	417	ALA	N-CA-C	12.13	129.26	108.76
1	A	407	GLU	O-C-N	-12.12	108.51	123.06
1	A	38	ASN	OD1-CG-ND2	-12.12	110.48	122.60
1	A	376	ARG	CB-CG-CD	12.09	139.11	111.30
1	A	76	ASN	CA-CB-CG	-12.07	100.53	112.60
1	A	449	ASN	CA-C-O	-12.07	107.32	121.44
1	A	375	THR	CA-CB-OG1	-12.03	91.55	109.60
1	A	312	THR	O-C-N	12.02	136.86	123.27
1	A	62	ASP	CA-C-O	12.00	134.84	119.12
1	E	132	ILE	N-CA-C	11.99	125.04	109.58
1	A	291	ILE	CA-C-O	-11.98	108.15	120.85
1	A	522	SER	N-CA-C	11.97	128.99	109.95
1	B	330	SER	CA-C-O	-11.97	103.39	120.51
1	A	546	ALA	O-C-N	11.96	136.96	122.48
1	A	470	ASN	CA-C-O	11.96	137.61	120.51
1	E	279	ASP	CA-CB-CG	11.93	124.53	112.60
1	A	17	LEU	CA-C-O	-11.93	108.30	120.82
1	A	183	TYR	CA-C-O	-11.92	105.06	119.49
1	D	47	ASN	CA-CB-CG	11.92	124.52	112.60
1	B	215	ARG	NE-CZ-NH1	11.92	133.42	121.50
1	B	465	THR	CA-C-O	-11.91	107.61	120.36
1	B	476	ALA	CA-C-O	11.91	134.67	120.14
1	A	132	ILE	N-CA-C	11.89	125.62	109.80
1	F	279	ASP	CA-CB-CG	11.89	124.49	112.60
1	B	143	HIS	O-C-N	11.88	136.88	122.27
1	B	545	ASN	CA-CB-CG	11.88	124.48	112.60
1	F	132	ILE	N-CA-C	11.87	124.90	109.58
1	B	92	GLN	CB-CG-CD	-11.86	92.44	112.60
1	B	11	GLN	CA-CB-CG	-11.85	90.40	114.10
1	B	99	PHE	CA-C-O	-11.85	108.69	120.90
1	A	309	ASP	CA-C-N	-11.84	103.98	122.10
1	A	309	ASP	C-N-CA	-11.84	103.98	122.10
1	B	270	VAL	CA-C-O	-11.83	106.45	121.48
1	B	485	ILE	O-C-N	-11.83	107.78	122.57
1	A	309	ASP	N-CA-C	-11.82	98.57	113.23
1	A	427	ASP	CA-CB-CG	-11.81	100.79	112.60
1	A	91	ASN	CA-C-N	-11.81	105.57	123.17
1	A	91	ASN	C-N-CA	-11.81	105.57	123.17
1	A	509	PHE	CA-CB-CG	11.80	125.60	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	LEU	N-CA-CB	-11.79	92.49	110.42
1	A	469	ASN	CA-C-O	-11.78	104.89	119.38
1	B	201	PHE	O-C-N	11.78	132.04	121.32
1	B	165	THR	CA-CB-OG1	-11.76	91.96	109.60
1	A	152	ASP	N-CA-CB	11.76	127.56	110.16
1	A	177	ARG	NE-CZ-NH2	11.76	129.78	119.20
1	A	279	ASP	CB-CA-C	11.75	126.40	110.06
1	A	375	THR	OG1-CB-CG2	11.74	132.79	109.30
1	A	263	LYS	N-CA-C	-11.73	95.42	111.96
1	A	275	ILE	CB-CA-C	-11.73	95.31	111.49
1	F	206	GLU	CG-CD-OE2	11.73	145.38	118.40
1	B	311	HIS	O-C-N	11.70	136.17	123.06
1	A	534	PRO	O-C-N	11.68	137.82	122.99
1	B	25	THR	OG1-CB-CG2	11.68	132.65	109.30
1	B	177	ARG	CA-C-O	11.68	137.21	120.51
1	A	94	LYS	CB-CA-C	11.67	133.13	109.67
1	B	416	VAL	CA-C-N	11.67	140.71	122.74
1	B	416	VAL	C-N-CA	11.67	140.71	122.74
1	A	34	ALA	O-C-N	11.66	135.86	122.22
1	B	125	HIS	CA-CB-CG	-11.65	102.14	113.80
1	B	443	ILE	CA-C-O	-11.65	108.07	120.53
1	A	157	ALA	N-CA-C	-11.64	98.61	111.07
1	A	271	ARG	O-C-N	11.61	132.53	121.38
1	A	373	THR	CA-CB-OG1	-11.61	92.19	109.60
1	B	231	PHE	CA-C-O	-11.61	108.81	121.00
1	A	299	ALA	CA-C-O	-11.60	108.62	120.80
1	A	441	GLU	CA-CB-CG	-11.59	90.92	114.10
1	B	296	ILE	N-CA-CB	11.59	124.11	110.55
1	A	360	LYS	CA-CB-CG	11.57	137.25	114.10
1	B	454	ARG	CA-CB-CG	11.55	137.19	114.10
1	A	465	THR	CA-C-O	-11.54	107.53	120.69
1	B	218	GLU	N-CA-CB	11.53	127.06	110.12
1	B	11	GLN	OE1-CD-NE2	11.51	134.11	122.60
1	B	370	HIS	CA-C-O	-11.51	106.85	120.43
1	B	494	THR	N-CA-C	11.51	128.10	111.87
1	A	417	ALA	N-CA-C	11.51	128.20	108.76
1	B	528	VAL	O-C-N	11.49	133.77	122.05
1	A	642	ILE	CA-C-O	-11.48	107.96	121.28
1	A	461	THR	O-C-N	-11.48	107.73	123.11
1	B	218	GLU	N-CA-C	-11.48	98.77	111.28
1	B	317	GLN	CB-CG-CD	11.47	132.10	112.60
1	A	534	PRO	CB-CA-C	-11.47	96.71	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	ASP	CA-C-O	-11.44	108.98	121.00
1	B	141	THR	CA-C-O	-11.44	108.69	121.28
1	B	458	ASN	CA-C-O	-11.43	108.59	120.71
1	B	583	TYR	CA-C-O	-11.43	108.23	120.46
1	A	92	GLN	CB-CG-CD	-11.42	93.18	112.60
1	B	311	HIS	CA-C-O	-11.42	107.65	121.36
1	B	497	GLU	N-CA-C	-11.41	98.59	111.82
1	B	390	ILE	N-CA-CB	11.39	128.54	110.31
1	B	555	LEU	N-CA-C	-11.39	96.52	112.13
1	A	179	GLN	N-CA-C	-11.39	86.54	110.80
1	A	145	PHE	CA-C-N	11.38	140.02	122.94
1	A	145	PHE	C-N-CA	11.38	140.02	122.94
1	B	487	ASP	N-CA-C	11.38	128.27	112.45
1	A	111	ASN	OD1-CG-ND2	11.36	133.96	122.60
1	A	555	LEU	CA-C-O	-11.36	104.27	120.51
1	E	558	TYR	N-CA-C	11.35	126.26	113.21
1	A	263	LYS	CA-C-N	-11.34	107.35	123.00
1	A	263	LYS	C-N-CA	-11.34	107.35	123.00
1	B	308	SER	CA-CB-OG	11.33	133.77	111.10
1	A	578	MET	CA-CB-CG	11.33	136.76	114.10
1	B	272	PRO	CA-C-O	-11.33	108.07	122.12
1	E	408	PHE	CA-CB-CG	11.33	125.13	113.80
1	B	161	GLN	OE1-CD-NE2	11.32	133.92	122.60
1	B	147	ASN	CA-CB-CG	-11.29	101.31	112.60
1	A	146	THR	CA-C-O	11.26	132.86	120.70
1	B	75	PHE	O-C-N	11.23	137.85	122.46
1	B	344	HIS	CG-CD2-NE2	-11.23	95.97	107.20
1	F	408	PHE	CA-CB-CG	11.22	125.02	113.80
1	A	137	LEU	CA-C-O	-11.21	108.36	120.92
1	B	369	GLU	CA-CB-CG	11.20	136.49	114.10
1	A	244	ASP	CA-CB-CG	11.19	123.79	112.60
1	A	423	ILE	CA-C-O	-11.18	108.25	120.43
1	B	489	ASN	N-CA-C	-11.18	86.99	110.80
1	B	102	ASN	CA-CB-CG	-11.18	101.42	112.60
1	A	474	ARG	NE-CZ-NH1	11.17	132.67	121.50
1	B	6	GLY	N-CA-C	-11.17	86.70	113.18
1	A	213	LEU	CA-C-O	-11.17	107.53	120.49
1	A	235	ARG	O-C-N	11.16	136.00	122.27
1	A	302	HIS	N-CA-CB	11.16	126.25	110.07
1	C	408	PHE	CA-CB-CG	11.12	124.92	113.80
1	B	62	ASP	O-C-N	11.11	140.19	122.41
1	A	147	ASN	CB-CG-OD1	-11.10	98.60	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	463	LYS	N-CA-CB	11.10	128.96	110.87
1	A	247	HIS	CA-CB-CG	-11.09	102.71	113.80
1	B	259	LEU	N-CA-CB	-11.08	95.34	112.08
1	A	240	LEU	O-C-N	-11.08	110.53	122.94
1	A	331	SER	O-C-N	11.08	136.32	122.14
1	B	298	GLU	CA-CB-CG	11.08	136.25	114.10
1	B	143	HIS	CA-C-O	-11.07	107.24	119.97
1	B	319	LYS	O-C-N	11.06	138.59	122.43
1	C	279	ASP	CA-CB-CG	11.06	123.66	112.60
1	B	196	THR	O-C-N	11.06	133.84	122.12
1	A	361	PHE	CA-C-O	-11.02	107.02	119.14
1	B	190	MET	CA-C-N	-11.01	105.30	120.38
1	B	190	MET	C-N-CA	-11.01	105.30	120.38
1	B	534	PRO	CB-CA-C	-11.01	93.40	111.56
1	B	40	LEU	N-CA-C	11.00	126.01	112.59
1	B	445	ASP	CA-C-N	10.98	136.81	123.19
1	B	445	ASP	C-N-CA	10.98	136.81	123.19
1	B	259	LEU	CB-CA-C	10.98	128.90	111.66
1	D	279	ASP	CA-CB-CG	10.96	123.56	112.60
1	B	504	GLU	O-C-N	10.95	136.40	122.93
1	A	635	VAL	O-C-N	10.89	135.23	121.94
1	B	417	ALA	N-CA-CB	-10.88	91.98	110.80
1	A	273	ASP	OD1-CG-OD2	-10.88	96.79	122.90
1	B	412	VAL	O-C-N	10.87	136.16	122.57
1	B	303	GLY	N-CA-C	-10.87	101.54	114.48
1	A	214	ASP	N-CA-C	10.87	124.28	111.02
1	A	206	GLU	OE1-CD-OE2	-10.86	96.83	122.90
1	B	215	ARG	NH1-CZ-NH2	-10.86	105.18	119.30
1	A	543	ALA	CA-C-O	10.86	131.88	120.70
1	D	487	ASP	N-CA-C	10.85	126.35	112.89
1	B	57	MET	O-C-N	10.84	133.68	122.08
1	B	359	GLY	CA-C-O	10.83	139.41	120.57
1	A	620	ARG	NE-CZ-NH2	10.81	128.93	119.20
1	B	413	VAL	CB-CA-C	10.81	123.73	111.08
1	A	361	PHE	O-C-N	10.81	136.97	122.49
1	B	412	VAL	CA-C-O	-10.80	107.28	120.78
1	A	612	HIS	CA-CB-CG	10.80	124.60	113.80
1	A	107	ARG	NH1-CZ-NH2	-10.79	105.27	119.30
1	A	407	GLU	CA-C-N	10.79	142.15	121.54
1	A	407	GLU	C-N-CA	10.79	142.15	121.54
1	B	13	ASP	O-C-N	-10.79	110.53	122.08
1	A	570	LEU	CA-C-O	-10.79	108.80	120.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	521	ARG	NE-CZ-NH2	-10.79	109.49	119.20
1	A	546	ALA	CA-C-N	-10.78	106.03	122.09
1	A	546	ALA	C-N-CA	-10.78	106.03	122.09
1	B	92	GLN	OE1-CD-NE2	10.78	133.38	122.60
1	A	496	ASP	N-CA-C	-10.77	87.86	110.80
1	A	313	ILE	CA-CB-CG2	10.76	128.79	110.50
1	B	285	HIS	CA-C-O	-10.76	110.15	121.55
1	A	25	THR	OG1-CB-CG2	10.75	130.80	109.30
1	A	322	GLU	CB-CG-CD	10.75	130.87	112.60
1	A	434	ILE	CA-C-O	-10.74	109.46	120.85
1	B	178	GLU	O-C-N	10.74	136.88	122.59
1	B	229	ALA	N-CA-CB	10.71	125.52	109.98
1	A	506	ASP	CA-CB-CG	10.71	123.31	112.60
1	A	47	ASN	N-CA-CB	10.70	125.33	110.56
1	B	16	HIS	CA-CB-CG	-10.70	103.11	113.80
1	B	75	PHE	CA-CB-CG	-10.69	103.11	113.80
1	A	328	ILE	O-C-N	-10.66	107.76	121.84
1	A	528	VAL	O-C-N	10.66	131.68	122.09
1	B	215	ARG	CB-CG-CD	10.65	135.80	111.30
1	A	387	MET	N-CA-CB	10.65	125.77	110.12
1	A	565	PRO	CA-C-O	-10.64	109.21	121.34
1	A	87	PHE	CA-C-O	10.64	132.29	120.90
1	B	499	ARG	CD-NE-CZ	10.64	139.29	124.40
1	A	441	GLU	CB-CG-CD	-10.63	94.53	112.60
1	A	547	VAL	N-CA-C	-10.63	102.30	112.83
1	B	496	ASP	N-CA-CB	10.63	128.46	110.49
1	B	253	ARG	CA-CB-CG	10.63	135.35	114.10
1	C	561	SER	N-CA-C	10.62	125.89	111.24
1	B	327	ILE	CA-C-O	-10.61	108.78	119.92
1	E	487	ASP	N-CA-C	10.61	126.39	113.23
1	E	370	HIS	CA-CB-CG	10.60	124.40	113.80
1	B	306	THR	OG1-CB-CG2	10.59	130.48	109.30
1	A	253	ARG	CA-C-O	-10.59	109.42	121.07
1	B	447	GLU	CA-C-O	-10.59	109.54	120.98
1	B	74	LEU	O-C-N	10.58	137.88	122.43
1	A	641	ASN	CA-CB-CG	-10.57	102.03	112.60
1	B	179	GLN	N-CA-C	-10.57	95.06	109.54
1	B	251	ILE	CA-C-O	-10.57	109.19	121.98
1	D	322	GLU	CA-CB-CG	10.57	135.23	114.10
1	E	390	ILE	N-CA-C	-10.57	100.38	111.58
1	B	359	GLY	O-C-N	-10.56	108.97	122.70
1	B	554	ASP	CB-CA-C	10.55	124.45	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	ASP	O-C-N	-10.55	109.96	122.93
1	B	363	LEU	N-CA-C	-10.54	96.69	110.39
1	A	108	GLU	CB-CG-CD	10.54	130.52	112.60
1	D	63	HIS	CA-CB-CG	10.54	124.34	113.80
1	B	585	ALA	O-C-N	10.53	135.59	123.27
1	F	390	ILE	N-CA-C	-10.52	100.43	111.58
1	C	370	HIS	CA-CB-CG	10.52	124.31	113.80
1	E	206	GLU	CG-CD-OE2	10.52	142.58	118.40
1	A	191	ASN	CA-CB-CG	10.51	123.11	112.60
1	C	63	HIS	CA-CB-CG	10.50	124.30	113.80
1	A	399	PRO	CB-CA-C	-10.50	101.52	111.39
1	A	317	GLN	O-C-N	-10.49	109.26	121.32
1	A	371	PHE	CA-C-O	-10.48	108.25	120.10
1	A	440	GLY	CA-C-O	-10.47	102.34	120.57
1	A	479	ARG	CD-NE-CZ	-10.47	109.73	124.40
1	A	73	SER	CA-C-O	-10.47	109.28	121.11
1	A	454	ARG	NE-CZ-NH2	10.47	128.62	119.20
1	B	126	SER	CA-C-O	10.46	132.88	121.16
1	E	63	HIS	CA-CB-CG	10.46	124.26	113.80
1	B	197	TRP	CA-C-O	-10.44	109.48	120.55
1	B	272	PRO	N-CA-C	-10.44	95.70	111.57
1	D	390	ILE	N-CA-C	-10.44	100.52	111.58
1	B	182	ALA	O-C-N	10.42	133.17	122.12
1	C	299	ALA	N-CA-C	-10.42	99.46	111.03
1	A	285	HIS	O-C-N	-10.42	110.56	122.86
1	B	364	PRO	O-C-N	10.42	133.75	121.46
1	B	183	TYR	O-C-N	10.41	133.16	122.12
1	F	370	HIS	CA-CB-CG	10.41	124.21	113.80
1	A	406	LEU	N-CA-C	10.40	123.89	111.82
1	C	390	ILE	N-CA-C	-10.40	100.56	111.58
1	B	422	LEU	CA-C-N	-10.39	107.68	122.75
1	B	422	LEU	C-N-CA	-10.39	107.68	122.75
1	A	220	PHE	CA-C-O	-10.38	110.09	121.00
1	B	227	LEU	O-C-N	10.38	132.77	122.07
1	B	200	ASP	CA-CB-CG	10.37	122.97	112.60
1	A	635	VAL	CA-C-O	-10.37	107.46	121.15
1	E	635	VAL	N-CA-C	10.37	120.88	110.82
1	F	522	SER	N-CA-C	10.34	126.82	110.17
1	A	208	SER	N-CA-C	-10.33	98.98	111.69
1	A	501	PHE	CA-C-N	10.33	135.41	120.95
1	A	501	PHE	C-N-CA	10.33	135.41	120.95
1	A	32	ASP	CA-C-O	-10.33	105.63	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	ASP	CB-CA-C	10.32	130.01	110.51
1	B	583	TYR	O-C-N	10.31	136.12	123.13
1	A	216	LYS	N-CA-CB	10.30	125.79	109.51
1	B	547	VAL	N-CA-C	-10.30	101.80	111.48
1	A	51	ALA	N-CA-C	-10.29	100.06	111.28
1	A	230	ARG	NE-CZ-NH1	-10.29	111.21	121.50
1	A	293	GLU	CG-CD-OE2	10.29	142.06	118.40
1	B	635	VAL	N-CA-C	10.28	120.79	110.82
1	B	141	THR	O-C-N	10.28	129.56	121.23
1	B	152	ASP	CA-C-O	-10.28	108.83	120.24
1	B	91	ASN	CA-C-N	-10.27	107.86	123.17
1	B	91	ASN	C-N-CA	-10.27	107.86	123.17
1	B	521	ARG	NH1-CZ-NH2	10.26	132.64	119.30
1	B	579	GLU	O-C-N	-10.26	111.16	123.27
1	A	385	LYS	N-CA-CB	10.26	127.83	110.49
1	A	442	ASN	CA-CB-CG	10.26	122.86	112.60
1	A	447	GLU	CA-C-O	10.25	131.20	120.54
1	B	553	LEU	CA-C-N	-10.25	105.81	121.40
1	B	553	LEU	C-N-CA	-10.25	105.81	121.40
1	B	181	VAL	CB-CA-C	10.25	128.10	111.29
1	E	241	ASP	CA-CB-CG	10.25	122.85	112.60
1	A	496	ASP	N-CA-CB	10.24	127.80	110.49
1	A	353	ARG	CA-C-O	10.24	132.53	119.12
1	A	329	GLU	O-C-N	10.23	136.89	122.36
1	A	63	HIS	N-CA-CB	10.23	127.78	110.49
1	F	63	HIS	CA-CB-CG	10.23	124.03	113.80
1	A	317	GLN	CA-C-O	10.22	134.17	120.16
1	A	608	GLN	N-CA-C	-10.22	100.34	113.12
1	B	164	GLY	N-CA-C	10.22	137.41	113.18
1	A	137	LEU	O-C-N	10.21	133.85	122.11
1	A	241	ASP	CA-CB-CG	10.21	122.81	112.60
1	A	32	ASP	N-CA-C	-10.20	100.77	113.01
1	A	328	ILE	N-CA-C	10.20	122.12	111.00
1	B	555	LEU	O-C-N	10.20	135.18	121.92
1	F	635	VAL	N-CA-C	10.20	120.71	110.82
1	A	419	ASP	N-CA-CB	-10.19	98.10	110.53
1	C	522	SER	N-CA-C	10.19	126.58	110.17
1	C	635	VAL	N-CA-C	10.19	120.70	110.82
1	B	539	LEU	O-C-N	10.19	137.30	122.43
1	B	612	HIS	CA-CB-CG	10.19	123.99	113.80
1	C	322	GLU	CA-CB-CG	10.18	134.47	114.10
1	B	503	ILE	O-C-N	-10.18	112.49	123.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	621	PRO	CB-CA-C	10.18	128.36	111.56
1	A	291	ILE	CA-C-N	10.18	133.67	120.44
1	A	291	ILE	C-N-CA	10.18	133.67	120.44
1	A	438	ASP	CA-C-O	10.18	132.04	120.54
1	F	61	ASN	CA-CB-CG	-10.17	102.43	112.60
1	F	322	GLU	CA-CB-CG	10.16	134.41	114.10
1	A	176	ASN	CA-CB-CG	10.15	122.75	112.60
1	D	385	LYS	N-CA-C	-10.14	100.19	111.14
1	D	494	THR	N-CA-C	10.14	132.40	110.80
1	B	375	THR	N-CA-C	-10.14	100.01	112.38
1	A	422	LEU	CA-C-N	-10.13	108.06	122.75
1	A	422	LEU	C-N-CA	-10.13	108.06	122.75
1	B	167	ASN	CA-C-O	10.13	131.78	120.43
1	F	494	THR	N-CA-C	10.13	132.38	110.80
1	B	360	LYS	N-CA-C	-10.13	100.67	113.23
1	D	407	GLU	N-CA-C	10.13	125.15	109.96
1	E	322	GLU	CA-CB-CG	10.12	134.35	114.10
1	C	61	ASN	CA-CB-CG	-10.12	102.48	112.60
1	B	316	ARG	CG-CD-NE	10.12	134.26	112.00
1	B	328	ILE	O-C-N	-10.12	111.41	121.83
1	B	582	LEU	CB-CA-C	10.11	126.46	109.48
1	A	25	THR	CB-CA-C	-10.10	90.95	109.54
1	A	445	ASP	CA-CB-CG	10.10	122.70	112.60
1	D	370	HIS	CA-CB-CG	10.10	123.90	113.80
1	B	114	GLU	N-CA-C	-10.10	99.00	111.11
1	A	238	ASN	OD1-CG-ND2	10.09	132.69	122.60
1	B	395	THR	O-C-N	10.09	132.81	122.12
1	C	363	LEU	N-CA-C	-10.09	97.19	110.40
1	B	180	ARG	O-C-N	10.07	132.60	121.93
1	E	61	ASN	CA-CB-CG	-10.07	102.53	112.60
1	B	121	VAL	CA-C-O	10.07	131.42	120.95
1	F	241	ASP	CA-CB-CG	10.06	122.66	112.60
1	C	241	ASP	CA-CB-CG	10.05	122.66	112.60
1	A	226	GLN	CB-CA-C	10.05	129.10	110.11
1	B	264	TYR	CA-C-O	-10.02	109.30	120.32
1	F	299	ALA	N-CA-C	-10.02	99.91	111.03
1	B	299	ALA	CB-CA-C	10.02	127.62	110.79
1	A	234	GLU	N-CA-CB	10.02	125.08	110.06
1	A	177	ARG	NH1-CZ-NH2	-10.02	106.28	119.30
1	B	68	GLN	CA-C-O	-10.00	110.19	121.89
1	A	363	LEU	N-CA-C	-10.00	96.50	110.29
1	B	132	ILE	N-CA-C	10.00	123.10	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	VAL	N-CA-C	9.99	122.08	108.89
1	C	494	THR	N-CA-C	9.99	132.09	110.80
1	A	281	ASP	CA-C-O	-9.99	110.07	120.96
1	B	613	GLY	O-C-N	9.99	134.29	122.50
1	A	439	SER	CA-C-N	-9.99	101.84	121.41
1	A	439	SER	C-N-CA	-9.99	101.84	121.41
1	A	584	VAL	CA-C-N	-9.99	106.55	122.73
1	A	584	VAL	C-N-CA	-9.99	106.55	122.73
1	A	14	ILE	CA-C-O	-9.98	109.60	121.18
1	B	477	THR	CA-CB-OG1	-9.98	94.63	109.60
1	F	363	LEU	N-CA-C	-9.98	97.33	110.40
1	A	522	SER	CA-C-O	9.97	132.43	121.16
1	B	386	TYR	O-C-N	-9.96	109.35	122.59
1	D	241	ASP	CA-CB-CG	9.95	122.55	112.60
1	A	190	MET	N-CA-CB	9.95	124.43	110.01
1	B	464	ILE	N-CA-CB	-9.94	99.08	111.31
1	A	638	GLY	CA-C-N	9.94	135.52	123.19
1	A	638	GLY	C-N-CA	9.94	135.52	123.19
1	A	623	GLY	N-CA-C	-9.94	100.82	115.63
1	B	578	MET	CA-C-N	-9.93	109.15	123.05
1	B	578	MET	C-N-CA	-9.93	109.15	123.05
1	B	342	SER	CA-C-O	9.92	138.47	122.20
1	D	61	ASN	CA-CB-CG	-9.92	102.68	112.60
1	D	635	VAL	N-CA-C	9.92	120.44	110.82
1	A	8	ALA	CA-C-N	9.90	140.45	121.54
1	A	8	ALA	C-N-CA	9.90	140.45	121.54
1	A	21	ILE	CA-C-O	-9.90	108.41	120.78
1	A	44	SER	N-CA-C	-9.89	99.60	114.64
1	C	199	MET	N-CA-C	-9.89	100.96	113.43
1	A	547	VAL	CA-C-N	-9.89	107.17	122.60
1	A	547	VAL	C-N-CA	-9.89	107.17	122.60
1	B	149	GLU	N-CA-CB	-9.89	95.53	110.07
1	B	16	HIS	CA-C-O	-9.89	110.52	120.70
1	B	313	ILE	CA-CB-CG2	9.89	127.31	110.50
1	B	197	TRP	O-C-N	9.88	132.59	122.12
1	B	414	ASN	OD1-CG-ND2	9.88	132.48	122.60
1	B	99	PHE	O-C-N	9.88	132.70	122.03
1	B	469	ASN	CA-C-O	-9.87	106.22	119.05
1	A	239	TRP	N-CA-C	-9.87	101.84	113.38
1	D	363	LEU	N-CA-C	-9.86	97.14	110.36
1	B	332	LYS	CA-C-O	-9.86	107.46	119.59
1	B	393	LYS	N-CA-CB	9.85	124.60	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	462	TYR	CA-C-O	-9.85	109.59	120.92
1	A	73	SER	O-C-N	9.85	135.99	123.19
1	A	535	SER	CB-CA-C	-9.85	91.08	113.33
1	A	16	HIS	N-CA-CB	9.84	124.27	110.01
1	B	443	ILE	CB-CA-C	9.83	125.31	110.96
1	B	226	GLN	CB-CA-C	9.83	128.69	110.70
1	B	473	GLU	N-CA-C	-9.82	92.64	108.55
1	E	199	MET	N-CA-C	-9.81	101.87	114.04
1	A	253	ARG	NE-CZ-NH1	9.81	131.31	121.50
1	B	571	PRO	CA-C-O	-9.81	108.48	122.31
1	F	487	ASP	N-CA-C	9.81	125.06	112.89
1	B	242	PRO	N-CA-CB	-9.80	92.96	103.25
1	A	199	MET	N-CA-C	-9.79	101.22	113.55
1	E	363	LEU	N-CA-C	-9.79	97.24	110.36
1	D	199	MET	N-CA-C	-9.78	101.91	114.04
1	B	338	GLN	O-C-N	9.78	135.96	122.46
1	B	226	GLN	CG-CD-NE2	-9.78	101.73	116.40
1	A	571	PRO	CA-C-O	9.77	135.05	122.15
1	B	388	ASP	CA-CB-CG	9.77	122.37	112.60
1	B	379	SER	CA-C-O	9.77	131.75	119.05
1	B	380	PHE	CA-C-O	9.76	131.07	120.82
1	A	9	GLN	O-C-N	9.76	135.56	122.59
1	B	281	ASP	CA-CB-CG	9.75	122.35	112.60
1	A	24	PRO	N-CD-CG	-9.74	88.58	103.20
1	A	372	GLU	CB-CG-CD	9.74	129.16	112.60
1	D	299	ALA	N-CA-C	-9.74	98.68	111.24
1	A	109	ARG	CA-C-O	9.73	130.59	118.43
1	B	307	ASP	CA-C-O	-9.73	109.23	121.88
1	B	460	PHE	CA-C-O	-9.73	110.82	121.33
1	D	470	ASN	CA-CB-CG	9.72	122.32	112.60
1	E	385	LYS	N-CA-C	-9.72	100.64	111.14
1	A	449	ASN	O-C-N	9.71	135.77	123.15
1	B	328	ILE	N-CA-C	9.71	120.53	110.72
1	A	227	LEU	N-CA-CB	9.70	126.89	110.49
1	A	457	HIS	O-C-N	9.70	135.50	122.59
1	B	292	THR	CB-CA-C	9.70	126.32	110.81
1	B	395	THR	CA-CB-OG1	-9.70	95.05	109.60
1	E	273	ASP	CA-CB-CG	9.70	122.30	112.60
1	B	295	ARG	CB-CG-CD	9.69	133.59	111.30
1	B	482	LEU	CA-C-O	-9.69	109.66	120.70
1	B	627	GLU	CG-CD-OE1	-9.69	96.12	118.40
1	B	274	ASN	CB-CG-ND2	9.68	130.92	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	ILE	CA-C-O	-9.68	108.68	120.78
1	A	360	LYS	N-CA-C	-9.68	101.60	113.50
1	B	497	GLU	N-CA-CB	9.68	125.28	110.28
1	A	302	HIS	CB-CA-C	-9.67	95.63	110.90
1	A	501	PHE	N-CA-CB	-9.66	95.37	110.44
1	B	306	THR	CA-CB-OG1	-9.65	95.12	109.60
1	A	554	ASP	N-CA-CB	9.65	125.08	110.70
1	A	343	LEU	CD1-CG-CD2	-9.64	89.59	110.80
1	B	271	ARG	CA-C-N	9.64	129.76	120.31
1	B	271	ARG	C-N-CA	9.64	129.76	120.31
1	E	643	LYS	CA-CB-CG	9.63	133.36	114.10
1	A	345	ASN	OD1-CG-ND2	-9.63	112.97	122.60
1	A	632	ASP	CB-CG-OD2	9.62	140.53	118.40
1	A	521	ARG	NE-CZ-NH2	-9.62	110.54	119.20
1	B	537	GLN	CB-CG-CD	-9.62	96.25	112.60
1	A	396	ASP	CA-C-O	-9.61	106.56	119.05
1	B	470	ASN	CA-C-O	9.61	131.73	121.55
1	A	442	ASN	OD1-CG-ND2	-9.60	113.00	122.60
1	A	441	GLU	CG-CD-OE2	-9.60	96.32	118.40
1	B	45	ILE	O-C-N	9.59	134.62	122.05
1	B	312	THR	CA-CB-OG1	-9.58	95.23	109.60
1	A	128	LEU	CA-C-O	-9.57	108.30	119.59
1	B	39	PRO	CB-CA-C	9.57	125.59	111.62
1	B	263	LYS	N-CA-CB	9.57	124.29	110.13
1	D	408	PHE	CA-CB-CG	9.57	123.37	113.80
1	B	88	ALA	O-C-N	9.56	134.82	122.39
1	A	166	PHE	CA-C-O	9.55	130.84	120.71
1	B	387	MET	CA-C-O	-9.55	110.31	120.63
1	B	644	HIS	CA-CB-CG	9.55	123.35	113.80
1	A	562	CYS	N-CA-C	9.55	121.77	111.36
1	E	644	HIS	CA-CB-CG	9.55	123.35	113.80
1	B	87	PHE	CA-CB-CG	9.54	123.34	113.80
1	A	27	TYR	CA-C-O	9.54	125.49	119.29
1	B	548	ASN	CB-CG-ND2	-9.53	102.10	116.40
1	B	319	LYS	N-CA-CB	9.53	126.42	110.41
1	B	80	ARG	NH1-CZ-NH2	9.53	131.69	119.30
1	B	78	ARG	CD-NE-CZ	9.52	137.73	124.40
1	B	165	THR	CA-CB-CG2	9.52	126.68	110.50
1	B	503	ILE	CA-CB-CG1	9.51	126.57	110.40
1	B	111	ASN	CA-CB-CG	9.51	122.11	112.60
1	B	217	GLY	O-C-N	9.51	135.06	122.70
1	B	376	ARG	N-CA-CB	9.50	123.85	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	VAL	CA-C-N	9.49	137.36	122.74
1	A	416	VAL	C-N-CA	9.49	137.36	122.74
1	B	231	PHE	O-C-N	9.49	131.90	122.03
1	B	503	ILE	CA-C-O	9.49	130.54	120.48
1	B	238	ASN	OD1-CG-ND2	9.49	132.09	122.60
1	A	391	PHE	N-CA-C	-9.48	99.83	111.40
1	F	547	VAL	N-CA-C	-9.48	89.62	109.34
1	A	222	TRP	N-CA-C	9.46	121.20	111.07
1	A	469	ASN	OD1-CG-ND2	-9.46	113.14	122.60
1	A	628	ARG	NE-CZ-NH2	-9.46	110.69	119.20
1	F	423	ILE	CB-CA-C	9.45	125.22	110.28
1	A	58	LYS	O-C-N	9.45	131.92	122.09
1	B	442	ASN	CA-C-N	9.45	135.41	123.12
1	B	442	ASN	C-N-CA	9.45	135.41	123.12
1	A	195	VAL	N-CA-CB	9.45	124.12	110.52
1	B	86	LEU	O-C-N	9.44	132.91	122.15
1	A	224	HIS	CA-C-O	9.44	130.65	119.60
1	B	197	TRP	N-CA-CB	9.44	124.00	110.12
1	B	623	GLY	N-CA-C	-9.44	101.56	115.63
1	A	505	LEU	N-CA-CB	-9.44	96.69	110.47
1	A	639	VAL	N-CA-C	-9.44	94.96	108.17
1	B	261	SER	CA-C-O	-9.43	110.07	121.11
1	D	643	LYS	CA-CB-CG	9.43	132.97	114.10
1	B	51	ALA	N-CA-C	-9.42	100.89	111.82
1	C	509	PHE	CA-CB-CG	9.42	123.22	113.80
1	B	32	ASP	O-C-N	9.42	135.06	122.43
1	B	74	LEU	CA-C-O	-9.42	107.05	119.11
1	A	621	PRO	CA-C-N	-9.42	109.86	123.05
1	A	621	PRO	C-N-CA	-9.42	109.86	123.05
1	C	643	LYS	CA-CB-CG	9.42	132.94	114.10
1	A	615	ALA	N-CA-CB	-9.42	94.58	110.49
1	B	301	ASP	CA-CB-CG	-9.42	103.18	112.60
1	B	496	ASP	N-CA-C	-9.41	90.76	110.80
1	B	544	ASP	CA-C-O	-9.40	110.84	120.90
1	A	406	LEU	O-C-N	-9.40	110.71	122.27
1	A	284	ALA	N-CA-CB	9.40	127.57	111.69
1	A	294	SER	O-C-N	9.40	132.24	122.09
1	E	522	SER	N-CA-C	9.40	125.30	110.17
1	B	381	PHE	CA-CB-CG	-9.39	104.41	113.80
1	A	180	ARG	CA-C-O	-9.39	106.70	118.43
1	A	219	LEU	CB-CA-C	9.39	125.62	110.88
1	A	278	GLU	OE1-CD-OE2	-9.38	100.38	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	ILE	N-CA-C	-9.38	92.62	106.88
1	A	512	VAL	CA-C-O	9.38	132.52	119.95
1	F	644	HIS	CA-CB-CG	9.38	123.18	113.80
1	B	93	CYS	O-C-N	9.37	133.56	123.06
1	A	250	ARG	NH1-CZ-NH2	9.36	131.47	119.30
1	A	442	ASN	N-CA-CB	9.36	125.78	111.84
1	B	364	PRO	CA-C-N	9.35	130.58	120.11
1	B	364	PRO	C-N-CA	9.35	130.58	120.11
1	B	436	ALA	N-CA-C	9.34	123.18	111.69
1	A	391	PHE	CA-CB-CG	9.34	123.14	113.80
1	C	358	HIS	CA-CB-CG	-9.32	104.48	113.80
1	A	423	ILE	CB-CA-C	9.32	125.00	110.28
1	D	358	HIS	CA-CB-CG	-9.32	104.48	113.80
1	B	77	THR	N-CA-CB	9.31	126.16	110.32
1	B	100	ARG	CB-CG-CD	9.31	132.72	111.30
1	A	38	ASN	CB-CG-OD1	9.31	139.42	120.80
1	A	32	ASP	O-C-N	9.31	135.31	122.46
1	B	278	GLU	CA-C-O	9.31	132.71	121.72
1	A	107	ARG	NE-CZ-NH2	9.29	127.56	119.20
1	B	273	ASP	OD1-CG-OD2	-9.29	100.59	122.90
1	A	537	GLN	N-CA-C	-9.29	101.14	111.07
1	A	16	HIS	O-C-N	9.28	131.62	122.07
1	E	358	HIS	CA-CB-CG	-9.27	104.53	113.80
1	A	374	ALA	O-C-N	-9.27	110.18	122.23
1	A	50	GLY	O-C-N	9.27	131.49	122.41
1	A	70	HIS	O-C-N	9.27	133.81	123.25
1	B	152	ASP	CA-CB-CG	9.27	121.86	112.60
1	B	271	ARG	CB-CA-C	9.26	121.93	109.42
1	B	55	THR	CA-C-O	-9.26	108.77	119.60
1	A	533	MET	CA-C-N	9.25	129.33	119.89
1	A	533	MET	C-N-CA	9.25	129.33	119.89
1	A	158	LYS	CA-C-O	-9.25	110.75	120.55
1	B	202	PRO	CA-C-O	-9.25	110.21	121.31
1	B	344	HIS	CB-CG-CD2	-9.25	119.18	131.20
1	B	130	ASP	N-CA-C	9.24	121.04	110.97
1	A	31	LYS	N-CA-C	9.24	121.04	110.97
1	A	67	GLU	CA-CB-CG	9.23	132.57	114.10
1	B	190	MET	CA-CB-CG	-9.23	95.63	114.10
1	A	80	ARG	N-CA-CB	9.23	123.79	110.13
1	A	613	GLY	O-C-N	9.22	133.12	122.33
1	B	458	ASN	N-CA-CB	-9.22	95.84	110.69
1	A	215	ARG	NE-CZ-NH1	-9.22	112.28	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	448	ILE	CA-C-O	-9.21	110.15	120.84
1	B	227	LEU	CA-C-O	-9.21	111.15	120.82
1	A	59	GLU	N-CA-CB	9.21	123.42	110.07
1	B	574	LYS	CA-C-O	9.21	130.11	120.63
1	B	407	GLU	CA-CB-CG	9.20	132.50	114.10
1	B	202	PRO	O-C-N	9.19	134.13	123.10
1	A	68	GLN	O-C-N	9.19	133.43	122.68
1	A	207	ASP	CB-CG-OD2	-9.19	97.26	118.40
1	A	629	ARG	NH1-CZ-NH2	-9.19	107.36	119.30
1	B	150	VAL	CA-C-O	-9.19	110.63	120.64
1	F	199	MET	N-CA-C	-9.18	102.59	113.88
1	B	65	LEU	CB-CA-C	9.18	124.94	109.80
1	B	415	GLY	O-C-N	9.18	131.98	123.54
1	A	193	HIS	CE1-NE2-CD2	-9.17	99.83	109.00
1	A	542	GLN	N-CA-C	9.17	122.46	111.82
1	A	608	GLN	O-C-N	9.16	135.57	122.20
1	B	296	ILE	CB-CA-C	-9.15	100.26	111.97
1	B	326	ASP	N-CA-C	-9.14	100.44	111.69
1	B	592	ASP	O-C-N	9.14	134.75	122.59
1	B	238	ASN	CA-CB-CG	-9.14	103.46	112.60
1	C	216	LYS	N-CA-C	-9.13	96.61	110.30
1	F	358	HIS	CA-CB-CG	-9.13	104.67	113.80
1	A	43	THR	CA-CB-OG1	-9.12	95.92	109.60
1	B	643	LYS	CA-CB-CG	9.12	132.34	114.10
1	D	509	PHE	CA-CB-CG	9.12	122.92	113.80
1	D	162	LYS	N-CA-C	-9.12	96.56	110.32
1	B	322	GLU	N-CA-CB	9.11	123.84	110.26
1	B	585	ALA	CA-C-O	-9.11	110.58	120.24
1	B	155	TYR	CA-C-O	9.11	130.44	119.97
1	F	643	LYS	CA-CB-CG	9.11	132.31	114.10
1	A	287	HIS	CA-C-O	9.10	130.06	120.42
1	A	619	ASN	CA-C-O	-9.10	109.13	119.41
1	B	460	PHE	CA-C-N	-9.10	108.43	122.62
1	B	460	PHE	C-N-CA	-9.10	108.43	122.62
1	B	132	ILE	CB-CA-C	-9.09	98.73	111.28
1	A	521	ARG	CA-C-O	-9.09	110.81	120.99
1	A	399	PRO	N-CA-CB	9.08	108.28	103.19
1	A	23	GLU	CA-C-O	9.08	128.21	119.13
1	A	97	TYR	CA-C-O	9.08	130.37	120.20
1	A	298	GLU	CA-C-O	9.07	129.89	119.27
1	B	501	PHE	CA-C-N	9.06	134.38	121.42
1	B	501	PHE	C-N-CA	9.06	134.38	121.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	388	ASP	O-C-N	9.05	131.76	122.08
1	A	83	ALA	N-CA-CB	9.05	123.63	110.06
1	A	505	LEU	CB-CA-C	9.04	125.06	109.24
1	B	435	ASN	OD1-CG-ND2	9.04	131.64	122.60
1	B	116	VAL	CA-CB-CG2	9.04	125.76	110.40
1	A	276	HIS	CA-CB-CG	-9.03	104.77	113.80
1	A	243	VAL	CA-C-O	9.02	131.14	120.85
1	B	203	PHE	O-C-N	-9.02	111.67	122.22
1	A	67	GLU	CB-CG-CD	-9.01	97.28	112.60
1	A	141	THR	CA-C-N	9.01	129.24	119.87
1	A	141	THR	C-N-CA	9.01	129.24	119.87
1	B	384	HIS	O-C-N	9.01	135.58	122.43
1	A	133	VAL	CA-C-O	-9.00	110.94	120.48
1	A	594	GLU	OE1-CD-OE2	9.00	144.50	122.90
1	A	237	SER	CA-C-N	-9.00	108.12	122.79
1	A	237	SER	C-N-CA	-9.00	108.12	122.79
1	A	269	PRO	CA-C-N	9.00	134.85	122.34
1	A	269	PRO	C-N-CA	9.00	134.85	122.34
1	B	224	HIS	CE1-NE2-CD2	-9.00	100.00	109.00
1	B	277	PHE	CB-CA-C	-8.99	92.52	110.42
1	B	170	PHE	CA-C-O	-8.99	105.52	120.80
1	E	279	ASP	CB-CA-C	8.99	123.11	110.16
1	A	415	GLY	CA-C-O	-8.98	111.69	121.48
1	A	353	ARG	CD-NE-CZ	8.98	136.97	124.40
1	B	507	LYS	CA-C-O	-8.98	109.47	119.98
1	A	570	LEU	O-C-N	8.98	131.59	121.53
1	B	314	ASP	CB-CG-OD2	8.97	139.04	118.40
1	B	376	ARG	CB-CA-C	-8.97	96.72	110.90
1	B	480	ILE	N-CA-CB	-8.97	100.62	112.10
1	B	165	THR	CA-C-N	8.97	135.93	122.93
1	B	165	THR	C-N-CA	8.97	135.93	122.93
1	A	230	ARG	NH1-CZ-NH2	8.96	130.95	119.30
1	B	106	PHE	CA-CB-CG	-8.96	104.84	113.80
1	B	244	ASP	CA-C-N	8.96	134.31	121.50
1	B	244	ASP	C-N-CA	8.96	134.31	121.50
1	B	487	ASP	CA-C-O	-8.96	109.07	120.00
1	B	151	ILE	O-C-N	8.95	131.05	121.83
1	B	581	ASN	N-CA-CB	-8.95	96.52	110.57
1	A	124	ILE	N-CA-C	8.95	122.24	111.05
1	A	161	GLN	CA-CB-CG	-8.95	96.20	114.10
1	B	579	GLU	CA-C-O	8.95	130.17	120.32
1	A	51	ALA	CA-C-N	-8.95	108.36	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	ALA	C-N-CA	-8.95	108.36	120.79
1	A	56	LEU	O-C-N	8.94	131.69	122.03
1	A	373	THR	N-CA-CB	-8.93	97.08	111.01
1	B	498	ALA	O-C-N	-8.93	110.72	122.42
1	A	308	SER	CA-CB-OG	-8.92	93.25	111.10
1	B	243	VAL	N-CA-C	8.92	121.09	109.58
1	E	299	ALA	N-CA-C	-8.92	99.73	111.24
1	A	27	TYR	CA-C-N	8.92	130.99	119.84
1	A	27	TYR	C-N-CA	8.92	130.99	119.84
1	A	149	GLU	CA-C-N	-8.92	109.10	120.60
1	A	149	GLU	C-N-CA	-8.92	109.10	120.60
1	C	385	LYS	N-CA-C	-8.92	101.51	111.14
1	A	122	SER	CA-C-N	-8.91	109.33	120.56
1	A	122	SER	C-N-CA	-8.91	109.33	120.56
1	A	190	MET	CA-C-N	-8.91	108.51	120.54
1	A	190	MET	C-N-CA	-8.91	108.51	120.54
1	B	195	VAL	CA-C-O	-8.91	111.16	121.05
1	B	578	MET	O-C-N	8.90	134.72	123.15
1	A	27	TYR	CB-CA-C	8.90	120.32	110.08
1	A	160	THR	OG1-CB-CG2	8.90	127.10	109.30
1	A	382	ARG	N-CA-C	-8.90	101.53	111.14
1	A	31	LYS	CB-CA-C	-8.89	97.27	110.96
1	A	402	THR	CA-CB-OG1	-8.89	96.26	109.60
1	C	555	LEU	CB-CA-C	8.89	126.35	111.23
1	F	279	ASP	CB-CA-C	8.89	122.96	110.16
1	A	295	ARG	CA-C-N	8.89	131.81	120.70
1	A	295	ARG	C-N-CA	8.89	131.81	120.70
1	A	431	TYR	CA-C-N	-8.89	109.61	122.94
1	A	431	TYR	C-N-CA	-8.89	109.61	122.94
1	B	305	ILE	CA-C-N	-8.88	110.05	122.93
1	B	305	ILE	C-N-CA	-8.88	110.05	122.93
1	C	644	HIS	CA-CB-CG	8.88	122.68	113.80
1	A	251	ILE	CA-CB-CG1	-8.88	95.31	110.40
1	A	278	GLU	CG-CD-OE2	8.87	138.79	118.40
1	B	406	LEU	O-C-N	-8.87	111.44	122.17
1	C	545	ASN	CA-CB-CG	8.87	121.47	112.60
1	D	443	ILE	N-CA-C	-8.87	95.75	108.17
1	A	505	LEU	O-C-N	-8.86	109.78	122.36
1	A	149	GLU	CA-CB-CG	8.86	131.81	114.10
1	B	269	PRO	CA-C-O	8.86	131.84	121.56
1	A	87	PHE	O-C-N	-8.86	112.88	122.09
1	A	179	GLN	CB-CA-C	8.86	128.04	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	THR	N-CA-C	-8.85	101.60	111.07
1	B	321	ILE	CA-C-O	-8.85	109.72	120.78
1	B	270	VAL	O-C-N	8.84	132.77	122.69
1	B	625	PRO	N-CA-CB	-8.84	92.88	102.60
1	B	235	ARG	NE-CZ-NH1	8.84	130.34	121.50
1	B	183	TYR	CA-C-N	8.83	138.40	121.54
1	B	183	TYR	C-N-CA	8.83	138.40	121.54
1	B	342	SER	O-C-N	-8.82	104.83	122.22
1	A	652	HIS	O-C-N	8.82	133.36	123.04
1	A	644	HIS	CA-CB-CG	8.81	122.61	113.80
1	B	233	PHE	N-CA-CB	8.81	123.07	109.94
1	A	211	TYR	N-CA-CB	-8.80	96.29	110.55
1	E	49	HIS	CA-C-N	8.80	133.40	120.11
1	E	49	HIS	C-N-CA	8.80	133.40	120.11
1	A	616	TYR	CA-C-O	-8.80	112.32	119.71
1	A	47	ASN	CA-C-O	-8.79	108.77	119.59
1	A	153	LYS	CA-C-N	8.80	132.40	120.44
1	A	153	LYS	C-N-CA	8.80	132.40	120.44
1	B	224	HIS	CA-C-N	-8.80	107.61	120.28
1	B	224	HIS	C-N-CA	-8.80	107.61	120.28
1	A	300	ILE	CA-C-N	-8.78	105.75	120.68
1	A	300	ILE	C-N-CA	-8.78	105.75	120.68
1	A	634	ARG	CB-CG-CD	8.78	131.49	111.30
1	B	530	VAL	N-CA-CB	-8.78	98.92	111.21
1	A	260	THR	CA-CB-CG2	8.77	125.41	110.50
1	A	231	PHE	N-CA-CB	8.77	122.71	109.91
1	A	110	MET	O-C-N	-8.77	112.99	123.16
1	C	243	VAL	N-CA-C	8.77	120.89	109.58
1	A	91	ASN	CA-C-O	-8.76	109.45	119.79
1	B	206	GLU	CG-CD-OE1	8.76	138.56	118.40
1	B	222	TRP	N-CA-C	8.76	121.63	111.11
1	A	278	GLU	O-C-N	8.76	133.44	123.19
1	F	47	ASN	CA-CB-CG	8.76	121.36	112.60
1	B	49	HIS	CA-CB-CG	-8.74	105.06	113.80
1	B	467	SER	CA-C-N	8.74	135.70	122.77
1	B	467	SER	C-N-CA	8.74	135.70	122.77
1	A	205	TRP	O-C-N	-8.73	112.59	123.06
1	B	529	THR	CA-CB-OG1	-8.73	96.51	109.60
1	B	539	LEU	CA-C-O	-8.72	107.95	119.11
1	F	509	PHE	CA-CB-CG	8.72	122.52	113.80
1	B	313	ILE	O-C-N	-8.72	114.57	123.03
1	A	478	PHE	CA-CB-CG	-8.72	105.08	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	273	ASP	CA-CB-CG	8.71	121.31	112.60
1	B	546	ALA	N-CA-C	-8.71	99.38	112.54
1	A	418	ILE	CA-C-N	8.71	134.94	122.05
1	A	418	ILE	C-N-CA	8.71	134.94	122.05
1	B	19	ASP	CA-CB-CG	8.70	121.30	112.60
1	B	73	SER	N-CA-CB	8.70	125.97	110.83
1	B	606	HIS	CA-CB-CG	-8.70	105.10	113.80
1	B	107	ARG	NE-CZ-NH2	8.69	127.03	119.20
1	A	213	LEU	CB-CA-C	8.69	124.54	110.29
1	A	124	ILE	O-C-N	-8.69	113.10	121.87
1	D	243	VAL	N-CA-C	8.69	120.78	109.58
1	B	265	GLY	O-C-N	-8.68	111.42	122.70
1	B	305	ILE	O-C-N	8.68	132.13	122.93
1	A	479	ARG	CA-C-O	-8.67	111.30	120.58
1	B	63	HIS	CA-C-O	-8.67	108.11	120.51
1	A	35	GLU	OE1-CD-OE2	-8.67	102.09	122.90
1	A	47	ASN	N-CA-C	-8.67	103.22	112.93
1	C	47	ASN	CA-CB-CG	8.67	121.27	112.60
1	E	243	VAL	N-CA-C	8.67	120.76	109.58
1	B	124	ILE	CA-C-O	-8.66	111.99	121.17
1	B	74	LEU	N-CA-C	-8.66	102.70	113.18
1	A	329	GLU	N-CA-C	-8.65	101.57	112.90
1	F	243	VAL	N-CA-C	8.65	120.74	109.58
1	B	560	ARG	NE-CZ-NH1	8.64	130.15	121.50
1	A	526	SER	N-CA-C	8.63	121.46	110.24
1	F	48	ASP	CA-CB-CG	8.63	121.23	112.60
1	A	47	ASN	OD1-CG-ND2	-8.63	113.97	122.60
1	A	387	MET	CB-CA-C	-8.63	96.47	110.79
1	E	224	HIS	CA-CB-CG	-8.63	105.17	113.80
1	C	67	GLU	CA-CB-CG	8.62	131.35	114.10
1	B	387	MET	CA-CB-CG	8.62	131.33	114.10
1	B	452	VAL	CA-C-N	8.61	134.82	122.85
1	B	452	VAL	C-N-CA	8.61	134.82	122.85
1	A	336	ASN	CA-CB-CG	8.60	121.20	112.60
1	B	25	THR	CB-CA-C	-8.60	93.63	109.46
1	B	217	GLY	CA-C-N	-8.60	108.75	120.28
1	B	217	GLY	C-N-CA	-8.60	108.75	120.28
1	A	46	TYR	O-C-N	8.59	133.12	123.16
1	B	587	THR	CA-CB-OG1	-8.59	96.72	109.60
1	D	206	GLU	CG-CD-OE1	8.58	138.14	118.40
1	A	467	SER	N-CA-C	8.58	124.37	109.96
1	D	276	HIS	CA-CB-CG	-8.58	105.22	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	MET	CA-CB-CG	8.57	131.25	114.10
1	A	641	ASN	OD1-CG-ND2	8.57	131.18	122.60
1	B	147	ASN	CA-C-O	-8.57	108.25	120.51
1	A	317	GLN	CG-CD-OE1	8.57	137.93	120.80
1	D	513	PRO	N-CA-C	8.57	130.12	112.47
1	F	179	GLN	N-CA-C	-8.57	92.55	110.80
1	F	254	GLU	N-CA-C	8.57	123.68	107.75
1	A	39	PRO	CB-CA-C	8.56	124.12	111.62
1	B	225	HIS	CA-C-O	8.56	129.78	120.10
1	B	489	ASN	CA-C-N	-8.56	107.03	120.91
1	B	489	ASN	C-N-CA	-8.56	107.03	120.91
1	D	56	LEU	N-CA-C	-8.56	100.20	111.24
1	D	125	HIS	CA-CB-CG	-8.56	105.24	113.80
1	B	100	ARG	NH1-CZ-NH2	-8.55	108.19	119.30
1	E	162	LYS	N-CA-C	-8.54	95.47	109.82
1	F	49	HIS	N-CA-C	-8.54	102.16	112.58
1	A	277	PHE	N-CA-CB	8.54	124.92	110.49
1	B	488	ASN	N-CA-CB	8.54	124.92	110.49
1	A	625	PRO	N-CD-CG	-8.53	93.56	103.80
1	A	628	ARG	CB-CA-C	8.54	126.22	109.66
1	C	179	GLN	N-CA-C	-8.54	92.62	110.80
1	E	67	GLU	CA-CB-CG	8.54	131.17	114.10
1	A	336	ASN	OD1-CG-ND2	-8.53	114.07	122.60
1	B	237	SER	CA-CB-OG	-8.53	94.05	111.10
1	D	644	HIS	CA-CB-CG	8.52	122.32	113.80
1	B	405	ASN	CA-C-N	8.52	134.94	120.71
1	B	405	ASN	C-N-CA	8.52	134.94	120.71
1	F	67	GLU	CA-CB-CG	8.52	131.14	114.10
1	B	350	MET	CG-SD-CE	-8.52	82.17	100.90
1	B	365	PRO	CA-C-O	-8.51	110.05	122.31
1	D	419	ASP	CB-CA-C	8.51	124.98	112.05
1	A	283	VAL	CB-CA-C	8.51	125.24	111.29
1	A	358	HIS	CB-CA-C	8.51	126.05	109.72
1	B	257	ALA	O-C-N	8.50	128.96	121.39
1	B	379	SER	O-C-N	-8.50	110.73	122.46
1	A	385	LYS	CA-C-O	-8.50	108.35	120.51
1	E	48	ASP	CA-CB-CG	8.50	121.10	112.60
1	B	117	TYR	O-C-N	8.50	130.87	122.03
1	A	471	ASP	CA-C-O	8.49	132.66	120.51
1	B	263	LYS	N-CA-C	-8.49	101.04	111.40
1	C	49	HIS	N-CA-C	-8.49	102.22	112.58
1	E	179	GLN	N-CA-C	-8.49	92.71	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	82	GLU	CA-C-O	8.49	129.91	121.00
1	A	62	ASP	OD1-CG-OD2	-8.49	102.53	122.90
1	A	8	ALA	CB-CA-C	-8.48	97.23	110.81
1	C	48	ASP	CA-CB-CG	8.48	121.08	112.60
1	A	12	GLN	O-C-N	-8.48	113.21	122.03
1	A	470	ASN	OD1-CG-ND2	8.47	131.07	122.60
1	E	637	ASP	CA-CB-CG	8.47	121.07	112.60
1	A	225	HIS	N-CA-C	-8.47	102.00	111.82
1	A	320	GLY	O-C-N	8.47	133.71	122.70
1	A	435	ASN	CB-CG-OD1	-8.46	103.87	120.80
1	D	67	GLU	CA-CB-CG	8.46	131.03	114.10
1	A	157	ALA	N-CA-CB	8.46	122.28	110.01
1	D	279	ASP	CB-CA-C	8.46	122.34	110.16
1	A	545	ASN	N-CA-C	-8.46	102.51	113.17
1	B	142	PRO	CA-C-O	8.46	130.53	118.86
1	A	83	ALA	CB-CA-C	-8.45	96.31	110.68
1	B	86	LEU	CB-CA-C	8.45	125.22	110.85
1	D	179	GLN	N-CA-C	-8.45	92.80	110.80
1	F	92	GLN	CA-CB-CG	8.45	130.99	114.10
1	E	145	PHE	CA-CB-CG	8.45	122.25	113.80
1	A	274	ASN	OD1-CG-ND2	8.44	131.04	122.60
1	A	356	ASP	OD1-CG-OD2	8.44	143.16	122.90
1	B	378	PRO	O-C-N	8.44	131.94	122.24
1	F	385	LYS	N-CA-C	-8.44	102.03	111.14
1	A	48	ASP	CA-C-O	8.43	128.56	119.03
1	A	175	LYS	O-C-N	8.43	136.50	123.00
1	B	485	ILE	N-CA-CB	8.43	125.14	111.23
1	B	497	GLU	O-C-N	8.43	132.64	122.27
1	A	261	SER	O-C-N	8.43	133.55	123.27
1	A	102	ASN	OD1-CG-ND2	8.42	131.02	122.60
1	B	36	ASN	N-CA-CB	-8.42	97.33	110.30
1	A	25	THR	CA-CB-OG1	-8.42	96.97	109.60
1	C	92	GLN	CA-CB-CG	8.42	130.93	114.10
1	B	112	GLU	CB-CG-CD	8.41	126.91	112.60
1	B	614	GLU	N-CA-CB	-8.41	96.27	110.49
1	B	496	ASP	CB-CG-OD2	8.41	137.75	118.40
1	A	243	VAL	CB-CA-C	-8.41	100.22	111.15
1	A	361	PHE	CA-CB-CG	-8.41	105.39	113.80
1	B	463	LYS	CB-CG-CD	8.41	130.64	111.30
1	A	542	GLN	CB-CG-CD	-8.40	98.31	112.60
1	B	226	GLN	CA-C-O	-8.40	110.91	120.24
1	C	206	GLU	CG-CD-OE1	8.40	137.72	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	645	VAL	N-CA-CB	-8.40	97.67	111.44
1	B	427	ASP	N-CA-CB	-8.40	96.30	110.49
1	A	66	LEU	CA-CB-CG	8.39	145.68	116.30
1	A	581	ASN	CA-CB-CG	8.38	120.98	112.60
1	B	33	ILE	CA-C-O	8.39	130.06	121.17
1	A	217	GLY	N-CA-C	-8.38	93.32	113.18
1	B	110	MET	N-CA-C	-8.38	97.43	110.42
1	B	309	ASP	CA-C-O	-8.38	109.21	119.18
1	A	365	PRO	CA-C-O	-8.38	111.48	121.95
1	B	268	PHE	CA-C-O	-8.38	112.30	119.59
1	B	191	ASN	O-C-N	8.37	131.00	122.12
1	A	585	ALA	CA-C-O	-8.37	111.04	120.66
1	A	510	GLN	OE1-CD-NE2	-8.37	114.23	122.60
1	B	315	ILE	O-C-N	-8.37	112.11	122.57
1	E	556	SER	N-CA-C	8.37	122.50	108.20
1	A	126	SER	CA-C-O	8.36	130.53	121.16
1	A	144	MET	O-C-N	8.36	133.53	122.33
1	B	562	CYS	N-CA-C	8.36	128.60	110.80
1	B	446	VAL	CB-CA-C	-8.36	98.38	110.83
1	A	582	LEU	O-C-N	8.35	132.71	123.27
1	C	279	ASP	CB-CA-C	8.35	122.18	110.16
1	B	396	ASP	CA-CB-CG	8.35	120.95	112.60
1	D	53	VAL	N-CA-C	-8.35	103.74	111.67
1	A	501	PHE	O-C-N	-8.34	111.03	122.46
1	B	141	THR	CA-C-N	8.34	128.54	119.87
1	B	141	THR	C-N-CA	8.34	128.54	119.87
1	A	143	HIS	CA-C-N	8.34	134.85	120.68
1	A	143	HIS	C-N-CA	8.34	134.85	120.68
1	A	383	LEU	CA-C-O	-8.33	110.39	119.97
1	A	410	GLY	CA-C-O	-8.33	106.08	120.57
1	B	85	MET	N-CA-CB	8.33	123.13	110.30
1	B	567	ARG	NE-CZ-NH2	-8.33	111.70	119.20
1	A	468	ASN	CA-C-O	-8.32	112.26	121.58
1	A	61	ASN	OD1-CG-ND2	8.32	130.92	122.60
1	C	558	TYR	N-CA-C	8.32	122.20	112.72
1	A	216	LYS	CA-CB-CG	8.31	130.73	114.10
1	A	562	CYS	CB-CA-C	-8.31	96.71	110.85
1	B	106	PHE	CA-C-O	-8.30	112.15	120.70
1	B	35	GLU	CG-CD-OE1	8.30	137.50	118.40
1	A	416	VAL	CB-CA-C	8.29	123.39	110.28
1	B	12	GLN	CB-CA-C	8.29	124.11	110.92
1	C	487	ASP	N-CA-C	8.29	123.39	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	554	ASP	N-CA-C	-8.29	103.28	112.72
1	B	43	THR	N-CA-C	-8.29	93.15	110.80
1	B	322	GLU	N-CA-C	-8.28	100.94	112.45
1	F	145	PHE	CA-CB-CG	8.28	122.08	113.80
1	B	214	ASP	O-C-N	-8.28	111.58	122.59
1	B	489	ASN	O-C-N	8.28	133.60	122.59
1	B	254	GLU	CB-CG-CD	8.28	126.67	112.60
1	B	443	ILE	CA-CB-CG2	8.27	124.57	110.50
1	A	202	PRO	CA-C-O	-8.27	111.97	121.56
1	B	496	ASP	O-C-N	8.27	133.59	122.59
1	B	31	LYS	N-CA-CB	8.27	122.27	110.12
1	B	84	LEU	CA-C-N	-8.27	106.62	120.68
1	B	84	LEU	C-N-CA	-8.27	106.62	120.68
1	A	391	PHE	N-CA-CB	8.26	122.36	110.13
1	A	140	ILE	CA-C-N	8.26	131.94	122.85
1	A	140	ILE	C-N-CA	8.26	131.94	122.85
1	A	548	ASN	N-CA-C	-8.26	102.22	112.88
1	B	573	SER	CA-CB-OG	-8.26	94.58	111.10
1	D	322	GLU	N-CA-CB	8.26	122.35	110.13
1	A	221	PHE	O-C-N	8.26	132.19	122.20
1	B	301	ASP	O-C-N	8.26	131.56	122.15
1	A	36	ASN	O-C-N	8.25	133.23	122.42
1	D	92	GLN	CA-CB-CG	8.25	130.60	114.10
1	A	286	VAL	O-C-N	8.24	130.20	121.87
1	B	186	GLU	O-C-N	-8.24	112.45	122.34
1	B	500	TRP	CB-CG-CD2	-8.24	115.26	126.80
1	A	193	HIS	ND1-CE1-NE2	8.24	116.64	108.40
1	B	163	PRO	CA-C-O	-8.24	111.27	122.15
1	A	101	SER	CB-CA-C	8.23	124.01	110.92
1	B	80	ARG	N-CA-CB	8.23	121.92	109.98
1	B	345	ASN	CB-CG-ND2	-8.22	104.06	116.40
1	B	407	GLU	CG-CD-OE2	8.22	137.31	118.40
1	B	397	SER	N-CA-C	-8.22	102.81	113.17
1	A	16	HIS	CA-CB-CG	-8.22	105.58	113.80
1	A	444	GLU	CA-CB-CG	8.22	130.53	114.10
1	A	503	ILE	CB-CG1-CD1	-8.22	96.55	113.80
1	A	567	ARG	CA-C-O	-8.21	110.82	120.10
1	B	49	HIS	CA-C-O	8.21	130.42	120.57
1	B	474	ARG	CG-CD-NE	8.21	130.06	112.00
1	D	273	ASP	CA-CB-CG	8.20	120.80	112.60
1	B	7	ASN	N-CA-CB	8.20	124.34	110.49
1	A	190	MET	N-CA-C	-8.20	102.30	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	456	ASN	CB-CG-OD1	-8.19	104.41	120.80
1	B	175	LYS	CA-CB-CG	8.19	130.48	114.10
1	B	474	ARG	NE-CZ-NH1	-8.19	113.31	121.50
1	B	198	HIS	CE1-NE2-CD2	8.19	117.19	109.00
1	B	607	ALA	CB-CA-C	8.19	124.72	110.64
1	B	619	ASN	CA-CB-CG	8.18	120.78	112.60
1	A	581	ASN	CA-C-O	-8.17	111.54	120.36
1	A	646	VAL	CA-C-O	-8.16	111.48	120.71
1	A	281	ASP	O-C-N	8.16	132.85	123.06
1	A	344	HIS	CA-C-O	-8.16	112.43	121.00
1	B	231	PHE	CE1-CZ-CE2	-8.16	105.32	120.00
1	B	556	SER	CA-C-N	8.15	137.11	121.54
1	B	556	SER	C-N-CA	8.15	137.11	121.54
1	A	186	GLU	CA-C-O	8.15	129.29	119.43
1	A	33	ILE	CA-C-N	8.15	132.01	120.28
1	A	33	ILE	C-N-CA	8.15	132.01	120.28
1	A	128	LEU	N-CA-CB	-8.15	98.10	110.73
1	A	73	SER	N-CA-CB	8.14	125.01	111.08
1	A	309	ASP	CA-C-O	-8.14	109.74	119.27
1	A	326	ASP	CB-CG-OD1	8.14	137.13	118.40
1	A	623	GLY	CA-C-N	8.14	132.47	120.83
1	A	623	GLY	C-N-CA	8.14	132.47	120.83
1	A	37	PHE	O-C-N	8.14	132.46	122.86
1	A	308	SER	N-CA-CB	8.13	124.08	110.41
1	A	588	ASP	CA-CB-CG	8.13	120.73	112.60
1	B	275	ILE	CB-CA-C	-8.13	97.96	111.29
1	B	112	GLU	CB-CA-C	-8.13	95.59	110.63
1	A	558	TYR	N-CA-CB	-8.13	98.01	110.44
1	B	385	LYS	N-CA-C	-8.13	102.36	111.14
1	A	362	ASN	CA-C-O	8.12	132.19	122.03
1	B	353	ARG	CD-NE-CZ	-8.12	113.03	124.40
1	C	216	LYS	N-CA-CB	8.13	122.61	109.28
1	B	358	HIS	CA-CB-CG	-8.12	105.68	113.80
1	B	387	MET	N-CA-CB	8.12	122.25	110.06
1	B	463	LYS	N-CA-CB	8.12	124.09	110.69
1	F	125	HIS	CA-CB-CG	-8.12	105.68	113.80
1	A	474	ARG	CD-NE-CZ	8.12	135.76	124.40
1	B	413	VAL	O-C-N	8.11	131.92	122.83
1	C	125	HIS	CA-CB-CG	-8.11	105.69	113.80
1	A	168	VAL	CA-C-N	8.11	139.31	121.80
1	A	168	VAL	C-N-CA	8.11	139.31	121.80
1	B	224	HIS	ND1-CE1-NE2	8.10	116.50	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	637	ASP	CA-CB-CG	8.10	120.70	112.60
1	A	233	PHE	CB-CA-C	-8.10	98.16	110.88
1	A	311	HIS	CA-CB-CG	-8.10	105.70	113.80
1	A	473	GLU	CB-CG-CD	8.10	126.36	112.60
1	F	562	CYS	N-CA-C	8.10	120.18	111.36
1	B	87	PHE	O-C-N	-8.09	113.54	122.12
1	A	520	GLU	OE1-CD-OE2	8.09	142.31	122.90
1	A	29	ASP	CB-CG-OD2	-8.08	99.81	118.40
1	A	316	ARG	CG-CD-NE	8.08	129.78	112.00
1	B	133	VAL	O-C-N	-8.08	113.64	123.10
1	A	310	GLY	N-CA-C	-8.08	103.85	115.64
1	A	624	TYR	CG-CD2-CE2	8.08	133.32	121.20
1	A	327	ILE	N-CA-C	-8.07	101.13	113.16
1	B	464	ILE	CA-C-O	-8.07	110.90	120.75
1	A	288	ASP	CA-CB-CG	-8.06	104.54	112.60
1	A	469	ASN	CA-CB-CG	8.06	120.66	112.60
1	B	637	ASP	CA-CB-CG	8.06	120.66	112.60
1	B	21	ILE	O-C-N	8.06	131.24	122.06
1	E	322	GLU	N-CA-CB	8.05	122.05	110.13
1	B	35	GLU	CA-C-O	8.05	130.94	120.07
1	B	345	ASN	CA-CB-CG	-8.05	104.55	112.60
1	B	47	ASN	OD1-CG-ND2	8.05	130.65	122.60
1	A	7	ASN	N-CA-CB	8.04	124.08	110.49
1	A	74	LEU	O-C-N	8.04	134.29	122.39
1	A	567	ARG	NE-CZ-NH2	-8.04	111.97	119.20
1	B	403	HIS	N-CA-C	-8.04	102.11	111.03
1	A	86	LEU	CA-C-O	-8.03	112.31	120.90
1	A	119	LEU	O-C-N	-8.03	113.74	122.09
1	A	594	GLU	CB-CG-CD	-8.03	98.95	112.60
1	C	637	ASP	CA-CB-CG	8.02	120.62	112.60
1	E	47	ASN	CA-CB-CG	8.02	120.62	112.60
1	B	218	GLU	CA-C-O	-8.02	112.05	120.55
1	E	125	HIS	CA-CB-CG	-8.02	105.78	113.80
1	B	365	PRO	CA-C-N	-8.01	115.34	122.47
1	B	365	PRO	C-N-CA	-8.01	115.34	122.47
1	B	429	PHE	N-CA-CB	-8.01	97.61	111.55
1	C	273	ASP	CA-CB-CG	8.01	120.61	112.60
1	A	435	ASN	O-C-N	8.01	133.51	122.46
1	A	281	ASP	CA-CB-CG	8.01	120.61	112.60
1	A	360	LYS	N-CA-CB	8.01	122.30	110.53
1	A	96	TRP	CA-C-O	-8.01	109.06	120.51
1	A	321	ILE	O-C-N	8.01	131.19	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	509	PHE	CA-CB-CG	8.01	121.81	113.80
1	A	24	PRO	O-C-N	8.00	133.44	122.64
1	D	224	HIS	CA-CB-CG	-8.00	105.80	113.80
1	A	169	SER	N-CA-CB	-8.00	97.79	110.19
1	A	478	PHE	CA-C-O	-8.00	112.30	121.66
1	B	208	SER	O-C-N	7.99	131.26	122.15
1	E	423	ILE	CB-CA-C	7.99	122.90	110.28
1	A	270	VAL	CA-C-O	7.99	130.88	121.93
1	B	494	THR	CA-CB-OG1	7.98	121.57	109.60
1	A	54	GLU	CB-CG-CD	-7.98	99.04	112.60
1	A	585	ALA	N-CA-C	-7.97	95.92	109.24
1	B	11	GLN	CB-CG-CD	-7.97	99.05	112.60
1	A	438	ASP	CB-CA-C	7.97	122.87	109.80
1	A	548	ASN	OD1-CG-ND2	-7.96	114.64	122.60
1	A	287	HIS	CG-CD2-NE2	-7.96	99.24	107.20
1	A	114	GLU	N-CA-C	-7.95	102.30	110.97
1	B	348	HIS	ND1-CE1-NE2	7.95	116.35	108.40
1	A	55	THR	CA-CB-OG1	-7.95	97.67	109.60
1	A	629	ARG	CA-CB-CG	7.95	130.00	114.10
1	B	10	LYS	CG-CD-CE	7.95	129.58	111.30
1	A	106	PHE	CA-CB-CG	-7.94	105.86	113.80
1	A	446	VAL	CA-C-O	-7.94	112.06	120.48
1	E	92	GLN	CA-CB-CG	7.94	129.99	114.10
1	A	558	TYR	CA-C-N	-7.93	110.07	121.42
1	A	558	TYR	C-N-CA	-7.93	110.07	121.42
1	B	139	GLN	CB-CA-C	7.93	122.40	109.07
1	B	178	GLU	CB-CA-C	-7.93	94.63	110.42
1	E	326	ASP	CA-CB-CG	7.93	120.53	112.60
1	A	395	THR	O-C-N	7.93	130.24	122.07
1	A	572	LYS	O-C-N	7.93	130.53	122.12
1	B	480	ILE	CA-C-O	-7.93	112.54	120.31
1	B	278	GLU	CA-CB-CG	-7.91	98.27	114.10
1	B	372	GLU	CG-CD-OE1	-7.91	100.20	118.40
1	E	303	GLY	N-CA-C	-7.91	105.07	114.48
1	F	326	ASP	CA-CB-CG	7.91	120.51	112.60
1	B	407	GLU	CA-C-O	7.90	129.88	121.19
1	B	611	VAL	N-CA-CB	-7.90	98.20	111.23
1	A	646	VAL	CA-C-N	7.90	136.18	121.97
1	A	646	VAL	C-N-CA	7.90	136.18	121.97
1	A	469	ASN	CB-CA-C	7.89	126.80	110.31
1	F	222	TRP	N-CA-C	7.89	119.51	111.07
1	A	37	PHE	CA-C-O	-7.89	112.96	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	HIS	O-C-N	7.89	130.61	122.09
1	B	257	ALA	N-CA-C	-7.89	96.78	109.40
1	B	220	PHE	O-C-N	-7.89	113.57	122.09
1	B	401	TYR	CA-CB-CG	7.89	128.10	113.90
1	A	42	ASP	CA-CB-CG	7.88	120.48	112.60
1	B	574	LYS	CB-CA-C	7.88	120.67	108.61
1	A	456	ASN	OD1-CG-ND2	-7.88	114.72	122.60
1	E	49	HIS	N-CA-C	-7.88	102.97	112.58
1	B	438	ASP	CA-CB-CG	-7.88	104.72	112.60
1	A	502	CYS	CA-C-O	7.88	129.87	120.81
1	B	229	ALA	CB-CA-C	-7.88	98.74	110.95
1	A	367	VAL	O-C-N	-7.88	113.95	121.90
1	B	302	HIS	CA-C-N	-7.87	114.27	123.08
1	B	302	HIS	C-N-CA	-7.87	114.27	123.08
1	A	314	ASP	CA-CB-CG	-7.86	104.74	112.60
1	A	322	GLU	CB-CA-C	7.86	125.08	110.70
1	A	514	SER	CA-C-N	-7.86	109.53	121.87
1	A	514	SER	C-N-CA	-7.86	109.53	121.87
1	B	596	HIS	CA-C-O	-7.86	107.44	120.80
1	A	210	GLY	N-CA-C	7.86	131.81	113.18
1	A	380	PHE	CB-CA-C	7.86	123.22	110.88
1	D	219	LEU	CB-CA-C	7.86	123.38	110.81
1	A	228	THR	CA-CB-CG2	7.85	123.84	110.50
1	B	432	SER	N-CA-CB	-7.85	98.23	110.55
1	B	424	THR	CA-C-O	-7.84	112.30	121.16
1	D	326	ASP	CA-CB-CG	7.84	120.44	112.60
1	B	193	HIS	CA-CB-CG	7.84	121.64	113.80
1	B	408	PHE	N-CA-CB	7.83	125.31	110.82
1	E	222	TRP	N-CA-C	7.83	119.45	111.07
1	C	443	ILE	N-CA-C	-7.83	97.18	108.53
1	B	112	GLU	N-CA-C	7.83	120.71	111.71
1	B	192	ILE	CA-CB-CG1	-7.83	97.09	110.40
1	A	29	ASP	O-C-N	7.83	131.64	122.17
1	A	94	LYS	CD-CE-NZ	7.82	136.94	111.90
1	B	221	PHE	CA-C-N	7.82	131.10	120.54
1	B	221	PHE	C-N-CA	7.82	131.10	120.54
1	A	440	GLY	O-C-N	7.82	132.87	122.70
1	A	363	LEU	N-CA-CB	-7.82	100.57	110.03
1	B	198	HIS	CB-CA-C	-7.82	97.28	110.81
1	B	479	ARG	CA-C-O	7.82	128.92	120.32
1	D	222	TRP	N-CA-C	7.82	119.43	111.07
1	A	10	LYS	O-C-N	7.81	130.44	122.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	442	ASN	CA-C-N	7.81	133.38	123.14
1	A	442	ASN	C-N-CA	7.81	133.38	123.14
1	B	556	SER	CA-CB-OG	7.81	126.72	111.10
1	A	293	GLU	CA-C-N	7.81	131.06	120.44
1	A	293	GLU	C-N-CA	7.81	131.06	120.44
1	A	149	GLU	CG-CD-OE2	-7.80	100.45	118.40
1	A	291	ILE	CB-CG1-CD1	-7.80	97.41	113.80
1	B	639	VAL	N-CA-C	-7.80	97.25	108.17
1	A	394	HIS	CA-CB-CG	-7.80	106.00	113.80
1	B	474	ARG	NE-CZ-NH2	7.80	126.22	119.20
1	A	367	VAL	CA-C-O	7.79	129.13	120.64
1	A	470	ASN	O-C-N	-7.79	112.22	122.59
1	A	177	ARG	O-C-N	-7.79	112.23	122.59
1	B	40	LEU	CA-C-O	-7.79	110.76	119.95
1	A	458	ASN	CB-CG-OD1	7.78	136.36	120.80
1	A	490	GLY	N-CA-C	-7.78	103.97	115.72
1	A	344	HIS	CE1-NE2-CD2	7.78	116.78	109.00
1	A	510	GLN	CB-CG-CD	-7.78	99.38	112.60
1	B	559	GLU	N-CA-CB	7.78	123.48	110.41
1	B	295	ARG	NE-CZ-NH1	-7.78	113.72	121.50
1	C	222	TRP	N-CA-C	7.77	119.39	111.07
1	A	115	PHE	CA-CB-CG	-7.77	106.03	113.80
1	A	289	LEU	O-C-N	7.77	130.42	122.03
1	C	326	ASP	CA-CB-CG	7.77	120.37	112.60
1	A	19	ASP	CA-CB-CG	7.77	120.37	112.60
1	A	417	ALA	CB-CA-C	-7.77	95.64	109.70
1	A	579	GLU	CA-C-O	7.76	128.86	120.32
1	B	376	ARG	O-C-N	7.76	130.47	122.09
1	E	219	LEU	CB-CA-C	7.76	123.23	110.81
1	A	515	GLY	N-CA-C	-7.76	96.51	112.34
1	B	290	GLU	CB-CG-CD	7.76	125.79	112.60
1	F	639	VAL	N-CA-C	-7.75	97.31	108.17
1	B	31	LYS	CA-C-N	-7.75	107.77	120.72
1	B	31	LYS	C-N-CA	-7.75	107.77	120.72
1	A	646	VAL	CB-CA-C	7.75	120.52	110.91
1	B	357	PRO	CA-C-N	-7.75	106.47	121.58
1	B	357	PRO	C-N-CA	-7.75	106.47	121.58
1	A	372	GLU	CA-C-O	7.75	128.80	119.43
1	B	345	ASN	CA-C-O	-7.75	112.55	121.07
1	B	62	ASP	N-CA-C	-7.75	103.97	113.19
1	A	344	HIS	ND1-CE1-NE2	-7.74	100.66	108.40
1	A	557	ALA	N-CA-CB	7.74	123.58	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	449	ASN	CA-CB-CG	-7.74	104.86	112.60
1	F	322	GLU	N-CA-CB	7.74	122.19	110.19
1	A	496	ASP	O-C-N	7.74	132.89	122.59
1	B	183	TYR	N-CA-CB	7.74	121.67	110.06
1	A	533	MET	O-C-N	7.74	130.57	121.21
1	B	260	THR	OG1-CB-CG2	7.74	124.78	109.30
1	A	368	MET	CA-C-N	-7.73	110.11	122.95
1	A	368	MET	C-N-CA	-7.73	110.11	122.95
1	A	181	VAL	CA-C-N	7.73	130.64	120.28
1	A	181	VAL	C-N-CA	7.73	130.64	120.28
1	A	405	ASN	CA-CB-CG	-7.73	104.87	112.60
1	C	281	ASP	CA-CB-CG	7.73	120.33	112.60
1	C	219	LEU	CB-CA-C	7.72	123.16	110.81
1	A	304	TYR	N-CA-C	7.72	121.19	109.23
1	B	201	PHE	CD1-CG-CD2	7.72	130.18	118.60
1	A	563	GLY	N-CA-C	7.72	131.47	113.18
1	B	549	GLY	O-C-N	-7.71	112.67	122.70
1	A	301	ASP	CA-CB-CG	7.71	120.31	112.60
1	B	261	SER	O-C-N	7.71	132.72	123.24
1	A	154	ALA	CA-C-O	-7.71	112.76	120.70
1	B	416	VAL	CA-CB-CG1	7.70	123.49	110.40
1	C	639	VAL	N-CA-C	-7.70	97.39	108.17
1	A	78	ARG	O-C-N	7.70	131.17	122.32
1	C	555	LEU	CA-CB-CG	7.70	143.24	116.30
1	E	434	ILE	N-CA-C	7.69	118.49	110.72
1	B	165	THR	O-C-N	-7.69	114.24	123.16
1	D	637	ASP	CA-CB-CG	7.69	120.29	112.60
1	C	322	GLU	N-CA-CB	7.69	122.11	110.19
1	B	269	PRO	CB-CA-C	7.69	121.07	111.23
1	B	595	GLY	CA-C-N	-7.69	107.86	121.70
1	B	595	GLY	C-N-CA	-7.69	107.86	121.70
1	A	350	MET	CA-C-O	-7.68	112.41	120.55
1	B	301	ASP	CA-C-O	-7.68	112.28	120.42
1	D	303	GLY	N-CA-C	-7.68	105.34	114.48
1	B	449	ASN	OD1-CG-ND2	7.68	130.28	122.60
1	B	194	HIS	CE1-NE2-CD2	7.67	116.67	109.00
1	D	420	GLY	N-CA-C	7.67	124.66	111.16
1	A	608	GLN	OE1-CD-NE2	7.67	130.26	122.60
1	A	207	ASP	CA-CB-CG	7.66	120.26	112.60
1	A	619	ASN	CA-CB-CG	-7.66	104.94	112.60
1	B	405	ASN	CB-CG-ND2	-7.66	104.91	116.40
1	D	281	ASP	CA-CB-CG	7.66	120.26	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	TYR	O-C-N	-7.66	115.03	121.23
1	D	639	VAL	N-CA-C	-7.66	97.45	108.17
1	F	561	SER	N-CA-C	7.65	127.10	110.80
1	A	40	LEU	N-CA-CB	-7.65	98.87	110.73
1	B	329	GLU	CA-C-N	7.65	136.16	121.54
1	B	329	GLU	C-N-CA	7.65	136.16	121.54
1	B	43	THR	N-CA-CB	-7.65	97.57	110.49
1	D	407	GLU	CA-C-O	7.65	129.60	120.81
1	A	401	TYR	CA-C-O	-7.64	112.13	120.92
1	B	292	THR	CA-CB-OG1	-7.64	98.14	109.60
1	A	142	PRO	N-CA-CB	7.64	110.59	103.41
1	A	109	ARG	CA-C-N	7.63	133.39	122.09
1	A	109	ARG	C-N-CA	7.63	133.39	122.09
1	B	257	ALA	CA-C-O	-7.63	111.90	119.69
1	B	159	MET	N-CA-CB	7.63	121.08	110.01
1	B	529	THR	N-CA-C	7.63	121.93	109.72
1	A	35	GLU	CG-CD-OE2	7.63	135.95	118.40
1	A	323	LEU	N-CA-C	-7.62	101.96	111.11
1	B	68	GLN	O-C-N	7.62	131.60	122.68
1	B	526	SER	CA-CB-OG	-7.62	95.85	111.10
1	A	253	ARG	NH1-CZ-NH2	-7.62	109.39	119.30
1	F	434	ILE	N-CA-C	7.62	118.42	110.72
1	A	653	LEU	N-CA-CB	-7.61	97.56	110.50
1	B	626	LEU	CA-C-O	-7.61	110.66	119.56
1	B	254	GLU	N-CA-C	7.61	122.33	107.57
1	A	543	ALA	O-C-N	-7.60	113.88	122.09
1	A	572	LYS	CA-C-O	-7.60	112.49	120.55
1	B	7	ASN	N-CA-C	-7.60	94.61	110.80
1	B	548	ASN	CB-CG-OD1	7.60	136.01	120.80
1	F	219	LEU	CB-CA-C	7.60	122.97	110.81
1	A	304	TYR	CA-C-O	7.60	129.88	121.06
1	A	526	SER	CA-CB-OG	-7.60	95.90	111.10
1	B	190	MET	O-C-N	7.60	131.37	122.17
1	B	393	LYS	CB-CA-C	-7.60	98.18	110.79
1	A	290	GLU	CB-CG-CD	7.59	125.51	112.60
1	A	363	LEU	CB-CA-C	7.59	119.80	108.86
1	A	463	LYS	N-CA-C	-7.59	91.84	107.70
1	B	305	ILE	CA-C-O	-7.59	112.03	120.84
1	A	510	GLN	CA-C-O	-7.59	111.93	120.66
1	A	114	GLU	O-C-N	7.58	129.91	122.03
1	A	132	ILE	CA-C-O	-7.58	113.78	121.59
1	B	505	LEU	O-C-N	-7.58	111.60	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	361	PHE	CA-CB-CG	-7.58	106.22	113.80
1	A	123	VAL	CB-CA-C	7.58	121.67	111.97
1	B	38	ASN	O-C-N	7.57	125.81	121.27
1	B	452	VAL	CA-C-O	7.57	131.31	121.32
1	A	237	SER	N-CA-C	-7.57	103.79	112.87
1	A	78	ARG	CD-NE-CZ	7.57	134.99	124.40
1	A	412	VAL	O-C-N	-7.56	115.24	123.03
1	B	510	GLN	OE1-CD-NE2	7.56	130.16	122.60
1	A	200	ASP	CA-C-N	-7.56	113.26	123.46
1	A	200	ASP	C-N-CA	-7.56	113.26	123.46
1	B	138	TYR	CA-C-N	-7.56	109.72	122.11
1	B	138	TYR	C-N-CA	-7.56	109.72	122.11
1	A	528	VAL	N-CA-C	7.56	119.39	112.29
1	A	18	LEU	N-CA-CB	-7.55	100.13	110.56
1	A	178	GLU	N-CA-C	-7.55	101.50	110.41
1	B	204	TRP	N-CA-C	7.55	122.14	113.15
1	B	198	HIS	CG-CD2-NE2	-7.55	99.65	107.20
1	B	216	LYS	N-CA-CB	7.55	123.25	110.49
1	E	639	VAL	N-CA-C	-7.55	97.60	108.17
1	A	254	GLU	CB-CA-C	-7.55	99.00	111.68
1	B	511	LYS	CA-C-O	-7.55	112.45	121.05
1	A	175	LYS	CA-C-O	-7.54	107.97	120.80
1	C	224	HIS	CA-CB-CG	-7.54	106.26	113.80
1	B	102	ASN	O-C-N	7.54	130.15	122.08
1	B	403	HIS	CA-CB-CG	7.54	121.34	113.80
1	A	207	ASP	OD1-CG-OD2	-7.54	104.81	122.90
1	A	312	THR	N-CA-C	-7.54	96.96	109.24
1	B	376	ARG	NE-CZ-NH2	-7.54	112.42	119.20
1	B	133	VAL	N-CA-CB	7.53	120.94	111.46
1	B	335	SER	CA-C-O	-7.52	111.89	120.24
1	B	448	ILE	CB-CG1-CD1	-7.52	98.01	113.80
1	B	466	MET	CB-CA-C	-7.52	97.62	109.72
1	A	53	VAL	CG1-CB-CG2	7.51	127.32	110.80
1	A	649	ILE	O-C-N	7.51	131.37	123.26
1	B	596	HIS	CA-CB-CG	-7.51	106.29	113.80
1	A	364	PRO	CA-C-N	7.51	127.95	119.92
1	A	364	PRO	C-N-CA	7.51	127.95	119.92
1	F	252	ILE	N-CA-C	-7.50	95.67	106.55
1	A	515	GLY	O-C-N	7.50	129.27	121.77
1	A	631	PRO	CA-C-O	-7.50	106.95	120.60
1	A	411	MET	CA-C-O	-7.50	113.45	120.95
1	A	639	VAL	O-C-N	7.50	131.05	123.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	THR	CA-C-O	7.50	129.54	120.92
1	B	251	ILE	CA-C-N	-7.50	113.65	122.95
1	B	251	ILE	C-N-CA	-7.50	113.65	122.95
1	B	423	ILE	N-CA-CB	-7.50	99.44	111.58
1	A	509	PHE	CA-C-N	7.49	134.87	122.73
1	A	509	PHE	C-N-CA	7.49	134.87	122.73
1	B	52	ALA	CA-C-N	7.49	130.72	120.46
1	B	52	ALA	C-N-CA	7.49	130.72	120.46
1	B	422	LEU	CB-CA-C	7.49	123.00	110.79
1	B	344	HIS	CA-CB-CG	-7.49	106.31	113.80
1	E	92	GLN	CB-CG-CD	-7.48	99.88	112.60
1	A	296	ILE	CB-CG1-CD1	-7.48	98.09	113.80
1	B	542	GLN	CA-CB-CG	7.48	129.06	114.10
1	E	279	ASP	N-CA-C	-7.48	98.82	109.96
1	A	533	MET	N-CA-CB	7.47	120.49	109.88
1	A	514	SER	CA-CB-OG	7.47	126.05	111.10
1	B	51	ALA	N-CA-CB	-7.47	98.70	110.28
1	C	556	SER	N-CA-C	-7.47	95.52	108.52
1	B	194	HIS	CG-CD2-NE2	-7.47	99.73	107.20
1	A	273	ASP	CB-CA-C	7.47	122.90	109.83
1	A	588	ASP	N-CA-C	7.47	122.17	108.58
1	B	66	LEU	O-C-N	-7.47	113.68	122.87
1	A	157	ALA	CA-C-O	-7.47	112.98	120.82
1	A	616	TYR	N-CA-C	-7.47	100.39	109.57
1	A	391	PHE	CA-C-O	-7.46	112.56	120.55
1	B	572	LYS	N-CA-C	7.46	119.50	111.36
1	A	649	ILE	CA-C-O	-7.46	112.55	120.39
1	F	279	ASP	N-CA-C	-7.46	98.84	109.96
1	B	24	PRO	O-C-N	7.46	132.71	122.64
1	B	86	LEU	N-CA-C	-7.46	103.23	111.36
1	B	294	SER	O-C-N	7.46	130.15	122.09
1	B	486	GLU	CG-CD-OE1	7.46	135.56	118.40
1	A	373	THR	N-CA-C	7.45	125.64	114.09
1	A	458	ASN	OD1-CG-ND2	-7.45	115.15	122.60
1	B	511	LYS	O-C-N	7.45	131.81	123.01
1	C	434	ILE	N-CA-C	7.45	118.25	110.72
1	A	49	HIS	O-C-N	7.45	132.39	122.41
1	B	15	ASN	CA-CB-CG	7.45	120.05	112.60
1	B	147	ASN	CB-CA-C	-7.45	95.60	110.42
1	B	502	CYS	CA-CB-SG	7.45	131.53	114.40
1	B	508	PHE	O-C-N	7.45	131.75	123.33
1	B	620	ARG	CD-NE-CZ	-7.45	113.98	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ARG	O-C-N	7.44	131.79	122.86
1	A	305	ILE	CA-CB-CG1	7.44	123.05	110.40
1	B	137	LEU	CA-C-O	-7.43	109.88	120.51
1	B	149	GLU	CA-C-O	7.43	128.60	120.80
1	B	162	LYS	N-CA-C	-7.43	99.10	110.32
1	B	492	THR	CA-CB-OG1	-7.43	98.45	109.60
1	B	584	VAL	CB-CA-C	7.43	121.81	110.96
1	C	303	GLY	N-CA-C	-7.43	105.64	114.48
1	D	279	ASP	N-CA-C	-7.43	98.89	109.96
1	B	243	VAL	CB-CA-C	-7.43	99.97	111.26
1	A	10	LYS	CB-CG-CD	7.43	128.38	111.30
1	F	281	ASP	CA-CB-CG	7.43	120.03	112.60
1	A	534	PRO	N-CD-CG	-7.42	92.06	103.20
1	B	162	LYS	CA-C-N	7.42	127.87	120.52
1	B	162	LYS	C-N-CA	7.42	127.87	120.52
1	B	100	ARG	NE-CZ-NH1	7.42	128.92	121.50
1	E	443	ILE	N-CA-C	-7.42	97.04	107.80
1	A	13	ASP	O-C-N	7.42	129.98	122.12
1	B	40	LEU	CB-CA-C	-7.42	99.08	111.02
1	B	411	MET	O-C-N	-7.42	112.73	122.59
1	B	134	LEU	CB-CA-C	7.41	120.23	109.11
1	B	239	TRP	CA-C-O	7.41	127.70	119.78
1	A	449	ASN	CA-C-N	-7.40	112.19	122.93
1	A	449	ASN	C-N-CA	-7.40	112.19	122.93
1	D	434	ILE	N-CA-C	7.40	118.20	110.72
1	A	295	ARG	NH1-CZ-NH2	7.40	128.92	119.30
1	A	327	ILE	CA-C-O	-7.40	111.13	119.42
1	A	575	PRO	CA-C-N	7.40	131.56	120.31
1	A	575	PRO	C-N-CA	7.40	131.56	120.31
1	B	532	ASP	N-CA-CB	7.40	120.52	110.38
1	A	281	ASP	N-CA-CB	7.40	120.95	109.48
1	B	441	GLU	CA-C-N	7.40	136.66	124.31
1	B	441	GLU	C-N-CA	7.40	136.66	124.31
1	A	32	ASP	N-CA-CB	7.40	123.33	110.39
1	A	378	PRO	CA-C-O	-7.39	108.31	119.55
1	A	54	GLU	OE1-CD-OE2	7.39	140.63	122.90
1	A	219	LEU	O-C-N	7.39	129.68	122.07
1	A	358	HIS	N-CA-C	-7.39	104.27	113.28
1	A	585	ALA	O-C-N	7.38	132.28	123.27
1	B	345	ASN	OD1-CG-ND2	7.38	129.98	122.60
1	B	329	GLU	CA-C-O	7.38	128.23	119.60
1	A	439	SER	CA-CB-OG	-7.37	96.35	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	423	ILE	CA-C-O	-7.37	112.40	120.43
1	B	402	THR	O-C-N	7.37	131.34	122.20
1	A	69	ARG	N-CA-CB	-7.37	100.51	111.71
1	E	281	ASP	CA-CB-CG	7.37	119.97	112.60
1	B	354	GLN	O-C-N	7.36	131.90	122.33
1	E	244	ASP	CA-CB-CG	7.36	119.96	112.60
1	A	41	GLY	O-C-N	7.36	132.26	122.70
1	A	129	GLY	CA-C-O	-7.36	107.77	120.57
1	A	371	PHE	CA-CB-CG	-7.36	106.44	113.80
1	B	311	HIS	CA-CB-CG	-7.36	106.44	113.80
1	B	376	ARG	CA-C-O	-7.36	113.12	120.70
1	F	547	VAL	CB-CA-C	7.36	123.36	111.29
1	B	624	TYR	CA-C-O	7.36	126.67	119.75
1	B	33	ILE	CB-CA-C	7.35	121.38	111.97
1	B	224	HIS	CG-CD2-NE2	7.35	114.55	107.20
1	A	328	ILE	CA-C-O	7.35	128.57	120.71
1	A	632	ASP	N-CA-CB	7.34	122.30	110.77
1	B	90	LEU	CA-C-O	7.34	131.01	120.51
1	A	78	ARG	CA-CB-CG	-7.34	99.42	114.10
1	B	6	GLY	O-C-N	7.34	132.24	122.70
1	A	79	GLN	CB-CA-C	7.34	124.69	110.46
1	A	194	HIS	O-C-N	-7.33	114.35	122.12
1	B	181	VAL	CA-C-O	7.33	129.94	120.78
1	A	534	PRO	CA-C-N	-7.32	109.79	121.86
1	A	534	PRO	C-N-CA	-7.32	109.79	121.86
1	B	5	THR	CB-CA-C	-7.31	93.01	109.10
1	B	418	ILE	O-C-N	7.31	131.65	123.10
1	F	92	GLN	CB-CG-CD	-7.31	100.17	112.60
1	A	489	ASN	CB-CA-C	7.31	124.96	110.42
1	B	414	ASN	N-CA-CB	7.31	121.54	110.14
1	C	92	GLN	CB-CG-CD	-7.31	100.18	112.60
1	C	279	ASP	N-CA-C	-7.31	99.07	109.96
1	A	144	MET	CA-C-N	-7.30	110.90	122.29
1	A	144	MET	C-N-CA	-7.30	110.90	122.29
1	D	32	ASP	N-CA-C	-7.30	104.18	113.23
1	B	11	GLN	CG-CD-OE1	-7.30	106.20	120.80
1	B	63	HIS	CA-CB-CG	7.30	121.10	113.80
1	B	375	THR	CA-CB-CG2	7.30	122.91	110.50
1	A	279	ASP	CB-CG-OD1	7.29	135.18	118.40
1	B	128	LEU	CA-C-O	-7.29	110.08	120.51
1	B	509	PHE	CA-CB-CG	7.29	121.09	113.80
1	B	9	GLN	CG-CD-NE2	-7.29	105.47	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	563	GLY	CA-C-N	-7.28	108.66	122.13
1	A	563	GLY	C-N-CA	-7.28	108.66	122.13
1	B	217	GLY	N-CA-C	-7.28	95.92	113.18
1	F	443	ILE	N-CA-C	-7.28	97.24	107.80
1	A	250	ARG	NE-CZ-NH2	-7.28	112.65	119.20
1	A	337	VAL	CA-CB-CG2	7.27	122.77	110.40
1	C	114	GLU	N-CA-C	-7.27	103.29	111.07
1	A	653	LEU	CB-CA-C	7.27	123.92	110.10
1	A	483	CYS	O-C-N	7.27	130.79	121.34
1	D	480	ILE	N-CA-C	7.27	119.45	107.24
1	A	373	THR	CA-C-O	7.27	127.00	118.79
1	A	621	PRO	CA-C-O	-7.26	107.38	120.60
1	E	114	GLU	N-CA-C	-7.26	103.30	111.07
1	B	277	PHE	CA-CB-CG	7.26	121.06	113.80
1	B	422	LEU	CA-C-O	7.26	128.23	120.46
1	E	360	LYS	CA-CB-CG	7.26	128.61	114.10
1	B	606	HIS	CA-C-O	7.25	133.13	120.80
1	A	298	GLU	N-CA-CB	-7.25	99.12	110.44
1	A	620	ARG	CA-CB-CG	7.25	128.61	114.10
1	C	244	ASP	CA-CB-CG	7.25	119.85	112.60
1	F	206	GLU	OE1-CD-OE2	-7.25	105.49	122.90
1	A	183	TYR	N-CA-CB	7.25	122.65	110.32
1	A	303	GLY	CA-C-O	-7.25	107.95	120.57
1	B	314	ASP	OD1-CG-OD2	-7.25	105.49	122.90
1	A	264	TYR	CB-CA-C	7.25	122.26	109.72
1	A	608	GLN	N-CA-CB	7.25	121.51	110.42
1	B	89	VAL	CB-CA-C	7.25	123.17	111.29
1	B	336	ASN	CB-CG-OD1	7.25	135.29	120.80
1	B	426	PHE	CA-C-O	7.25	129.70	120.57
1	B	138	TYR	CA-CB-CG	7.25	126.94	113.90
1	A	188	ILE	CA-CB-CG2	7.24	122.81	110.50
1	A	400	PRO	O-C-N	7.24	131.67	122.91
1	B	195	VAL	N-CA-C	-7.24	103.72	110.53
1	F	546	ALA	N-CA-C	7.24	121.42	112.59
1	B	334	SER	O-C-N	7.24	131.75	123.06
1	A	139	GLN	N-CA-CB	7.24	121.17	110.53
1	A	292	THR	CA-CB-CG2	7.24	122.80	110.50
1	B	139	GLN	CA-CB-CG	7.24	128.57	114.10
1	B	398	PHE	CA-C-O	7.23	128.84	120.96
1	A	22	TYR	O-C-N	-7.23	113.11	122.37
1	A	309	ASP	O-C-N	7.23	132.37	122.46
1	B	292	THR	CA-C-N	7.23	131.67	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	THR	C-N-CA	7.23	131.67	120.82
1	A	93	CYS	CA-C-O	7.23	129.78	121.47
1	B	512	VAL	CA-C-N	7.23	127.27	119.89
1	B	512	VAL	C-N-CA	7.23	127.27	119.89
1	A	430	GLN	N-CA-CB	-7.23	99.42	110.77
1	B	594	GLU	CB-CG-CD	-7.23	100.31	112.60
1	F	491	ILE	N-CA-C	7.23	120.12	111.09
1	A	251	ILE	CA-CB-CG2	7.23	122.78	110.50
1	D	114	GLU	N-CA-C	-7.22	103.34	111.07
1	F	114	GLU	N-CA-C	-7.22	103.34	111.07
1	A	104	ALA	N-CA-C	-7.22	95.42	110.80
1	B	505	LEU	CA-C-O	7.21	127.56	119.41
1	A	491	ILE	CB-CG1-CD1	-7.21	98.65	113.80
1	A	197	TRP	N-CA-C	-7.21	103.42	111.28
1	B	90	LEU	O-C-N	-7.21	113.00	122.59
1	A	571	PRO	O-C-N	-7.21	114.39	123.04
1	A	580	PHE	N-CA-C	-7.21	99.57	109.95
1	E	179	GLN	CA-C-O	7.21	130.82	120.51
1	B	100	ARG	CD-NE-CZ	-7.21	114.31	124.40
1	B	131	GLY	O-C-N	7.21	129.61	122.19
1	B	466	MET	CA-C-O	-7.20	112.17	120.31
1	D	474	ARG	CB-CG-CD	7.20	127.86	111.30
1	A	390	ILE	N-CA-CB	7.20	123.72	110.40
1	A	421	GLU	CA-C-N	-7.20	107.80	121.54
1	A	421	GLU	C-N-CA	-7.20	107.80	121.54
1	B	533	MET	N-CA-CB	7.20	122.04	110.10
1	D	496	ASP	N-CA-CB	7.19	122.64	110.49
1	D	216	LYS	N-CA-CB	7.19	122.64	110.49
1	A	254	GLU	CA-C-N	-7.19	113.35	121.83
1	A	254	GLU	C-N-CA	-7.19	113.35	121.83
1	A	445	ASP	CA-C-O	-7.18	113.04	120.80
1	A	416	VAL	CA-C-O	7.18	128.25	120.43
1	A	40	LEU	N-CA-C	7.17	122.14	112.88
1	A	254	GLU	CG-CD-OE1	-7.17	101.90	118.40
1	F	419	ASP	CA-CB-CG	7.17	119.78	112.60
1	B	276	HIS	CA-C-O	-7.17	113.11	120.71
1	C	218	GLU	N-CA-C	-7.17	103.55	111.36
1	C	560	ARG	CA-C-N	7.17	133.21	122.68
1	C	560	ARG	C-N-CA	7.17	133.21	122.68
1	D	218	GLU	N-CA-C	-7.16	103.55	111.36
1	A	202	PRO	O-C-N	7.16	131.89	123.01
1	B	23	GLU	CA-C-N	7.16	128.79	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	GLU	C-N-CA	7.16	128.79	119.84
1	A	159	MET	O-C-N	-7.15	114.54	122.12
1	D	244	ASP	CA-CB-CG	7.15	119.75	112.60
1	B	210	GLY	O-C-N	-7.15	113.41	122.70
1	B	404	ASP	CA-CB-CG	-7.15	105.45	112.60
1	A	63	HIS	O-C-N	7.14	132.09	122.59
1	B	416	VAL	CB-CA-C	7.14	119.83	110.12
1	A	49	HIS	N-CA-CB	7.14	122.92	112.13
1	A	376	ARG	NH1-CZ-NH2	7.14	128.58	119.30
1	A	414	ASN	N-CA-CB	7.14	121.35	110.42
1	A	463	LYS	CA-C-N	7.14	131.80	122.95
1	A	463	LYS	C-N-CA	7.14	131.80	122.95
1	A	651	HIS	CA-C-N	-7.14	111.29	121.50
1	A	651	HIS	C-N-CA	-7.14	111.29	121.50
1	A	182	ALA	CA-C-N	7.14	132.02	120.60
1	A	182	ALA	C-N-CA	7.14	132.02	120.60
1	A	624	TYR	CB-CG-CD1	7.14	131.51	120.80
1	A	192	ILE	CB-CA-C	7.13	122.99	111.29
1	E	213	LEU	CB-CA-C	7.13	120.96	110.26
1	A	10	LYS	N-CA-C	-7.13	102.32	111.02
1	A	434	ILE	CA-CB-CG2	7.13	122.62	110.50
1	B	364	PRO	CB-CA-C	7.13	119.62	110.92
1	A	68	GLN	CA-C-O	-7.13	113.55	121.89
1	A	628	ARG	N-CA-CB	-7.13	99.65	111.20
1	C	480	ILE	N-CA-C	7.13	119.22	107.24
1	B	67	GLU	CB-CG-CD	-7.13	100.49	112.60
1	A	305	ILE	CA-C-O	-7.12	111.61	121.51
1	A	163	PRO	O-C-N	7.12	132.25	122.64
1	A	572	LYS	N-CA-C	7.12	119.04	111.28
1	B	344	HIS	CA-C-O	-7.12	110.33	120.51
1	B	7	ASN	OD1-CG-ND2	-7.12	115.48	122.60
1	A	117	TYR	O-C-N	-7.11	114.75	122.07
1	E	216	LYS	N-CA-CB	7.11	122.51	110.49
1	A	53	VAL	CA-CB-CG2	-7.11	98.31	110.40
1	A	184	PHE	CA-C-O	7.11	128.16	120.55
1	A	333	TYR	CB-CG-CD1	7.11	131.46	120.80
1	B	104	ALA	CA-C-N	7.11	130.13	120.54
1	B	104	ALA	C-N-CA	7.11	130.13	120.54
1	B	134	LEU	N-CA-CB	-7.11	100.45	110.04
1	A	162	LYS	O-C-N	7.10	130.86	121.70
1	A	431	TYR	CA-C-O	-7.10	113.30	121.68
1	B	51	ALA	CB-CA-C	7.10	124.31	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	504	GLU	CA-C-O	-7.10	112.65	120.81
1	B	626	LEU	O-C-N	7.10	130.86	122.34
1	F	179	GLN	CA-C-O	7.10	130.66	120.51
1	A	285	HIS	CA-C-O	7.09	129.29	121.56
1	C	310	GLY	N-CA-C	-7.09	104.39	115.67
1	A	467	SER	CB-CA-C	-7.09	97.83	109.53
1	F	480	ILE	N-CA-C	7.09	119.15	107.24
1	B	139	GLN	O-C-N	-7.09	113.90	122.48
1	A	270	VAL	O-C-N	-7.09	113.86	122.36
1	B	611	VAL	N-CA-C	7.08	124.08	109.34
1	A	398	PHE	N-CA-CB	7.08	119.85	110.29
1	B	219	LEU	CB-CA-C	7.08	122.14	110.81
1	A	132	ILE	CB-CA-C	-7.08	101.51	111.28
1	A	406	LEU	CA-C-O	7.08	128.11	119.97
1	B	131	GLY	CA-C-O	-7.08	113.23	120.45
1	B	482	LEU	O-C-N	7.08	132.21	123.01
1	B	570	LEU	N-CA-CB	7.08	117.95	109.74
1	B	278	GLU	CB-CG-CD	-7.07	100.58	112.60
1	A	107	ARG	CB-CG-CD	7.07	127.57	111.30
1	A	361	PHE	N-CA-CB	-7.07	100.14	110.53
1	B	78	ARG	NH1-CZ-NH2	-7.07	110.11	119.30
1	A	450	ALA	CA-C-N	-7.07	113.03	123.00
1	A	450	ALA	C-N-CA	-7.07	113.03	123.00
1	B	507	LYS	O-C-N	7.07	131.84	123.36
1	B	520	GLU	CA-C-O	-7.07	112.72	120.36
1	D	92	GLN	CB-CG-CD	-7.07	100.58	112.60
1	E	480	ILE	N-CA-C	7.07	119.12	107.24
1	A	480	ILE	N-CA-C	7.07	118.07	107.75
1	B	161	GLN	CA-C-O	-7.07	111.51	120.55
1	E	218	GLU	N-CA-C	-7.06	103.66	111.36
1	A	518	THR	CA-CB-CG2	7.06	122.50	110.50
1	A	548	ASN	CB-CA-C	7.06	122.65	110.72
1	F	310	GLY	N-CA-C	-7.06	104.45	115.67
1	B	71	TRP	CA-C-O	7.05	129.85	121.88
1	F	244	ASP	CA-CB-CG	7.05	119.66	112.60
1	D	35	GLU	CG-CD-OE2	7.05	134.62	118.40
1	A	69	ARG	CB-CG-CD	7.05	127.52	111.30
1	A	319	LYS	CA-C-O	7.05	130.19	118.91
1	E	310	GLY	N-CA-C	-7.05	104.46	115.67
1	B	497	GLU	CA-C-N	-7.05	110.07	122.26
1	B	497	GLU	C-N-CA	-7.05	110.07	122.26
1	A	196	THR	CA-C-O	7.04	128.24	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	218	GLU	N-CA-C	-7.04	103.68	111.36
1	B	279	ASP	N-CA-C	-7.04	99.47	109.96
1	D	213	LEU	CB-CA-C	7.04	120.82	110.26
1	B	362	ASN	O-C-N	-7.04	114.38	123.32
1	A	43	THR	OG1-CB-CG2	7.04	123.38	109.30
1	A	123	VAL	CA-C-O	-7.04	113.71	121.17
1	B	373	THR	N-CA-C	7.04	125.11	113.50
1	A	15	ASN	CB-CG-ND2	7.04	126.96	116.40
1	B	364	PRO	N-CA-CB	-7.04	96.25	103.08
1	B	491	ILE	CA-C-O	-7.04	110.71	119.43
1	B	26	LYS	CA-CB-CG	-7.03	100.03	114.10
1	D	310	GLY	N-CA-C	-7.03	104.49	115.67
1	A	579	GLU	CA-C-N	-7.03	110.26	123.27
1	A	579	GLU	C-N-CA	-7.03	110.26	123.27
1	A	208	SER	O-C-N	7.03	131.37	122.23
1	A	444	GLU	CA-C-O	7.02	128.09	120.43
1	B	231	PHE	CD1-CE1-CZ	7.02	132.64	120.00
1	B	169	SER	N-CA-CB	-7.02	99.68	110.42
1	B	518	THR	N-CA-CB	7.02	123.60	111.74
1	A	112	GLU	CB-CG-CD	7.01	124.53	112.60
1	A	149	GLU	CG-CD-OE1	7.01	134.53	118.40
1	B	407	GLU	CG-CD-OE1	-7.01	102.27	118.40
1	A	211	TYR	N-CA-C	-7.01	99.14	108.19
1	F	216	LYS	N-CA-CB	7.01	122.34	110.49
1	B	319	LYS	N-CA-C	-7.01	104.70	113.18
1	A	614	GLU	CA-C-O	7.01	128.71	120.58
1	B	388	ASP	CA-C-O	-7.01	113.36	121.07
1	C	179	GLN	CA-C-O	7.01	130.53	120.51
1	C	360	LYS	CA-CB-CG	7.01	128.11	114.10
1	A	154	ALA	N-CA-C	-7.00	103.57	111.14
1	D	588	ASP	N-CA-C	7.00	121.13	108.17
1	A	254	GLU	CG-CD-OE2	7.00	134.51	118.40
1	B	7	ASN	O-C-N	7.00	131.90	122.59
1	B	53	VAL	N-CA-CB	-7.00	101.02	110.54
1	B	176	ASN	OD1-CG-ND2	-7.00	115.60	122.60
1	B	136	PRO	CA-C-O	-7.00	112.73	120.92
1	B	218	GLU	CB-CG-CD	7.00	124.50	112.60
1	E	548	ASN	N-CA-C	-7.00	99.12	109.62
1	A	196	THR	O-C-N	-7.00	114.70	122.12
1	A	632	ASP	CB-CA-C	6.99	121.33	110.14
1	E	444	GLU	CA-CB-CG	6.99	128.09	114.10
1	A	180	ARG	NH1-CZ-NH2	6.99	128.39	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	219	LEU	CA-C-N	6.99	129.95	120.44
1	B	219	LEU	C-N-CA	6.99	129.95	120.44
1	B	495	LEU	N-CA-CB	6.98	121.60	111.62
1	A	72	TYR	CA-C-O	-6.98	111.62	120.14
1	C	496	ASP	N-CA-CB	6.98	122.29	110.49
1	B	445	ASP	CA-CB-CG	6.98	119.58	112.60
1	B	478	PHE	CA-CB-CG	-6.98	106.82	113.80
1	C	423	ILE	CB-CA-C	6.98	121.30	110.28
1	A	108	GLU	N-CA-C	6.97	121.49	113.19
1	A	616	TYR	CA-C-N	6.97	126.68	119.64
1	A	616	TYR	C-N-CA	6.97	126.68	119.64
1	C	63	HIS	N-CA-CB	6.97	122.27	110.49
1	A	442	ASN	O-C-N	6.97	131.53	122.40
1	B	138	TYR	CG-CD2-CE2	6.97	131.66	121.20
1	E	252	ILE	N-CA-C	-6.97	96.44	106.55
1	E	620	ARG	CA-CB-CG	6.97	128.04	114.10
1	C	443	ILE	CA-C-O	-6.97	112.78	120.72
1	B	119	LEU	CA-C-O	-6.97	113.68	121.00
1	A	161	GLN	CG-CD-NE2	-6.96	105.95	116.40
1	B	474	ARG	CD-NE-CZ	-6.96	114.65	124.40
1	D	179	GLN	CA-C-O	6.96	130.47	120.51
1	B	259	LEU	O-C-N	-6.96	111.03	122.23
1	B	18	LEU	CB-CA-C	-6.95	100.28	111.06
1	B	391	PHE	CA-CB-CG	6.95	120.75	113.80
1	B	588	ASP	N-CA-C	6.95	121.23	108.58
1	A	78	ARG	N-CA-CB	6.95	120.98	110.14
1	B	346	THR	O-C-N	6.95	129.32	122.09
1	A	295	ARG	CA-C-O	-6.95	113.47	120.90
1	B	49	HIS	N-CA-CB	6.95	123.03	112.47
1	B	353	ARG	N-CA-C	-6.95	104.68	113.02
1	A	190	MET	CA-C-O	-6.95	113.53	120.82
1	A	542	GLN	O-C-N	6.94	130.81	122.27
1	C	537	GLN	N-CA-C	-6.94	103.71	111.28
1	F	63	HIS	N-CA-CB	6.94	122.22	110.49
1	E	612	HIS	CA-CB-CG	6.94	120.74	113.80
1	A	336	ASN	CB-CG-OD1	6.94	134.68	120.80
1	E	496	ASP	N-CA-CB	6.94	122.21	110.49
1	A	15	ASN	CB-CG-OD1	-6.93	106.93	120.80
1	B	186	GLU	CB-CG-CD	6.93	124.39	112.60
1	E	254	GLU	N-CA-C	6.93	120.65	107.75
1	B	123	VAL	N-CA-C	-6.93	103.44	111.00
1	B	432	SER	N-CA-C	6.93	119.82	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	583	TYR	CA-C-N	-6.93	114.11	123.12
1	B	583	TYR	C-N-CA	-6.93	114.11	123.12
1	A	215	ARG	CB-CA-C	6.93	123.37	111.45
1	A	535	SER	CA-C-O	6.93	130.40	121.67
1	A	251	ILE	CB-CA-C	-6.93	103.97	111.59
1	A	398	PHE	CA-CB-CG	-6.93	106.87	113.80
1	B	423	ILE	O-C-N	6.93	130.55	123.07
1	A	436	ALA	N-CA-C	6.92	118.61	111.14
1	B	414	ASN	CA-C-N	-6.92	111.43	121.26
1	B	414	ASN	C-N-CA	-6.92	111.43	121.26
1	D	556	SER	N-CA-C	-6.92	96.06	110.80
1	B	67	GLU	CB-CA-C	-6.92	95.49	109.68
1	A	158	LYS	CG-CD-CE	-6.92	95.39	111.30
1	A	382	ARG	CA-CB-CG	-6.92	100.27	114.10
1	B	264	TYR	N-CA-C	-6.92	97.25	108.52
1	B	358	HIS	CB-CA-C	6.92	123.71	109.95
1	B	473	GLU	CA-CB-CG	6.91	127.92	114.10
1	C	213	LEU	CB-CA-C	6.91	120.62	110.26
1	A	126	SER	N-CA-CB	6.91	120.12	109.97
1	A	238	ASN	CB-CG-ND2	-6.91	106.04	116.40
1	B	213	LEU	CA-C-N	6.91	134.74	121.54
1	B	213	LEU	C-N-CA	6.91	134.74	121.54
1	B	285	HIS	CA-CB-CG	-6.91	106.89	113.80
1	A	45	ILE	CA-C-N	6.90	132.31	122.09
1	A	45	ILE	C-N-CA	6.90	132.31	122.09
1	B	238	ASN	CB-CA-C	6.90	122.20	111.02
1	F	213	LEU	CB-CA-C	6.90	120.61	110.26
1	D	419	ASP	N-CA-C	-6.90	95.75	108.24
1	A	408	PHE	CA-C-O	6.90	130.37	120.51
1	B	420	GLY	CA-C-O	-6.89	108.57	120.57
1	B	411	MET	N-CA-CB	-6.89	98.84	110.49
1	B	179	GLN	CA-C-N	6.89	134.02	121.41
1	B	179	GLN	C-N-CA	6.89	134.02	121.41
1	B	360	LYS	N-CA-CB	6.89	121.19	110.44
1	F	423	ILE	N-CA-CB	-6.89	100.42	111.58
1	F	496	ASP	N-CA-CB	6.89	122.13	110.49
1	A	606	HIS	CA-CB-CG	-6.88	106.92	113.80
1	B	91	ASN	OD1-CG-ND2	-6.88	115.72	122.60
1	B	299	ALA	N-CA-CB	-6.88	99.94	110.13
1	B	453	HIS	CA-C-O	6.88	128.28	120.84
1	B	577	GLY	CA-C-N	-6.88	111.78	122.59
1	B	577	GLY	C-N-CA	-6.88	111.78	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	221	PHE	CA-C-N	6.88	129.39	120.44
1	E	221	PHE	C-N-CA	6.88	129.39	120.44
1	A	147	ASN	CB-CA-C	-6.88	96.73	110.42
1	A	443	ILE	N-CA-C	-6.88	98.48	108.11
1	C	588	ASP	N-CA-C	6.88	120.89	108.17
1	B	451	ARG	NE-CZ-NH1	-6.88	114.62	121.50
1	B	504	GLU	N-CA-CB	6.88	120.09	109.85
1	A	412	VAL	N-CA-C	6.87	118.02	107.78
1	B	348	HIS	O-C-N	-6.87	114.14	122.11
1	C	331	SER	N-CA-C	-6.87	99.71	110.36
1	B	117	TYR	N-CA-CB	6.87	119.94	109.91
1	F	303	GLY	N-CA-C	-6.87	106.31	114.48
1	A	324	LEU	N-CA-CB	6.87	119.97	110.01
1	E	328	ILE	N-CA-C	6.87	116.99	110.53
1	B	459	GLU	N-CA-CB	6.87	120.90	109.92
1	D	29	ASP	CA-CB-CG	6.86	119.46	112.60
1	A	292	THR	CA-C-O	-6.86	113.62	120.82
1	B	38	ASN	OD1-CG-ND2	6.86	129.46	122.60
1	A	40	LEU	O-C-N	-6.86	114.09	122.25
1	B	234	GLU	O-C-N	6.86	129.97	122.15
1	B	305	ILE	CB-CG1-CD1	-6.86	99.40	113.80
1	A	407	GLU	CG-CD-OE2	6.85	134.16	118.40
1	B	16	HIS	N-CA-CB	6.85	120.00	110.07
1	A	271	ARG	NE-CZ-NH1	6.85	128.35	121.50
1	A	254	GLU	N-CA-C	6.84	120.85	107.98
1	B	95	GLU	N-CA-CB	-6.84	100.74	111.56
1	B	279	ASP	CB-CA-C	6.84	120.02	110.16
1	C	10	LYS	N-CA-C	-6.84	102.90	111.11
1	A	353	ARG	O-C-N	-6.84	112.26	122.39
1	A	56	LEU	N-CA-C	-6.84	103.44	111.03
1	A	629	ARG	CA-C-O	-6.84	113.12	120.92
1	A	100	ARG	CA-C-O	6.84	129.02	121.02
1	A	499	ARG	O-C-N	-6.84	115.03	122.07
1	B	213	LEU	CB-CA-C	6.84	120.52	110.26
1	E	30	LEU	CB-CA-C	6.83	122.30	110.68
1	B	319	LYS	CB-CA-C	-6.83	96.35	109.95
1	B	594	GLU	CA-CB-CG	6.83	127.77	114.10
1	E	588	ASP	N-CA-C	6.83	120.81	108.17
1	B	162	LYS	N-CA-CB	-6.83	96.31	110.45
1	B	332	LYS	CB-CG-CD	-6.83	95.59	111.30
1	C	561	SER	CA-C-N	6.83	130.12	120.28
1	C	561	SER	C-N-CA	6.83	130.12	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	410	GLY	N-CA-C	-6.83	96.99	113.18
1	A	289	LEU	N-CA-C	-6.83	103.45	111.03
1	A	479	ARG	NH1-CZ-NH2	6.83	128.17	119.30
1	C	466	MET	N-CA-C	6.83	118.77	108.46
1	A	295	ARG	CB-CG-CD	6.82	126.99	111.30
1	A	225	HIS	O-C-N	-6.82	113.88	122.27
1	C	213	LEU	N-CA-C	-6.82	99.56	109.59
1	B	294	SER	CA-CB-OG	-6.82	97.47	111.10
1	A	220	PHE	CA-C-N	6.82	132.03	121.19
1	A	220	PHE	C-N-CA	6.82	132.03	121.19
1	A	372	GLU	CA-C-N	-6.82	110.61	121.44
1	A	372	GLU	C-N-CA	-6.82	110.61	121.44
1	A	542	GLN	CG-CD-OE1	-6.82	107.17	120.80
1	A	560	ARG	CA-CB-CG	6.82	127.73	114.10
1	D	558	TYR	N-CA-C	6.82	118.15	108.54
1	B	60	LEU	O-C-N	6.81	129.97	122.20
1	A	238	ASN	O-C-N	6.81	131.33	122.20
1	A	594	GLU	CG-CD-OE1	-6.81	102.73	118.40
1	B	401	TYR	O-C-N	6.81	130.94	123.10
1	E	263	LYS	N-CA-C	-6.81	102.45	111.24
1	B	190	MET	N-CA-CB	6.81	120.21	110.13
1	B	330	SER	N-CA-CB	6.81	122.00	110.49
1	B	545	ASN	N-CA-C	-6.81	105.38	113.21
1	E	279	ASP	N-CA-CB	-6.81	98.76	109.51
1	F	588	ASP	N-CA-C	6.81	120.76	108.17
1	A	303	GLY	N-CA-C	-6.80	97.05	113.18
1	A	260	THR	O-C-N	-6.80	114.59	123.16
1	A	503	ILE	CA-CB-CG1	6.80	121.97	110.40
1	B	544	ASP	O-C-N	6.80	129.16	122.09
1	F	360	LYS	CA-CB-CG	6.80	127.70	114.10
1	B	510	GLN	CA-C-O	-6.80	112.84	120.66
1	C	467	SER	N-CA-C	6.80	120.75	109.46
1	B	358	HIS	N-CA-C	-6.80	104.95	113.18
1	B	456	ASN	CB-CG-ND2	6.80	126.60	116.40
1	F	213	LEU	N-CA-C	-6.80	99.60	109.59
1	A	520	GLU	CG-CD-OE1	-6.80	102.76	118.40
1	A	414	ASN	CA-C-O	-6.80	111.56	119.78
1	B	118	ALA	CA-C-O	6.79	127.75	120.55
1	A	193	HIS	CB-CA-C	-6.79	99.56	110.84
1	C	263	LYS	N-CA-C	-6.79	102.48	111.24
1	A	405	ASN	O-C-N	6.79	129.43	122.09
1	B	370	HIS	O-C-N	6.79	131.22	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	544	ASP	CA-CB-CG	6.79	119.39	112.60
1	D	10	LYS	N-CA-C	-6.79	102.96	111.11
1	B	559	GLU	CA-CB-CG	6.79	127.68	114.10
1	B	108	GLU	CG-CD-OE1	6.79	134.01	118.40
1	B	505	LEU	N-CA-CB	-6.79	100.56	110.47
1	B	617	PRO	CB-CA-C	-6.79	102.20	112.11
1	A	111	ASN	CB-CG-OD1	-6.79	107.23	120.80
1	A	182	ALA	N-CA-C	6.79	118.67	111.28
1	B	298	GLU	CG-CD-OE2	6.79	134.01	118.40
1	E	31	LYS	CA-C-O	-6.79	112.71	120.24
1	A	12	GLN	CB-CA-C	6.78	121.41	110.96
1	A	113	GLY	CA-C-N	6.78	129.60	120.65
1	A	113	GLY	C-N-CA	6.78	129.60	120.65
1	A	624	TYR	CZ-CE2-CD2	-6.78	107.39	119.60
1	E	555	LEU	N-CA-C	-6.78	100.19	110.70
1	D	63	HIS	N-CA-CB	6.78	121.95	110.49
1	A	141	THR	CA-C-O	-6.78	113.82	121.28
1	A	290	GLU	CA-C-N	-6.78	110.80	120.42
1	A	290	GLU	C-N-CA	-6.78	110.80	120.42
1	F	608	GLN	N-CA-C	-6.78	103.67	112.68
1	A	358	HIS	CA-CB-CG	-6.78	107.03	113.80
1	A	505	LEU	CA-C-O	6.77	127.06	119.41
1	C	620	ARG	CA-CB-CG	6.77	127.65	114.10
1	F	620	ARG	CA-CB-CG	6.77	127.65	114.10
1	D	360	LYS	CA-CB-CG	6.77	127.64	114.10
1	E	78	ARG	N-CA-CB	6.77	120.69	110.19
1	E	213	LEU	N-CA-C	-6.77	99.63	109.59
1	A	382	ARG	CB-CA-C	6.77	121.60	110.90
1	D	608	GLN	N-CA-C	-6.77	103.68	112.68
1	E	380	PHE	CA-CB-CG	-6.77	107.03	113.80
1	B	426	PHE	CA-CB-CG	6.77	120.57	113.80
1	A	395	THR	CA-CB-OG1	-6.76	99.45	109.60
1	B	70	HIS	O-C-N	6.76	130.96	123.25
1	B	251	ILE	O-C-N	6.76	130.98	122.52
1	C	328	ILE	N-CA-C	6.76	116.89	110.53
1	A	390	ILE	CB-CA-C	-6.76	103.42	111.94
1	D	263	LYS	N-CA-C	-6.76	102.52	111.24
1	A	608	GLN	CG-CD-OE1	-6.76	107.28	120.80
1	F	263	LYS	N-CA-C	-6.76	102.52	111.24
1	A	391	PHE	CA-C-N	-6.76	110.51	120.38
1	A	391	PHE	C-N-CA	-6.76	110.51	120.38
1	A	206	GLU	CA-C-O	-6.76	113.40	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	452	VAL	CA-C-N	6.75	133.14	123.14
1	A	452	VAL	C-N-CA	6.75	133.14	123.14
1	D	112	GLU	N-CA-C	6.75	118.64	111.28
1	B	324	LEU	N-CA-CB	6.75	119.80	110.01
1	A	537	GLN	CB-CG-CD	-6.75	101.13	112.60
1	A	161	GLN	N-CA-C	6.75	120.81	111.90
1	B	376	ARG	CB-CG-CD	6.74	126.81	111.30
1	B	218	GLU	CB-CA-C	-6.74	99.60	110.79
1	D	580	PHE	N-CA-C	-6.74	100.25	109.95
1	A	8	ALA	CA-C-O	6.73	128.10	120.90
1	A	245	GLU	OE1-CD-OE2	-6.73	106.74	122.90
1	B	382	ARG	NE-CZ-NH1	6.73	128.23	121.50
1	E	520	GLU	CA-CB-CG	6.73	127.56	114.10
1	A	216	LYS	N-CA-C	-6.72	99.94	109.96
1	B	250	ARG	N-CA-CB	-6.72	100.38	110.60
1	B	326	ASP	CA-C-N	6.72	131.24	120.82
1	B	326	ASP	C-N-CA	6.72	131.24	120.82
1	A	277	PHE	CB-CA-C	-6.72	97.05	110.42
1	C	162	LYS	CB-CA-C	6.72	117.40	109.47
1	A	297	HIS	CA-CB-CG	-6.72	107.08	113.80
1	A	444	GLU	CA-C-N	6.72	131.94	121.26
1	A	444	GLU	C-N-CA	6.72	131.94	121.26
1	A	296	ILE	N-CA-CB	6.71	117.94	110.62
1	B	410	GLY	N-CA-C	-6.71	97.27	113.18
1	B	507	LYS	N-CA-CB	6.71	120.17	110.37
1	B	586	VAL	CA-C-O	6.71	127.37	120.39
1	B	587	THR	CA-C-O	-6.71	113.19	121.78
1	B	620	ARG	CA-CB-CG	6.71	127.52	114.10
1	F	10	LYS	N-CA-C	-6.71	103.06	111.11
1	C	78	ARG	N-CA-CB	6.71	120.58	110.19
1	A	78	ARG	CA-C-N	-6.71	110.59	120.38
1	A	78	ARG	C-N-CA	-6.71	110.59	120.38
1	A	94	LYS	N-CA-CB	-6.70	100.28	110.33
1	B	69	ARG	CA-CB-CG	-6.70	100.69	114.10
1	C	112	GLU	N-CA-C	6.70	118.59	111.28
1	C	580	PHE	N-CA-C	-6.70	100.54	110.46
1	A	139	GLN	CA-CB-CG	6.70	127.50	114.10
1	A	299	ALA	CB-CA-C	6.70	121.92	110.86
1	C	221	PHE	CA-C-N	6.70	129.15	120.44
1	C	221	PHE	C-N-CA	6.70	129.15	120.44
1	B	419	ASP	CA-CB-CG	-6.70	105.90	112.60
1	E	63	HIS	N-CA-CB	6.70	121.81	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	221	PHE	CA-C-N	6.70	129.15	120.44
1	F	221	PHE	C-N-CA	6.70	129.15	120.44
1	F	380	PHE	CA-CB-CG	-6.70	107.10	113.80
1	D	213	LEU	N-CA-C	-6.69	99.75	109.59
1	A	585	ALA	CB-CA-C	6.69	122.60	109.35
1	B	352	GLY	CA-C-N	-6.69	111.06	122.56
1	B	352	GLY	C-N-CA	-6.69	111.06	122.56
1	A	32	ASP	CA-C-N	-6.69	109.85	120.55
1	A	32	ASP	C-N-CA	-6.69	109.85	120.55
1	A	215	ARG	CA-C-N	-6.69	111.12	121.02
1	A	215	ARG	C-N-CA	-6.69	111.12	121.02
1	B	316	ARG	O-C-N	6.69	131.91	122.68
1	B	594	GLU	CA-C-O	-6.69	110.95	120.51
1	A	136	PRO	CB-CA-C	-6.68	104.27	111.56
1	C	608	GLN	N-CA-C	-6.68	103.79	112.68
1	B	214	ASP	N-CA-C	6.68	125.03	110.80
1	F	279	ASP	N-CA-CB	-6.68	98.95	109.51
1	A	65	LEU	CB-CA-C	6.68	123.14	110.51
1	F	612	HIS	CA-CB-CG	6.68	120.48	113.80
1	B	251	ILE	CB-CA-C	-6.68	104.24	111.59
1	B	377	ASP	CA-CB-CG	-6.68	105.92	112.60
1	B	473	GLU	N-CA-CB	6.67	122.80	110.99
1	D	216	LYS	N-CA-C	-6.67	96.58	110.80
1	A	518	THR	CB-CA-C	6.67	120.44	111.70
1	A	194	HIS	CE1-NE2-CD2	6.67	115.67	109.00
1	A	574	LYS	CB-CA-C	6.67	119.28	109.08
1	F	328	ILE	N-CA-C	6.67	116.80	110.53
1	A	406	LEU	CA-C-N	6.66	130.58	121.05
1	A	406	LEU	C-N-CA	6.66	130.58	121.05
1	B	206	GLU	N-CA-CB	6.66	122.47	111.08
1	B	47	ASN	CB-CG-ND2	-6.66	106.41	116.40
1	F	216	LYS	N-CA-C	-6.66	96.62	110.80
1	F	443	ILE	CA-C-O	-6.66	113.41	120.53
1	D	78	ARG	N-CA-CB	6.66	120.51	110.19
1	A	629	ARG	CD-NE-CZ	-6.66	115.08	124.40
1	C	442	ASN	CA-CB-CG	-6.66	105.94	112.60
1	D	532	ASP	N-CA-C	-6.66	101.75	110.53
1	A	596	HIS	CA-CB-CG	-6.65	107.15	113.80
1	B	447	GLU	O-C-N	6.65	131.48	122.57
1	A	212	HIS	CA-CB-CG	6.65	120.45	113.80
1	A	494	THR	CA-C-O	-6.65	113.50	121.34
1	B	225	HIS	CA-CB-CG	-6.65	107.15	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	565	PRO	O-C-N	6.65	131.07	123.03
1	D	331	SER	N-CA-C	-6.64	99.56	109.86
1	F	78	ARG	N-CA-CB	6.64	120.49	110.19
1	B	39	PRO	O-C-N	6.64	131.87	122.37
1	A	428	GLU	OE1-CD-OE2	6.64	138.83	122.90
1	A	158	LYS	CB-CA-C	6.63	121.80	110.79
1	D	620	ARG	CA-CB-CG	6.63	127.37	114.10
1	A	357	PRO	N-CD-CG	-6.63	93.25	103.20
1	B	125	HIS	CG-CD2-NE2	-6.63	100.57	107.20
1	A	292	THR	CB-CA-C	6.63	121.29	110.88
1	A	414	ASN	N-CA-C	-6.63	104.84	113.12
1	B	46	TYR	N-CA-C	6.63	120.30	109.76
1	A	513	PRO	N-CA-CB	-6.62	94.60	103.15
1	B	363	LEU	CB-CA-C	6.62	118.75	108.61
1	A	225	HIS	CB-CG-CD2	-6.62	122.59	131.20
1	A	314	ASP	CA-C-O	-6.62	113.74	121.16
1	B	285	HIS	N-CA-C	6.62	119.36	110.35
1	B	399	PRO	CB-CA-C	6.62	119.00	110.92
1	A	632	ASP	N-CA-C	-6.62	97.49	108.34
1	B	175	LYS	N-CA-CB	6.61	121.74	110.50
1	E	572	LYS	N-CA-C	6.61	118.57	111.36
1	A	556	SER	N-CA-CB	6.61	121.66	110.49
1	B	499	ARG	NE-CZ-NH2	6.61	125.15	119.20
1	E	112	GLU	N-CA-C	6.60	118.48	111.28
1	E	467	SER	N-CA-C	6.60	120.42	109.46
1	A	272	PRO	CB-CA-C	6.60	119.71	110.60
1	A	305	ILE	CB-CG1-CD1	-6.60	99.94	113.80
1	B	295	ARG	CD-NE-CZ	-6.60	115.16	124.40
1	B	422	LEU	N-CA-C	-6.60	96.31	107.99
1	D	36	ASN	CA-CB-CG	-6.60	106.00	112.60
1	D	470	ASN	N-CA-C	-6.60	100.19	109.69
1	A	152	ASP	CA-CB-CG	6.59	119.19	112.60
1	E	290	GLU	CB-CG-CD	6.59	123.81	112.60
1	A	38	ASN	CA-CB-CG	6.59	119.19	112.60
1	A	191	ASN	CB-CA-C	6.59	121.36	110.81
1	A	619	ASN	OD1-CG-ND2	6.59	129.19	122.60
1	B	390	ILE	CA-CB-CG1	6.59	121.60	110.40
1	B	403	HIS	CB-CA-C	-6.58	100.75	110.95
1	D	62	ASP	N-CA-C	-6.58	105.36	113.19
1	E	331	SER	N-CA-C	-6.58	99.66	109.86
1	B	177	ARG	CB-CG-CD	-6.58	96.16	111.30
1	A	376	ARG	CD-NE-CZ	-6.58	115.19	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	ASN	CA-C-N	-6.58	110.07	120.60
1	B	76	ASN	C-N-CA	-6.58	110.07	120.60
1	B	421	GLU	O-C-N	6.58	130.77	123.33
1	D	328	ILE	N-CA-C	6.58	116.72	110.53
1	B	192	ILE	CA-C-N	6.58	130.69	120.82
1	B	192	ILE	C-N-CA	6.58	130.69	120.82
1	A	260	THR	CB-CA-C	6.58	121.41	109.37
1	A	475	LEU	CA-C-O	-6.58	114.38	121.94
1	B	10	LYS	N-CA-C	-6.58	100.59	111.37
1	B	244	ASP	CA-CB-CG	6.58	119.17	112.60
1	D	212	HIS	CA-CB-CG	6.58	120.38	113.80
1	E	608	GLN	N-CA-C	-6.58	103.94	112.68
1	F	112	GLU	N-CA-C	6.58	118.45	111.28
1	A	429	PHE	N-CA-CB	-6.57	99.41	111.37
1	A	9	GLN	CG-CD-OE1	6.57	133.94	120.80
1	B	258	PRO	CA-C-O	6.57	132.56	120.60
1	B	302	HIS	CE1-NE2-CD2	-6.57	102.43	109.00
1	F	290	GLU	CB-CG-CD	6.57	123.77	112.60
1	B	98	CYS	CB-CA-C	6.57	123.78	110.38
1	D	489	ASN	CB-CA-C	6.57	123.49	110.42
1	E	216	LYS	N-CA-C	-6.57	96.81	110.80
1	B	377	ASP	CA-C-O	-6.57	113.23	119.80
1	F	442	ASN	CA-CB-CG	-6.56	106.04	112.60
1	B	280	VAL	N-CA-CB	6.56	119.94	111.67
1	B	606	HIS	CB-CA-C	-6.56	97.63	110.10
1	B	302	HIS	N-CA-CB	6.56	119.58	110.07
1	E	10	LYS	N-CA-C	-6.56	103.24	111.11
1	B	140	ILE	CB-CA-C	-6.56	103.17	112.22
1	B	468	ASN	CB-CG-ND2	-6.56	106.56	116.40
1	A	295	ARG	NE-CZ-NH2	-6.56	113.30	119.20
1	A	344	HIS	CA-CB-CG	-6.55	107.25	113.80
1	A	479	ARG	NE-CZ-NH1	-6.55	114.95	121.50
1	B	251	ILE	CA-CB-CG1	-6.55	99.26	110.40
1	B	570	LEU	CA-CB-CG	6.55	139.24	116.30
1	E	181	VAL	N-CA-C	-6.55	104.93	111.88
1	A	422	LEU	N-CA-CB	-6.55	99.42	110.49
1	A	523	SER	CA-C-N	6.55	129.59	120.29
1	A	523	SER	C-N-CA	6.55	129.59	120.29
1	B	333	TYR	CB-CG-CD1	6.55	130.62	120.80
1	B	554	ASP	N-CA-CB	6.55	119.93	110.37
1	A	616	TYR	CB-CA-C	6.54	119.51	109.50
1	A	193	HIS	CA-C-N	-6.54	111.42	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	HIS	C-N-CA	-6.54	111.42	120.38
1	A	472	GLY	N-CA-C	6.54	128.69	113.18
1	A	130	ASP	N-CA-C	6.54	118.29	111.03
1	A	509	PHE	O-C-N	-6.54	115.76	123.22
1	A	204	TRP	N-CA-C	6.54	121.26	113.28
1	E	169	SER	N-CA-CB	-6.54	100.42	110.42
1	E	532	ASP	N-CA-C	-6.54	101.87	110.43
1	A	474	ARG	O-C-N	6.54	131.28	122.59
1	E	177	ARG	N-CA-C	6.54	124.72	110.80
1	B	302	HIS	ND1-CE1-NE2	6.53	114.93	108.40
1	C	62	ASP	N-CA-C	-6.53	105.42	113.19
1	A	5	THR	N-CA-CB	-6.53	100.40	111.50
1	B	14	ILE	O-C-N	-6.53	115.41	121.94
1	A	52	ALA	N-CA-CB	6.53	119.74	109.82
1	B	92	GLN	CG-CD-OE1	-6.53	107.75	120.80
1	B	503	ILE	CB-CG1-CD1	-6.52	100.10	113.80
1	B	31	LYS	N-CA-C	6.52	118.39	111.28
1	A	385	LYS	O-C-N	6.52	131.26	122.59
1	B	54	GLU	CA-C-O	6.52	127.47	119.97
1	B	191	ASN	N-CA-CB	6.52	119.84	110.06
1	D	268	PHE	O-C-N	6.52	126.72	121.38
1	A	524	LYS	CA-C-N	-6.51	109.28	122.31
1	A	524	LYS	C-N-CA	-6.51	109.28	122.31
1	A	612	HIS	N-CA-C	6.51	121.06	111.87
1	C	473	GLU	CB-CG-CD	6.51	123.68	112.60
1	D	221	PHE	CA-C-N	6.51	128.91	120.44
1	D	221	PHE	C-N-CA	6.51	128.91	120.44
1	A	347	ALA	N-CA-CB	6.51	120.42	110.14
1	A	469	ASN	N-CA-C	-6.51	104.60	112.54
1	A	435	ASN	CA-CB-CG	6.51	119.11	112.60
1	A	591	LYS	CA-CB-CG	6.50	127.11	114.10
1	B	510	GLN	CB-CG-CD	-6.50	101.54	112.60
1	D	177	ARG	N-CA-C	6.50	124.65	110.80
1	F	177	ARG	N-CA-C	6.50	124.65	110.80
1	A	349	VAL	N-CA-C	6.50	119.22	111.09
1	C	612	HIS	CA-CB-CG	6.50	120.30	113.80
1	B	375	THR	O-C-N	6.50	130.84	122.39
1	F	62	ASP	N-CA-C	-6.50	105.46	113.19
1	F	560	ARG	CA-C-N	6.50	133.95	121.54
1	F	560	ARG	C-N-CA	6.50	133.95	121.54
1	B	437	VAL	CA-C-O	-6.50	113.37	120.71
1	A	68	GLN	N-CA-C	-6.49	101.17	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	HIS	ND1-CG-CD2	6.49	112.59	106.10
1	E	62	ASP	N-CA-C	-6.49	105.46	113.19
1	B	24	PRO	N-CD-CG	-6.49	93.46	103.20
1	A	19	ASP	CB-CG-OD2	6.49	133.32	118.40
1	A	584	VAL	CA-CB-CG1	-6.49	99.37	110.40
1	E	443	ILE	CA-C-O	-6.49	113.59	120.53
1	A	86	LEU	N-CA-C	-6.49	103.33	111.11
1	A	226	GLN	O-C-N	-6.49	112.75	122.28
1	B	492	THR	O-C-N	-6.49	113.96	122.59
1	B	501	PHE	N-CA-CB	-6.48	99.52	110.41
1	C	95	GLU	CA-CB-CG	6.48	127.06	114.10
1	B	462	TYR	N-CA-CB	6.48	120.72	110.23
1	A	382	ARG	O-C-N	-6.47	115.10	122.09
1	C	532	ASP	N-CA-C	-6.47	101.95	110.43
1	F	278	GLU	CA-C-O	6.47	127.98	120.80
1	B	263	LYS	CA-CB-CG	6.47	127.04	114.10
1	A	77	THR	N-CA-C	6.47	120.03	111.75
1	A	159	MET	N-CA-CB	6.47	119.63	110.12
1	F	463	LYS	CB-CA-C	6.47	121.13	111.17
1	A	33	ILE	CA-C-O	6.47	127.63	120.71
1	A	242	PRO	N-CA-CB	-6.47	96.46	103.25
1	B	27	TYR	CA-C-O	6.47	124.79	119.36
1	B	443	ILE	N-CA-C	-6.47	98.42	107.80
1	A	474	ARG	NE-CZ-NH2	-6.46	113.38	119.20
1	A	567	ARG	CG-CD-NE	6.46	126.22	112.00
1	B	336	ASN	CA-CB-CG	6.46	119.06	112.60
1	C	279	ASP	N-CA-CB	-6.46	99.30	109.51
1	D	37	PHE	CA-CB-CG	6.46	120.26	113.80
1	B	64	ARG	N-CA-C	-6.46	103.52	112.30
1	B	190	MET	CB-CG-SD	-6.46	93.32	112.70
1	B	462	TYR	CB-CG-CD2	6.46	130.49	120.80
1	B	619	ASN	CA-C-O	-6.46	112.06	118.97
1	B	168	VAL	CA-C-N	6.46	134.92	122.53
1	B	168	VAL	C-N-CA	6.46	134.92	122.53
1	B	614	GLU	O-C-N	-6.45	114.01	122.59
1	A	388	ASP	O-C-N	6.45	128.74	122.03
1	B	412	VAL	CA-C-N	-6.45	112.77	121.80
1	B	412	VAL	C-N-CA	-6.45	112.77	121.80
1	A	193	HIS	O-C-N	6.45	130.00	122.20
1	B	93	CYS	CA-C-O	-6.45	113.63	121.36
1	D	443	ILE	CA-C-O	-6.45	113.65	120.48
1	D	572	LYS	N-CA-C	6.44	118.38	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	278	GLU	CA-C-O	6.44	127.95	120.80
1	D	612	HIS	CA-CB-CG	6.44	120.24	113.80
1	A	574	LYS	CB-CG-CD	6.44	126.11	111.30
1	A	193	HIS	CB-CG-ND1	6.44	132.36	122.70
1	B	185	GLY	CA-C-O	6.44	127.35	120.40
1	B	12	GLN	CG-CD-OE1	6.43	133.67	120.80
1	B	447	GLU	CA-C-N	-6.43	113.71	122.91
1	B	447	GLU	C-N-CA	-6.43	113.71	122.91
1	A	110	MET	CA-C-O	6.43	128.32	120.92
1	B	181	VAL	CA-C-N	6.43	128.90	120.28
1	B	181	VAL	C-N-CA	6.43	128.90	120.28
1	A	460	PHE	CB-CA-C	-6.43	96.62	110.45
1	B	5	THR	N-CA-CB	6.43	122.43	111.50
1	B	607	ALA	N-CA-C	-6.43	103.87	112.94
1	A	226	GLN	CB-CG-CD	6.43	123.53	112.60
1	A	81	LYS	N-CA-C	6.43	119.11	111.33
1	A	336	ASN	CA-C-O	-6.43	110.24	121.62
1	C	31	LYS	CA-C-O	-6.43	113.11	120.24
1	E	238	ASN	CA-CB-CG	-6.43	106.17	112.60
1	F	532	ASP	N-CA-C	-6.43	102.01	110.43
1	A	259	LEU	CB-CA-C	6.43	121.75	111.66
1	B	330	SER	O-C-N	6.43	131.14	122.59
1	C	290	GLU	CB-CG-CD	6.43	123.52	112.60
1	C	278	GLU	CA-C-O	6.42	127.93	120.80
1	C	254	GLU	N-CA-C	6.42	120.05	107.98
1	B	139	GLN	N-CA-C	-6.42	105.75	113.97
1	E	466	MET	N-CA-C	6.42	118.15	108.46
1	A	441	GLU	CB-CA-C	-6.42	97.65	110.42
1	A	252	ILE	N-CA-C	-6.41	97.34	107.15
1	A	279	ASP	N-CA-C	-6.41	100.68	110.30
1	A	449	ASN	N-CA-C	6.41	119.46	109.52
1	B	57	MET	N-CA-CB	6.41	119.57	109.82
1	F	181	VAL	N-CA-C	-6.41	105.08	111.88
1	A	158	LYS	N-CA-C	6.41	118.27	111.28
1	E	515	GLY	CA-C-N	6.41	127.85	119.84
1	E	515	GLY	C-N-CA	6.41	127.85	119.84
1	A	187	ASP	CB-CA-C	6.41	120.28	109.84
1	F	31	LYS	CA-C-O	-6.41	113.13	120.24
1	A	252	ILE	N-CA-CB	6.41	118.96	111.66
1	D	278	GLU	CA-C-O	6.41	127.91	120.80
1	A	516	PRO	CA-C-O	6.40	132.25	120.60
1	A	30	LEU	CB-CA-C	6.40	122.88	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	462	TYR	N-CA-CB	6.40	121.07	110.63
1	A	194	HIS	CB-CA-C	6.40	121.56	110.68
1	D	279	ASP	N-CA-CB	-6.40	99.40	109.51
1	B	425	PHE	CA-C-N	-6.40	113.47	123.13
1	B	425	PHE	C-N-CA	-6.40	113.47	123.13
1	D	523	SER	N-CA-C	-6.40	103.59	111.33
1	A	307	ASP	O-C-N	6.40	129.72	121.79
1	C	472	GLY	CA-C-N	6.40	131.43	121.26
1	C	472	GLY	C-N-CA	6.40	131.43	121.26
1	A	297	HIS	ND1-CG-CD2	6.39	112.49	106.10
1	A	468	ASN	CA-C-N	-6.39	110.04	120.72
1	A	468	ASN	C-N-CA	-6.39	110.04	120.72
1	B	332	LYS	CA-CB-CG	-6.39	101.31	114.10
1	B	399	PRO	N-CA-C	-6.39	102.90	110.70
1	B	421	GLU	CA-C-N	-6.39	114.03	123.11
1	B	421	GLU	C-N-CA	-6.39	114.03	123.11
1	A	354	GLN	N-CA-C	-6.39	104.03	112.34
1	A	519	ILE	O-C-N	-6.39	115.18	122.72
1	B	454	ARG	NE-CZ-NH1	6.39	127.89	121.50
1	A	271	ARG	CA-C-O	-6.39	113.73	119.86
1	B	30	LEU	CA-C-N	-6.39	111.72	120.28
1	B	30	LEU	C-N-CA	-6.39	111.72	120.28
1	B	69	ARG	NE-CZ-NH1	6.39	127.89	121.50
1	B	197	TRP	CE3-CZ3-CH2	-6.39	112.80	121.10
1	B	421	GLU	CA-C-O	-6.39	113.83	120.99
1	B	561	SER	N-CA-CB	-6.39	100.46	110.30
1	A	32	ASP	CB-CA-C	6.39	123.20	110.17
1	A	292	THR	O-C-N	6.39	128.65	122.07
1	A	479	ARG	CA-CB-CG	-6.39	101.33	114.10
1	C	138	TYR	CA-CB-CG	6.39	125.39	113.90
1	F	49	HIS	CA-C-O	6.39	128.24	120.57
1	A	165	THR	CB-CA-C	6.38	120.06	109.53
1	A	434	ILE	N-CA-C	6.38	117.17	110.72
1	E	496	ASP	N-CA-C	-6.38	97.20	110.80
1	B	426	PHE	O-C-N	-6.38	113.26	122.96
1	A	475	LEU	O-C-N	6.38	130.49	122.65
1	B	14	ILE	N-CA-CB	-6.38	103.43	110.51
1	B	149	GLU	CG-CD-OE2	-6.38	103.74	118.40
1	B	215	ARG	CA-CB-CG	6.38	126.85	114.10
1	B	314	ASP	CA-CB-CG	-6.38	106.22	112.60
1	B	328	ILE	CA-CB-CG1	-6.38	99.56	110.40
1	B	105	TYR	O-C-N	6.37	128.72	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	420	GLY	N-CA-C	-6.37	101.79	110.20
1	D	432	SER	N-CA-C	6.37	119.33	109.07
1	A	465	THR	CA-C-N	-6.37	109.38	121.54
1	A	465	THR	C-N-CA	-6.37	109.38	121.54
1	A	538	SER	O-C-N	-6.36	115.37	122.12
1	B	216	LYS	N-CA-C	-6.36	97.24	110.80
1	B	405	ASN	CB-CG-OD1	6.36	133.53	120.80
1	B	321	ILE	CA-C-N	-6.36	108.09	121.64
1	B	321	ILE	C-N-CA	-6.36	108.09	121.64
1	B	385	LYS	CB-CA-C	6.36	120.95	110.90
1	A	158	LYS	N-CA-CB	-6.36	100.77	110.12
1	B	508	PHE	CA-C-O	-6.36	113.87	120.99
1	B	617	PRO	N-CA-C	6.36	121.90	113.57
1	C	212	HIS	CA-CB-CG	6.36	120.16	113.80
1	F	238	ASN	CA-CB-CG	-6.36	106.24	112.60
1	B	288	ASP	CA-C-O	6.36	127.32	120.20
1	D	181	VAL	CA-C-N	6.36	129.31	120.29
1	D	181	VAL	C-N-CA	6.36	129.31	120.29
1	A	184	PHE	CB-CA-C	-6.35	100.12	110.79
1	B	324	LEU	O-C-N	6.35	128.61	122.07
1	B	190	MET	CA-C-O	-6.35	113.75	120.55
1	A	125	HIS	CA-CB-CG	-6.34	107.46	113.80
1	A	193	HIS	CB-CG-CD2	-6.34	122.96	131.20
1	B	247	HIS	CG-CD2-NE2	-6.34	100.86	107.20
1	B	438	ASP	CB-CG-OD2	-6.34	103.82	118.40
1	C	177	ARG	N-CA-C	6.34	124.30	110.80
1	A	121	VAL	CA-CB-CG2	-6.34	99.63	110.40
1	A	69	ARG	CA-CB-CG	-6.34	101.43	114.10
1	A	618	ASP	CA-C-N	6.33	133.43	122.09
1	A	618	ASP	C-N-CA	6.33	133.43	122.09
1	A	121	VAL	O-C-N	6.33	128.12	121.91
1	A	212	HIS	CA-C-N	-6.33	112.54	121.72
1	A	212	HIS	C-N-CA	-6.33	112.54	121.72
1	A	43	THR	O-C-N	6.33	131.01	122.59
1	B	272	PRO	CA-N-CD	-6.33	103.14	112.00
1	F	496	ASP	N-CA-C	-6.33	97.32	110.80
1	B	376	ARG	CA-CB-CG	6.33	126.75	114.10
1	B	543	ALA	N-CA-C	-6.33	102.93	112.04
1	A	291	ILE	O-C-N	-6.32	115.32	121.83
1	B	104	ALA	N-CA-C	-6.32	97.33	110.80
1	D	290	GLU	CB-CG-CD	6.32	123.35	112.60
1	A	531	PRO	O-C-N	6.32	130.86	123.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	646	VAL	CA-CB-CG1	6.32	121.14	110.40
1	B	591	LYS	O-C-N	6.32	130.13	122.48
1	D	9	GLN	O-C-N	6.32	127.98	121.79
1	E	387	MET	N-CA-CB	6.32	119.36	109.94
1	A	13	ASP	CA-C-O	-6.32	113.81	120.63
1	A	42	ASP	N-CA-C	-6.32	97.34	110.80
1	A	105	TYR	CA-CB-CG	-6.32	102.53	113.90
1	A	381	PHE	CA-C-O	6.32	127.14	119.31
1	E	489	ASN	CB-CA-C	6.32	122.99	110.42
1	A	38	ASN	O-C-N	6.31	126.68	121.44
1	B	206	GLU	OE1-CD-OE2	-6.31	107.75	122.90
1	A	297	HIS	CA-C-O	-6.31	111.85	119.49
1	A	557	ALA	N-CA-C	-6.31	97.36	110.80
1	E	152	ASP	CA-CB-CG	6.31	118.91	112.60
1	A	337	VAL	N-CA-C	-6.31	104.80	113.00
1	F	218	GLU	N-CA-CB	6.31	119.49	110.16
1	A	620	ARG	NH1-CZ-NH2	-6.30	111.10	119.30
1	D	27	TYR	CB-CA-C	6.30	116.11	110.44
1	D	218	GLU	N-CA-CB	6.30	119.49	110.16
1	A	30	LEU	N-CA-C	-6.30	103.68	111.75
1	A	284	ALA	O-C-N	6.30	129.08	123.41
1	B	23	GLU	CA-C-O	6.30	126.33	119.91
1	B	544	ASP	N-CA-C	-6.30	103.55	111.11
1	C	207	ASP	CA-CB-CG	6.30	118.90	112.60
1	D	42	ASP	CA-CB-CG	6.30	118.90	112.60
1	D	423	ILE	CB-CA-C	6.29	120.23	110.28
1	A	285	HIS	ND1-CE1-NE2	6.29	114.69	108.40
1	B	532	ASP	CA-C-O	-6.29	114.82	121.99
1	B	224	HIS	CA-CB-CG	-6.29	107.51	113.80
1	B	263	LYS	CA-C-O	-6.29	113.82	120.55
1	B	474	ARG	N-CA-CB	-6.29	99.74	111.13
1	D	138	TYR	CA-CB-CG	6.29	125.23	113.90
1	E	218	GLU	N-CA-CB	6.29	119.47	110.16
1	A	350	MET	CA-CB-CG	-6.29	101.53	114.10
1	A	454	ARG	NE-CZ-NH1	-6.29	115.21	121.50
1	C	49	HIS	CA-C-O	6.28	128.11	120.57
1	C	496	ASP	N-CA-C	-6.28	97.42	110.80
1	D	27	TYR	CA-C-N	6.28	127.69	119.84
1	D	27	TYR	C-N-CA	6.28	127.69	119.84
1	E	556	SER	CA-C-O	6.28	127.07	120.54
1	B	94	LYS	O-C-N	6.28	129.77	122.17
1	B	548	ASN	CA-CB-CG	-6.28	106.32	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	387	MET	N-CA-CB	6.28	119.30	109.94
1	F	276	HIS	CA-CB-CG	-6.28	107.52	113.80
1	F	331	SER	N-CA-C	-6.27	100.14	109.86
1	A	513	PRO	CA-C-O	-6.27	113.87	122.15
1	B	32	ASP	CA-CB-CG	6.27	118.87	112.60
1	B	194	HIS	CA-C-O	6.27	127.61	120.90
1	A	253	ARG	CA-CB-CG	6.27	126.63	114.10
1	D	380	PHE	CA-CB-CG	-6.27	107.53	113.80
1	F	543	ALA	CA-C-N	6.27	128.68	120.28
1	F	543	ALA	C-N-CA	6.27	128.68	120.28
1	A	177	ARG	CB-CG-CD	-6.26	96.89	111.30
1	A	293	GLU	O-C-N	-6.26	115.48	122.12
1	B	296	ILE	CB-CG1-CD1	-6.26	100.64	113.80
1	A	323	LEU	O-C-N	6.26	128.60	122.09
1	B	540	LYS	N-CA-C	-6.26	103.16	111.24
1	A	140	ILE	CB-CA-C	-6.26	103.85	112.24
1	A	490	GLY	CA-C-N	-6.26	111.23	121.19
1	A	490	GLY	C-N-CA	-6.26	111.23	121.19
1	B	463	LYS	CA-C-N	6.26	130.32	122.43
1	B	463	LYS	C-N-CA	6.26	130.32	122.43
1	B	231	PHE	N-CA-CB	6.26	119.05	109.91
1	B	497	GLU	CA-C-O	-6.26	112.77	119.97
1	D	254	GLU	N-CA-C	6.26	119.75	107.98
1	A	651	HIS	CG-CD2-NE2	6.26	113.46	107.20
1	B	184	PHE	CZ-CE2-CD2	-6.26	108.73	120.00
1	D	181	VAL	N-CA-C	-6.26	105.25	111.88
1	D	496	ASP	N-CA-C	-6.26	97.47	110.80
1	A	357	PRO	N-CA-CB	-6.26	96.43	103.44
1	E	31	LYS	CA-CB-CG	6.26	126.61	114.10
1	E	276	HIS	CA-CB-CG	-6.26	107.54	113.80
1	A	545	ASN	CA-CB-CG	6.25	118.85	112.60
1	F	49	HIS	CA-C-N	6.25	133.66	121.41
1	F	49	HIS	C-N-CA	6.25	133.66	121.41
1	A	218	GLU	N-CA-C	-6.25	104.57	111.82
1	B	353	ARG	O-C-N	6.25	130.45	122.39
1	B	246	LEU	O-C-N	6.24	130.50	122.89
1	A	374	ALA	CB-CA-C	6.24	122.12	110.70
1	A	555	LEU	N-CA-CB	-6.24	99.95	110.49
1	F	422	LEU	CA-C-N	-6.24	113.70	122.75
1	F	422	LEU	C-N-CA	-6.24	113.70	122.75
1	A	107	ARG	CA-CB-CG	6.24	126.57	114.10
1	C	56	LEU	N-CA-C	-6.24	104.11	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	LYS	O-C-N	6.24	129.31	122.20
1	B	313	ILE	CB-CG1-CD1	-6.24	100.71	113.80
1	A	496	ASP	CA-C-N	-6.23	110.84	120.31
1	A	496	ASP	C-N-CA	-6.23	110.84	120.31
1	A	587	THR	CA-C-N	6.23	132.48	122.32
1	A	587	THR	C-N-CA	6.23	132.48	122.32
1	B	137	LEU	O-C-N	6.23	130.88	122.59
1	C	276	HIS	CA-CB-CG	-6.23	107.57	113.80
1	F	226	GLN	CB-CA-C	6.23	122.11	110.70
1	A	567	ARG	NH1-CZ-NH2	-6.23	111.20	119.30
1	B	452	VAL	CA-CB-CG1	6.23	120.99	110.40
1	C	387	MET	N-CA-CB	6.23	119.22	109.94
1	F	517	GLU	N-CA-CB	6.23	121.33	111.43
1	B	90	LEU	CD1-CG-CD2	-6.23	97.10	110.80
1	C	169	SER	N-CA-CB	-6.23	100.89	110.42
1	B	147	ASN	O-C-N	6.22	130.87	122.59
1	B	314	ASP	O-C-N	6.22	130.53	122.87
1	F	580	PHE	N-CA-C	-6.22	101.25	110.46
1	B	266	GLY	N-CA-C	-6.22	102.13	110.97
1	B	366	GLY	O-C-N	-6.22	117.88	123.29
1	A	414	ASN	CA-C-N	-6.22	112.43	121.26
1	A	414	ASN	C-N-CA	-6.22	112.43	121.26
1	A	146	THR	CA-CB-CG2	6.22	121.07	110.50
1	A	422	LEU	CA-C-O	-6.22	111.62	120.51
1	B	302	HIS	CG-CD2-NE2	6.21	113.41	107.20
1	C	218	GLU	N-CA-CB	6.21	119.36	110.16
1	F	30	LEU	CB-CA-C	6.21	121.24	110.68
1	B	414	ASN	CB-CG-OD1	-6.21	108.38	120.80
1	B	289	LEU	N-CA-CB	-6.21	100.94	110.07
1	B	346	THR	N-CA-CB	6.21	119.19	109.94
1	C	432	SER	N-CA-C	6.21	119.06	109.07
1	A	372	GLU	CG-CD-OE2	-6.21	104.13	118.40
1	B	357	PRO	O-C-N	6.21	131.02	122.64
1	B	580	PHE	N-CA-C	-6.21	100.80	110.17
1	C	49	HIS	CA-C-N	6.21	133.57	121.41
1	C	49	HIS	C-N-CA	6.21	133.57	121.41
1	F	581	ASN	CA-CB-CG	6.20	118.80	112.60
1	B	23	GLU	CA-CB-CG	6.20	126.50	114.10
1	B	142	PRO	N-CA-C	6.20	121.66	114.03
1	A	401	TYR	O-C-N	6.20	130.35	123.16
1	B	235	ARG	CA-C-O	-6.20	113.85	120.42
1	A	253	ARG	CA-C-N	6.20	132.25	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ARG	C-N-CA	6.20	132.25	122.34
1	E	162	LYS	CB-CA-C	6.20	118.56	109.08
1	C	9	GLN	O-C-N	6.19	127.86	121.79
1	A	62	ASP	CB-CG-OD1	-6.19	104.16	118.40
1	A	112	GLU	CB-CA-C	-6.19	98.78	110.67
1	A	384	HIS	N-CA-CB	6.19	120.18	110.46
1	D	226	GLN	CB-CA-C	6.19	122.03	110.70
1	B	274	ASN	N-CA-CB	6.19	121.48	112.13
1	B	318	PRO	O-C-N	6.19	130.20	122.22
1	B	82	GLU	CA-C-N	6.19	131.03	121.19
1	B	82	GLU	C-N-CA	6.19	131.03	121.19
1	F	169	SER	N-CA-CB	-6.19	100.95	110.42
1	F	212	HIS	CA-CB-CG	6.18	119.98	113.80
1	A	138	TYR	CA-CB-CG	6.18	125.03	113.90
1	B	313	ILE	N-CA-CB	6.18	120.01	112.10
1	C	30	LEU	CB-CA-C	6.18	121.19	110.68
1	B	411	MET	CA-CB-CG	-6.18	101.74	114.10
1	A	297	HIS	CB-CA-C	-6.18	97.28	110.32
1	A	248	TRP	CA-C-O	-6.18	111.20	119.11
1	A	632	ASP	CB-CG-OD1	-6.18	104.19	118.40
1	A	637	ASP	N-CA-C	6.18	120.28	112.87
1	B	377	ASP	CA-C-N	6.18	126.36	119.32
1	B	377	ASP	C-N-CA	6.18	126.36	119.32
1	C	302	HIS	CA-CB-CG	6.18	119.98	113.80
1	F	201	PHE	O-C-N	6.18	126.94	121.32
1	A	285	HIS	N-CA-CB	-6.17	101.28	110.17
1	B	538	SER	CA-CB-OG	-6.17	98.75	111.10
1	C	181	VAL	N-CA-C	-6.17	105.33	111.88
1	F	56	LEU	N-CA-C	-6.17	104.18	111.03
1	B	311	HIS	CA-C-N	-6.17	112.15	122.64
1	B	311	HIS	C-N-CA	-6.17	112.15	122.64
1	A	144	MET	N-CA-CB	6.17	119.81	110.30
1	B	372	GLU	CG-CD-OE2	6.17	132.59	118.40
1	B	547	VAL	CA-C-O	6.17	125.95	120.70
1	A	295	ARG	CB-CA-C	6.17	120.68	110.81
1	C	558	TYR	N-CA-CB	-6.17	101.51	110.70
1	B	161	GLN	N-CA-CB	-6.16	103.10	112.28
1	A	236	LEU	CA-C-O	6.16	127.47	121.00
1	B	237	SER	CA-C-N	-6.16	112.81	122.49
1	B	237	SER	C-N-CA	-6.16	112.81	122.49
1	D	559	GLU	CA-CB-CG	6.16	126.42	114.10
1	E	581	ASN	CA-CB-CG	6.16	118.76	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	512	VAL	O-C-N	6.16	126.27	121.46
1	B	267	GLU	O-C-N	-6.16	116.02	123.16
1	C	363	LEU	CB-CA-C	6.15	118.38	109.09
1	A	407	GLU	OE1-CD-OE2	-6.15	108.13	122.90
1	E	206	GLU	OE1-CD-OE2	-6.15	108.14	122.90
1	A	47	ASN	CB-CG-OD1	6.15	133.10	120.80
1	A	460	PHE	CE1-CZ-CE2	-6.15	108.93	120.00
1	A	557	ALA	CA-C-O	6.15	129.31	120.51
1	E	56	LEU	N-CA-C	-6.15	104.20	111.03
1	B	423	ILE	CA-C-N	-6.15	112.97	122.87
1	B	423	ILE	C-N-CA	-6.15	112.97	122.87
1	A	258	PRO	CA-C-N	-6.15	113.04	122.08
1	A	258	PRO	C-N-CA	-6.15	113.04	122.08
1	A	460	PHE	N-CA-CB	-6.14	101.40	111.66
1	B	21	ILE	N-CA-C	6.14	120.74	111.89
1	D	277	PHE	CA-CB-CG	6.14	119.94	113.80
1	E	501	PHE	CA-CB-CG	6.14	119.94	113.80
1	B	93	CYS	CA-C-N	-6.13	110.47	120.71
1	B	93	CYS	C-N-CA	-6.13	110.47	120.71
1	F	466	MET	N-CA-C	6.13	117.72	108.46
1	A	566	ASP	N-CA-C	6.13	118.75	111.33
1	B	216	LYS	CB-CA-C	-6.13	98.22	110.42
1	A	362	ASN	N-CA-CB	-6.13	102.05	111.74
1	A	479	ARG	CA-C-N	-6.13	114.94	123.10
1	A	479	ARG	C-N-CA	-6.13	114.94	123.10
1	A	480	ILE	CA-CB-CG2	6.13	120.92	110.50
1	B	312	THR	CB-CA-C	6.13	119.86	109.50
1	D	489	ASN	N-CA-C	-6.13	97.74	110.80
1	A	476	ALA	CA-C-O	-6.13	113.25	120.60
1	B	344	HIS	CG-ND1-CE1	-6.13	98.88	109.30
1	A	306	THR	CA-CB-OG1	-6.13	100.41	109.60
1	B	103	ALA	CA-C-O	-6.13	111.75	120.51
1	A	235	ARG	CB-CG-CD	-6.12	97.21	111.30
1	A	362	ASN	O-C-N	-6.12	115.62	122.91
1	B	402	THR	CA-C-O	-6.12	114.41	121.82
1	A	179	GLN	CA-C-O	6.12	129.26	120.51
1	F	9	GLN	O-C-N	6.12	127.79	121.79
1	A	102	ASN	CB-CG-ND2	-6.12	107.22	116.40
1	C	226	GLN	CB-CA-C	6.12	121.89	110.70
1	A	267	GLU	CG-CD-OE1	-6.11	104.34	118.40
1	B	217	GLY	CA-C-O	-6.11	109.93	120.57
1	B	421	GLU	OE1-CD-OE2	6.11	137.57	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	HIS	CA-CB-CG	-6.11	107.69	113.80
1	A	229	ALA	O-C-N	6.11	128.38	122.03
1	C	201	PHE	O-C-N	6.11	126.88	121.32
1	C	488	ASN	N-CA-C	-6.11	105.13	112.58
1	D	387	MET	N-CA-CB	6.11	119.04	109.94
1	B	25	THR	N-CA-CB	6.10	119.56	110.29
1	D	264	TYR	N-CA-C	-6.10	98.57	108.52
1	A	61	ASN	CA-C-O	-6.10	113.47	120.24
1	D	581	ASN	CA-CB-CG	6.10	118.70	112.60
1	B	84	LEU	CB-CA-C	6.10	123.05	110.31
1	B	443	ILE	CA-C-N	-6.10	112.19	122.92
1	B	443	ILE	C-N-CA	-6.10	112.19	122.92
1	D	91	ASN	CA-C-O	-6.10	113.96	120.42
1	B	302	HIS	CA-C-O	-6.10	114.42	120.70
1	D	216	LYS	CA-CB-CG	6.10	126.29	114.10
1	A	316	ARG	CB-CG-CD	6.09	125.32	111.30
1	B	407	GLU	N-CA-C	6.09	119.06	110.23
1	B	456	ASN	OD1-CG-ND2	6.09	128.69	122.60
1	B	322	GLU	CA-C-N	-6.08	112.05	120.38
1	B	322	GLU	C-N-CA	-6.08	112.05	120.38
1	A	67	GLU	CB-CA-C	-6.08	97.06	109.65
1	A	247	HIS	CB-CA-C	-6.08	97.35	109.33
1	A	250	ARG	CA-C-O	-6.08	114.24	121.60
1	A	541	GLU	CA-C-N	6.08	129.55	120.31
1	A	541	GLU	C-N-CA	6.08	129.55	120.31
1	D	201	PHE	O-C-N	6.08	126.85	121.32
1	A	530	VAL	CA-C-N	6.08	127.29	120.66
1	A	530	VAL	C-N-CA	6.08	127.29	120.66
1	B	461	THR	CA-C-O	-6.08	114.00	121.11
1	A	225	HIS	ND1-CG-CD2	6.07	112.17	106.10
1	A	324	LEU	CA-C-O	-6.07	114.44	120.82
1	A	504	GLU	CB-CG-CD	-6.07	102.27	112.60
1	E	201	PHE	O-C-N	6.07	126.85	121.32
1	E	580	PHE	N-CA-C	-6.07	101.47	110.46
1	A	206	GLU	N-CA-C	-6.07	99.50	109.40
1	B	154	ALA	CA-C-O	-6.07	113.99	120.42
1	B	272	PRO	N-CA-CB	6.07	110.09	103.23
1	B	286	VAL	CA-C-O	6.07	127.38	119.85
1	B	611	VAL	CA-CB-CG1	6.07	120.72	110.40
1	E	138	TYR	CA-CB-CG	6.07	124.83	113.90
1	E	226	GLN	CB-CA-C	6.07	121.81	110.70
1	B	142	PRO	O-C-N	-6.07	113.86	122.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	207	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	103	ALA	O-C-N	-6.06	114.52	122.59
1	B	607	ALA	CA-C-O	6.06	126.64	119.48
1	A	627	GLU	CA-C-N	-6.06	112.62	122.81
1	A	627	GLU	C-N-CA	-6.06	112.62	122.81
1	A	12	GLN	OE1-CD-NE2	6.06	128.66	122.60
1	B	364	PRO	N-CA-C	-6.06	103.31	110.70
1	A	266	GLY	CA-C-O	-6.05	116.14	122.01
1	A	438	ASP	CA-C-N	6.05	133.10	121.54
1	A	438	ASP	C-N-CA	6.05	133.10	121.54
1	B	103	ALA	O-C-N	6.05	130.64	122.59
1	A	506	ASP	O-C-N	-6.05	117.97	123.41
1	A	560	ARG	N-CA-CB	-6.05	100.27	110.49
1	B	506	ASP	CA-CB-CG	-6.05	106.55	112.60
1	A	262	TYR	O-C-N	-6.05	115.21	122.65
1	B	294	SER	CA-C-N	6.05	128.70	120.54
1	B	294	SER	C-N-CA	6.05	128.70	120.54
1	B	413	VAL	CA-C-N	6.05	132.88	121.81
1	B	413	VAL	C-N-CA	6.05	132.88	121.81
1	E	489	ASN	N-CA-C	-6.05	97.92	110.80
1	B	370	HIS	CA-CB-CG	6.04	119.84	113.80
1	C	268	PHE	O-C-N	6.04	126.34	121.38
1	B	412	VAL	CA-CB-CG1	6.04	120.67	110.40
1	F	138	TYR	CA-CB-CG	6.04	124.78	113.90
1	B	496	ASP	OD1-CG-OD2	-6.04	108.40	122.90
1	E	9	GLN	O-C-N	6.04	127.71	121.79
1	E	217	GLY	N-CA-C	-6.04	98.86	113.18
1	A	338	GLN	O-C-N	6.04	131.25	122.43
1	B	109	ARG	NE-CZ-NH1	-6.04	115.46	121.50
1	B	260	THR	N-CA-CB	-6.04	101.19	110.85
1	B	215	ARG	O-C-N	6.04	129.48	121.99
1	B	232	ASP	OD1-CG-OD2	-6.04	108.41	122.90
1	C	497	GLU	N-CA-C	-6.04	104.78	111.36
1	A	332	LYS	N-CA-C	6.04	120.33	113.15
1	D	574	LYS	CB-CA-C	6.04	117.92	108.63
1	A	193	HIS	CG-CD2-NE2	6.03	113.23	107.20
1	F	152	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	404	ASP	CA-CB-CG	-6.03	106.57	112.60
1	B	124	ILE	O-C-N	6.03	127.82	121.91
1	A	93	CYS	N-CA-CB	-6.03	101.13	110.29
1	F	216	LYS	CA-CB-CG	6.03	126.15	114.10
1	F	363	LEU	CB-CA-C	6.03	118.19	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	GLN	CG-CD-NE2	-6.02	107.37	116.40
1	B	353	ARG	CA-C-N	-6.02	110.93	120.63
1	B	353	ARG	C-N-CA	-6.02	110.93	120.63
1	D	48	ASP	N-CA-C	-6.02	105.23	113.30
1	D	217	GLY	N-CA-C	-6.02	98.91	113.18
1	F	217	GLY	N-CA-C	-6.02	98.91	113.18
1	F	489	ASN	CB-CA-C	6.02	122.41	110.42
1	F	572	LYS	N-CA-C	6.02	117.92	111.36
1	A	403	HIS	CA-C-O	6.02	127.32	121.00
1	A	272	PRO	N-CA-C	-6.02	102.42	111.57
1	B	124	ILE	N-CA-CB	6.02	117.59	110.55
1	A	584	VAL	CG1-CB-CG2	6.02	124.04	110.80
1	B	230	ARG	CA-C-O	6.02	127.66	120.92
1	A	137	LEU	CA-C-N	6.01	129.16	120.38
1	A	137	LEU	C-N-CA	6.01	129.16	120.38
1	A	369	GLU	CB-CG-CD	6.01	122.82	112.60
1	A	591	LYS	O-C-N	6.01	129.75	122.35
1	B	195	VAL	N-CA-CB	6.01	118.26	110.57
1	B	279	ASP	N-CA-CB	-6.01	100.01	109.51
1	B	502	CYS	N-CA-CB	6.01	119.13	110.06
1	B	508	PHE	CA-C-N	-6.01	114.78	122.77
1	B	508	PHE	C-N-CA	-6.01	114.78	122.77
1	D	444	GLU	CA-C-N	6.01	129.29	120.82
1	D	444	GLU	C-N-CA	6.01	129.29	120.82
1	D	273	ASP	CB-CA-C	6.01	119.78	109.51
1	B	564	ILE	N-CA-CB	6.01	119.62	111.21
1	D	69	ARG	CB-CG-CD	6.01	125.11	111.30
1	A	159	MET	CA-CB-CG	6.00	126.11	114.10
1	B	619	ASN	CB-CG-ND2	6.00	125.41	116.40
1	A	375	THR	CA-C-O	6.00	129.09	120.51
1	B	410	GLY	O-C-N	6.00	130.50	122.70
1	A	524	LYS	O-C-N	6.00	128.99	122.15
1	C	217	GLY	N-CA-C	-6.00	98.96	113.18
1	B	79	GLN	CG-CD-NE2	-6.00	107.40	116.40
1	B	152	ASP	N-CA-CB	6.00	119.14	110.20
1	F	558	TYR	N-CA-C	6.00	120.21	112.41
1	A	280	VAL	CA-CB-CG1	6.00	120.59	110.40
1	C	555	LEU	N-CA-CB	-6.00	102.50	111.25
1	A	451	ARG	CD-NE-CZ	-5.99	116.01	124.40
1	B	344	HIS	CE1-NE2-CD2	5.99	114.99	109.00
1	B	385	LYS	CA-C-O	5.99	126.87	120.70
1	A	194	HIS	CG-CD2-NE2	-5.99	101.21	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466	MET	CA-C-N	5.99	131.62	122.93
1	B	466	MET	C-N-CA	5.99	131.62	122.93
1	A	296	ILE	CA-C-O	5.99	127.70	121.29
1	A	309	ASP	CB-CG-OD2	-5.99	104.63	118.40
1	A	26	LYS	CD-CE-NZ	5.98	131.04	111.90
1	A	357	PRO	CA-C-N	-5.98	110.93	122.06
1	A	357	PRO	C-N-CA	-5.98	110.93	122.06
1	B	354	GLN	CB-CG-CD	5.98	122.77	112.60
1	B	365	PRO	CB-CG-CD	-5.98	86.96	106.10
1	A	56	LEU	CA-C-O	-5.98	114.74	120.90
1	A	92	GLN	CA-CB-CG	5.98	126.06	114.10
1	A	182	ALA	CA-C-O	5.98	126.89	120.55
1	A	611	VAL	CA-CB-CG2	5.98	120.57	110.40
1	B	526	SER	N-CA-C	5.98	118.67	110.24
1	B	143	HIS	CE1-NE2-CD2	5.98	114.98	109.00
1	C	216	LYS	CA-CB-CG	5.98	126.06	114.10
1	B	244	ASP	CB-CG-OD1	5.97	132.14	118.40
1	F	497	GLU	N-CA-C	-5.97	104.85	111.36
1	B	500	TRP	CB-CG-CD1	5.97	135.86	126.90
1	E	49	HIS	CA-C-O	5.97	127.74	120.57
1	B	616	TYR	CA-C-O	-5.97	114.69	119.71
1	A	144	MET	CA-C-O	-5.97	112.75	119.79
1	A	325	GLY	CA-C-N	-5.97	110.53	120.68
1	A	325	GLY	C-N-CA	-5.97	110.53	120.68
1	B	427	ASP	CA-C-O	5.97	129.05	120.51
1	C	264	TYR	N-CA-C	-5.97	98.79	108.52
1	A	560	ARG	CB-CA-C	5.97	122.30	110.42
1	B	507	LYS	CB-CA-C	-5.97	103.30	110.94
1	A	36	ASN	CA-CB-CG	-5.97	106.63	112.60
1	B	362	ASN	CA-C-O	5.97	130.21	122.45
1	A	27	TYR	CB-CG-CD1	5.96	129.75	120.80
1	A	560	ARG	NE-CZ-NH2	-5.96	113.83	119.20
1	D	169	SER	N-CA-CB	-5.96	101.29	110.42
1	A	85	MET	N-CA-CB	5.96	119.27	110.33
1	A	309	ASP	N-CA-CB	5.96	119.74	110.44
1	B	621	PRO	CA-C-O	-5.96	109.75	120.60
1	A	139	GLN	O-C-N	5.96	130.47	122.49
1	B	64	ARG	CD-NE-CZ	-5.96	116.06	124.40
1	A	251	ILE	CA-C-N	-5.95	115.04	122.48
1	A	251	ILE	C-N-CA	-5.95	115.04	122.48
1	A	463	LYS	CB-CG-CD	5.95	124.99	111.30
1	B	69	ARG	NH1-CZ-NH2	-5.95	111.56	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	622	LEU	N-CA-C	5.95	118.43	108.73
1	B	411	MET	N-CA-C	5.95	123.48	110.80
1	F	432	SER	N-CA-C	5.95	118.65	109.07
1	B	612	HIS	N-CA-C	5.95	119.85	112.59
1	D	42	ASP	N-CA-C	-5.95	98.13	110.80
1	D	555	LEU	N-CA-C	-5.95	104.55	112.94
1	A	313	ILE	N-CA-C	-5.95	99.18	107.80
1	A	395	THR	N-CA-CB	5.95	118.64	110.01
1	B	461	THR	O-C-N	5.95	130.56	123.24
1	C	69	ARG	CB-CG-CD	5.95	124.98	111.30
1	A	484	PRO	O-C-N	5.95	130.67	122.64
1	B	438	ASP	CA-C-O	-5.95	114.08	120.92
1	A	593	THR	CA-CB-OG1	-5.95	100.68	109.60
1	B	621	PRO	CA-C-N	-5.95	114.86	122.77
1	B	621	PRO	C-N-CA	-5.95	114.86	122.77
1	F	69	ARG	CB-CG-CD	5.95	124.98	111.30
1	A	422	LEU	CD1-CG-CD2	-5.94	97.72	110.80
1	B	570	LEU	CA-C-N	5.94	125.92	120.21
1	B	570	LEU	C-N-CA	5.94	125.92	120.21
1	B	336	ASN	CB-CG-ND2	-5.94	107.49	116.40
1	B	44	SER	O-C-N	5.94	130.49	122.59
1	B	531	PRO	CA-C-N	-5.94	109.89	121.06
1	B	531	PRO	C-N-CA	-5.94	109.89	121.06
1	A	56	LEU	CB-CA-C	5.94	120.16	110.95
1	A	426	PHE	N-CA-C	5.94	119.63	107.69
1	E	216	LYS	CA-CB-CG	5.94	125.98	114.10
1	A	412	VAL	CA-C-O	-5.94	114.37	120.25
1	B	28	PRO	CB-CA-C	-5.94	101.76	111.56
1	B	66	LEU	CA-C-N	5.94	131.78	120.97
1	B	66	LEU	C-N-CA	5.94	131.78	120.97
1	B	224	HIS	CA-C-O	5.94	126.80	119.79
1	B	512	VAL	CA-CB-CG1	-5.94	100.31	110.40
1	A	188	ILE	CB-CG1-CD1	-5.93	101.34	113.80
1	A	437	VAL	CA-C-N	-5.93	113.83	122.19
1	A	437	VAL	C-N-CA	-5.93	113.83	122.19
1	B	587	THR	CA-CB-CG2	5.93	120.58	110.50
1	A	421	GLU	N-CA-CB	5.93	120.08	110.77
1	B	125	HIS	N-CA-C	5.93	120.67	112.90
1	C	225	HIS	N-CA-C	-5.93	104.82	111.28
1	A	93	CYS	CB-CA-C	5.93	120.37	109.46
1	B	17	LEU	CB-CG-CD2	-5.93	92.92	110.70
1	A	102	ASN	CA-CB-CG	-5.93	106.67	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	112	GLU	CB-CA-C	-5.92	100.96	110.79
1	B	102	ASN	CB-CG-ND2	-5.92	107.52	116.40
1	B	274	ASN	CB-CG-OD1	-5.92	108.96	120.80
1	B	468	ASN	N-CA-CB	-5.92	100.70	110.53
1	A	216	LYS	CA-C-O	-5.92	113.89	120.70
1	A	356	ASP	N-CA-CB	-5.92	99.84	110.37
1	B	207	ASP	CB-CG-OD1	5.92	132.01	118.40
1	C	562	CYS	N-CA-C	5.92	118.52	111.71
1	A	506	ASP	CA-C-N	5.92	130.39	121.40
1	A	506	ASP	C-N-CA	5.92	130.39	121.40
1	B	466	MET	N-CA-C	5.92	117.39	108.46
1	F	273	ASP	CB-CA-C	5.92	120.18	109.83
1	B	143	HIS	ND1-CE1-NE2	-5.91	102.49	108.40
1	C	32	ASP	N-CA-C	-5.91	104.91	111.71
1	D	214	ASP	N-CA-C	5.91	123.40	110.80
1	E	632	ASP	CB-CA-C	5.91	119.60	110.14
1	A	247	HIS	CG-CD2-NE2	-5.91	101.29	107.20
1	A	571	PRO	CB-CA-C	5.91	119.50	110.75
1	A	616	TYR	O-C-N	5.91	126.22	121.38
1	B	362	ASN	CA-CB-CG	5.91	118.51	112.60
1	B	461	THR	CA-CB-CG2	5.91	120.55	110.50
1	C	91	ASN	CA-C-O	-5.91	114.16	120.42
1	E	497	GLU	N-CA-C	-5.91	104.92	111.36
1	B	50	GLY	CA-C-O	5.90	130.84	120.57
1	B	211	TYR	CA-C-O	5.90	127.63	121.31
1	D	65	LEU	N-CA-CB	-5.90	101.01	110.63
1	D	442	ASN	CA-CB-CG	-5.90	106.70	112.60
1	B	371	PHE	N-CA-C	5.90	119.67	112.23
1	B	35	GLU	OE1-CD-OE2	-5.90	108.74	122.90
1	C	49	HIS	CA-CB-CG	-5.90	107.90	113.80
1	A	41	GLY	N-CA-C	-5.90	99.20	113.18
1	F	403	HIS	N-CA-C	-5.90	104.54	110.97
1	B	204	TRP	CA-C-O	5.89	128.31	119.23
1	C	581	ASN	CA-CB-CG	5.89	118.49	112.60
1	A	204	TRP	CA-C-O	5.89	126.18	119.18
1	B	207	ASP	N-CA-C	-5.88	106.19	113.19
1	A	117	TYR	CG-CD1-CE1	5.88	130.02	121.20
1	F	264	TYR	N-CA-C	-5.88	98.93	108.52
1	B	490	GLY	CA-C-N	-5.88	111.39	121.09
1	B	490	GLY	C-N-CA	-5.88	111.39	121.09
1	A	508	PHE	CA-CB-CG	5.88	119.68	113.80
1	A	250	ARG	NE-CZ-NH1	-5.88	115.62	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	112	GLU	CB-CA-C	-5.88	101.04	110.79
1	A	238	ASN	CB-CA-C	5.87	120.56	111.28
1	B	68	GLN	CB-CG-CD	-5.87	102.62	112.60
1	E	91	ASN	CA-C-O	-5.87	114.19	120.42
1	A	235	ARG	N-CA-CB	5.87	119.38	110.28
1	C	181	VAL	CA-C-N	5.87	128.63	120.29
1	C	181	VAL	C-N-CA	5.87	128.63	120.29
1	A	216	LYS	CG-CD-CE	-5.87	97.80	111.30
1	A	301	ASP	O-C-N	-5.87	114.47	122.33
1	A	618	ASP	CA-CB-CG	5.87	118.47	112.60
1	D	139	GLN	CA-CB-CG	5.87	125.83	114.10
1	A	494	THR	N-CA-CB	-5.87	102.75	111.43
1	A	150	VAL	O-C-N	5.86	127.80	121.94
1	A	497	GLU	N-CA-CB	5.86	119.37	110.28
1	B	56	LEU	N-CA-C	-5.86	104.48	111.69
1	A	645	VAL	CB-CA-C	5.86	119.53	110.50
1	A	651	HIS	CE1-NE2-CD2	-5.86	103.14	109.00
1	B	128	LEU	CB-CA-C	-5.86	98.76	110.42
1	B	184	PHE	CA-C-N	5.86	127.47	120.14
1	B	184	PHE	C-N-CA	5.86	127.47	120.14
1	B	560	ARG	CB-CA-C	5.86	119.17	110.62
1	F	91	ASN	CA-C-O	-5.86	114.21	120.42
1	A	113	GLY	O-C-N	5.86	127.87	122.19
1	B	424	THR	CA-CB-CG2	5.86	120.45	110.50
1	B	528	VAL	N-CA-CB	-5.86	105.54	112.39
1	F	42	ASP	CA-CB-CG	5.86	118.45	112.60
1	A	348	HIS	N-CA-C	-5.85	103.69	111.24
1	C	632	ASP	CB-CA-C	5.85	119.50	110.14
1	A	393	LYS	N-CA-CB	5.85	119.23	110.22
1	B	614	GLU	CA-C-O	5.85	128.87	120.51
1	A	499	ARG	NE-CZ-NH1	-5.85	115.65	121.50
1	A	149	GLU	CB-CG-CD	5.84	122.53	112.60
1	A	469	ASN	O-C-N	5.84	130.26	122.43
1	A	590	ASP	CA-CB-CG	5.84	118.44	112.60
1	B	368	MET	N-CA-CB	-5.84	100.59	110.41
1	F	554	ASP	N-CA-C	-5.84	102.62	111.56
1	F	632	ASP	CB-CA-C	5.84	119.49	110.14
1	B	101	SER	CB-CA-C	5.84	122.05	110.42
1	B	289	LEU	N-CA-C	-5.84	103.71	111.24
1	B	557	ALA	CA-C-N	-5.84	113.38	122.67
1	B	557	ALA	C-N-CA	-5.84	113.38	122.67
1	E	432	SER	N-CA-C	5.84	118.48	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	LEU	CA-C-N	5.84	129.77	121.42
1	A	65	LEU	C-N-CA	5.84	129.77	121.42
1	A	147	ASN	CB-CG-ND2	5.84	125.16	116.40
1	A	388	ASP	CA-CB-CG	5.84	118.44	112.60
1	C	444	GLU	CA-CB-CG	5.84	125.77	114.10
1	C	139	GLN	CA-CB-CG	5.83	125.77	114.10
1	F	32	ASP	N-CA-C	-5.83	105.00	111.71
1	A	181	VAL	CB-CA-C	5.83	120.86	111.29
1	A	457	HIS	CA-C-O	-5.83	112.17	120.51
1	E	65	LEU	N-CA-CB	-5.83	101.12	110.63
1	A	163	PRO	CA-CB-CG	-5.83	93.42	104.50
1	A	221	PHE	CA-C-N	5.83	128.02	120.44
1	A	221	PHE	C-N-CA	5.83	128.02	120.44
1	A	143	HIS	N-CA-CB	-5.83	100.71	110.39
1	A	97	TYR	O-C-N	-5.83	115.56	122.20
1	B	540	LYS	CB-CG-CD	5.83	124.70	111.30
1	F	181	VAL	CA-C-N	5.83	128.56	120.29
1	F	181	VAL	C-N-CA	5.83	128.56	120.29
1	A	12	GLN	CA-C-N	5.82	128.36	120.38
1	A	12	GLN	C-N-CA	5.82	128.36	120.38
1	B	67	GLU	N-CA-CB	5.82	118.69	110.36
1	A	626	LEU	N-CA-CB	-5.82	102.06	110.56
1	B	9	GLN	O-C-N	5.82	130.33	122.59
1	F	225	HIS	N-CA-C	-5.82	104.53	111.69
1	A	100	ARG	CA-C-N	-5.82	112.70	120.79
1	A	100	ARG	C-N-CA	-5.82	112.70	120.79
1	B	476	ALA	O-C-N	-5.82	116.79	123.42
1	E	558	TYR	N-CA-CB	-5.82	102.14	110.57
1	A	569	LEU	CA-C-O	-5.81	112.20	120.51
1	B	302	HIS	O-C-N	5.81	128.37	122.09
1	B	25	THR	CA-C-O	-5.81	114.79	121.47
1	A	97	TYR	CA-C-N	5.81	130.51	120.58
1	A	97	TYR	C-N-CA	5.81	130.51	120.58
1	A	245	GLU	CG-CD-OE2	5.81	131.76	118.40
1	B	608	GLN	O-C-N	5.81	129.80	122.19
1	E	69	ARG	CB-CG-CD	5.81	124.66	111.30
1	A	321	ILE	CA-C-O	-5.81	113.00	120.03
1	B	276	HIS	O-C-N	5.81	130.59	123.21
1	A	16	HIS	CB-CG-CD2	-5.81	123.65	131.20
1	E	408	PHE	N-CA-C	-5.81	100.86	109.11
1	A	112	GLU	N-CA-C	5.80	118.55	111.82
1	A	443	ILE	CB-CA-C	5.80	119.22	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	ASN	N-CA-CB	5.80	118.75	110.16
1	B	360	LYS	CA-C-O	-5.80	112.48	119.27
1	C	42	ASP	CA-CB-CG	5.80	118.41	112.60
1	B	545	ASN	N-CA-CB	5.80	118.98	110.57
1	B	573	SER	CA-C-O	5.80	128.81	120.51
1	B	548	ASN	N-CA-CB	5.80	120.30	110.49
1	A	549	GLY	CA-C-O	5.80	130.66	120.57
1	E	214	ASP	N-CA-C	5.80	123.15	110.80
1	F	251	ILE	O-C-N	5.80	128.51	122.54
1	B	322	GLU	O-C-N	5.80	130.80	122.28
1	B	462	TYR	CB-CG-CD1	-5.79	112.11	120.80
1	D	49	HIS	CA-CB-CG	-5.79	108.01	113.80
1	B	166	PHE	O-C-N	-5.79	115.86	123.21
1	B	196	THR	CA-C-O	-5.79	114.41	120.55
1	B	227	LEU	N-CA-CB	5.79	118.41	110.01
1	D	238	ASN	CA-CB-CG	-5.79	106.81	112.60
1	E	537	GLN	N-CA-C	-5.79	105.05	111.36
1	A	205	TRP	CA-C-O	5.79	127.27	120.96
1	B	225	HIS	CB-CA-C	5.79	121.34	110.63
1	A	306	THR	O-C-N	-5.79	116.54	123.31
1	A	572	LYS	N-CA-CB	5.78	118.62	110.12
1	B	454	ARG	NE-CZ-NH2	-5.78	114.00	119.20
1	D	409	SER	N-CA-C	5.78	120.91	111.37
1	D	112	GLU	CB-CA-C	-5.78	101.19	110.79
1	A	45	ILE	O-C-N	5.78	129.00	122.18
1	B	540	LYS	CG-CD-CE	5.78	124.60	111.30
1	B	624	TYR	CB-CG-CD1	5.78	129.47	120.80
1	B	291	ILE	N-CA-CB	5.78	119.25	110.58
1	B	187	ASP	CA-C-O	5.78	127.45	120.81
1	B	486	GLU	CG-CD-OE2	-5.78	105.11	118.40
1	C	387	MET	CA-CB-CG	5.78	125.66	114.10
1	A	544	ASP	CB-CG-OD1	-5.78	105.12	118.40
1	A	593	THR	CA-C-O	5.78	128.77	120.51
1	B	373	THR	OG1-CB-CG2	5.77	120.85	109.30
1	B	431	TYR	CB-CA-C	5.77	121.09	110.24
1	A	267	GLU	O-C-N	5.77	129.85	123.16
1	B	212	HIS	N-CA-CB	-5.77	101.65	110.65
1	F	78	ARG	CB-CG-CD	5.77	124.57	111.30
1	A	276	HIS	ND1-CE1-NE2	-5.77	102.63	108.40
1	F	444	GLU	CA-C-N	5.77	129.56	121.02
1	F	444	GLU	C-N-CA	5.77	129.56	121.02
1	B	61	ASN	CB-CG-ND2	-5.77	107.75	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	ILE	CA-C-N	5.76	130.35	121.19
1	A	192	ILE	C-N-CA	5.76	130.35	121.19
1	A	643	LYS	CA-C-N	-5.76	113.86	122.74
1	A	643	LYS	C-N-CA	-5.76	113.86	122.74
1	F	67	GLU	CB-CA-C	-5.76	97.86	109.68
1	F	95	GLU	CA-CB-CG	5.76	125.63	114.10
1	F	545	ASN	CA-CB-CG	5.76	118.36	112.60
1	A	241	ASP	CB-CG-OD1	-5.76	105.15	118.40
1	C	89	VAL	CB-CA-C	5.76	120.73	111.29
1	B	203	PHE	N-CA-C	-5.76	105.09	111.71
1	B	414	ASN	O-C-N	5.76	128.94	122.32
1	C	112	GLU	CB-CA-C	-5.76	101.23	110.79
1	D	632	ASP	CB-CA-C	5.76	119.35	110.14
1	E	78	ARG	CB-CG-CD	5.76	124.54	111.30
1	F	369	GLU	CA-CB-CG	5.75	125.61	114.10
1	A	502	CYS	CA-C-N	5.75	131.14	122.91
1	A	502	CYS	C-N-CA	5.75	131.14	122.91
1	C	517	GLU	N-CA-CB	5.75	119.68	111.05
1	D	275	ILE	CB-CA-C	-5.75	105.26	111.59
1	A	62	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	207	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	274	ASN	CA-C-O	-5.75	114.44	121.28
1	B	277	PHE	N-CA-C	5.75	123.05	110.80
1	B	453	HIS	O-C-N	-5.75	115.80	122.87
1	D	207	ASP	CA-CB-CG	5.75	118.35	112.60
1	D	225	HIS	N-CA-C	-5.75	105.01	111.28
1	A	326	ASP	CA-C-O	-5.75	113.00	119.79
1	C	65	LEU	N-CA-CB	-5.75	101.26	110.63
1	B	71	TRP	CA-C-N	-5.75	111.83	121.94
1	B	71	TRP	C-N-CA	-5.75	111.83	121.94
1	B	357	PRO	N-CD-CG	-5.75	94.58	103.20
1	B	362	ASN	CB-CA-C	5.75	122.87	112.30
1	D	85	MET	N-CA-CB	5.75	118.76	110.20
1	A	429	PHE	O-C-N	5.75	130.31	123.24
1	B	206	GLU	N-CA-C	-5.75	100.53	109.72
1	B	241	ASP	CA-CB-CG	5.75	118.34	112.60
1	A	176	ASN	CA-C-O	-5.74	112.30	120.51
1	A	371	PHE	O-C-N	5.74	128.94	122.22
1	A	637	ASP	CA-C-O	-5.74	111.86	119.10
1	D	67	GLU	CB-CA-C	-5.74	97.91	109.68
1	E	212	HIS	CA-CB-CG	5.74	119.54	113.80
1	E	264	TYR	N-CA-C	-5.74	99.16	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	305	ILE	N-CA-C	-5.74	100.16	108.71
1	B	568	MET	N-CA-C	5.74	120.13	113.18
1	A	122	SER	O-C-N	5.74	127.98	122.07
1	D	617	PRO	N-CA-C	5.74	121.09	113.57
1	B	111	ASN	CA-C-O	-5.74	115.31	121.56
1	B	514	SER	CA-C-N	5.74	130.88	121.87
1	B	514	SER	C-N-CA	5.74	130.88	121.87
1	A	474	ARG	N-CA-C	5.74	123.02	110.80
1	A	37	PHE	CA-C-N	5.73	129.17	122.52
1	A	37	PHE	C-N-CA	5.73	129.17	122.52
1	A	137	LEU	N-CA-CB	5.73	119.12	109.78
1	F	85	MET	N-CA-CB	5.73	118.74	110.20
1	A	522	SER	N-CA-CB	-5.73	101.68	110.85
1	E	369	GLU	CA-CB-CG	5.73	125.56	114.10
1	A	277	PHE	CA-CB-CG	5.73	119.53	113.80
1	B	123	VAL	CB-CA-C	5.73	119.92	112.24
1	C	238	ASN	CA-CB-CG	-5.73	106.87	112.60
1	D	422	LEU	N-CA-C	-5.73	98.60	110.80
1	A	288	ASP	CA-C-O	-5.72	113.63	120.10
1	D	78	ARG	CB-CG-CD	5.72	124.47	111.30
1	F	472	GLY	N-CA-C	5.72	126.75	113.18
1	F	489	ASN	N-CA-C	-5.72	98.61	110.80
1	A	45	ILE	CA-C-O	-5.72	113.01	119.42
1	A	309	ASP	OD1-CG-OD2	5.72	136.63	122.90
1	B	101	SER	CA-C-O	-5.72	112.33	120.51
1	B	237	SER	N-CA-CB	-5.72	100.35	110.42
1	D	275	ILE	N-CA-C	5.72	116.29	110.05
1	E	38	ASN	O-C-N	5.72	126.19	121.44
1	A	91	ASN	N-CA-CB	5.72	119.11	110.30
1	B	122	SER	CA-C-O	5.72	126.48	120.42
1	A	318	PRO	CA-C-O	-5.72	110.86	119.55
1	B	30	LEU	CA-CB-CG	-5.72	96.30	116.30
1	E	442	ASN	CA-CB-CG	-5.72	106.88	112.60
1	A	362	ASN	CB-CA-C	5.71	120.45	112.11
1	B	177	ARG	O-C-N	-5.71	114.99	122.59
1	B	322	GLU	CA-C-O	-5.71	113.03	120.00
1	E	85	MET	N-CA-CB	5.71	118.72	110.20
1	A	61	ASN	CB-CG-OD1	-5.71	109.37	120.80
1	D	497	GLU	N-CA-C	-5.71	105.13	111.36
1	E	271	ARG	CA-C-N	5.71	125.91	120.31
1	E	271	ARG	C-N-CA	5.71	125.91	120.31
1	B	247	HIS	N-CA-CB	5.71	120.84	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	464	ILE	CB-CG1-CD1	-5.71	101.81	113.80
1	C	85	MET	N-CA-CB	5.71	118.71	110.20
1	C	214	ASP	N-CA-C	5.71	122.96	110.80
1	A	10	LYS	CA-C-N	5.70	128.24	120.54
1	A	10	LYS	C-N-CA	5.70	128.24	120.54
1	E	67	GLU	CB-CA-C	-5.70	97.99	109.68
1	F	214	ASP	N-CA-C	5.70	122.95	110.80
1	C	348	HIS	N-CA-CB	5.70	118.20	110.10
1	A	201	PHE	CE1-CZ-CE2	5.70	130.26	120.00
1	A	99	PHE	O-C-N	5.70	130.17	122.59
1	F	387	MET	CA-CB-CG	5.70	125.50	114.10
1	B	346	THR	CA-CB-CG2	-5.70	100.82	110.50
1	B	549	GLY	N-CA-C	5.69	126.67	113.18
1	C	617	PRO	N-CA-C	5.69	121.03	113.57
1	B	253	ARG	O-C-N	5.69	128.17	122.08
1	B	285	HIS	ND1-CE1-NE2	5.69	114.09	108.40
1	E	49	HIS	CA-CB-CG	-5.69	108.11	113.80
1	E	363	LEU	CB-CA-C	5.69	118.42	109.37
1	F	65	LEU	N-CA-CB	-5.69	101.36	110.63
1	F	444	GLU	CA-CB-CG	5.69	125.48	114.10
1	A	120	TYR	CA-C-O	5.69	126.79	120.82
1	A	127	LYS	N-CA-CB	-5.69	100.88	110.49
1	A	301	ASP	CA-C-N	5.69	128.17	120.44
1	A	301	ASP	C-N-CA	5.69	128.17	120.44
1	A	460	PHE	CD1-CG-CD2	-5.69	110.07	118.60
1	D	128	LEU	N-CA-C	5.69	121.22	113.37
1	E	302	HIS	CA-CB-CG	5.69	119.49	113.80
1	F	32	ASP	CB-CA-C	5.69	121.15	110.63
1	A	20	LYS	CA-C-O	5.68	128.64	120.51
1	B	345	ASN	O-C-N	5.68	128.16	122.08
1	C	32	ASP	CB-CA-C	5.68	121.15	110.63
1	D	488	ASN	N-CA-C	-5.68	104.30	111.92
1	D	155	TYR	N-CA-CB	5.68	119.09	110.28
1	A	148	SER	CA-C-N	5.68	130.08	120.88
1	A	148	SER	C-N-CA	5.68	130.08	120.88
1	B	442	ASN	CB-CG-ND2	5.68	124.92	116.40
1	C	277	PHE	CA-CB-CG	5.68	119.48	113.80
1	B	518	THR	N-CA-C	-5.68	97.34	107.28
1	C	161	GLN	N-CA-CB	-5.68	103.67	112.30
1	A	428	GLU	CA-C-O	5.68	127.87	120.21
1	A	590	ASP	N-CA-C	5.68	118.24	111.71
1	D	540	LYS	N-CA-C	-5.68	103.92	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401	TYR	CB-CG-CD2	5.67	129.31	120.80
1	B	498	ALA	CA-C-O	5.67	125.62	119.15
1	B	514	SER	N-CA-C	5.67	122.88	110.80
1	A	219	LEU	N-CA-C	-5.67	105.00	111.07
1	B	146	THR	CA-CB-OG1	-5.67	101.10	109.60
1	B	575	PRO	N-CA-C	-5.67	106.77	113.86
1	B	58	LYS	CA-C-N	-5.67	111.25	120.71
1	B	58	LYS	C-N-CA	-5.67	111.25	120.71
1	B	555	LEU	CA-C-O	-5.67	111.72	120.16
1	C	78	ARG	CB-CG-CD	5.67	124.33	111.30
1	A	312	THR	CA-C-O	-5.67	114.25	120.43
1	B	373	THR	N-CA-CB	-5.66	99.80	111.07
1	A	215	ARG	N-CA-CB	-5.66	103.14	111.51
1	B	318	PRO	CB-CA-C	-5.66	103.38	112.21
1	B	365	PRO	CA-N-CD	-5.66	104.08	112.00
1	C	23	GLU	CA-CB-CG	5.66	125.42	114.10
1	C	67	GLU	CB-CA-C	-5.66	98.08	109.68
1	F	442	ASN	CB-CA-C	5.66	120.45	111.23
1	B	234	GLU	CB-CG-CD	5.66	122.22	112.60
1	B	161	GLN	CB-CA-C	-5.66	102.49	111.48
1	B	485	ILE	CA-C-O	-5.66	113.71	120.78
1	E	295	ARG	CB-CG-CD	5.66	124.31	111.30
1	F	407	GLU	N-CA-C	5.66	118.39	109.96
1	D	596	HIS	CA-CB-CG	-5.65	108.15	113.80
1	B	177	ARG	N-CA-C	5.65	122.84	110.80
1	B	398	PHE	CB-CA-C	5.65	118.36	109.37
1	B	439	SER	N-CA-CB	-5.65	101.31	110.81
1	B	486	GLU	CA-C-N	5.65	133.68	121.64
1	B	486	GLU	C-N-CA	5.65	133.68	121.64
1	B	152	ASP	O-C-N	5.65	129.58	122.23
1	E	442	ASN	CB-CA-C	5.65	120.44	111.23
1	F	206	GLU	N-CA-C	-5.65	100.49	109.59
1	B	102	ASN	CA-C-O	-5.65	114.86	121.07
1	D	444	GLU	CA-CB-CG	5.65	125.40	114.10
1	B	497	GLU	CB-CG-CD	5.65	122.20	112.60
1	B	588	ASP	CB-CA-C	-5.64	102.24	111.50
1	E	505	LEU	N-CA-CB	-5.64	102.23	110.47
1	E	532	ASP	CA-CB-CG	5.64	118.25	112.60
1	A	365	PRO	CA-N-CD	-5.64	104.10	112.00
1	E	390	ILE	N-CA-CB	5.64	120.84	110.40
1	B	37	PHE	CB-CA-C	5.64	119.72	109.62
1	B	410	GLY	CA-C-O	-5.64	110.75	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	407	GLU	N-CA-C	5.64	118.37	109.96
1	A	71	TRP	N-CA-CB	5.64	118.11	110.38
1	A	107	ARG	NE-CZ-NH1	5.64	127.14	121.50
1	B	78	ARG	N-CA-CB	5.64	119.81	110.33
1	C	128	LEU	N-CA-C	5.64	121.15	113.37
1	B	95	GLU	CG-CD-OE2	-5.64	105.43	118.40
1	B	537	GLN	N-CA-C	-5.64	105.28	111.82
1	D	53	VAL	CB-CA-C	5.64	118.45	111.80
1	A	577	GLY	O-C-N	5.64	129.18	122.64
1	B	72	TYR	CB-CA-C	5.63	120.84	109.68
1	E	207	ASP	CA-CB-CG	5.63	118.23	112.60
1	B	290	GLU	CG-CD-OE2	-5.63	105.44	118.40
1	B	43	THR	CB-CA-C	5.63	121.62	110.42
1	B	76	ASN	CA-CB-CG	5.63	118.23	112.60
1	E	561	SER	N-CA-C	5.63	117.49	110.91
1	A	73	SER	N-CA-C	-5.63	100.72	109.72
1	A	450	ALA	CB-CA-C	5.63	119.51	109.38
1	D	505	LEU	N-CA-CB	-5.63	102.26	110.47
1	F	89	VAL	CB-CA-C	5.63	120.52	111.29
1	A	282	GLY	CA-C-N	-5.62	111.84	121.97
1	A	282	GLY	C-N-CA	-5.62	111.84	121.97
1	B	82	GLU	CB-CA-C	5.62	119.62	110.96
1	A	641	ASN	N-CA-C	5.62	118.93	112.97
1	A	354	GLN	CA-CB-CG	-5.62	102.86	114.10
1	B	547	VAL	CB-CA-C	5.62	116.49	111.71
1	A	95	GLU	CB-CG-CD	5.62	122.15	112.60
1	A	175	LYS	N-CA-C	-5.62	95.27	111.00
1	A	392	LYS	N-CA-C	5.62	118.94	111.75
1	F	115	PHE	CA-CB-CG	-5.62	108.18	113.80
1	B	22	TYR	CA-C-O	-5.62	110.58	119.23
1	B	117	TYR	CA-C-N	5.62	127.81	120.28
1	B	117	TYR	C-N-CA	5.62	127.81	120.28
1	B	259	LEU	CA-C-N	5.62	131.91	122.87
1	B	259	LEU	C-N-CA	5.62	131.91	122.87
1	B	581	ASN	CA-C-O	-5.62	114.25	120.38
1	B	606	HIS	N-CA-C	5.62	126.73	111.00
1	F	501	PHE	CA-CB-CG	5.62	119.42	113.80
1	B	408	PHE	CA-C-O	5.62	131.53	120.69
1	B	104	ALA	CA-C-O	5.62	128.54	120.51
1	B	533	MET	CA-C-O	5.62	126.42	120.63
1	B	471	ASP	CA-CB-CG	5.61	118.21	112.60
1	D	409	SER	CA-C-O	-5.61	114.63	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	390	ILE	N-CA-CB	5.61	120.78	110.40
1	F	488	ASN	N-CA-C	-5.61	103.53	111.56
1	F	540	LYS	N-CA-C	-5.61	104.00	111.24
1	A	76	ASN	CA-C-O	-5.61	113.98	120.49
1	A	523	SER	CA-C-O	5.61	128.53	120.51
1	B	192	ILE	CB-CA-C	5.61	120.49	111.29
1	A	512	VAL	CB-CA-C	5.61	121.56	111.36
1	F	505	LEU	N-CA-CB	-5.61	102.29	110.47
1	A	557	ALA	CB-CA-C	-5.60	99.27	110.42
1	A	60	LEU	O-C-N	5.60	128.59	122.20
1	B	10	LYS	CA-C-O	5.60	127.58	121.02
1	B	471	ASP	N-CA-C	-5.60	104.80	111.69
1	D	466	MET	N-CA-C	5.60	116.92	108.46
1	B	293	GLU	CA-C-N	5.60	128.06	120.44
1	B	293	GLU	C-N-CA	5.60	128.06	120.44
1	C	179	GLN	CA-C-N	5.60	131.26	121.52
1	C	179	GLN	C-N-CA	5.60	131.26	121.52
1	A	63	HIS	CB-CA-C	-5.60	99.28	110.42
1	D	7	ASN	CB-CA-C	5.60	121.56	110.42
1	A	75	PHE	CA-CB-CG	-5.59	108.21	113.80
1	A	507	LYS	O-C-N	5.59	130.07	123.36
1	B	193	HIS	O-C-N	5.59	128.54	122.11
1	B	627	GLU	OE1-CD-OE2	5.59	136.33	122.90
1	D	398	PHE	CB-CA-C	5.59	117.50	109.11
1	A	312	THR	N-CA-CB	5.59	119.55	110.43
1	B	342	SER	N-CA-C	5.59	117.83	107.60
1	C	555	LEU	N-CA-C	-5.59	103.20	111.81
1	B	287	HIS	CA-C-N	-5.59	112.22	120.38
1	B	287	HIS	C-N-CA	-5.59	112.22	120.38
1	D	387	MET	CA-CB-CG	5.59	125.28	114.10
1	A	211	TYR	CB-CA-C	5.59	125.89	114.10
1	A	285	HIS	N-CA-C	5.59	118.38	110.50
1	F	128	LEU	N-CA-C	5.59	121.08	113.37
1	B	36	ASN	O-C-N	-5.59	114.84	122.33
1	A	313	ILE	CB-CG1-CD1	-5.58	102.07	113.80
1	A	348	HIS	CA-C-N	-5.58	111.14	120.30
1	A	348	HIS	C-N-CA	-5.58	111.14	120.30
1	B	211	TYR	CA-C-N	-5.58	115.12	123.00
1	B	211	TYR	C-N-CA	-5.58	115.12	123.00
1	A	231	PHE	CB-CA-C	-5.58	102.36	110.96
1	B	594	GLU	CG-CD-OE1	-5.58	105.56	118.40
1	F	617	PRO	N-CA-C	5.58	120.88	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	ASN	CB-CA-C	5.58	121.53	110.42
1	A	186	GLU	N-CA-C	5.58	119.71	113.02
1	B	125	HIS	ND1-CG-CD2	5.58	111.68	106.10
1	B	107	ARG	CD-NE-CZ	-5.58	116.59	124.40
1	D	363	LEU	CB-CA-C	5.58	118.24	109.37
1	B	110	MET	CA-C-N	5.58	129.69	120.94
1	B	110	MET	C-N-CA	5.58	129.69	120.94
1	B	375	THR	CB-CA-C	5.58	122.09	110.32
1	E	227	LEU	N-CA-C	-5.58	104.42	111.11
1	B	479	ARG	NE-CZ-NH1	-5.57	115.93	121.50
1	B	569	LEU	CA-C-O	-5.57	112.54	120.51
1	A	253	ARG	O-C-N	5.57	128.04	122.08
1	D	407	GLU	CA-C-N	5.57	131.98	123.23
1	D	407	GLU	C-N-CA	5.57	131.98	123.23
1	E	50	GLY	N-CA-C	5.57	121.61	113.48
1	A	627	GLU	CB-CG-CD	5.57	122.07	112.60
1	F	49	HIS	CA-CB-CG	-5.57	108.23	113.80
1	A	29	ASP	OD1-CG-OD2	5.57	136.26	122.90
1	B	293	GLU	OE1-CD-OE2	5.57	136.27	122.90
1	A	134	LEU	CA-C-O	-5.57	115.59	120.60
1	A	188	ILE	CA-C-O	-5.57	113.30	120.03
1	A	215	ARG	N-CA-C	-5.57	103.75	110.88
1	A	399	PRO	N-CA-C	-5.57	105.13	110.47
1	A	400	PRO	CA-C-N	-5.57	113.85	122.09
1	A	400	PRO	C-N-CA	-5.57	113.85	122.09
1	A	514	SER	CB-CA-C	5.57	121.03	109.95
1	B	274	ASN	N-CA-C	-5.56	104.23	111.74
1	A	291	ILE	N-CA-CB	5.56	118.92	110.58
1	A	453	HIS	CA-CB-CG	5.56	119.36	113.80
1	B	434	ILE	CA-C-N	-5.56	110.92	121.54
1	B	434	ILE	C-N-CA	-5.56	110.92	121.54
1	C	43	THR	N-CA-C	-5.56	98.95	110.80
1	A	201	PHE	O-C-N	5.56	126.42	121.36
1	A	210	GLY	O-C-N	-5.56	115.47	122.70
1	B	185	GLY	O-C-N	-5.56	116.35	122.24
1	C	405	ASN	N-CA-C	5.56	117.20	111.03
1	F	193	HIS	CA-CB-CG	5.56	119.36	113.80
1	B	176	ASN	CA-C-O	-5.56	112.56	120.51
1	E	7	ASN	CB-CA-C	5.56	121.48	110.42
1	A	105	TYR	O-C-N	5.55	127.87	122.09
1	B	19	ASP	CB-CG-OD2	5.55	131.17	118.40
1	B	177	ARG	NH1-CZ-NH2	-5.55	112.08	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	7	ASN	CB-CA-C	5.55	121.47	110.42
1	C	390	ILE	N-CA-CB	5.55	120.67	110.40
1	D	411	MET	N-CA-C	5.55	122.62	110.80
1	B	494	THR	CB-CA-C	-5.55	102.51	111.28
1	E	398	PHE	CB-CA-C	5.55	117.43	109.11
1	F	7	ASN	CB-CA-C	5.55	121.46	110.42
1	B	209	TYR	CA-C-O	-5.54	112.58	120.51
1	A	233	PHE	CA-CB-CG	-5.54	108.26	113.80
1	A	268	PHE	O-C-N	5.54	126.23	121.30
1	A	224	HIS	CA-CB-CG	-5.54	108.26	113.80
1	A	378	PRO	CA-C-N	-5.54	108.56	121.52
1	A	378	PRO	C-N-CA	-5.54	108.56	121.52
1	D	390	ILE	N-CA-CB	5.54	120.64	110.40
1	F	421	GLU	N-CA-C	-5.54	100.10	108.46
1	B	121	VAL	CB-CA-C	5.54	119.61	112.14
1	B	632	ASP	CB-CA-C	5.54	119.00	110.14
1	B	643	LYS	CB-CG-CD	5.54	124.03	111.30
1	C	38	ASN	O-C-N	5.54	126.03	121.44
1	A	406	LEU	CB-CA-C	5.53	121.29	110.67
1	A	504	GLU	OE1-CD-OE2	5.53	136.18	122.90
1	A	367	VAL	CA-CB-CG1	5.53	119.80	110.40
1	A	288	ASP	O-C-N	5.53	128.69	122.22
1	B	499	ARG	CA-C-O	5.53	126.41	120.55
1	B	191	ASN	CA-C-O	-5.53	114.66	120.63
1	A	267	GLU	CG-CD-OE2	5.53	131.11	118.40
1	A	293	GLU	CG-CD-OE1	-5.53	105.69	118.40
1	B	86	LEU	CA-C-N	-5.53	112.81	120.38
1	B	86	LEU	C-N-CA	-5.53	112.81	120.38
1	C	295	ARG	CB-CG-CD	5.53	124.01	111.30
1	E	494	THR	N-CA-CB	-5.53	103.25	111.43
1	B	233	PHE	CB-CA-C	-5.52	101.97	110.81
1	E	139	GLN	CA-CB-CG	5.52	125.15	114.10
1	B	200	ASP	CA-C-N	-5.52	115.41	122.98
1	B	200	ASP	C-N-CA	-5.52	115.41	122.98
1	F	139	GLN	CA-CB-CG	5.52	125.15	114.10
1	C	115	PHE	CA-CB-CG	-5.52	108.28	113.80
1	A	128	LEU	CB-CG-CD2	-5.52	94.14	110.70
1	D	115	PHE	CA-CB-CG	-5.52	108.28	113.80
1	F	471	ASP	N-CA-C	5.52	119.18	112.23
1	F	596	HIS	CA-CB-CG	-5.52	108.28	113.80
1	D	488	ASN	CA-C-N	5.52	132.08	121.54
1	D	488	ASN	C-N-CA	5.52	132.08	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	130	ASP	N-CA-C	5.52	116.98	110.97
1	A	158	LYS	CD-CE-NZ	-5.51	94.25	111.90
1	B	401	TYR	CA-C-O	-5.51	114.77	121.28
1	B	307	ASP	CB-CG-OD2	5.51	131.08	118.40
1	C	155	TYR	N-CA-CB	5.51	118.83	110.28
1	F	227	LEU	N-CA-C	-5.51	104.50	111.11
1	A	438	ASP	CB-CG-OD2	-5.51	105.72	118.40
1	B	10	LYS	CB-CA-C	5.51	119.99	110.84
1	B	205	TRP	CG-CD1-NE1	5.51	117.36	110.20
1	F	179	GLN	CA-C-N	5.51	131.11	121.52
1	F	179	GLN	C-N-CA	5.51	131.11	121.52
1	B	574	LYS	O-C-N	-5.51	110.63	121.59
1	C	572	LYS	N-CA-C	5.51	117.28	111.28
1	D	537	GLN	N-CA-C	-5.51	104.97	110.97
1	D	636	ILE	CA-C-N	5.51	131.23	120.99
1	D	636	ILE	C-N-CA	5.51	131.23	120.99
1	B	94	LYS	CB-CG-CD	5.50	123.96	111.30
1	D	554	ASP	CA-CB-CG	-5.50	107.09	112.60
1	F	162	LYS	CB-CA-C	5.50	116.85	109.42
1	A	7	ASN	CB-CA-C	5.50	121.37	110.42
1	A	536	PHE	CA-C-N	5.50	127.59	120.44
1	A	536	PHE	C-N-CA	5.50	127.59	120.44
1	E	130	ASP	N-CA-C	5.50	116.97	110.97
1	A	134	LEU	CB-CA-C	5.50	116.78	108.86
1	A	405	ASN	N-CA-CB	5.50	118.04	110.07
1	A	270	VAL	N-CA-CB	-5.50	101.58	112.24
1	A	547	VAL	CB-CA-C	5.50	120.61	111.37
1	B	575	PRO	N-CA-CB	-5.50	98.23	103.51
1	C	505	LEU	N-CA-CB	-5.50	102.45	110.47
1	A	537	GLN	CA-C-O	-5.49	115.05	120.82
1	B	72	TYR	CA-C-N	-5.49	114.70	122.94
1	B	72	TYR	C-N-CA	-5.49	114.70	122.94
1	C	596	HIS	CA-CB-CG	-5.49	108.31	113.80
1	D	488	ASN	N-CA-CB	5.49	121.08	112.46
1	B	253	ARG	CD-NE-CZ	-5.49	116.71	124.40
1	D	385	LYS	N-CA-CB	5.49	118.03	110.07
1	E	115	PHE	CA-CB-CG	-5.49	108.31	113.80
1	E	387	MET	CA-CB-CG	5.49	125.08	114.10
1	A	436	ALA	CA-C-N	5.49	131.28	122.50
1	A	436	ALA	C-N-CA	5.49	131.28	122.50
1	B	342	SER	N-CA-CB	-5.49	102.55	112.27
1	B	93	CYS	CA-CB-SG	-5.49	101.78	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	ASP	CB-CG-OD2	-5.49	105.78	118.40
1	B	585	ALA	CA-C-N	-5.49	115.80	123.10
1	B	585	ALA	C-N-CA	-5.49	115.80	123.10
1	F	43	THR	N-CA-C	-5.49	99.11	110.80
1	D	486	GLU	CA-C-N	5.49	130.74	121.14
1	D	486	GLU	C-N-CA	5.49	130.74	121.14
1	F	295	ARG	CB-CG-CD	5.49	123.92	111.30
1	C	540	LYS	N-CA-C	-5.48	104.17	111.24
1	D	35	GLU	OE1-CD-OE2	-5.48	109.74	122.90
1	A	417	ALA	CA-C-O	5.48	126.41	120.32
1	B	177	ARG	NE-CZ-NH1	5.48	126.98	121.50
1	B	418	ILE	CA-CB-CG2	5.48	119.82	110.50
1	B	536	PHE	O-C-N	5.48	128.40	122.15
1	A	491	ILE	CA-CB-CG1	-5.48	101.08	110.40
1	B	25	THR	N-CA-C	5.48	118.59	110.48
1	E	124	ILE	N-CA-C	5.48	115.68	110.42
1	B	82	GLU	O-C-N	-5.48	116.33	122.03
1	A	109	ARG	CD-NE-CZ	-5.48	116.73	124.40
1	B	27	TYR	O-C-N	5.48	126.34	121.19
1	C	206	GLU	OE1-CD-OE2	-5.48	109.76	122.90
1	E	643	LYS	CB-CG-CD	5.48	123.90	111.30
1	E	162	LYS	O-C-N	5.48	126.00	121.35
1	A	456	ASN	O-C-N	-5.47	118.04	123.46
1	B	267	GLU	CA-C-N	5.47	131.65	121.69
1	B	267	GLU	C-N-CA	5.47	131.65	121.69
1	F	31	LYS	CA-CB-CG	5.47	125.05	114.10
1	A	405	ASN	CA-C-O	-5.47	115.06	120.70
1	A	408	PHE	CA-CB-CG	-5.47	108.33	113.80
1	A	471	ASP	O-C-N	-5.47	115.31	122.59
1	B	190	MET	N-CA-C	-5.47	104.73	111.40
1	B	336	ASN	OD1-CG-ND2	-5.47	117.13	122.60
1	A	298	GLU	N-CA-C	-5.47	106.45	113.23
1	A	301	ASP	CB-CA-C	5.47	121.53	110.38
1	B	58	LYS	CA-CB-CG	-5.47	103.17	114.10
1	C	95	GLU	CB-CG-CD	5.47	121.89	112.60
1	C	179	GLN	CB-CA-C	5.47	121.30	110.42
1	B	576	GLU	CA-CB-CG	-5.46	103.17	114.10
1	A	284	ALA	CA-C-O	5.46	127.12	121.06
1	B	614	GLU	CA-C-N	5.46	129.10	121.02
1	B	614	GLU	C-N-CA	5.46	129.10	121.02
1	D	124	ILE	N-CA-C	5.46	115.66	110.42
1	D	641	ASN	N-CA-C	5.46	119.49	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	277	PHE	CA-CB-CG	5.46	119.26	113.80
1	D	227	LEU	N-CA-C	-5.46	104.56	111.11
1	A	245	GLU	CA-CB-CG	5.46	125.01	114.10
1	A	409	SER	CA-CB-OG	-5.46	100.19	111.10
1	A	345	ASN	CA-CB-CG	5.46	118.06	112.60
1	A	92	GLN	N-CA-C	5.45	120.21	111.81
1	A	155	TYR	CA-C-O	5.45	126.26	120.10
1	B	226	GLN	CA-CB-CG	-5.45	103.19	114.10
1	C	227	LEU	N-CA-C	-5.45	104.57	111.11
1	D	193	HIS	CA-CB-CG	5.45	119.25	113.80
1	A	406	LEU	CA-CB-CG	-5.45	97.22	116.30
1	B	286	VAL	CA-C-N	-5.45	111.41	120.68
1	B	286	VAL	C-N-CA	-5.45	111.41	120.68
1	A	250	ARG	CG-CD-NE	-5.45	100.01	112.00
1	A	500	TRP	CB-CG-CD1	5.45	135.08	126.90
1	B	83	ALA	CA-C-O	5.45	127.40	121.02
1	B	513	PRO	CA-C-N	5.45	131.95	121.54
1	B	513	PRO	C-N-CA	5.45	131.95	121.54
1	C	369	GLU	CA-CB-CG	5.45	125.00	114.10
1	D	522	SER	N-CA-C	5.45	118.99	110.32
1	B	9	GLN	CA-C-N	-5.45	112.53	121.19
1	B	9	GLN	C-N-CA	-5.45	112.53	121.19
1	B	123	VAL	O-C-N	5.45	129.03	121.84
1	B	129	GLY	O-C-N	-5.45	115.62	122.70
1	B	608	GLN	N-CA-C	-5.45	105.43	112.68
1	D	382	ARG	N-CA-C	-5.45	105.42	111.36
1	A	162	LYS	CA-C-O	-5.45	113.79	120.05
1	A	641	ASN	CA-C-O	-5.45	112.50	119.80
1	B	101	SER	CA-CB-OG	-5.45	100.21	111.10
1	D	446	VAL	N-CA-C	-5.45	100.49	108.11
1	B	38	ASN	CA-CB-CG	-5.44	107.16	112.60
1	A	252	ILE	CA-C-N	-5.44	113.23	120.79
1	A	252	ILE	C-N-CA	-5.44	113.23	120.79
1	A	194	HIS	CA-C-O	-5.44	114.76	120.63
1	B	155	TYR	CA-CB-CG	5.44	123.69	113.90
1	B	179	GLN	CA-C-O	5.44	131.07	121.94
1	B	260	THR	O-C-N	-5.44	116.31	123.16
1	C	636	ILE	CA-C-N	5.44	131.10	120.99
1	C	636	ILE	C-N-CA	5.44	131.10	120.99
1	A	333	TYR	CB-CG-CD2	-5.43	112.65	120.80
1	C	305	ILE	N-CA-C	-5.43	100.61	108.71
1	E	179	GLN	CA-C-N	5.43	130.97	121.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	179	GLN	C-N-CA	5.43	130.97	121.52
1	B	81	LYS	N-CA-CB	5.43	118.03	109.94
1	F	305	ILE	N-CA-C	-5.43	100.62	108.71
1	A	554	ASP	CA-C-N	-5.43	111.18	121.54
1	A	554	ASP	C-N-CA	-5.43	111.18	121.54
1	A	80	ARG	NH1-CZ-NH2	5.42	126.35	119.30
1	B	242	PRO	N-CD-CG	-5.42	95.06	103.20
1	B	435	ASN	CB-CG-OD1	-5.42	109.95	120.80
1	B	562	CYS	CB-CA-C	-5.42	99.62	110.42
1	C	501	PHE	CA-CB-CG	5.42	119.22	113.80
1	F	23	GLU	CA-CB-CG	5.42	124.95	114.10
1	F	532	ASP	CA-CB-CG	5.42	118.03	112.60
1	F	161	GLN	N-CA-CB	-5.42	104.06	112.30
1	A	611	VAL	CA-C-O	-5.42	114.00	120.78
1	B	9	GLN	CG-CD-OE1	5.42	131.65	120.80
1	B	194	HIS	ND1-CG-CD2	5.42	111.52	106.10
1	B	289	LEU	CD1-CG-CD2	-5.42	98.87	110.80
1	D	206	GLU	OE1-CD-OE2	-5.42	109.89	122.90
1	F	445	ASP	N-CA-C	5.42	118.04	109.96
1	F	537	GLN	N-CA-C	-5.42	105.45	111.36
1	B	82	GLU	CG-CD-OE2	5.42	130.86	118.40
1	B	23	GLU	CB-CA-C	5.42	118.05	109.55
1	B	389	ASN	CA-CB-CG	5.42	118.02	112.60
1	C	382	ARG	N-CA-C	-5.42	105.46	111.36
1	E	491	ILE	N-CA-C	5.42	120.03	112.50
1	F	382	ARG	N-CA-C	-5.42	105.46	111.36
1	A	280	VAL	CA-CB-CG2	-5.41	101.20	110.40
1	A	313	ILE	O-C-N	-5.41	116.77	123.10
1	B	169	SER	CA-C-O	-5.41	113.23	119.78
1	B	585	ALA	N-CA-CB	5.41	119.27	110.77
1	A	81	LYS	CG-CD-CE	-5.41	98.85	111.30
1	A	628	ARG	CA-C-N	-5.41	113.19	120.82
1	A	628	ARG	C-N-CA	-5.41	113.19	120.82
1	B	519	ILE	N-CA-CB	5.41	116.96	110.31
1	A	198	HIS	N-CA-C	5.41	119.74	113.20
1	A	424	THR	O-C-N	5.41	130.26	123.23
1	B	547	VAL	O-C-N	5.41	125.96	121.85
1	B	455	LEU	O-C-N	5.41	129.01	122.85
1	D	434	ILE	CA-C-O	-5.41	115.12	120.85
1	F	124	ILE	N-CA-C	5.41	115.61	110.42
1	A	221	PHE	CA-C-O	-5.40	114.70	121.02
1	A	522	SER	O-C-N	-5.40	116.35	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	ARG	CG-CD-NE	-5.40	100.11	112.00
1	B	619	ASN	CB-CG-OD1	-5.40	109.99	120.80
1	A	318	PRO	CB-CA-C	5.40	120.64	112.21
1	A	407	GLU	N-CA-C	5.40	118.18	110.24
1	A	462	TYR	CB-CG-CD1	5.40	128.91	120.80
1	B	381	PHE	CA-C-O	-5.40	113.76	119.97
1	B	537	GLN	CA-C-N	-5.40	113.42	120.44
1	B	537	GLN	C-N-CA	-5.40	113.42	120.44
1	B	620	ARG	CG-CD-NE	-5.40	100.11	112.00
1	E	617	PRO	N-CA-C	5.40	120.64	113.57
1	A	47	ASN	O-C-N	5.40	129.28	122.37
1	A	236	LEU	O-C-N	5.40	127.64	122.03
1	A	496	ASP	CB-CG-OD2	5.40	130.81	118.40
1	C	643	LYS	CB-CG-CD	5.40	123.72	111.30
1	A	525	ASP	CA-C-N	-5.40	112.89	120.82
1	A	525	ASP	C-N-CA	-5.40	112.89	120.82
1	A	544	ASP	O-C-N	-5.40	115.91	122.22
1	E	161	GLN	N-CA-CB	-5.40	104.10	112.30
1	A	422	LEU	CB-CG-CD1	5.39	126.88	110.70
1	B	313	ILE	N-CA-C	-5.39	98.18	107.24
1	D	179	GLN	CA-C-N	5.39	130.91	121.52
1	D	179	GLN	C-N-CA	5.39	130.91	121.52
1	D	305	ILE	N-CA-C	-5.39	100.67	108.71
1	F	422	LEU	CB-CA-C	5.39	119.41	110.78
1	B	110	MET	CB-CA-C	5.39	118.70	109.80
1	B	179	GLN	CB-CA-C	5.39	124.39	111.83
1	B	483	CYS	CA-C-O	-5.39	113.54	121.46
1	C	124	ILE	N-CA-C	5.39	115.59	110.42
1	A	545	ASN	CB-CG-ND2	-5.39	108.31	116.40
1	D	369	GLU	CA-CB-CG	5.39	124.88	114.10
1	A	369	GLU	OE1-CD-OE2	-5.39	109.97	122.90
1	A	388	ASP	N-CA-CB	5.38	117.77	109.91
1	B	166	PHE	CA-CB-CG	-5.38	108.42	113.80
1	E	382	ARG	N-CA-C	-5.38	105.49	111.36
1	A	161	GLN	CB-CA-C	-5.38	103.21	111.66
1	A	559	GLU	O-C-N	5.38	129.36	123.01
1	B	92	GLN	CA-CB-CG	5.38	124.87	114.10
1	C	7	ASN	N-CA-CB	5.38	119.59	110.49
1	E	407	GLU	CA-C-N	5.38	130.00	122.79
1	E	407	GLU	C-N-CA	5.38	130.00	122.79
1	E	181	VAL	CA-C-N	5.38	127.93	120.29
1	E	181	VAL	C-N-CA	5.38	127.93	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	THR	CA-C-N	-5.38	113.31	120.63
1	A	55	THR	C-N-CA	-5.38	113.31	120.63
1	A	257	ALA	N-CA-C	-5.38	100.79	109.40
1	A	473	GLU	CA-CB-CG	5.38	124.86	114.10
1	B	558	TYR	CB-CA-C	5.38	119.68	111.02
1	A	380	PHE	CG-CD1-CE1	5.38	129.84	120.70
1	B	10	LYS	O-C-N	-5.38	115.69	122.20
1	B	417	ALA	CB-CA-C	-5.38	99.97	109.70
1	D	405	ASN	N-CA-C	5.38	116.95	111.14
1	E	77	THR	CA-C-O	-5.38	113.27	119.61
1	D	177	ARG	CA-C-O	5.38	128.20	120.51
1	F	574	LYS	CB-CA-C	5.38	117.13	108.91
1	D	91	ASN	CA-C-N	-5.37	114.03	122.95
1	D	91	ASN	C-N-CA	-5.37	114.03	122.95
1	E	434	ILE	CA-C-O	-5.37	115.15	120.85
1	A	77	THR	CA-C-N	5.37	131.64	121.81
1	A	77	THR	C-N-CA	5.37	131.64	121.81
1	E	43	THR	N-CA-C	-5.37	99.36	110.80
1	F	398	PHE	CB-CA-C	5.37	117.17	109.11
1	A	575	PRO	O-C-N	5.37	129.52	122.27
1	B	372	GLU	N-CA-C	-5.37	106.76	113.15
1	D	643	LYS	CB-CG-CD	5.37	123.65	111.30
1	A	160	THR	CA-CB-CG2	-5.37	101.37	110.50
1	A	564	ILE	CA-C-O	5.37	127.14	119.95
1	F	38	ASN	O-C-N	5.37	125.90	121.44
1	A	159	MET	CA-C-O	5.37	126.24	120.55
1	A	385	LYS	N-CA-C	-5.37	99.37	110.80
1	C	77	THR	CA-C-O	-5.37	113.28	119.61
1	A	249	ASP	CB-CA-C	5.36	119.66	110.01
1	A	438	ASP	CB-CG-OD1	5.36	130.73	118.40
1	C	532	ASP	CA-CB-CG	5.36	117.96	112.60
1	F	643	LYS	CB-CG-CD	5.36	123.64	111.30
1	A	488	ASN	N-CA-C	-5.36	99.38	110.80
1	B	504	GLU	CB-CA-C	-5.36	101.31	109.89
1	D	420	GLY	CA-C-O	5.36	127.24	120.54
1	F	307	ASP	CA-C-N	5.36	128.00	120.28
1	F	307	ASP	C-N-CA	5.36	128.00	120.28
1	A	138	TYR	N-CA-CB	5.36	118.60	110.14
1	A	634	ARG	CA-C-N	-5.36	114.35	120.88
1	A	634	ARG	C-N-CA	-5.36	114.35	120.88
1	A	635	VAL	CB-CA-C	-5.36	104.87	111.94
1	D	272	PRO	CA-C-O	-5.36	115.08	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	398	PHE	CB-CA-C	5.35	117.14	109.11
1	A	343	LEU	O-C-N	-5.35	115.47	122.59
1	C	204	TRP	N-CA-C	5.35	119.68	113.20
1	E	277	PHE	CA-CB-CG	5.35	119.15	113.80
1	B	453	HIS	CA-CB-CG	-5.35	108.45	113.80
1	D	77	THR	CA-C-O	-5.35	113.30	119.61
1	D	399	PRO	N-CA-C	-5.35	104.17	110.70
1	E	128	LEU	N-CA-C	5.35	120.75	113.37
1	F	636	ILE	CA-C-N	5.35	130.94	120.99
1	F	636	ILE	C-N-CA	5.35	130.94	120.99
1	A	451	ARG	O-C-N	-5.35	117.07	123.27
1	A	540	LYS	N-CA-C	-5.35	105.09	111.03
1	C	91	ASN	CA-C-N	-5.35	114.07	122.95
1	C	91	ASN	C-N-CA	-5.35	114.07	122.95
1	E	210	GLY	N-CA-C	5.35	125.85	113.18
1	E	636	ILE	CA-C-N	5.35	130.94	120.99
1	E	636	ILE	C-N-CA	5.35	130.94	120.99
1	F	210	GLY	N-CA-C	5.35	125.85	113.18
1	A	243	VAL	N-CA-CB	5.35	116.36	110.53
1	B	299	ALA	N-CA-C	-5.34	104.88	111.40
1	B	288	ASP	O-C-N	5.34	128.29	122.20
1	A	439	SER	CB-CA-C	-5.34	99.79	110.42
1	B	216	LYS	CA-CB-CG	5.34	124.78	114.10
1	E	95	GLU	CA-CB-CG	5.34	124.78	114.10
1	B	43	THR	OG1-CB-CG2	5.34	119.97	109.30
1	F	470	ASN	CA-CB-CG	5.34	117.94	112.60
1	B	641	ASN	N-CA-C	5.33	119.34	113.21
1	F	434	ILE	CA-C-O	-5.33	115.19	120.85
1	A	211	TYR	CG-CD2-CE2	5.33	129.20	121.20
1	D	177	ARG	CA-C-N	5.33	131.73	121.54
1	D	177	ARG	C-N-CA	5.33	131.73	121.54
1	E	25	THR	N-CA-CB	5.33	117.88	109.83
1	B	36	ASN	CB-CA-C	5.33	121.26	110.38
1	B	376	ARG	CD-NE-CZ	-5.33	116.94	124.40
1	B	565	PRO	CA-C-O	-5.33	115.26	121.34
1	B	596	HIS	ND1-CE1-NE2	5.33	113.73	108.40
1	A	618	ASP	CB-CG-OD1	5.33	130.66	118.40
1	C	434	ILE	CA-C-O	-5.33	115.20	120.85
1	D	170	PHE	CA-CB-CG	5.33	119.13	113.80
1	A	588	ASP	N-CA-CB	-5.32	101.58	110.42
1	C	273	ASP	CB-CA-C	5.32	119.15	109.83
1	E	577	GLY	O-C-N	5.32	127.42	122.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	25	THR	N-CA-CB	5.32	117.87	109.83
1	A	93	CYS	CA-C-N	-5.32	111.73	121.52
1	A	93	CYS	C-N-CA	-5.32	111.73	121.52
1	B	275	ILE	CA-CB-CG2	5.32	119.54	110.50
1	B	474	ARG	CA-CB-CG	5.32	124.74	114.10
1	B	534	PRO	N-CA-CB	-5.32	97.67	103.25
1	B	258	PRO	N-CA-CB	-5.32	97.67	103.25
1	B	282	GLY	CA-C-N	-5.32	112.40	121.97
1	B	282	GLY	C-N-CA	-5.32	112.40	121.97
1	B	393	LYS	CG-CD-CE	5.32	123.53	111.30
1	A	380	PHE	CA-CB-CG	-5.32	108.48	113.80
1	B	248	TRP	CZ3-CH2-CZ2	-5.32	114.59	121.50
1	A	10	LYS	CA-C-O	-5.31	115.23	121.07
1	A	476	ALA	CA-C-N	-5.31	115.70	122.77
1	A	476	ALA	C-N-CA	-5.31	115.70	122.77
1	D	204	TRP	N-CA-C	5.31	119.63	113.20
1	B	560	ARG	CB-CG-CD	5.31	123.52	111.30
1	A	247	HIS	ND1-CG-CD2	5.31	111.41	106.10
1	B	380	PHE	CA-CB-CG	-5.31	108.49	113.80
1	C	289	LEU	CB-CA-C	5.31	119.62	110.86
1	A	452	VAL	CA-CB-CG2	-5.30	101.38	110.40
1	F	77	THR	CA-C-O	-5.30	113.35	119.61
1	A	331	SER	N-CA-C	-5.30	101.62	109.94
1	B	307	ASP	CB-CG-OD1	-5.30	106.21	118.40
1	D	234	GLU	CB-CG-CD	5.30	121.61	112.60
1	A	198	HIS	ND1-CG-CD2	5.30	111.40	106.10
1	B	193	HIS	CE1-NE2-CD2	5.30	114.30	109.00
1	B	379	SER	CA-CB-OG	5.30	121.70	111.10
1	D	179	GLN	CB-CA-C	5.30	120.96	110.42
1	B	384	HIS	CA-C-O	-5.30	112.33	119.11
1	E	89	VAL	CB-CA-C	5.30	119.98	111.29
1	A	360	LYS	CG-CD-CE	-5.29	99.12	111.30
1	B	247	HIS	ND1-CG-CD2	5.29	111.39	106.10
1	A	326	ASP	N-CA-C	-5.29	105.56	112.23
1	A	364	PRO	N-CA-C	-5.29	104.24	110.70
1	B	144	MET	O-C-N	-5.29	114.56	122.39
1	E	305	ILE	N-CA-C	-5.29	100.82	108.71
1	A	453	HIS	CA-C-O	5.29	126.73	120.70
1	A	361	PHE	CA-C-N	-5.29	115.02	122.63
1	A	361	PHE	C-N-CA	-5.29	115.02	122.63
1	B	150	VAL	O-C-N	5.29	127.24	121.90
1	C	444	GLU	CA-C-N	5.29	128.85	121.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	444	GLU	C-N-CA	5.29	128.85	121.02
1	F	399	PRO	N-CA-C	-5.29	104.25	110.70
1	A	63	HIS	CA-CB-CG	5.29	119.08	113.80
1	A	118	ALA	O-C-N	-5.29	116.59	122.09
1	A	396	ASP	CA-C-N	5.29	133.89	121.52
1	A	396	ASP	C-N-CA	5.29	133.89	121.52
1	B	446	VAL	N-CA-CB	5.29	118.44	111.25
1	A	439	SER	O-C-N	-5.28	115.56	122.59
1	B	90	LEU	N-CA-CB	-5.28	101.56	110.49
1	B	113	GLY	CA-C-N	-5.28	113.41	120.54
1	B	113	GLY	C-N-CA	-5.28	113.41	120.54
1	C	210	GLY	N-CA-C	5.28	125.70	113.18
1	D	142	PRO	N-CA-C	5.28	120.79	113.98
1	A	38	ASN	CA-C-N	-5.28	114.64	119.82
1	A	38	ASN	C-N-CA	-5.28	114.64	119.82
1	D	555	LEU	O-C-N	5.28	128.58	122.19
1	A	112	GLU	CG-CD-OE2	-5.28	106.26	118.40
1	B	253	ARG	NH1-CZ-NH2	5.28	126.16	119.30
1	C	307	ASP	CA-C-N	5.28	127.88	120.28
1	C	307	ASP	C-N-CA	5.28	127.88	120.28
1	D	247	HIS	N-CA-CB	5.28	120.11	111.08
1	F	268	PHE	O-C-N	5.28	125.71	121.38
1	F	356	ASP	CA-CB-CG	5.28	117.88	112.60
1	B	169	SER	CA-CB-OG	-5.28	100.54	111.10
1	B	324	LEU	CA-C-O	-5.28	115.28	120.82
1	B	403	HIS	O-C-N	5.28	127.73	122.03
1	D	532	ASP	CA-CB-CG	5.28	117.88	112.60
1	E	403	HIS	N-CA-C	-5.28	105.22	110.97
1	A	91	ASN	CA-CB-CG	5.28	117.88	112.60
1	A	458	ASN	CB-CG-ND2	-5.28	108.48	116.40
1	C	23	GLU	O-C-N	5.28	125.95	121.84
1	B	462	TYR	N-CA-C	-5.27	101.10	109.96
1	A	302	HIS	CA-C-N	-5.27	111.08	121.41
1	A	302	HIS	C-N-CA	-5.27	111.08	121.41
1	B	121	VAL	CA-CB-CG1	5.27	119.36	110.40
1	B	366	GLY	CA-C-O	5.27	127.83	121.77
1	A	53	VAL	CA-C-N	-5.27	111.47	121.54
1	A	53	VAL	C-N-CA	-5.27	111.47	121.54
1	B	14	ILE	CB-CG1-CD1	5.27	124.87	113.80
1	B	533	MET	CA-CB-CG	5.27	124.64	114.10
1	B	148	SER	N-CA-CB	5.27	118.23	110.33
1	B	353	ARG	NE-CZ-NH2	-5.27	114.46	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	210	GLY	N-CA-C	5.27	125.66	113.18
1	B	431	TYR	CZ-CE2-CD2	-5.27	110.12	119.60
1	F	438	ASP	CB-CA-C	5.26	118.43	109.80
1	B	486	GLU	O-C-N	-5.26	115.80	122.43
1	A	629	ARG	O-C-N	5.26	129.47	122.95
1	B	382	ARG	CD-NE-CZ	-5.26	117.04	124.40
1	C	289	LEU	N-CA-C	-5.26	104.46	111.24
1	B	304	TYR	CB-CG-CD1	-5.26	112.92	120.80
1	B	500	TRP	CB-CA-C	5.26	120.41	109.95
1	B	514	SER	CA-C-O	-5.26	112.99	120.51
1	C	399	PRO	N-CA-C	-5.26	104.29	110.70
1	B	636	ILE	CA-C-N	5.25	130.76	120.99
1	B	636	ILE	C-N-CA	5.25	130.76	120.99
1	D	33	ILE	N-CA-C	-5.25	105.41	110.72
1	B	96	TRP	CB-CA-C	5.25	119.46	110.74
1	B	489	ASN	CA-CB-CG	-5.25	107.35	112.60
1	A	259	LEU	N-CA-CB	-5.25	104.15	112.08
1	F	559	GLU	N-CA-C	5.25	118.81	112.93
1	F	48	ASP	N-CA-CB	5.25	118.54	110.61
1	A	155	TYR	N-CA-CB	5.25	118.30	110.22
1	A	388	ASP	OD1-CG-OD2	5.25	135.49	122.90
1	B	108	GLU	CA-CB-CG	5.25	124.59	114.10
1	B	334	SER	CB-CA-C	5.25	117.71	109.84
1	F	162	LYS	O-C-N	5.25	126.06	121.39
1	A	365	PRO	CB-CG-CD	-5.25	89.32	106.10
1	D	32	ASP	CB-CA-C	5.25	120.20	109.55
1	A	58	LYS	N-CA-CB	5.24	117.75	109.94
1	B	295	ARG	O-C-N	5.24	127.54	122.09
1	B	451	ARG	CD-NE-CZ	-5.24	117.06	124.40
1	D	161	GLN	CB-CA-C	-5.24	104.29	111.73
1	F	91	ASN	CA-C-N	-5.24	114.25	122.95
1	F	91	ASN	C-N-CA	-5.24	114.25	122.95
1	A	84	LEU	CA-C-N	-5.24	111.88	121.52
1	A	84	LEU	C-N-CA	-5.24	111.88	121.52
1	A	316	ARG	N-CA-C	-5.24	104.05	110.65
1	B	438	ASP	CB-CA-C	5.24	118.17	109.53
1	B	517	GLU	CB-CG-CD	5.24	121.50	112.60
1	D	578	MET	O-C-N	5.24	129.22	123.25
1	A	648	LYS	CG-CD-CE	5.23	123.34	111.30
1	B	39	PRO	CA-C-N	5.23	130.99	122.67
1	B	39	PRO	C-N-CA	5.23	130.99	122.67
1	B	149	GLU	CB-CA-C	5.23	119.49	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	574	LYS	CB-CA-C	5.23	116.92	108.91
1	A	512	VAL	O-C-N	-5.23	115.14	121.10
1	C	206	GLU	N-CA-C	-5.23	101.17	109.59
1	B	492	THR	OG1-CB-CG2	5.23	119.76	109.30
1	B	326	ASP	CA-C-O	-5.23	114.44	120.24
1	B	586	VAL	CA-C-N	-5.23	113.70	123.05
1	B	586	VAL	C-N-CA	-5.23	113.70	123.05
1	F	7	ASN	N-CA-CB	5.23	119.32	110.49
1	B	295	ARG	CA-C-O	-5.22	115.31	120.90
1	B	387	MET	N-CA-C	-5.22	105.01	111.33
1	D	289	LEU	N-CA-C	-5.22	104.50	111.24
1	E	142	PRO	N-CA-C	5.22	120.72	113.98
1	C	164	GLY	CA-C-N	5.22	129.55	122.19
1	C	164	GLY	C-N-CA	5.22	129.55	122.19
1	A	576	GLU	CA-C-O	5.22	125.97	119.97
1	A	263	LYS	O-C-N	-5.22	116.03	122.19
1	A	283	VAL	O-C-N	5.22	129.09	122.57
1	A	310	GLY	O-C-N	5.22	128.29	122.50
1	A	413	VAL	CA-CB-CG1	-5.22	101.53	110.40
1	B	592	ASP	CB-CA-C	5.22	120.80	110.42
1	B	572	LYS	CA-C-O	5.22	125.95	120.42
1	C	234	GLU	CB-CG-CD	5.21	121.47	112.60
1	A	620	ARG	CB-CG-CD	5.21	123.29	111.30
1	B	116	VAL	CG1-CB-CG2	-5.21	99.33	110.80
1	B	215	ARG	N-CA-C	-5.21	104.09	110.61
1	B	5	THR	OG1-CB-CG2	5.21	119.72	109.30
1	C	6	GLY	N-CA-C	-5.21	100.83	113.18
1	C	512	VAL	O-C-N	5.21	126.10	121.41
1	D	23	GLU	CA-CB-CG	5.21	124.52	114.10
1	C	198	HIS	CB-CA-C	-5.21	101.80	110.81
1	A	542	GLN	CA-CB-CG	-5.21	103.68	114.10
1	D	289	LEU	CB-CA-C	5.21	119.46	110.86
1	F	155	TYR	N-CA-CB	5.21	118.36	110.28
1	C	150	VAL	CB-CA-C	5.21	118.86	112.04
1	A	66	LEU	O-C-N	5.20	129.15	123.01
1	A	157	ALA	CA-C-N	-5.20	113.31	120.28
1	A	157	ALA	C-N-CA	-5.20	113.31	120.28
1	F	289	LEU	CB-CA-C	5.20	119.45	110.86
1	C	213	LEU	CA-C-N	5.20	131.48	121.54
1	C	213	LEU	C-N-CA	5.20	131.48	121.54
1	A	636	ILE	CA-C-N	5.20	130.66	120.99
1	A	636	ILE	C-N-CA	5.20	130.66	120.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	513	PRO	CA-C-O	-5.20	111.14	120.60
1	B	441	GLU	N-CA-C	5.20	117.64	108.75
1	D	218	GLU	CA-CB-CG	5.20	124.49	114.10
1	A	617	PRO	N-CA-C	5.20	121.40	114.18
1	A	123	VAL	N-CA-C	-5.19	105.44	110.42
1	A	431	TYR	O-C-N	5.19	130.37	122.94
1	B	554	ASP	OD1-CG-OD2	-5.19	110.44	122.90
1	A	558	TYR	CA-C-O	-5.19	113.00	119.28
1	B	583	TYR	N-CA-CB	5.19	119.09	110.47
1	A	396	ASP	N-CA-CB	-5.19	101.31	110.39
1	A	356	ASP	CA-C-O	5.19	127.26	120.16
1	B	94	LYS	CB-CA-C	5.19	119.50	110.79
1	B	619	ASN	O-C-N	5.19	128.75	122.48
1	B	448	ILE	N-CA-C	5.18	116.43	108.71
1	C	177	ARG	CA-C-O	5.18	127.92	120.51
1	A	180	ARG	N-CA-C	-5.18	106.76	114.64
1	A	200	ASP	N-CA-C	-5.18	105.28	111.03
1	B	473	GLU	CA-C-O	-5.18	114.32	120.43
1	C	226	GLN	CA-C-O	-5.18	114.49	120.24
1	E	289	LEU	CB-CA-C	5.18	119.41	110.86
1	F	291	ILE	N-CA-CB	5.18	116.61	110.55
1	B	308	SER	CB-CA-C	-5.18	100.11	110.42
1	B	47	ASN	CA-C-O	-5.18	109.98	119.36
1	D	7	ASN	N-CA-CB	5.18	119.24	110.49
1	F	218	GLU	CA-CB-CG	5.18	124.46	114.10
1	D	525	ASP	N-CA-C	-5.18	107.01	113.38
1	A	256	PHE	O-C-N	5.18	129.05	123.10
1	A	349	VAL	O-C-N	-5.18	115.95	121.80
1	B	468	ASN	O-C-N	5.18	128.94	122.63
1	C	19	ASP	CA-CB-CG	5.18	117.78	112.60
1	D	376	ARG	CA-C-N	5.18	127.61	120.67
1	D	376	ARG	C-N-CA	5.18	127.61	120.67
1	E	91	ASN	CA-C-N	-5.18	114.36	122.95
1	E	91	ASN	C-N-CA	-5.18	114.36	122.95
1	F	439	SER	N-CA-C	-5.18	99.97	108.41
1	D	445	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	499	ARG	CA-C-N	5.17	131.67	121.58
1	A	499	ARG	C-N-CA	5.17	131.67	121.58
1	A	376	ARG	NE-CZ-NH1	-5.17	116.33	121.50
1	B	516	PRO	N-CA-CB	-5.17	97.82	103.25
1	C	78	ARG	CA-CB-CG	-5.17	103.76	114.10
1	E	273	ASP	CB-CA-C	5.17	120.28	110.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	348	HIS	N-CA-CB	5.17	117.67	110.07
1	E	272	PRO	N-CA-C	-5.17	103.72	111.57
1	C	25	THR	N-CA-CB	5.17	117.63	109.83
1	B	304	TYR	N-CA-C	5.17	117.24	109.23
1	A	72	TYR	O-C-N	5.16	129.31	123.42
1	A	80	ARG	N-CA-C	-5.16	105.10	111.40
1	A	617	PRO	O-C-N	5.16	129.56	122.38
1	B	123	VAL	CA-C-O	-5.16	115.19	120.71
1	B	395	THR	CA-C-O	-5.16	115.05	120.63
1	E	247	HIS	N-CA-CB	5.16	119.91	111.08
1	F	226	GLN	CA-CB-CG	-5.16	103.78	114.10
1	B	349	VAL	CA-C-O	5.16	126.25	119.85
1	A	179	GLN	CB-CG-CD	5.16	121.37	112.60
1	E	438	ASP	CB-CA-C	5.16	118.26	109.80
1	F	213	LEU	CA-C-N	5.16	131.40	121.54
1	F	213	LEU	C-N-CA	5.16	131.40	121.54
1	A	26	LYS	N-CA-C	-5.16	107.03	113.38
1	A	36	ASN	CA-C-O	-5.16	113.27	119.15
1	A	263	LYS	CA-CB-CG	5.16	124.42	114.10
1	B	204	TRP	CB-CA-C	-5.16	100.82	110.36
1	D	515	GLY	O-C-N	5.16	126.93	121.77
1	A	352	GLY	CA-C-O	-5.16	115.13	120.90
1	C	177	ARG	CA-C-N	5.16	131.39	121.54
1	C	177	ARG	C-N-CA	5.16	131.39	121.54
1	F	177	ARG	CA-C-N	5.16	131.39	121.54
1	F	177	ARG	C-N-CA	5.16	131.39	121.54
1	A	473	GLU	CG-CD-OE2	5.15	130.25	118.40
1	B	47	ASN	N-CA-CB	5.15	118.04	110.57
1	A	191	ASN	O-C-N	5.15	127.45	122.09
1	A	629	ARG	CB-CA-C	5.15	117.93	109.90
1	B	372	GLU	CA-C-N	-5.15	112.24	120.17
1	B	372	GLU	C-N-CA	-5.15	112.24	120.17
1	B	583	TYR	CA-CB-CG	-5.15	104.63	113.90
1	C	48	ASP	N-CA-CB	5.15	118.39	110.61
1	B	187	ASP	CA-C-N	5.15	129.46	120.86
1	B	187	ASP	C-N-CA	5.15	129.46	120.86
1	C	247	HIS	N-CA-CB	5.15	119.89	111.08
1	C	23	GLU	CB-CA-C	-5.15	102.06	109.63
1	E	78	ARG	CA-CB-CG	-5.15	103.81	114.10
1	B	512	VAL	CA-C-O	5.14	125.50	119.89
1	C	142	PRO	N-CA-C	5.14	120.62	113.98
1	C	471	ASP	CA-CB-CG	5.14	117.75	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	488	ASN	CA-C-O	5.14	127.36	120.98
1	F	247	HIS	N-CA-CB	5.14	119.88	111.08
1	A	649	ILE	CA-CB-CG1	-5.14	101.66	110.40
1	B	63	HIS	CB-CA-C	-5.14	100.19	110.42
1	B	340	TYR	N-CA-C	5.14	119.19	113.02
1	C	31	LYS	CA-CB-CG	5.14	124.38	114.10
1	D	25	THR	N-CA-CB	5.14	117.59	109.83
1	D	489	ASN	CA-C-N	5.14	129.24	120.91
1	D	489	ASN	C-N-CA	5.14	129.24	120.91
1	E	399	PRO	N-CA-C	-5.14	104.43	110.70
1	A	7	ASN	CB-CG-OD1	-5.14	110.52	120.80
1	A	201	PHE	CD1-CG-CD2	5.14	126.31	118.60
1	A	461	THR	CB-CA-C	5.14	119.63	109.66
1	B	453	HIS	N-CA-CB	-5.14	101.91	110.39
1	E	494	THR	CA-C-O	-5.14	115.27	121.34
1	F	179	GLN	CB-CA-C	5.14	120.65	110.42
1	A	284	ALA	CA-C-N	-5.14	112.87	120.94
1	A	284	ALA	C-N-CA	-5.14	112.87	120.94
1	A	622	LEU	N-CA-C	5.14	116.90	108.52
1	B	48	ASP	CA-C-O	5.14	124.70	119.05
1	E	155	TYR	N-CA-CB	5.14	118.25	110.28
1	B	229	ALA	CA-C-N	-5.14	113.11	120.82
1	B	229	ALA	C-N-CA	-5.14	113.11	120.82
1	B	250	ARG	O-C-N	-5.14	115.36	122.76
1	A	432	SER	N-CA-C	5.14	117.77	109.40
1	A	587	THR	CA-CB-OG1	-5.14	101.90	109.60
1	E	622	LEU	N-CA-C	5.14	117.10	108.73
1	F	522	SER	CA-C-O	5.14	127.34	121.28
1	A	380	PHE	CD1-CE1-CZ	-5.13	110.76	120.00
1	D	78	ARG	CA-CB-CG	-5.13	103.83	114.10
1	F	562	CYS	CB-CA-C	-5.13	102.12	110.85
1	A	44	SER	O-C-N	5.13	127.37	121.93
1	A	46	TYR	CA-C-O	-5.13	115.02	120.92
1	F	289	LEU	N-CA-C	-5.13	104.62	111.24
1	A	111	ASN	CB-CA-C	5.13	118.81	109.62
1	C	130	ASP	N-CA-C	5.13	116.56	110.97
1	D	130	ASP	N-CA-C	5.13	116.56	110.97
1	E	179	GLN	CB-CA-C	5.13	120.63	110.42
1	A	50	GLY	N-CA-C	5.13	121.85	114.10
1	A	191	ASN	CA-C-N	-5.13	112.74	121.97
1	A	191	ASN	C-N-CA	-5.13	112.74	121.97
1	A	394	HIS	O-C-N	5.13	129.82	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	ASN	CB-CG-OD1	-5.13	110.54	120.80
1	E	32	ASP	CB-CA-C	5.13	120.52	110.67
1	F	467	SER	N-CA-C	5.13	118.58	109.96
1	B	83	ALA	N-CA-C	-5.13	102.96	111.37
1	F	162	LYS	N-CA-C	-5.13	101.19	109.40
1	B	13	ASP	CA-C-O	5.13	126.71	121.07
1	B	115	PHE	CA-CB-CG	-5.13	108.67	113.80
1	C	371	PHE	N-CA-C	5.13	117.77	111.82
1	A	197	TRP	N-CA-CB	5.12	117.65	110.12
1	A	84	LEU	CB-CA-C	5.12	119.85	110.11
1	D	623	GLY	N-CA-C	-5.12	108.00	115.63
1	F	577	GLY	O-C-N	5.12	127.23	122.47
1	D	361	PHE	CA-CB-CG	-5.12	108.68	113.80
1	E	234	GLU	CB-CG-CD	5.12	121.31	112.60
1	A	263	LYS	N-CA-CB	5.12	119.44	110.27
1	B	295	ARG	N-CA-C	-5.12	104.97	111.11
1	A	490	GLY	O-C-N	5.12	128.28	122.55
1	B	488	ASN	O-C-N	5.12	129.40	122.59
1	A	444	GLU	CB-CG-CD	5.12	121.30	112.60
1	B	190	MET	CG-SD-CE	-5.12	89.64	100.90
1	F	140	ILE	CA-C-N	5.12	128.16	122.74
1	F	140	ILE	C-N-CA	5.12	128.16	122.74
1	A	445	ASP	O-C-N	5.12	130.08	123.07
1	B	500	TRP	O-C-N	5.12	129.90	122.43
1	C	226	GLN	CA-CB-CG	-5.12	103.87	114.10
1	F	78	ARG	CA-CB-CG	-5.12	103.87	114.10
1	F	559	GLU	CB-CA-C	-5.12	101.96	110.81
1	A	19	ASP	N-CA-C	-5.11	102.19	110.32
1	A	581	ASN	CA-C-N	-5.11	115.66	122.72
1	A	581	ASN	C-N-CA	-5.11	115.66	122.72
1	B	596	HIS	CE1-NE2-CD2	-5.11	103.89	109.00
1	E	226	GLN	CA-C-O	-5.11	114.56	120.24
1	D	168	VAL	CA-C-N	5.11	132.34	122.53
1	D	168	VAL	C-N-CA	5.11	132.34	122.53
1	E	291	ILE	N-CA-CB	5.11	116.53	110.55
1	B	624	TYR	O-C-N	-5.11	116.75	121.30
1	A	10	LYS	CB-CA-C	5.11	119.04	110.92
1	B	521	ARG	CA-C-N	-5.11	114.64	122.87
1	B	521	ARG	C-N-CA	-5.11	114.64	122.87
1	C	622	LEU	N-CA-C	5.11	117.06	108.73
1	A	519	ILE	N-CA-C	5.11	116.16	109.21
1	B	194	HIS	ND1-CE1-NE2	-5.11	103.29	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	264	TYR	CB-CA-C	5.11	118.57	110.19
1	D	622	LEU	N-CA-C	5.11	117.06	108.73
1	A	580	PHE	CA-C-N	-5.11	115.79	122.99
1	A	580	PHE	C-N-CA	-5.11	115.79	122.99
1	B	198	HIS	ND1-CG-CD2	5.11	111.20	106.10
1	B	409	SER	CA-C-N	-5.11	111.40	121.41
1	B	409	SER	C-N-CA	-5.11	111.40	121.41
1	C	170	PHE	CA-CB-CG	5.11	118.91	113.80
1	A	338	GLN	N-CA-CB	5.10	118.98	110.41
1	A	560	ARG	CB-CG-CD	-5.10	99.56	111.30
1	B	95	GLU	CB-CG-CD	5.10	121.28	112.60
1	A	406	LEU	CD1-CG-CD2	-5.10	99.58	110.80
1	B	245	GLU	CG-CD-OE2	5.10	130.13	118.40
1	A	7	ASN	N-CA-C	-5.10	99.94	110.80
1	A	343	LEU	CA-C-N	5.10	127.38	120.65
1	A	343	LEU	C-N-CA	5.10	127.38	120.65
1	A	480	ILE	CB-CG1-CD1	-5.10	103.09	113.80
1	A	630	ILE	O-C-N	5.10	126.91	121.10
1	B	78	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	C	641	ASN	N-CA-C	5.10	119.07	113.21
1	A	226	GLN	N-CA-C	-5.10	105.36	112.45
1	B	350	MET	O-C-N	5.10	129.16	122.33
1	B	406	LEU	CD1-CG-CD2	-5.10	99.59	110.80
1	F	408	PHE	N-CA-C	-5.10	101.87	109.11
1	A	17	LEU	CB-CG-CD2	-5.10	95.41	110.70
1	A	234	GLU	CG-CD-OE2	5.09	130.12	118.40
1	D	291	ILE	N-CA-CB	5.09	116.51	110.55
1	E	177	ARG	CA-C-N	5.09	131.27	121.54
1	E	177	ARG	C-N-CA	5.09	131.27	121.54
1	D	140	ILE	CA-C-N	5.09	128.14	122.74
1	D	140	ILE	C-N-CA	5.09	128.14	122.74
1	B	247	HIS	CE1-NE2-CD2	5.09	114.09	109.00
1	D	295	ARG	CB-CG-CD	5.09	123.01	111.30
1	D	467	SER	N-CA-C	5.09	118.51	109.96
1	D	524	LYS	N-CA-C	5.09	119.12	113.01
1	F	471	ASP	CA-C-O	-5.09	113.78	119.79
1	A	155	TYR	O-C-N	-5.09	116.27	122.22
1	C	408	PHE	N-CA-C	-5.09	101.88	109.11
1	D	206	GLU	N-CA-C	-5.09	101.40	109.59
1	A	223	VAL	N-CA-C	5.09	117.41	111.05
1	A	359	GLY	CA-C-O	5.09	129.42	120.57
1	A	586	VAL	CA-C-O	5.09	127.30	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	560	ARG	CA-C-O	5.09	126.66	120.25
1	A	237	SER	CA-C-O	-5.09	112.69	119.10
1	A	510	GLN	O-C-N	5.09	129.47	123.27
1	B	28	PRO	CA-N-CD	-5.09	104.88	112.00
1	E	439	SER	N-CA-C	-5.09	100.12	108.41
1	D	532	ASP	N-CA-CB	5.08	117.63	110.36
1	A	12	GLN	CG-CD-NE2	-5.08	108.78	116.40
1	A	417	ALA	N-CA-CB	-5.08	102.01	110.80
1	B	226	GLN	CA-C-N	-5.08	113.83	120.44
1	B	226	GLN	C-N-CA	-5.08	113.83	120.44
1	F	177	ARG	CA-C-O	5.08	127.78	120.51
1	A	537	GLN	CA-C-N	-5.08	113.47	120.28
1	A	537	GLN	C-N-CA	-5.08	113.47	120.28
1	B	14	ILE	CA-C-O	5.08	126.55	121.27
1	C	401	TYR	CA-CB-CG	5.08	123.04	113.90
1	A	544	ASP	CA-C-O	5.08	125.84	120.10
1	B	159	MET	N-CA-C	-5.08	105.64	111.07
1	C	190	MET	O-C-N	5.08	127.58	122.09
1	E	289	LEU	N-CA-C	-5.08	104.69	111.24
1	D	401	TYR	CA-CB-CG	5.08	123.04	113.90
1	B	28	PRO	CA-C-O	-5.08	111.36	120.60
1	B	310	GLY	O-C-N	5.08	128.39	122.45
1	E	517	GLU	CA-CB-CG	5.08	124.25	114.10
1	F	141	THR	CA-C-N	5.08	124.79	119.82
1	F	141	THR	C-N-CA	5.08	124.79	119.82
1	D	382	ARG	CB-CA-C	5.07	119.47	110.85
1	B	38	ASN	CB-CA-C	5.07	116.96	110.98
1	A	429	PHE	CA-C-N	-5.07	115.62	122.77
1	A	429	PHE	C-N-CA	-5.07	115.62	122.77
1	A	627	GLU	N-CA-C	-5.07	107.07	113.20
1	A	643	LYS	CB-CA-C	-5.07	100.74	109.86
1	B	191	ASN	N-CA-C	-5.07	105.20	111.33
1	B	446	VAL	CA-C-N	-5.07	113.96	122.17
1	B	446	VAL	C-N-CA	-5.07	113.96	122.17
1	C	298	GLU	CA-CB-CG	5.07	124.24	114.10
1	E	407	GLU	N-CA-C	5.07	117.51	109.96
1	E	35	GLU	CG-CD-OE1	5.07	130.05	118.40
1	F	226	GLN	CA-C-O	-5.07	114.62	120.24
1	A	317	GLN	CB-CG-CD	5.06	121.21	112.60
1	A	358	HIS	CA-C-O	5.06	125.20	119.18
1	C	218	GLU	CA-CB-CG	5.06	124.23	114.10
1	F	622	LEU	N-CA-C	5.06	116.98	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	641	ASN	N-CA-C	5.06	119.03	113.21
1	A	376	ARG	CA-CB-CG	5.06	124.22	114.10
1	A	652	HIS	N-CA-CB	5.06	117.79	109.95
1	B	306	THR	O-C-N	5.06	129.64	123.21
1	A	90	LEU	N-CA-CB	-5.06	101.94	110.49
1	A	286	VAL	CA-C-N	5.06	127.47	120.29
1	A	286	VAL	C-N-CA	5.06	127.47	120.29
1	B	303	GLY	O-C-N	5.06	127.88	122.22
1	A	546	ALA	N-CA-C	-5.06	107.50	113.97
1	A	518	THR	OG1-CB-CG2	-5.05	99.19	109.30
1	A	566	ASP	O-C-N	-5.05	116.76	122.12
1	B	306	THR	CA-CB-CG2	-5.05	101.91	110.50
1	C	193	HIS	CA-CB-CG	5.05	118.86	113.80
1	F	6	GLY	N-CA-C	-5.05	101.20	113.18
1	B	576	GLU	N-CA-CB	-5.05	102.52	110.30
1	E	140	ILE	CA-C-N	5.05	128.10	122.74
1	E	140	ILE	C-N-CA	5.05	128.10	122.74
1	B	213	LEU	N-CA-C	-5.05	102.16	109.59
1	B	444	GLU	CA-C-N	5.05	128.50	121.02
1	B	444	GLU	C-N-CA	5.05	128.50	121.02
1	D	89	VAL	CB-CA-C	5.05	119.58	111.29
1	F	371	PHE	N-CA-C	5.05	117.68	111.82
1	A	421	GLU	CB-CG-CD	5.05	121.18	112.60
1	A	574	LYS	CA-CB-CG	-5.05	104.00	114.10
1	A	624	TYR	CB-CG-CD2	-5.05	113.23	120.80
1	B	513	PRO	CA-C-O	-5.05	115.78	121.43
1	A	339	TYR	CB-CA-C	5.04	118.00	110.08
1	A	287	HIS	CE1-NE2-CD2	5.04	114.04	109.00
1	B	397	SER	O-C-N	5.04	128.65	122.34
1	A	580	PHE	CB-CA-C	5.04	121.11	111.48
1	C	381	PHE	CA-CB-CG	-5.04	108.76	113.80
1	A	590	ASP	CA-C-N	-5.04	114.25	122.26
1	A	590	ASP	C-N-CA	-5.04	114.25	122.26
1	B	312	THR	N-CA-C	-5.04	102.06	110.17
1	E	226	GLN	CA-CB-CG	-5.04	104.02	114.10
1	B	445	ASP	O-C-N	5.04	129.71	123.01
1	B	560	ARG	N-CA-CB	5.04	118.76	110.90
1	C	382	ARG	CB-CA-C	5.04	119.41	110.85
1	D	458	ASN	CA-C-O	-5.04	115.26	120.70
1	B	67	GLU	CA-C-O	-5.04	116.03	121.87
1	D	19	ASP	CA-CB-CG	5.04	117.64	112.60
1	E	356	ASP	CA-CB-CG	5.04	117.64	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	420	GLY	O-C-N	5.04	129.99	124.00
1	B	591	LYS	N-CA-C	-5.04	107.52	113.97
1	C	291	ILE	N-CA-CB	5.04	116.44	110.55
1	D	525	ASP	CA-CB-CG	-5.04	107.56	112.60
1	E	177	ARG	CA-C-O	5.04	127.71	120.51
1	B	231	PHE	CZ-CE2-CD2	5.03	129.06	120.00
1	A	411	MET	N-CA-C	5.03	117.77	110.42
1	B	33	ILE	CA-CB-CG2	-5.03	101.95	110.50
1	B	632	ASP	N-CA-CB	5.03	118.67	110.77
1	C	498	ALA	N-CA-C	5.03	119.57	113.38
1	D	512	VAL	CA-C-O	5.03	122.46	119.19
1	B	70	HIS	ND1-CG-CD2	5.03	111.13	106.10
1	B	148	SER	O-C-N	5.03	129.50	122.36
1	B	227	LEU	CB-CA-C	-5.03	102.99	110.88
1	E	522	SER	CA-C-O	5.03	127.21	121.28
1	E	641	ASN	N-CA-C	5.03	118.99	113.21
1	B	355	GLY	N-CA-C	-5.03	107.82	115.66
1	B	522	SER	N-CA-CB	-5.03	102.81	110.85
1	A	58	LYS	CA-C-O	-5.02	115.53	120.90
1	A	230	ARG	CB-CA-C	5.02	119.22	110.68
1	A	400	PRO	N-CA-CB	-5.02	98.67	103.39
1	B	40	LEU	O-C-N	5.02	128.44	122.26
1	B	431	TYR	O-C-N	-5.02	115.76	122.94
1	D	141	THR	CA-C-N	5.02	124.74	119.82
1	D	141	THR	C-N-CA	5.02	124.74	119.82
1	B	180	ARG	NH1-CZ-NH2	5.02	125.83	119.30
1	C	426	PHE	N-CA-C	5.02	117.78	107.69
1	D	321	ILE	CA-C-O	-5.02	114.51	120.78
1	D	426	PHE	N-CA-C	5.02	117.78	107.69
1	E	32	ASP	N-CA-C	-5.02	106.00	111.82
1	A	526	SER	CB-CA-C	-5.02	100.76	109.64
1	B	352	GLY	O-C-N	-5.02	116.18	122.70
1	E	371	PHE	N-CA-C	5.02	117.64	111.82
1	F	142	PRO	N-CA-C	5.02	120.45	113.98
1	A	194	HIS	CA-C-N	5.01	127.91	120.74
1	A	194	HIS	C-N-CA	5.01	127.91	120.74
1	B	409	SER	CA-C-O	5.01	126.67	121.15
1	D	85	MET	N-CA-C	-5.01	105.52	111.69
1	E	268	PHE	O-C-N	5.01	125.49	121.38
1	A	132	ILE	O-C-N	5.01	127.93	122.57
1	B	114	GLU	CB-CG-CD	-5.01	104.08	112.60
1	B	143	HIS	CG-CD2-NE2	-5.01	102.19	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	426	PHE	N-CA-C	5.01	117.76	107.69
1	A	326	ASP	N-CA-CB	5.01	118.02	110.30
1	A	444	GLU	CB-CA-C	5.01	118.01	109.75
1	F	190	MET	O-C-N	5.01	127.50	122.09
1	B	5	THR	CA-C-O	-5.01	112.29	120.80
1	A	403	HIS	O-C-N	-5.01	116.82	122.03
1	D	26	LYS	CA-CB-CG	-5.01	104.09	114.10
1	F	234	GLU	CB-CG-CD	5.01	121.11	112.60
1	C	393	LYS	N-CA-CB	5.00	117.93	110.22
1	A	155	TYR	CA-CB-CG	5.00	122.90	113.90
1	A	423	ILE	N-CA-C	-5.00	100.87	108.17
1	A	503	ILE	O-C-N	5.00	128.23	122.93
1	E	361	PHE	CA-CB-CG	-5.00	108.80	113.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	295	ARG	Sidechain
1	B	177	ARG	Sidechain
1	B	521	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	A	5173	0	4888	706	0
1	B	5173	0	4886	674	1
1	C	5173	0	4888	436	3
1	D	5173	0	4888	492	1
1	E	5173	0	4888	447	0
1	F	5173	0	4888	439	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2	0	0	0	0
3	A	186	0	0	40	0
3	B	186	0	0	16	0
3	C	186	0	0	12	0
3	D	186	0	0	11	0
3	E	186	0	0	10	0
3	F	186	0	0	9	0
All	All	32166	0	29326	3112	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 52.

All (3112) 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:161:GLN:OE1	1:B:443:ILE:HD13	1.28	1.29
1:A:422:LEU:CD2	1:A:570:LEU:HD21	1.66	1.23
1:A:316:ARG:HD3	3:A:829:HOH:O	1.41	1.19
1:A:165:THR:CG2	1:A:449:ASN:HB2	1.73	1.17
1:B:456:ASN:HD22	1:B:457:HIS:N	1.42	1.17
1:A:456:ASN:HD22	1:A:457:HIS:N	1.43	1.16
1:A:411:MET:HG3	3:A:834:HOH:O	0.96	1.13
1:A:513:PRO:CG	1:A:517:GLU:HG3	1.79	1.13
1:A:135:PRO:HB2	1:A:140:ILE:HD11	1.24	1.11
1:A:422:LEU:HD22	1:A:570:LEU:HD21	1.18	1.10
1:B:95:GLU:HA	1:B:128:LEU:HD21	1.32	1.10
1:A:313:ILE:HD11	1:A:323:LEU:HD13	1.33	1.10
1:A:412:VAL:O	1:A:412:VAL:HG22	1.47	1.09
1:B:368:MET:HE1	1:B:380:PHE:HA	1.18	1.09
1:A:56:LEU:HD11	1:A:110:MET:HE3	1.32	1.07
1:A:533:MET:HB3	1:A:534:PRO:HD2	1.33	1.07
1:D:165:THR:HG22	1:D:449:ASN:HB2	1.33	1.06
1:C:165:THR:HG22	1:C:449:ASN:HB2	1.36	1.05
1:A:253:ARG:NH1	3:A:701:HOH:O	1.90	1.05
1:A:313:ILE:CD1	1:A:323:LEU:HD13	1.87	1.04
1:A:634:ARG:NH1	1:A:634:ARG:HG2	1.53	1.04
1:A:412:VAL:HG13	1:A:467:SER:O	1.55	1.04
1:A:634:ARG:HH11	1:A:634:ARG:CG	1.71	1.04
1:B:456:ASN:ND2	1:B:457:HIS:H	1.54	1.04
1:B:168:VAL:HG21	1:B:452:VAL:HG12	1.39	1.04
1:C:175:LYS:HB2	1:D:491:ILE:HG12	1.40	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:MET:HE3	1:A:512:VAL:CG1	1.88	1.03
1:A:456:ASN:ND2	1:A:457:HIS:H	1.56	1.03
1:A:416:VAL:HG22	1:A:645:VAL:HG11	1.41	1.02
1:A:513:PRO:HG3	1:A:517:GLU:CG	1.91	1.01
1:D:634:ARG:HH21	1:F:64:ARG:HD2	1.22	1.01
1:C:368:MET:HE1	1:C:380:PHE:HA	1.42	1.01
1:D:150:VAL:HG21	1:D:168:VAL:HG12	1.40	1.01
1:A:373:THR:O	1:A:376:ARG:HB2	1.59	1.01
1:D:456:ASN:HD22	1:D:457:HIS:N	1.59	1.00
1:B:417:ALA:HB3	1:B:463:LYS:O	1.58	1.00
1:B:185:GLY:O	1:B:375:THR:HG22	1.61	1.00
1:B:120:TYR:CD2	1:B:134:LEU:HD13	1.95	0.99
1:B:611:VAL:HG12	1:B:612:HIS:HD2	1.25	0.99
1:E:239:TRP:CH2	1:E:574:LYS:HD3	1.97	0.99
1:F:423:ILE:HD11	1:F:652:HIS:NE2	1.77	0.99
1:C:472:GLY:HA2	1:C:514:SER:HB2	1.45	0.99
1:C:456:ASN:HD22	1:C:457:HIS:N	1.60	0.99
1:F:456:ASN:HD22	1:F:457:HIS:N	1.59	0.99
1:B:606:HIS:HD2	1:B:608:GLN:HG2	1.27	0.99
1:B:416:VAL:HG22	1:B:645:VAL:HG11	1.45	0.99
1:D:421:GLU:HG2	1:D:422:LEU:H	1.28	0.98
1:E:456:ASN:HD22	1:E:457:HIS:N	1.60	0.98
1:D:46:TYR:CZ	1:D:53:VAL:HG21	1.98	0.98
1:E:423:ILE:HD11	1:E:652:HIS:NE2	1.78	0.98
1:C:150:VAL:HG21	1:C:168:VAL:HG12	1.44	0.98
1:B:56:LEU:HD21	1:B:110:MET:HE3	1.45	0.98
1:E:368:MET:HE1	1:E:380:PHE:HA	1.45	0.98
1:F:165:THR:HG22	1:F:449:ASN:HB2	1.45	0.98
1:B:423:ILE:HD11	1:B:652:HIS:NE2	1.79	0.97
1:D:272:PRO:HG2	1:E:272:PRO:HG2	1.41	0.97
1:E:606:HIS:HD2	1:E:608:GLN:HG2	1.29	0.97
1:E:56:LEU:HD11	1:E:110:MET:HE3	1.47	0.97
1:A:423:ILE:HD11	1:A:652:HIS:CE1	1.98	0.97
1:D:368:MET:HE1	1:D:380:PHE:HA	1.45	0.97
1:F:56:LEU:HD11	1:F:110:MET:HE3	1.46	0.97
1:A:165:THR:HG22	1:A:449:ASN:HB2	1.43	0.96
1:F:368:MET:HE1	1:F:380:PHE:HA	1.45	0.96
1:A:89:VAL:O	1:A:92:GLN:N	1.98	0.96
1:A:120:TYR:CD2	1:A:134:LEU:HD13	1.99	0.96
1:A:423:ILE:HD11	1:A:652:HIS:NE2	1.79	0.96
1:B:135:PRO:HB2	1:B:140:ILE:HD11	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:THR:HG22	1:E:449:ASN:HB2	1.45	0.96
1:A:135:PRO:CB	1:A:140:ILE:HD11	1.96	0.95
1:A:513:PRO:HG3	1:A:517:GLU:HG3	0.96	0.95
1:B:283:VAL:HG11	1:B:349:VAL:HB	1.44	0.95
1:A:477:THR:HG23	1:A:509:PHE:CD1	2.02	0.95
1:C:56:LEU:HD11	1:C:110:MET:HE3	1.46	0.95
1:F:150:VAL:HG21	1:F:168:VAL:HG12	1.47	0.95
1:A:634:ARG:HG2	1:A:634:ARG:HH11	0.78	0.95
1:E:5:THR:HG22	1:E:6:GLY:H	1.30	0.95
1:A:31:LYS:O	1:A:34:ALA:HB3	1.67	0.95
1:A:48:ASP:HB3	1:A:92:GLN:NE2	1.81	0.94
1:C:423:ILE:HD11	1:C:652:HIS:NE2	1.81	0.94
1:D:56:LEU:HD11	1:D:110:MET:HE3	1.47	0.94
1:C:606:HIS:HD2	1:C:608:GLN:HG2	1.32	0.94
1:F:493:LEU:HD13	1:F:498:ALA:HB2	1.49	0.94
1:D:95:GLU:HG2	1:D:96:TRP:H	1.30	0.94
1:B:65:LEU:HD12	1:B:82:GLU:HG2	1.49	0.94
1:F:239:TRP:CH2	1:F:574:LYS:HD3	2.01	0.94
1:A:440:GLY:C	1:A:441:GLU:CG	2.38	0.94
1:B:76:ASN:HD22	1:B:79:GLN:H	1.15	0.94
1:D:413:VAL:HA	1:D:466:MET:HB3	1.48	0.94
1:A:560:ARG:NH2	1:A:606:HIS:N	2.14	0.94
1:B:143:HIS:CE1	1:B:151:ILE:HG21	2.03	0.94
1:C:8:ALA:HB1	1:C:546:ALA:HB3	1.50	0.94
1:C:239:TRP:CH2	1:C:574:LYS:HD3	2.03	0.94
1:C:493:LEU:HD13	1:C:498:ALA:HB2	1.50	0.94
1:E:456:ASN:ND2	1:E:457:HIS:H	1.65	0.94
1:D:239:TRP:CH2	1:D:574:LYS:HD3	2.03	0.94
1:E:150:VAL:HG21	1:E:168:VAL:HG12	1.49	0.93
1:A:21:ILE:HG13	1:A:21:ILE:O	1.65	0.93
1:C:272:PRO:HG2	1:F:272:PRO:HG2	1.51	0.93
1:F:317:GLN:HB2	1:F:318:PRO:HD2	1.50	0.93
1:F:606:HIS:HD2	1:F:608:GLN:HG2	1.31	0.93
1:B:48:ASP:HB3	1:B:92:GLN:NE2	1.83	0.93
1:D:423:ILE:HD11	1:D:652:HIS:NE2	1.84	0.92
1:A:161:GLN:OE1	1:B:443:ILE:CD1	2.17	0.92
1:A:411:MET:HE3	1:A:512:VAL:HG11	1.49	0.92
1:B:89:VAL:O	1:B:92:GLN:N	2.03	0.92
1:D:493:LEU:HD13	1:D:498:ALA:HB2	1.51	0.92
1:F:456:ASN:ND2	1:F:457:HIS:H	1.66	0.92
1:D:317:GLN:HB2	1:D:318:PRO:HD2	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:95:GLU:HA	1:F:128:LEU:HD21	1.50	0.92
1:A:411:MET:HE3	1:A:512:VAL:HB	1.50	0.92
1:B:18:LEU:HD21	1:B:119:LEU:HD23	1.49	0.92
1:B:548:ASN:H	1:B:548:ASN:ND2	1.67	0.92
1:A:470:ASN:ND2	1:A:474:ARG:HD3	1.83	0.92
1:B:76:ASN:ND2	1:B:79:GLN:HG3	1.86	0.92
1:C:317:GLN:HB2	1:C:318:PRO:HD2	1.50	0.91
1:C:456:ASN:ND2	1:C:457:HIS:H	1.66	0.91
1:B:121:VAL:HG23	1:B:199:MET:HG2	1.52	0.91
1:E:317:GLN:HB2	1:E:318:PRO:HD2	1.50	0.91
1:D:456:ASN:ND2	1:D:457:HIS:H	1.66	0.91
1:A:248:TRP:CH2	1:A:289:LEU:HD13	2.06	0.91
1:A:422:LEU:HD22	1:A:570:LEU:CD2	2.00	0.91
1:D:411:MET:HE1	1:D:512:VAL:HB	1.48	0.91
1:D:606:HIS:HD2	1:D:608:GLN:HG2	1.34	0.91
1:A:411:MET:HE3	1:A:512:VAL:CB	2.00	0.90
1:E:408:PHE:N	1:E:641:ASN:OD1	2.04	0.90
1:A:155:TYR:CG	1:B:159:MET:HE1	2.05	0.90
1:F:168:VAL:HG21	1:F:452:VAL:HG12	1.54	0.90
1:A:50:GLY:O	1:A:53:VAL:HG23	1.72	0.90
1:A:412:VAL:O	1:A:412:VAL:CG2	2.18	0.90
1:A:543:ALA:O	1:A:547:VAL:HG22	1.70	0.90
1:B:487:ASP:CB	1:B:491:ILE:H	1.84	0.90
1:E:493:LEU:HD13	1:E:498:ALA:HB2	1.55	0.89
1:A:165:THR:CB	1:A:449:ASN:HB2	2.01	0.89
1:B:60:LEU:HD11	1:B:109:ARG:HG3	1.54	0.89
1:B:74:LEU:HG	1:B:74:LEU:O	1.69	0.89
1:F:313:ILE:HD11	1:F:323:LEU:HD13	1.54	0.89
1:B:589:GLY:O	1:B:593:THR:OG1	1.89	0.89
1:A:462:TYR:O	1:A:520:GLU:HA	1.72	0.89
1:A:305:ILE:HG13	1:A:315:ILE:HG21	1.54	0.89
1:B:611:VAL:HG12	1:B:612:HIS:CD2	2.07	0.89
1:C:414:ASN:HD22	1:C:466:MET:HA	1.38	0.89
1:C:168:VAL:HG21	1:C:452:VAL:HG12	1.53	0.88
1:E:168:VAL:HG21	1:E:452:VAL:HG12	1.53	0.88
1:C:313:ILE:HD11	1:C:323:LEU:HD13	1.54	0.88
1:B:239:TRP:CH2	1:B:574:LYS:HD3	2.08	0.88
1:E:48:ASP:HB3	1:E:92:GLN:NE2	1.88	0.88
1:F:543:ALA:HA	1:F:553:LEU:HD11	1.54	0.88
1:A:411:MET:CE	1:A:512:VAL:HB	2.03	0.88
1:A:468:ASN:OD1	1:A:470:ASN:HB2	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ASP:HB3	1:B:92:GLN:HE21	1.39	0.88
1:E:411:MET:HG3	3:E:834:HOH:O	1.74	0.88
1:A:440:GLY:C	1:A:441:GLU:HG2	1.69	0.87
1:B:487:ASP:HB2	1:B:491:ILE:H	1.38	0.87
1:A:150:VAL:HG21	1:A:168:VAL:HG12	1.53	0.87
1:B:416:VAL:HG22	1:B:645:VAL:CG1	2.02	0.87
1:B:522:SER:O	1:B:523:SER:C	2.14	0.87
1:D:95:GLU:HG2	1:D:96:TRP:N	1.86	0.87
1:D:508:PHE:CE2	1:D:521:ARG:HD2	2.09	0.87
1:A:11:GLN:O	1:A:15:ASN:ND2	2.08	0.87
1:A:639:VAL:HG23	1:A:641:ASN:ND2	1.89	0.87
1:A:159:MET:HE1	1:B:155:TYR:CG	2.09	0.87
1:D:543:ALA:O	1:D:547:VAL:HG23	1.74	0.86
1:F:8:ALA:HA	1:F:553:LEU:HD12	1.58	0.86
1:D:313:ILE:HD11	1:D:323:LEU:HD13	1.56	0.86
1:E:543:ALA:O	1:E:547:VAL:HG23	1.75	0.86
1:B:255:GLY:HA2	1:B:271:ARG:NH1	1.90	0.86
1:E:95:GLU:HA	1:E:128:LEU:HD21	1.58	0.86
1:A:408:PHE:CB	1:A:641:ASN:OD1	2.24	0.86
1:C:7:ASN:C	1:C:9:GLN:H	1.81	0.86
1:C:150:VAL:HG12	1:C:433:LEU:HD11	1.56	0.86
1:B:5:THR:HG22	1:B:10:LYS:HD3	1.57	0.85
1:B:329:GLU:HA	1:B:344:HIS:HB3	1.56	0.85
1:E:7:ASN:C	1:E:9:GLN:H	1.79	0.85
1:B:634:ARG:HG2	1:B:634:ARG:HH11	1.41	0.85
1:A:493:LEU:HD13	1:A:498:ALA:HB2	1.58	0.85
1:B:29:ASP:O	1:B:33:ILE:HG13	1.77	0.85
1:E:553:LEU:HD22	1:E:555:LEU:HG	1.59	0.85
1:B:493:LEU:HB3	1:B:497:GLU:HB2	1.59	0.85
1:D:185:GLY:O	1:D:375:THR:HG22	1.77	0.85
1:A:417:ALA:HB3	1:A:463:LYS:O	1.77	0.85
1:F:422:LEU:HD22	1:F:570:LEU:HD21	1.58	0.85
1:E:634:ARG:HG2	1:E:634:ARG:HH11	1.42	0.84
1:E:606:HIS:CD2	1:E:608:GLN:HG2	2.12	0.84
1:F:414:ASN:HD22	1:F:466:MET:HA	1.42	0.84
1:C:576:GLU:OE1	1:D:576:GLU:OE1	1.95	0.84
1:D:150:VAL:HG12	1:D:433:LEU:HD11	1.56	0.84
1:F:7:ASN:C	1:F:9:GLN:H	1.80	0.84
1:B:533:MET:HE3	1:B:533:MET:H	1.42	0.84
1:E:43:THR:HG23	1:E:49:HIS:C	2.02	0.84
1:D:7:ASN:C	1:D:9:GLN:H	1.80	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:HIS:HB3	1:A:211:TYR:OH	1.78	0.84
1:D:413:VAL:HA	1:D:466:MET:CB	2.07	0.84
1:F:606:HIS:CD2	1:F:608:GLN:HG2	2.13	0.84
1:A:594:GLU:O	1:A:594:GLU:HG2	1.76	0.84
1:B:487:ASP:HB2	1:B:491:ILE:N	1.92	0.84
1:F:43:THR:HG23	1:F:49:HIS:C	2.03	0.84
1:E:313:ILE:HD11	1:E:323:LEU:HD13	1.60	0.84
1:A:591:LYS:HA	1:A:594:GLU:HB2	1.59	0.83
1:B:66:LEU:HD22	1:B:67:GLU:O	1.79	0.83
1:E:185:GLY:O	1:E:375:THR:HG22	1.78	0.83
1:A:256:PHE:C	1:A:256:PHE:CD1	2.54	0.83
1:B:101:SER:O	1:B:104:ALA:HB3	1.77	0.83
1:B:39:PRO:HB3	1:B:102:ASN:HD21	1.43	0.83
1:B:570:LEU:HB3	1:B:571:PRO:HD2	1.59	0.83
1:F:560:ARG:NH1	1:F:606:HIS:N	2.27	0.83
1:A:255:GLY:HA2	1:A:271:ARG:NH1	1.92	0.83
1:F:185:GLY:O	1:F:375:THR:HG22	1.78	0.83
1:A:200:ASP:O	1:A:202:PRO:HD3	1.78	0.83
1:B:570:LEU:HB3	1:B:571:PRO:CD	2.08	0.83
1:B:20:LYS:N	1:B:435:ASN:HD21	1.76	0.83
1:C:185:GLY:O	1:C:375:THR:HG22	1.77	0.83
1:A:418:ILE:HD11	1:A:462:TYR:CE1	2.14	0.83
1:A:86:LEU:HD23	1:A:90:LEU:HD22	1.59	0.83
1:C:43:THR:HG23	1:C:49:HIS:C	2.03	0.83
1:A:74:LEU:O	1:A:74:LEU:HG	1.77	0.82
1:B:59:GLU:OE1	1:B:64:ARG:HD3	1.79	0.82
1:D:133:VAL:HG22	1:D:558:TYR:O	1.77	0.82
1:F:634:ARG:HG2	1:F:634:ARG:HH11	1.43	0.82
1:B:555:LEU:HD23	1:B:556:SER:H	1.44	0.82
1:B:606:HIS:CD2	1:B:608:GLN:HG2	2.14	0.82
1:C:634:ARG:HH11	1:C:634:ARG:HG2	1.43	0.82
1:B:535:SER:OG	1:B:536:PHE:N	2.12	0.82
1:D:168:VAL:HG21	1:D:452:VAL:HG12	1.58	0.82
1:F:269:PRO:HB3	1:F:363:LEU:HD23	1.61	0.82
1:C:380:PHE:CE1	1:C:384:HIS:CE1	2.68	0.82
1:B:313:ILE:C	1:B:313:ILE:HD12	2.04	0.82
1:A:533:MET:CE	1:A:533:MET:H	1.91	0.82
1:A:554:ASP:O	1:A:555:LEU:C	2.20	0.82
1:C:422:LEU:HD22	1:C:570:LEU:HD21	1.60	0.82
1:C:606:HIS:CD2	1:C:608:GLN:HG2	2.14	0.82
1:D:634:ARG:HG2	1:D:634:ARG:HH11	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:TYR:OH	1:B:234:GLU:OE1	1.98	0.81
1:E:560:ARG:NH1	1:E:606:HIS:N	2.28	0.81
1:A:414:ASN:HD22	1:A:466:MET:HA	1.46	0.81
1:A:533:MET:HB3	1:A:534:PRO:CD	2.10	0.81
1:B:477:THR:HG23	1:B:509:PHE:CD1	2.16	0.81
1:D:606:HIS:CD2	1:D:608:GLN:HG2	2.15	0.81
1:A:185:GLY:O	1:A:375:THR:HG22	1.81	0.81
1:B:178:GLU:HG3	1:B:178:GLU:O	1.78	0.81
1:B:486:GLU:HA	1:B:492:THR:HA	1.61	0.81
1:C:560:ARG:HG2	1:C:609:CYS:HB3	1.61	0.81
1:E:411:MET:CE	1:E:468:ASN:HD22	1.94	0.81
1:A:284:ALA:O	1:A:350:MET:HE1	1.80	0.81
1:B:522:SER:O	1:B:524:LYS:N	2.13	0.81
1:B:588:ASP:OD1	1:B:588:ASP:O	1.97	0.81
1:C:175:LYS:HB2	1:D:491:ILE:CG1	2.11	0.81
1:A:479:ARG:NH2	1:A:618:ASP:OD2	2.14	0.81
1:A:508:PHE:CE2	1:A:521:ARG:CD	2.63	0.81
1:C:8:ALA:CB	1:C:546:ALA:HB3	2.11	0.81
1:C:175:LYS:CB	1:D:491:ILE:HG12	2.10	0.81
1:A:606:HIS:HD2	1:A:608:GLN:HG2	1.44	0.80
1:E:18:LEU:HD21	1:E:119:LEU:HD23	1.64	0.80
1:E:419:ASP:HB2	1:E:463:LYS:HD2	1.62	0.80
1:F:18:LEU:HD21	1:F:119:LEU:HD23	1.63	0.80
1:A:243:VAL:HG23	1:A:385:LYS:HD3	1.63	0.80
1:E:414:ASN:HD22	1:E:466:MET:HA	1.47	0.80
1:A:422:LEU:HD23	1:A:570:LEU:HD21	1.60	0.80
1:B:61:ASN:C	1:B:63:HIS:H	1.84	0.80
1:A:72:TYR:HA	1:A:79:GLN:OE1	1.81	0.80
1:B:606:HIS:HB3	1:B:608:GLN:H	1.47	0.80
1:C:18:LEU:HD21	1:C:119:LEU:HD23	1.64	0.80
1:B:175:LYS:O	1:B:176:ASN:HB2	1.80	0.80
1:E:150:VAL:HG12	1:E:433:LEU:HD11	1.64	0.80
1:E:486:GLU:HA	1:E:492:THR:HA	1.64	0.80
1:A:553:LEU:HD22	1:A:555:LEU:HG	1.63	0.79
1:B:356:ASP:CG	1:B:359:GLY:HA2	2.06	0.79
1:D:456:ASN:HD22	1:D:457:HIS:H	0.81	0.79
1:F:150:VAL:HG12	1:F:433:LEU:HD11	1.63	0.79
1:A:368:MET:HE1	1:A:380:PHE:CD2	2.16	0.79
1:D:448:ILE:C	1:D:449:ASN:HD22	1.89	0.79
1:D:18:LEU:HD21	1:D:119:LEU:HD23	1.63	0.79
1:E:269:PRO:HB3	1:E:363:LEU:HD23	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:PHE:HB3	1:A:216:LYS:CD	2.13	0.79
1:B:248:TRP:CH2	1:B:289:LEU:HD13	2.18	0.79
1:A:85:MET:HE1	3:A:808:HOH:O	1.81	0.79
1:A:252:ILE:HG13	1:A:275:ILE:HG22	1.63	0.79
1:A:300:ILE:CD1	1:A:390:ILE:HG22	2.13	0.79
1:C:456:ASN:HD22	1:C:457:HIS:H	0.81	0.79
1:D:40:LEU:HD12	1:D:53:VAL:HG12	1.65	0.79
1:A:237:SER:HA	1:A:574:LYS:HE3	1.65	0.78
1:A:439:SER:O	1:B:160:THR:HG22	1.83	0.78
1:A:159:MET:HE1	1:B:155:TYR:CD1	2.18	0.78
1:A:56:LEU:HD11	1:A:110:MET:CE	2.11	0.78
1:A:86:LEU:HD12	1:A:110:MET:SD	2.23	0.78
1:A:220:PHE:CE2	1:A:329:GLU:HB2	2.19	0.78
1:B:591:LYS:HB2	1:B:591:LYS:HZ2	1.49	0.78
1:F:466:MET:HE2	3:F:834:HOH:O	1.82	0.78
1:B:56:LEU:HD21	1:B:110:MET:CE	2.13	0.78
1:B:158:LYS:HG2	1:B:437:VAL:CG2	2.14	0.78
1:B:413:VAL:HG12	1:B:643:LYS:CG	2.13	0.78
1:A:69:ARG:HG2	1:A:264:TYR:CE2	2.19	0.77
1:A:120:TYR:O	1:A:124:ILE:HG13	1.84	0.77
1:A:178:GLU:OE1	3:A:705:HOH:O	2.01	0.77
1:C:487:ASP:HB2	1:C:491:ILE:O	1.83	0.77
1:B:591:LYS:HB2	1:B:591:LYS:NZ	2.00	0.77
1:B:330:SER:HB2	1:B:342:SER:OG	1.84	0.77
1:A:76:ASN:HB3	1:A:79:GLN:HB2	1.66	0.77
1:B:26:LYS:HE2	1:B:440:GLY:O	1.83	0.77
1:E:423:ILE:HD11	1:E:652:HIS:CE1	2.19	0.77
1:F:411:MET:HG3	3:F:834:HOH:O	1.83	0.77
1:A:418:ILE:HD11	1:A:462:TYR:CD1	2.18	0.77
1:C:411:MET:HG3	3:C:834:HOH:O	1.85	0.77
1:A:56:LEU:CD1	1:A:110:MET:HE3	2.14	0.77
1:A:323:LEU:HD11	3:A:849:HOH:O	1.84	0.77
1:B:356:ASP:OD2	1:B:359:GLY:HA2	1.84	0.77
1:C:408:PHE:N	1:C:641:ASN:OD1	2.17	0.77
1:A:86:LEU:CD2	1:A:90:LEU:HD22	2.15	0.77
1:A:165:THR:HB	1:A:449:ASN:CB	2.14	0.77
1:A:434:ILE:HD11	1:A:447:GLU:HA	1.67	0.77
1:F:408:PHE:N	1:F:641:ASN:OD1	2.18	0.77
1:B:78:ARG:NH1	1:B:82:GLU:OE2	2.16	0.77
1:A:168:VAL:HG21	1:A:452:VAL:HG12	1.65	0.76
1:A:226:GLN:O	1:A:227:LEU:C	2.23	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:PHE:CE2	1:A:521:ARG:HD3	2.20	0.76
1:B:468:ASN:ND2	1:B:512:VAL:O	2.17	0.76
1:D:330:SER:OG	1:D:341:GLY:O	2.03	0.76
1:B:548:ASN:H	1:B:548:ASN:HD22	1.31	0.76
1:D:272:PRO:CG	1:E:272:PRO:HG2	2.15	0.76
1:A:252:ILE:HG13	1:A:275:ILE:CG2	2.15	0.76
1:B:305:ILE:HD12	1:B:315:ILE:HG21	1.66	0.76
1:E:60:LEU:HD21	1:E:109:ARG:HD2	1.66	0.76
1:A:155:TYR:CD1	1:B:159:MET:HE1	2.19	0.76
1:A:533:MET:H	1:A:533:MET:HE3	1.50	0.76
1:D:423:ILE:HD11	1:D:652:HIS:CE1	2.21	0.76
1:B:37:PHE:CE2	1:B:101:SER:HB3	2.21	0.76
1:F:423:ILE:HD11	1:F:652:HIS:CE1	2.20	0.76
1:D:60:LEU:HD21	1:D:109:ARG:HD2	1.68	0.76
1:D:634:ARG:HH21	1:F:64:ARG:CD	1.98	0.76
1:B:316:ARG:HG3	1:B:398:PHE:HE1	1.51	0.75
1:B:565:PRO:HB2	1:B:568:MET:HG2	1.66	0.75
1:A:165:THR:HB	1:A:449:ASN:HB2	1.69	0.75
1:A:220:PHE:CZ	1:A:329:GLU:HB2	2.21	0.75
1:B:74:LEU:O	1:B:74:LEU:CG	2.32	0.75
1:B:150:VAL:HG12	1:B:433:LEU:HD11	1.67	0.75
1:B:489:ASN:HB3	1:B:491:ILE:HD11	1.66	0.75
1:D:59:GLU:OE1	1:D:64:ARG:HD3	1.87	0.75
1:E:313:ILE:C	1:E:313:ILE:HD12	2.11	0.75
1:A:300:ILE:HD11	1:A:390:ILE:HG22	1.68	0.75
1:B:29:ASP:OD1	1:B:29:ASP:N	2.18	0.75
1:B:423:ILE:HD11	1:B:652:HIS:CE1	2.20	0.75
1:D:634:ARG:HE	1:F:64:ARG:NE	1.83	0.75
1:B:11:GLN:HG2	1:B:132:ILE:HG23	1.67	0.75
1:B:19:ASP:O	1:B:20:LYS:C	2.29	0.75
1:B:425:PHE:N	1:B:456:ASN:O	2.18	0.75
1:C:165:THR:HA	1:C:449:ASN:O	1.87	0.75
1:A:606:HIS:CD2	1:A:608:GLN:HG2	2.21	0.75
1:C:60:LEU:HD21	1:C:109:ARG:HD2	1.68	0.75
1:B:466:MET:HE2	3:B:834:HOH:O	1.85	0.75
1:B:220:PHE:O	1:B:221:PHE:C	2.27	0.74
1:B:592:ASP:C	1:B:594:GLU:H	1.95	0.74
1:C:11:GLN:HG3	1:C:15:ASN:HD21	1.52	0.74
1:D:5:THR:HG22	1:D:6:GLY:H	1.52	0.74
1:A:190:MET:HG2	1:A:568:MET:HE2	1.66	0.74
1:A:641:ASN:HD22	1:A:641:ASN:C	1.93	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:TRP:CH2	1:C:289:LEU:HD13	2.21	0.74
1:D:487:ASP:HB3	1:D:491:ILE:H	1.50	0.74
1:E:185:GLY:HA2	1:E:375:THR:CG2	2.17	0.74
1:A:11:GLN:HG3	1:A:15:ASN:HD21	1.52	0.74
1:D:40:LEU:CD1	1:D:53:VAL:HG12	2.17	0.74
1:B:243:VAL:HG23	1:B:385:LYS:HD2	1.68	0.74
1:D:11:GLN:HG3	1:D:15:ASN:HD21	1.51	0.74
1:D:313:ILE:C	1:D:313:ILE:HD12	2.13	0.74
1:A:317:GLN:HB2	1:A:318:PRO:HD2	1.67	0.74
1:B:244:ASP:O	1:B:382:ARG:HG3	1.87	0.74
1:C:533:MET:HE3	1:C:533:MET:H	1.53	0.74
1:E:120:TYR:O	1:E:124:ILE:HG13	1.88	0.74
1:A:17:LEU:HD21	1:A:103:ALA:O	1.88	0.74
1:A:50:GLY:C	1:A:53:VAL:HG23	2.12	0.74
1:B:446:VAL:O	1:B:446:VAL:HG13	1.86	0.74
1:D:248:TRP:CH2	1:D:289:LEU:HD13	2.22	0.74
1:D:422:LEU:HD22	1:D:570:LEU:HD21	1.68	0.74
1:E:59:GLU:OE1	1:E:64:ARG:HD3	1.88	0.74
1:A:533:MET:CB	1:A:534:PRO:HD2	2.02	0.74
1:B:148:SER:HB2	1:B:259:LEU:O	1.87	0.74
1:D:411:MET:HE1	1:D:512:VAL:CB	2.18	0.74
1:D:185:GLY:HA2	1:D:375:THR:CG2	2.18	0.74
1:A:133:VAL:CG2	1:A:555:LEU:HD13	2.18	0.73
1:A:368:MET:HE1	1:A:380:PHE:HA	1.69	0.73
1:B:62:ASP:HB2	1:B:64:ARG:HG2	1.70	0.73
1:C:508:PHE:CE2	1:C:521:ARG:HD2	2.23	0.73
1:E:411:MET:HE1	1:E:468:ASN:HD22	1.52	0.73
1:A:139:GLN:NE2	1:A:432:SER:H	1.86	0.73
1:E:48:ASP:HB3	1:E:92:GLN:HE21	1.48	0.73
1:F:329:GLU:HA	1:F:344:HIS:HB3	1.70	0.73
1:A:557:ALA:HB3	1:A:558:TYR:CD2	2.22	0.73
1:B:72:TYR:HA	1:B:79:GLN:OE1	1.88	0.73
1:C:48:ASP:HB3	1:C:92:GLN:NE2	2.03	0.73
1:F:512:VAL:HG11	3:F:834:HOH:O	1.87	0.73
1:A:48:ASP:HB3	1:A:92:GLN:HE21	1.51	0.73
1:A:374:ALA:C	1:A:376:ARG:H	1.94	0.73
1:C:247:HIS:HB2	1:C:250:ARG:HG2	1.69	0.73
1:D:177:ARG:HG2	1:E:360:LYS:HB3	1.68	0.73
1:E:130:ASP:O	1:E:559:GLU:OE1	2.06	0.73
1:F:330:SER:OG	1:F:341:GLY:O	2.06	0.73
1:F:533:MET:HE3	1:F:533:MET:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:547:VAL:HG23	1:F:548:ASN:ND2	2.02	0.73
1:C:59:GLU:OE1	1:C:64:ARG:HD3	1.87	0.73
1:C:185:GLY:HA2	1:C:375:THR:CG2	2.17	0.73
1:D:533:MET:HE3	1:D:533:MET:H	1.53	0.73
1:E:248:TRP:CH2	1:E:289:LEU:HD13	2.23	0.73
1:B:76:ASN:HD22	1:B:79:GLN:HG3	1.52	0.73
1:B:239:TRP:CZ3	1:B:574:LYS:NZ	2.56	0.73
1:B:416:VAL:CG2	1:B:645:VAL:HG11	2.18	0.73
1:D:69:ARG:HG2	1:D:264:TYR:CE2	2.24	0.73
1:E:247:HIS:HB2	1:E:250:ARG:HG2	1.69	0.73
1:F:59:GLU:OE1	1:F:64:ARG:HD3	1.87	0.73
1:B:61:ASN:C	1:B:63:HIS:N	2.42	0.73
1:D:197:TRP:NE1	1:D:223:VAL:HG21	2.04	0.73
1:F:48:ASP:HB3	1:F:92:GLN:NE2	2.03	0.73
1:F:248:TRP:CH2	1:F:289:LEU:HD13	2.23	0.73
1:A:7:ASN:HA	1:A:10:LYS:HB2	1.71	0.73
1:B:374:ALA:C	1:B:376:ARG:N	2.45	0.73
1:F:46:TYR:CE2	1:F:53:VAL:HG21	2.24	0.73
1:B:196:THR:HG21	1:B:561:SER:HB2	1.70	0.73
1:C:478:PHE:CZ	1:C:519:ILE:HD12	2.23	0.73
1:D:466:MET:HE2	3:D:834:HOH:O	1.88	0.73
1:B:65:LEU:CD1	1:B:82:GLU:HG2	2.19	0.72
1:C:560:ARG:HD3	1:C:609:CYS:O	1.89	0.72
1:E:329:GLU:HA	1:E:344:HIS:HB3	1.69	0.72
1:E:456:ASN:HD22	1:E:457:HIS:H	0.80	0.72
1:C:491:ILE:HG12	1:D:175:LYS:HB2	1.71	0.72
1:D:120:TYR:O	1:D:124:ILE:HG13	1.89	0.72
1:F:60:LEU:HD21	1:F:109:ARG:HD2	1.69	0.72
1:B:456:ASN:ND2	1:B:457:HIS:N	2.25	0.72
1:D:48:ASP:N	1:D:92:GLN:HE21	1.87	0.72
1:F:120:TYR:O	1:F:124:ILE:HG13	1.89	0.72
1:B:262:TYR:CE1	1:B:268:PHE:CE1	2.76	0.72
1:C:69:ARG:HG2	1:C:264:TYR:CE2	2.25	0.72
1:C:120:TYR:O	1:C:124:ILE:HG13	1.89	0.72
1:F:247:HIS:HB2	1:F:250:ARG:HG2	1.69	0.72
1:D:486:GLU:HA	1:D:492:THR:HA	1.72	0.72
1:E:533:MET:H	1:E:533:MET:HE3	1.54	0.72
1:F:185:GLY:HA2	1:F:375:THR:CG2	2.18	0.72
1:A:354:GLN:HA	1:A:354:GLN:NE2	2.04	0.72
1:A:456:ASN:HD22	1:A:457:HIS:H	0.77	0.72
1:B:185:GLY:HA2	1:B:375:THR:HG23	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:LEU:HD13	1:B:498:ALA:HB2	1.69	0.72
1:B:406:LEU:HB2	1:B:639:VAL:HG11	1.71	0.72
1:C:5:THR:HG22	1:C:6:GLY:H	1.55	0.72
1:C:423:ILE:HD11	1:C:652:HIS:CE1	2.24	0.72
1:A:135:PRO:HB2	1:A:140:ILE:CD1	2.12	0.72
1:B:466:MET:O	1:B:466:MET:CG	2.36	0.72
1:C:368:MET:HE1	1:C:380:PHE:HD1	1.55	0.72
1:E:11:GLN:HG3	1:E:15:ASN:HD21	1.54	0.72
1:B:353:ARG:NE	1:B:369:GLU:OE2	2.21	0.72
1:A:42:ASP:O	1:A:45:ILE:HD11	1.90	0.72
1:A:522:SER:O	1:A:523:SER:C	2.33	0.72
1:B:69:ARG:N	1:B:112:GLU:OE2	2.22	0.72
1:E:162:LYS:O	1:E:446:VAL:HG21	1.90	0.72
1:E:367:VAL:O	1:E:373:THR:HG22	1.90	0.72
1:F:11:GLN:HG3	1:F:15:ASN:HD21	1.55	0.72
1:D:247:HIS:HB2	1:D:250:ARG:HG2	1.71	0.71
1:E:466:MET:HE2	3:E:834:HOH:O	1.89	0.71
1:A:125:HIS:CB	1:A:211:TYR:OH	2.37	0.71
1:A:427:ASP:HB3	1:A:567:ARG:HH12	1.54	0.71
1:E:256:PHE:CD1	1:E:256:PHE:C	2.66	0.71
1:A:441:GLU:H	1:A:443:ILE:HG22	1.54	0.71
1:B:132:ILE:HG22	1:B:133:VAL:N	2.05	0.71
1:B:466:MET:O	1:B:466:MET:HG3	1.89	0.71
1:D:634:ARG:NH2	1:F:64:ARG:HD2	2.02	0.71
1:B:313:ILE:HD11	1:B:323:LEU:HD13	1.72	0.71
1:B:592:ASP:O	1:B:619:ASN:ND2	2.16	0.71
1:A:169:SER:O	1:A:170:PHE:HB2	1.90	0.71
1:A:283:VAL:HG11	1:A:349:VAL:HB	1.72	0.71
1:B:374:ALA:C	1:B:376:ARG:H	1.98	0.71
1:C:313:ILE:C	1:C:313:ILE:HD12	2.15	0.71
1:D:421:GLU:CG	1:D:422:LEU:H	2.01	0.71
1:E:508:PHE:CE2	1:E:521:ARG:HD2	2.26	0.71
1:A:440:GLY:O	1:A:441:GLU:OE1	2.08	0.71
1:F:5:THR:HG22	1:F:6:GLY:H	1.54	0.71
1:A:260:THR:HG22	1:A:268:PHE:CE1	2.26	0.71
1:A:470:ASN:HD22	1:A:474:ARG:HD3	1.55	0.71
1:B:147:ASN:HD22	1:B:149:GLU:HB3	1.53	0.71
1:C:46:TYR:CE2	1:C:53:VAL:HG21	2.26	0.71
1:E:373:THR:O	1:E:376:ARG:HB2	1.91	0.71
1:F:508:PHE:CE2	1:F:521:ARG:HD2	2.25	0.71
1:A:244:ASP:CG	1:A:382:ARG:HD3	2.15	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:MET:HE1	1:B:380:PHE:CA	2.10	0.71
1:C:95:GLU:HA	1:C:128:LEU:HD21	1.72	0.71
1:F:69:ARG:HG2	1:F:264:TYR:CE2	2.26	0.71
1:C:237:SER:HA	1:C:574:LYS:HE3	1.73	0.71
1:F:256:PHE:CD1	1:F:256:PHE:C	2.68	0.71
1:A:408:PHE:HB3	1:A:641:ASN:OD1	1.91	0.71
1:B:386:TYR:O	1:B:387:MET:C	2.30	0.71
1:C:197:TRP:NE1	1:C:223:VAL:HG21	2.06	0.71
1:B:72:TYR:HD2	1:B:79:GLN:HB3	1.56	0.70
1:B:256:PHE:CD1	1:B:256:PHE:C	2.69	0.70
1:F:367:VAL:O	1:F:373:THR:HG22	1.91	0.70
1:B:301:ASP:OD2	1:B:393:LYS:NZ	2.24	0.70
1:B:412:VAL:HB	1:B:640:SER:HB2	1.73	0.70
1:C:634:ARG:HH21	1:E:64:ARG:HD2	1.54	0.70
1:D:203:PHE:HB3	1:D:329:GLU:OE2	1.91	0.70
1:D:373:THR:O	1:D:376:ARG:HB2	1.91	0.70
1:E:560:ARG:HH12	1:E:606:HIS:N	1.89	0.70
1:A:201:PHE:HB3	1:A:216:LYS:HD3	1.73	0.70
1:B:193:HIS:ND1	1:B:562:CYS:O	2.24	0.70
1:C:491:ILE:CD1	1:D:175:LYS:HB2	2.22	0.70
1:F:197:TRP:NE1	1:F:223:VAL:HG21	2.07	0.70
1:A:374:ALA:O	1:A:376:ARG:N	2.25	0.70
1:D:53:VAL:HG22	1:D:89:VAL:HG13	1.73	0.70
1:A:493:LEU:HB2	1:A:497:GLU:HB2	1.73	0.70
1:A:620:ARG:HG3	1:A:624:TYR:CG	2.26	0.70
1:B:547:VAL:C	1:B:549:GLY:H	1.99	0.70
1:C:367:VAL:O	1:C:373:THR:HG22	1.92	0.70
1:E:120:TYR:CD2	1:E:134:LEU:HD13	2.27	0.70
1:B:89:VAL:O	1:B:90:LEU:C	2.35	0.70
1:B:482:LEU:HB2	1:B:505:LEU:HD22	1.73	0.70
1:C:165:THR:HG22	1:C:449:ASN:CB	2.19	0.70
1:C:256:PHE:CD1	1:C:256:PHE:C	2.70	0.70
1:B:398:PHE:HB3	1:B:399:PRO:HD2	1.74	0.70
1:B:368:MET:CE	1:B:380:PHE:HA	2.11	0.70
1:D:161:GLN:OE1	1:E:443:ILE:HD13	1.92	0.70
1:A:40:LEU:HD21	1:A:54:GLU:HG3	1.73	0.69
1:A:200:ASP:C	1:A:202:PRO:HD3	2.17	0.69
1:A:466:MET:HG3	1:A:466:MET:O	1.91	0.69
1:B:8:ALA:HA	1:B:553:LEU:HD12	1.73	0.69
1:B:248:TRP:CZ2	1:B:289:LEU:HD13	2.27	0.69
1:B:278:GLU:H	1:B:354:GLN:HE22	1.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:517:GLU:HG2	1:F:518:THR:H	1.55	0.69
1:A:112:GLU:O	1:A:116:VAL:HG23	1.92	0.69
1:A:356:ASP:CG	1:A:359:GLY:HA2	2.17	0.69
1:B:461:THR:OG1	1:B:521:ARG:O	2.07	0.69
1:D:183:TYR:OH	1:D:234:GLU:OE1	2.10	0.69
1:B:193:HIS:O	1:B:197:TRP:N	2.18	0.69
1:A:183:TYR:OH	1:A:234:GLU:OE1	2.11	0.69
1:A:554:ASP:O	1:A:556:SER:N	2.26	0.69
1:E:197:TRP:NE1	1:E:223:VAL:HG21	2.07	0.69
1:F:243:VAL:O	1:F:385:LYS:HD3	1.92	0.69
1:F:313:ILE:C	1:F:313:ILE:HD12	2.16	0.69
1:F:373:THR:O	1:F:376:ARG:HB2	1.93	0.69
1:B:425:PHE:CE1	1:B:456:ASN:HB3	2.27	0.69
1:B:475:LEU:HB3	1:B:589:GLY:HA3	1.74	0.69
1:D:130:ASP:O	1:D:559:GLU:OE1	2.10	0.69
1:D:256:PHE:C	1:D:256:PHE:CD1	2.70	0.69
1:D:329:GLU:HA	1:D:344:HIS:HB3	1.74	0.69
1:E:69:ARG:HG2	1:E:264:TYR:CE2	2.27	0.69
1:F:120:TYR:CD2	1:F:134:LEU:HD13	2.27	0.69
1:F:592:ASP:C	1:F:594:GLU:H	2.00	0.69
1:A:47:ASN:ND2	1:A:94:LYS:HG2	2.07	0.69
1:A:641:ASN:ND2	1:A:641:ASN:N	2.36	0.69
1:C:272:PRO:CG	1:F:272:PRO:HG2	2.22	0.69
1:E:48:ASP:CB	1:E:92:GLN:HE21	2.05	0.69
1:A:447:GLU:HG3	3:A:726:HOH:O	1.93	0.69
1:B:8:ALA:HB1	1:B:546:ALA:HB3	1.74	0.69
1:B:66:LEU:HD13	1:B:111:ASN:ND2	2.07	0.69
1:B:218:GLU:HG2	1:B:321:ILE:CG2	2.21	0.69
1:C:466:MET:HE2	3:C:834:HOH:O	1.93	0.69
1:C:533:MET:H	1:C:533:MET:CE	2.06	0.69
1:D:177:ARG:CG	1:E:360:LYS:HB3	2.23	0.69
1:A:238:ASN:OD1	3:A:695:HOH:O	2.11	0.69
1:A:353:ARG:C	1:A:355:GLY:N	2.50	0.69
1:B:237:SER:HA	1:B:574:LYS:HE3	1.73	0.69
1:B:533:MET:HE3	1:B:533:MET:N	2.08	0.69
1:D:367:VAL:O	1:D:373:THR:HG22	1.92	0.69
1:A:111:ASN:C	1:A:111:ASN:OD1	2.36	0.69
1:D:7:ASN:C	1:D:9:GLN:N	2.50	0.69
1:D:454:ARG:HG3	1:D:567:ARG:NH1	2.08	0.69
1:C:368:MET:CE	1:C:380:PHE:HA	2.22	0.68
1:D:353:ARG:C	1:D:355:GLY:H	2.01	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LYS:HD3	1:A:446:VAL:HG11	1.74	0.68
1:B:5:THR:HG22	1:B:10:LYS:CD	2.23	0.68
1:B:255:GLY:H	1:B:273:ASP:HB3	1.58	0.68
1:D:592:ASP:C	1:D:594:GLU:H	2.01	0.68
1:B:20:LYS:N	1:B:435:ASN:ND2	2.41	0.68
1:B:89:VAL:O	1:B:91:ASN:N	2.27	0.68
1:D:260:THR:HG22	1:D:268:PHE:CE1	2.29	0.68
1:C:255:GLY:HA2	1:C:271:ARG:NH1	2.07	0.68
1:D:95:GLU:CG	1:D:96:TRP:H	2.06	0.68
1:E:533:MET:H	1:E:533:MET:CE	2.06	0.68
1:A:16:HIS:CD2	1:A:27:TYR:CE2	2.82	0.68
1:A:422:LEU:HB3	1:A:649:ILE:HG12	1.74	0.68
1:B:7:ASN:C	1:B:9:GLN:H	2.02	0.68
1:C:243:VAL:O	1:C:385:LYS:HD3	1.94	0.68
1:A:165:THR:HA	1:A:449:ASN:O	1.94	0.68
1:A:620:ARG:NE	3:A:839:HOH:O	2.26	0.68
1:C:120:TYR:CD2	1:C:134:LEU:HD13	2.29	0.68
1:D:159:MET:HE1	1:E:155:TYR:CD1	2.28	0.68
1:F:61:ASN:C	1:F:63:HIS:H	2.01	0.68
1:B:135:PRO:CB	1:B:140:ILE:HD11	2.23	0.68
1:A:255:GLY:HA2	1:A:271:ARG:HH12	1.59	0.68
1:A:300:ILE:HG12	1:A:324:LEU:HD11	1.75	0.68
1:B:120:TYR:O	1:B:124:ILE:HG13	1.93	0.68
1:B:195:VAL:HG22	1:B:196:THR:N	2.07	0.68
1:A:425:PHE:N	1:A:456:ASN:O	2.22	0.68
1:A:477:THR:HG23	1:A:509:PHE:CE1	2.29	0.68
1:E:46:TYR:CE2	1:E:53:VAL:HG21	2.29	0.68
1:A:374:ALA:C	1:A:376:ARG:N	2.51	0.67
1:B:588:ASP:OD1	1:B:588:ASP:C	2.36	0.67
1:D:413:VAL:HG23	1:D:466:MET:SD	2.34	0.67
1:B:247:HIS:HB2	1:B:250:ARG:HG2	1.76	0.67
1:B:260:THR:HG22	1:B:268:PHE:CE2	2.28	0.67
1:B:412:VAL:O	1:B:412:VAL:CG2	2.42	0.67
1:C:203:PHE:HB3	1:C:329:GLU:OE2	1.94	0.67
1:E:61:ASN:C	1:E:63:HIS:H	2.02	0.67
1:B:255:GLY:HA2	1:B:271:ARG:HH12	1.59	0.67
1:B:470:ASN:HD22	1:B:474:ARG:HG3	1.59	0.67
1:B:487:ASP:HB3	1:B:491:ILE:H	1.59	0.67
1:F:12:GLN:NE2	1:F:544:ASP:OD1	2.27	0.67
1:C:353:ARG:O	1:C:356:ASP:N	2.23	0.67
1:C:491:ILE:CG1	1:D:175:LYS:HB2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:VAL:O	1:D:385:LYS:HD3	1.94	0.67
1:A:522:SER:O	1:A:525:ASP:N	2.27	0.67
1:B:158:LYS:HG2	1:B:437:VAL:HG21	1.75	0.67
1:B:207:ASP:OD2	1:B:212:HIS:HB2	1.95	0.67
1:B:533:MET:H	1:B:533:MET:CE	2.07	0.67
1:C:305:ILE:HG13	1:C:315:ILE:HG21	1.77	0.67
1:A:19:ASP:O	1:A:20:LYS:C	2.37	0.67
1:C:37:PHE:CE2	1:C:101:SER:HB3	2.30	0.67
1:D:353:ARG:O	1:D:356:ASP:N	2.20	0.67
1:D:533:MET:H	1:D:533:MET:CE	2.07	0.67
1:E:412:VAL:HB	1:E:640:SER:HB2	1.75	0.67
1:F:456:ASN:HD22	1:F:457:HIS:H	0.80	0.67
1:A:368:MET:CE	1:A:380:PHE:CD2	2.78	0.67
1:B:487:ASP:HB3	1:B:490:GLY:H	1.60	0.67
1:C:329:GLU:HA	1:C:344:HIS:HB3	1.75	0.67
1:F:533:MET:H	1:F:533:MET:CE	2.07	0.67
1:C:454:ARG:HG3	1:C:567:ARG:NH1	2.10	0.67
1:A:185:GLY:O	1:A:375:THR:CG2	2.43	0.67
1:A:258:PRO:O	1:A:259:LEU:C	2.33	0.67
1:A:272:PRO:HG2	1:B:272:PRO:HG2	1.76	0.67
1:B:5:THR:CG2	1:B:10:LYS:HE3	2.25	0.67
1:B:488:ASN:N	1:B:490:GLY:H	1.93	0.67
1:F:7:ASN:C	1:F:9:GLN:N	2.50	0.67
1:F:72:TYR:CD2	1:F:79:GLN:HB3	2.29	0.67
1:A:468:ASN:HD22	1:A:514:SER:HA	1.59	0.66
1:B:95:GLU:HA	1:B:128:LEU:CD2	2.18	0.66
1:C:183:TYR:OH	1:C:234:GLU:OE1	2.10	0.66
1:F:37:PHE:CE2	1:F:101:SER:HB3	2.30	0.66
1:A:471:ASP:OD1	1:A:474:ARG:NH1	2.27	0.66
1:B:289:LEU:O	1:B:290:GLU:C	2.38	0.66
1:B:402:THR:O	1:B:405:ASN:HB2	1.94	0.66
1:C:313:ILE:CD1	1:C:323:LEU:HD13	2.24	0.66
1:C:576:GLU:CD	1:D:576:GLU:OE1	2.39	0.66
1:E:243:VAL:O	1:E:385:LYS:HD3	1.94	0.66
1:A:573:SER:OG	1:A:574:LYS:N	2.29	0.66
1:B:495:LEU:HD23	1:B:630:ILE:HG21	1.75	0.66
1:B:573:SER:HA	1:B:578:MET:CE	2.25	0.66
1:D:61:ASN:C	1:D:63:HIS:H	2.02	0.66
1:E:183:TYR:OH	1:E:234:GLU:OE1	2.11	0.66
1:F:72:TYR:HA	1:F:79:GLN:OE1	1.96	0.66
1:C:353:ARG:C	1:C:355:GLY:H	2.03	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:SER:HA	1:D:574:LYS:HE3	1.77	0.66
1:D:411:MET:HE2	3:D:834:HOH:O	1.95	0.66
1:A:411:MET:CE	1:A:512:VAL:CG1	2.70	0.66
1:A:491:ILE:CG1	1:F:175:LYS:HB2	2.26	0.66
1:A:353:ARG:O	1:A:354:GLN:C	2.36	0.66
1:C:61:ASN:C	1:C:63:HIS:H	2.01	0.66
1:C:269:PRO:HB3	1:C:363:LEU:HD23	1.76	0.66
1:A:491:ILE:HD11	1:F:175:LYS:HB2	1.78	0.66
1:B:86:LEU:HD22	1:B:90:LEU:HD22	1.78	0.66
1:C:373:THR:O	1:C:376:ARG:HB2	1.96	0.66
1:D:120:TYR:CD2	1:D:134:LEU:HD13	2.31	0.66
1:A:239:TRP:CH2	1:A:574:LYS:HD3	2.30	0.66
1:A:307:ASP:OD2	1:A:311:HIS:HB2	1.94	0.66
1:A:427:ASP:CB	1:A:567:ARG:HH12	2.09	0.66
1:B:60:LEU:HD21	1:B:109:ARG:HD2	1.77	0.66
1:E:37:PHE:CE2	1:E:101:SER:HB3	2.31	0.66
1:F:313:ILE:CD1	1:F:323:LEU:HD13	2.25	0.66
1:A:639:VAL:HG23	1:A:641:ASN:HD21	1.60	0.66
1:B:593:THR:C	1:B:595:GLY:H	2.04	0.66
1:D:368:MET:CE	1:D:380:PHE:HA	2.22	0.66
1:D:408:PHE:CD1	1:D:588:ASP:HB2	2.30	0.66
1:A:423:ILE:HD11	1:A:652:HIS:CD2	2.30	0.65
1:A:641:ASN:ND2	1:A:641:ASN:H	1.94	0.65
1:B:9:GLN:O	1:B:10:LYS:C	2.39	0.65
1:B:165:THR:HG22	1:B:449:ASN:HB2	1.78	0.65
1:B:293:GLU:O	1:B:297:HIS:HB2	1.96	0.65
1:C:592:ASP:C	1:C:594:GLU:H	2.01	0.65
1:E:86:LEU:HD12	1:E:110:MET:SD	2.36	0.65
1:F:305:ILE:HG13	1:F:315:ILE:HG21	1.77	0.65
1:A:60:LEU:HD21	1:A:109:ARG:HD2	1.78	0.65
1:A:89:VAL:O	1:A:91:ASN:N	2.29	0.65
1:A:585:ALA:HB1	1:A:642:ILE:HG12	1.78	0.65
1:B:76:ASN:ND2	1:B:79:GLN:H	1.91	0.65
1:E:7:ASN:C	1:E:9:GLN:N	2.48	0.65
1:E:11:GLN:HE22	1:E:133:VAL:H	1.44	0.65
1:F:368:MET:CE	1:F:380:PHE:HA	2.24	0.65
1:A:313:ILE:HD13	1:A:323:LEU:HD13	1.78	0.65
1:B:46:TYR:OH	1:B:53:VAL:HG11	1.96	0.65
1:B:239:TRP:CH2	1:B:574:LYS:CD	2.78	0.65
1:C:65:LEU:HD12	1:C:82:GLU:HG2	1.78	0.65
1:D:65:LEU:HD12	1:D:82:GLU:HG2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:ILE:CD1	1:D:323:LEU:HD13	2.25	0.65
1:A:256:PHE:C	1:A:256:PHE:HD1	1.99	0.65
1:A:416:VAL:HG22	1:A:645:VAL:CG1	2.23	0.65
1:B:190:MET:O	1:B:191:ASN:C	2.37	0.65
1:B:313:ILE:HD11	1:B:323:LEU:CD1	2.27	0.65
1:C:330:SER:OG	1:C:341:GLY:O	2.09	0.65
1:D:86:LEU:HD12	1:D:110:MET:SD	2.37	0.65
1:E:368:MET:CE	1:E:380:PHE:HA	2.24	0.65
1:F:237:SER:HA	1:F:574:LYS:HE3	1.78	0.65
1:C:260:THR:HG22	1:C:268:PHE:CE1	2.31	0.65
1:D:269:PRO:HB3	1:D:363:LEU:HD23	1.78	0.65
1:F:553:LEU:CD2	1:F:555:LEU:HD13	2.27	0.65
1:A:133:VAL:HG21	1:A:555:LEU:HD13	1.79	0.65
1:A:375:THR:HB	3:A:747:HOH:O	1.95	0.65
1:B:187:ASP:OD1	1:B:189:GLY:N	2.28	0.65
1:B:307:ASP:C	1:B:307:ASP:OD1	2.37	0.65
1:C:462:TYR:O	1:C:520:GLU:HA	1.96	0.65
1:E:65:LEU:HD12	1:E:82:GLU:HG2	1.79	0.65
1:B:392:LYS:O	1:B:396:ASP:HB2	1.97	0.65
1:E:330:SER:OG	1:E:341:GLY:O	2.12	0.65
1:F:65:LEU:HD12	1:F:82:GLU:HG2	1.78	0.65
1:A:493:LEU:HA	1:A:497:GLU:OE1	1.97	0.65
1:B:480:ILE:HG12	1:B:584:VAL:HG22	1.79	0.65
1:F:17:LEU:HD21	1:F:103:ALA:O	1.97	0.65
1:F:165:THR:CG2	1:F:449:ASN:HB2	2.22	0.65
1:F:168:VAL:CG2	1:F:452:VAL:HG12	2.26	0.65
1:F:513:PRO:HG3	1:F:517:GLU:OE2	1.97	0.65
1:A:269:PRO:HB3	1:A:363:LEU:HD23	1.79	0.65
1:A:353:ARG:O	1:A:355:GLY:N	2.30	0.65
1:A:412:VAL:CG1	1:A:467:SER:O	2.39	0.65
1:A:570:LEU:HB2	3:A:858:HOH:O	1.96	0.65
1:B:86:LEU:CD2	1:B:90:LEU:HD22	2.27	0.65
1:D:434:ILE:HD11	1:D:447:GLU:HA	1.79	0.65
1:D:513:PRO:O	1:D:514:SER:HB3	1.96	0.65
1:F:29:ASP:O	1:F:33:ILE:HG13	1.96	0.65
1:F:195:VAL:HG11	1:F:372:GLU:HB3	1.78	0.65
1:A:408:PHE:N	1:A:641:ASN:OD1	2.29	0.64
1:B:68:GLN:HB3	1:B:69:ARG:NH1	2.12	0.64
1:B:408:PHE:N	1:B:641:ASN:OD1	2.29	0.64
1:B:412:VAL:O	1:B:412:VAL:HG22	1.97	0.64
1:D:513:PRO:O	1:D:514:SER:CB	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:VAL:CG2	1:A:452:VAL:HG12	2.26	0.64
1:A:260:THR:C	1:A:268:PHE:HD1	2.05	0.64
1:C:491:ILE:HG12	1:D:175:LYS:CB	2.27	0.64
1:A:464:ILE:HG22	1:A:464:ILE:O	1.96	0.64
1:B:575:PRO:HD2	1:B:576:GLU:HG3	1.78	0.64
1:E:168:VAL:CG2	1:E:452:VAL:HG12	2.25	0.64
1:B:197:TRP:NE1	1:B:223:VAL:HG21	2.12	0.64
1:C:560:ARG:HG2	1:C:609:CYS:CB	2.27	0.64
1:D:17:LEU:HD21	1:D:103:ALA:O	1.96	0.64
1:D:95:GLU:HA	1:D:128:LEU:HD21	1.80	0.64
1:D:478:PHE:CZ	1:D:519:ILE:HD12	2.32	0.64
1:F:330:SER:HB2	1:F:342:SER:OG	1.98	0.64
1:B:163:PRO:HG3	1:B:446:VAL:HG23	1.79	0.64
1:C:17:LEU:HD21	1:C:103:ALA:O	1.97	0.64
1:C:86:LEU:HD12	1:C:110:MET:SD	2.37	0.64
1:E:305:ILE:HG13	1:E:315:ILE:HG21	1.79	0.64
1:A:639:VAL:CG2	1:A:641:ASN:HD21	2.11	0.64
1:C:560:ARG:CG	1:C:609:CYS:HB3	2.28	0.64
1:E:5:THR:HG22	1:E:6:GLY:N	2.10	0.64
1:E:17:LEU:HD21	1:E:103:ALA:O	1.98	0.64
1:E:408:PHE:HB3	1:E:641:ASN:OD1	1.97	0.64
1:E:425:PHE:CE1	1:E:456:ASN:HB3	2.33	0.64
1:C:22:TYR:C	1:C:69:ARG:HH21	2.05	0.64
1:C:29:ASP:O	1:C:33:ILE:HG13	1.97	0.64
1:C:86:LEU:CD2	1:C:90:LEU:HD22	2.28	0.64
1:C:380:PHE:HE1	1:C:384:HIS:CE1	2.15	0.64
1:C:578:MET:HE3	1:C:580:PHE:HZ	1.62	0.64
1:D:53:VAL:CG2	1:D:89:VAL:HG13	2.27	0.64
1:D:165:THR:CG2	1:D:449:ASN:HB2	2.17	0.64
1:D:191:ASN:O	1:D:195:VAL:HG13	1.98	0.64
1:D:353:ARG:C	1:D:355:GLY:N	2.53	0.64
1:E:269:PRO:HB3	1:E:363:LEU:CD2	2.28	0.64
1:E:313:ILE:CD1	1:E:323:LEU:HD13	2.27	0.64
1:E:592:ASP:C	1:E:594:GLU:H	2.05	0.64
1:A:455:LEU:HG	1:A:456:ASN:H	1.62	0.64
1:A:633:GLU:O	1:A:635:VAL:N	2.31	0.64
1:A:639:VAL:CG2	1:A:641:ASN:ND2	2.61	0.64
1:C:191:ASN:O	1:C:195:VAL:HG13	1.97	0.64
1:C:244:ASP:O	1:C:382:ARG:HG3	1.98	0.64
1:F:86:LEU:HD12	1:F:110:MET:SD	2.38	0.64
1:A:269:PRO:O	3:A:708:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:PRO:HB2	1:C:140:ILE:HD11	1.80	0.64
1:C:491:ILE:HD11	1:D:175:LYS:HB2	1.80	0.64
1:D:244:ASP:O	1:D:382:ARG:HG3	1.98	0.64
1:D:466:MET:HE1	1:D:586:VAL:HG11	1.78	0.64
1:E:195:VAL:HG11	1:E:372:GLU:HB3	1.80	0.64
1:F:252:ILE:HB	1:F:275:ILE:HG22	1.79	0.64
1:F:255:GLY:HA2	1:F:271:ARG:NH1	2.13	0.64
1:E:468:ASN:HD21	1:E:474:ARG:HG2	1.61	0.64
1:F:68:GLN:HB3	1:F:69:ARG:NH1	2.13	0.64
1:F:269:PRO:HB3	1:F:363:LEU:CD2	2.26	0.64
1:F:454:ARG:HG3	1:F:567:ARG:NH1	2.13	0.64
1:F:575:PRO:HD2	1:F:576:GLU:HG3	1.80	0.64
1:F:244:ASP:O	1:F:382:ARG:HG3	1.98	0.63
1:A:456:ASN:ND2	1:A:457:HIS:N	2.28	0.63
1:B:82:GLU:O	1:B:85:MET:N	2.27	0.63
1:B:220:PHE:CZ	1:B:329:GLU:HB2	2.34	0.63
1:B:477:THR:HB	1:B:479:ARG:NH1	2.14	0.63
1:E:68:GLN:HB3	1:E:69:ARG:NH1	2.13	0.63
1:A:160:THR:C	1:A:161:GLN:HG3	2.23	0.63
1:A:278:GLU:H	1:A:354:GLN:HE22	1.46	0.63
1:B:72:TYR:CD2	1:B:79:GLN:HB3	2.33	0.63
1:B:316:ARG:HG3	1:B:398:PHE:CE1	2.33	0.63
1:B:423:ILE:HD11	1:B:652:HIS:CD2	2.33	0.63
1:D:40:LEU:HD13	1:D:57:MET:HG3	1.80	0.63
1:D:207:ASP:OD2	1:D:212:HIS:HB2	1.99	0.63
1:F:8:ALA:HB1	1:F:546:ALA:HB3	1.80	0.63
1:F:86:LEU:CD2	1:F:90:LEU:HD22	2.29	0.63
1:F:165:THR:HA	1:F:449:ASN:O	1.97	0.63
1:F:425:PHE:CE1	1:F:456:ASN:HB3	2.33	0.63
1:B:43:THR:HG23	1:B:49:HIS:C	2.24	0.63
1:B:56:LEU:HD11	1:B:65:LEU:HD21	1.80	0.63
1:B:620:ARG:HG3	1:B:624:TYR:CG	2.33	0.63
1:D:300:ILE:HG12	1:D:324:LEU:HD11	1.80	0.63
1:A:281:ASP:OD2	1:A:358:HIS:HB3	1.99	0.63
1:A:592:ASP:C	1:A:594:GLU:H	2.06	0.63
1:B:300:ILE:HD11	1:B:390:ILE:HG22	1.79	0.63
1:B:353:ARG:C	1:B:355:GLY:N	2.55	0.63
1:B:456:ASN:HD22	1:B:457:HIS:H	0.69	0.63
1:D:634:ARG:HE	1:F:64:ARG:CZ	2.11	0.63
1:A:85:MET:HB3	3:A:826:HOH:O	1.98	0.63
1:A:248:TRP:CZ2	1:A:289:LEU:HD13	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:SER:OG	1:A:267:GLU:HG2	1.98	0.63
1:B:573:SER:HA	1:B:578:MET:HE2	1.79	0.63
1:C:414:ASN:ND2	1:C:466:MET:HA	2.11	0.63
1:A:51:ALA:O	1:A:52:ALA:C	2.37	0.63
1:A:329:GLU:HA	1:A:344:HIS:HB3	1.80	0.63
1:A:418:ILE:CD1	1:A:462:TYR:CD1	2.81	0.63
1:A:504:GLU:OE1	3:A:791:HOH:O	2.15	0.63
1:A:633:GLU:C	1:A:635:VAL:N	2.52	0.63
1:C:68:GLN:HB3	1:C:69:ARG:NH1	2.13	0.63
1:A:533:MET:HG3	3:A:781:HOH:O	1.97	0.63
1:B:166:PHE:O	1:B:451:ARG:N	2.28	0.63
1:D:578:MET:HE3	1:D:580:PHE:HZ	1.63	0.63
1:B:211:TYR:CE2	1:B:612:HIS:HA	2.34	0.63
1:C:300:ILE:HG12	1:C:324:LEU:HD11	1.80	0.63
1:E:255:GLY:HA2	1:E:271:ARG:NH1	2.13	0.63
1:A:106:PHE:O	1:A:107:ARG:C	2.40	0.62
1:A:506:ASP:OD2	1:A:521:ARG:NE	2.25	0.62
1:C:72:TYR:HA	1:C:79:GLN:OE1	1.99	0.62
1:C:425:PHE:CE1	1:C:456:ASN:HB3	2.34	0.62
1:D:68:GLN:HB3	1:D:69:ARG:NH1	2.14	0.62
1:E:423:ILE:CD1	1:E:652:HIS:CE1	2.82	0.62
1:E:620:ARG:HG3	1:E:624:TYR:CG	2.33	0.62
1:A:248:TRP:CZ3	1:A:289:LEU:HD13	2.34	0.62
1:B:188:ILE:O	1:B:192:ILE:HG12	1.99	0.62
1:E:169:SER:O	1:E:170:PHE:HB2	1.98	0.62
1:A:630:ILE:HD13	1:A:636:ILE:HG12	1.79	0.62
1:D:425:PHE:CE1	1:D:456:ASN:HB3	2.34	0.62
1:F:300:ILE:HG12	1:F:324:LEU:HD11	1.80	0.62
1:A:97:TYR:O	1:A:101:SER:HB2	2.00	0.62
1:A:611:VAL:HG12	1:A:612:HIS:CD2	2.34	0.62
1:B:338:GLN:HE22	1:F:316:ARG:HH21	1.45	0.62
1:C:620:ARG:HG3	1:C:624:TYR:CG	2.34	0.62
1:E:244:ASP:O	1:E:382:ARG:HG3	1.99	0.62
1:C:195:VAL:HG11	1:C:372:GLU:HB3	1.82	0.62
1:D:419:ASP:HB3	1:D:463:LYS:HD2	1.82	0.62
1:E:203:PHE:HB3	1:E:329:GLU:OE2	1.99	0.62
1:F:207:ASP:OD2	1:F:212:HIS:HB2	2.00	0.62
1:F:423:ILE:CD1	1:F:652:HIS:CE1	2.83	0.62
1:D:255:GLY:HA2	1:D:271:ARG:NH1	2.14	0.62
1:D:316:ARG:HH21	1:F:338:GLN:HE22	1.47	0.62
1:E:454:ARG:HG3	1:E:567:ARG:NH1	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:533:MET:HB3	1:F:534:PRO:HD2	1.82	0.62
1:A:530:VAL:HG21	1:A:561:SER:HB3	1.81	0.62
1:B:69:ARG:NH1	1:B:69:ARG:HG3	2.15	0.62
1:F:620:ARG:HG3	1:F:624:TYR:CG	2.34	0.62
1:A:95:GLU:HG3	1:A:96:TRP:N	2.15	0.62
1:A:262:TYR:CE1	1:A:268:PHE:CE2	2.87	0.62
1:B:252:ILE:HD11	1:B:277:PHE:CD1	2.34	0.62
1:B:522:SER:C	1:B:524:LYS:N	2.54	0.62
1:D:403:HIS:NE2	1:D:407:GLU:OE1	2.33	0.62
1:E:487:ASP:HB3	1:E:491:ILE:H	1.65	0.62
1:A:40:LEU:HD11	1:A:54:GLU:HA	1.82	0.62
1:A:592:ASP:O	1:A:619:ASN:ND2	2.33	0.62
1:B:56:LEU:CD2	1:B:110:MET:HE3	2.27	0.62
1:B:141:THR:O	1:B:141:THR:OG1	2.07	0.62
1:B:256:PHE:CE2	1:B:377:ASP:HA	2.35	0.62
1:B:461:THR:OG1	1:B:462:TYR:N	2.33	0.62
1:F:183:TYR:OH	1:F:234:GLU:OE1	2.11	0.62
1:A:177:ARG:HD3	1:A:179:GLN:HG3	1.82	0.61
1:A:292:THR:OG1	3:A:787:HOH:O	2.15	0.61
1:A:392:LYS:O	1:A:396:ASP:HB2	2.00	0.61
1:A:560:ARG:HH21	1:A:606:HIS:N	1.97	0.61
1:B:37:PHE:CZ	1:B:101:SER:HB3	2.35	0.61
1:B:43:THR:HG23	1:B:49:HIS:O	2.00	0.61
1:D:411:MET:HE3	1:D:468:ASN:CG	2.24	0.61
1:E:207:ASP:OD2	1:E:212:HIS:HB2	2.00	0.61
1:C:207:ASP:OD2	1:C:212:HIS:HB2	2.00	0.61
1:E:611:VAL:HG12	1:E:612:HIS:HD2	1.64	0.61
1:F:367:VAL:HA	1:F:373:THR:CG2	2.31	0.61
1:A:634:ARG:HH21	1:C:64:ARG:HD2	1.65	0.61
1:B:300:ILE:HG12	1:B:324:LEU:HD11	1.81	0.61
1:D:330:SER:HB2	1:D:342:SER:OG	1.99	0.61
1:D:392:LYS:O	1:D:396:ASP:HB2	1.99	0.61
1:E:300:ILE:HG12	1:E:324:LEU:HD11	1.80	0.61
1:A:177:ARG:NH1	1:A:179:GLN:HG3	2.15	0.61
1:B:168:VAL:CG2	1:B:452:VAL:HG12	2.25	0.61
1:B:416:VAL:CG2	1:B:645:VAL:CG1	2.75	0.61
1:B:610:GLY:HA2	1:B:614:GLU:HB2	1.82	0.61
1:E:462:TYR:O	1:E:520:GLU:HA	2.01	0.61
1:E:611:VAL:HG12	1:E:612:HIS:CD2	2.36	0.61
1:B:220:PHE:CE2	1:B:329:GLU:HB2	2.35	0.61
1:B:548:ASN:HD22	1:B:548:ASN:N	1.89	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:ALA:HA	1:D:553:LEU:HD12	1.82	0.61
1:B:177:ARG:NH1	1:B:179:GLN:HG3	2.14	0.61
1:B:317:GLN:HB2	1:B:318:PRO:HD2	1.83	0.61
1:D:168:VAL:CG2	1:D:452:VAL:HG12	2.30	0.61
1:F:412:VAL:HB	1:F:640:SER:HB2	1.82	0.61
1:E:533:MET:HB3	1:E:534:PRO:HD2	1.83	0.61
1:A:60:LEU:HD22	1:A:106:PHE:HE1	1.66	0.61
1:A:180:ARG:HG3	1:A:180:ARG:O	1.99	0.61
1:D:155:TYR:O	1:D:159:MET:HG3	2.01	0.61
1:F:46:TYR:CZ	1:F:53:VAL:HG21	2.36	0.61
1:C:69:ARG:NH1	1:C:69:ARG:HG3	2.14	0.61
1:C:168:VAL:CG2	1:C:452:VAL:HG12	2.26	0.61
1:E:252:ILE:HB	1:E:275:ILE:HG22	1.81	0.61
1:A:7:ASN:O	1:A:11:GLN:N	2.31	0.61
1:A:59:GLU:OE1	1:A:64:ARG:HD3	2.01	0.61
1:A:408:PHE:CE2	1:A:411:MET:HG2	2.36	0.61
1:A:423:ILE:CD1	1:A:652:HIS:CE1	2.79	0.61
1:A:446:VAL:HG13	1:A:446:VAL:O	2.01	0.61
1:A:620:ARG:CZ	3:A:839:HOH:O	2.49	0.61
1:D:195:VAL:HG11	1:D:372:GLU:HB3	1.83	0.61
1:E:69:ARG:NH1	1:E:69:ARG:HG3	2.16	0.61
1:F:169:SER:O	1:F:170:PHE:HB2	1.99	0.61
1:F:547:VAL:HG23	1:F:548:ASN:H	1.65	0.61
1:A:456:ASN:ND2	1:A:457:HIS:O	2.34	0.60
1:A:512:VAL:HG13	1:A:513:PRO:HD2	1.81	0.60
1:B:143:HIS:CE1	1:B:151:ILE:CG2	2.79	0.60
1:B:237:SER:OG	1:B:578:MET:HE1	2.01	0.60
1:C:412:VAL:HB	1:C:640:SER:HB2	1.82	0.60
1:E:86:LEU:CD2	1:E:90:LEU:HD22	2.31	0.60
1:E:158:LYS:HD3	1:E:446:VAL:CG1	2.31	0.60
1:F:468:ASN:HB3	1:F:514:SER:HA	1.84	0.60
1:B:555:LEU:O	1:B:556:SER:C	2.44	0.60
1:C:367:VAL:HA	1:C:373:THR:CG2	2.31	0.60
1:C:533:MET:HB3	1:C:534:PRO:HD2	1.83	0.60
1:D:367:VAL:HA	1:D:373:THR:CG2	2.30	0.60
1:E:330:SER:HB2	1:E:342:SER:OG	2.01	0.60
1:A:477:THR:HG23	1:A:509:PHE:HD1	1.66	0.60
1:B:413:VAL:HG12	1:B:643:LYS:HG3	1.82	0.60
1:C:399:PRO:O	1:C:628:ARG:HD3	2.01	0.60
1:C:575:PRO:HD2	1:C:576:GLU:HG3	1.82	0.60
1:D:135:PRO:HB2	1:D:140:ILE:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:GLN:HA	1:D:354:GLN:NE2	2.16	0.60
1:D:533:MET:HB3	1:D:534:PRO:HD2	1.84	0.60
1:E:237:SER:HA	1:E:574:LYS:HE3	1.81	0.60
1:E:293:GLU:HG3	3:E:861:HOH:O	2.01	0.60
1:E:406:LEU:HB2	1:E:639:VAL:HG11	1.83	0.60
1:A:508:PHE:CE2	1:A:521:ARG:HD2	2.35	0.60
1:B:175:LYS:O	1:B:176:ASN:CB	2.49	0.60
1:B:222:TRP:CD1	1:B:622:LEU:HD23	2.36	0.60
1:C:46:TYR:CZ	1:C:53:VAL:HG21	2.36	0.60
1:C:576:GLU:OE1	1:D:576:GLU:CD	2.44	0.60
1:D:69:ARG:NH1	1:D:69:ARG:HG3	2.16	0.60
1:D:177:ARG:HD3	1:D:179:GLN:HG3	1.83	0.60
1:F:22:TYR:C	1:F:69:ARG:HH21	2.09	0.60
1:F:591:LYS:NZ	1:F:591:LYS:HB2	2.16	0.60
1:A:243:VAL:O	1:A:244:ASP:C	2.42	0.60
1:B:285:HIS:HB2	1:B:288:ASP:CG	2.26	0.60
1:B:413:VAL:HG12	1:B:643:LYS:HG2	1.82	0.60
1:C:293:GLU:HG3	3:C:861:HOH:O	2.01	0.60
1:D:48:ASP:OD2	1:D:92:GLN:HG3	2.01	0.60
1:D:72:TYR:HA	1:D:79:GLN:OE1	2.02	0.60
1:D:508:PHE:CE2	1:D:521:ARG:CD	2.84	0.60
1:B:553:LEU:O	1:B:554:ASP:HB2	2.02	0.60
1:C:48:ASP:HB3	1:C:92:GLN:HE21	1.65	0.60
1:F:69:ARG:NH1	1:F:69:ARG:HG3	2.16	0.60
1:F:392:LYS:O	1:F:396:ASP:HB2	2.01	0.60
1:F:399:PRO:O	1:F:628:ARG:HD3	2.01	0.60
1:A:256:PHE:HD1	1:A:256:PHE:O	1.84	0.60
1:B:593:THR:O	1:B:595:GLY:N	2.34	0.60
1:C:158:LYS:HD3	1:C:446:VAL:CG1	2.32	0.60
1:C:353:ARG:NE	1:C:369:GLU:OE2	2.35	0.60
1:E:57:MET:HE3	1:E:61:ASN:HD21	1.67	0.60
1:E:367:VAL:HA	1:E:373:THR:CG2	2.30	0.60
1:F:553:LEU:HD22	1:F:555:LEU:HD13	1.83	0.60
1:F:560:ARG:HH12	1:F:606:HIS:N	2.00	0.60
1:A:281:ASP:OD2	1:A:358:HIS:HA	2.02	0.60
1:A:594:GLU:O	1:A:594:GLU:CG	2.46	0.60
1:E:392:LYS:O	1:E:396:ASP:HB2	2.02	0.60
1:E:399:PRO:O	1:E:628:ARG:HD3	2.02	0.60
1:F:408:PHE:HB3	1:F:641:ASN:OD1	2.02	0.60
1:F:479:ARG:NH1	1:F:587:THR:OG1	2.35	0.60
1:C:408:PHE:HB3	1:C:641:ASN:OD1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ARG:O	1:D:78:ARG:NH1	2.35	0.60
1:D:316:ARG:HH21	1:F:338:GLN:NE2	1.99	0.60
1:D:366:GLY:H	1:D:369:GLU:HG3	1.67	0.60
1:E:8:ALA:HA	1:E:553:LEU:HD12	1.83	0.60
1:E:191:ASN:O	1:E:195:VAL:HG13	2.02	0.60
1:F:611:VAL:HG12	1:F:612:HIS:HD2	1.67	0.60
1:B:113:GLY:O	1:B:114:GLU:C	2.38	0.60
1:B:143:HIS:HE1	1:B:151:ILE:HG21	1.62	0.60
1:B:487:ASP:HB3	1:B:490:GLY:N	2.17	0.60
1:E:160:THR:O	1:E:161:GLN:HB2	2.02	0.60
1:E:366:GLY:H	1:E:369:GLU:HG3	1.67	0.60
1:F:366:GLY:H	1:F:369:GLU:HG3	1.66	0.60
1:A:43:THR:HG22	1:A:43:THR:O	2.02	0.59
1:A:425:PHE:CE1	1:A:456:ASN:HB3	2.37	0.59
1:B:60:LEU:CD1	1:B:109:ARG:HG3	2.30	0.59
1:C:18:LEU:CD2	1:C:119:LEU:HD23	2.32	0.59
1:C:392:LYS:O	1:C:396:ASP:HB2	2.02	0.59
1:C:591:LYS:HB2	1:C:591:LYS:NZ	2.17	0.59
1:D:18:LEU:CD2	1:D:119:LEU:HD23	2.32	0.59
1:D:305:ILE:HG13	1:D:315:ILE:HG21	1.83	0.59
1:E:72:TYR:HA	1:E:79:GLN:OE1	2.01	0.59
1:F:11:GLN:HE22	1:F:133:VAL:H	1.50	0.59
1:F:293:GLU:HG3	3:F:861:HOH:O	2.01	0.59
1:A:349:VAL:HG21	3:A:756:HOH:O	2.01	0.59
1:B:146:THR:HG21	1:B:433:LEU:HD21	1.84	0.59
1:B:218:GLU:HG2	1:B:321:ILE:HG23	1.84	0.59
1:D:620:ARG:HG3	1:D:624:TYR:CG	2.37	0.59
1:D:632:ASP:OD1	1:D:635:VAL:HG23	2.02	0.59
1:A:29:ASP:O	1:A:33:ILE:HG13	2.03	0.59
1:A:421:GLU:O	1:A:422:LEU:C	2.45	0.59
1:C:423:ILE:CD1	1:C:652:HIS:CE1	2.85	0.59
1:D:317:GLN:HB2	1:D:318:PRO:CD	2.30	0.59
1:E:18:LEU:CD2	1:E:119:LEU:HD23	2.32	0.59
1:E:479:ARG:NH1	1:E:587:THR:OG1	2.35	0.59
1:E:543:ALA:HA	1:E:553:LEU:HD11	1.83	0.59
1:F:135:PRO:HB2	1:F:140:ILE:HD11	1.83	0.59
1:B:59:GLU:HG3	1:B:85:MET:HE1	1.84	0.59
1:B:89:VAL:C	1:B:91:ASN:N	2.60	0.59
1:C:165:THR:CG2	1:C:449:ASN:HB2	2.22	0.59
1:C:353:ARG:C	1:C:355:GLY:N	2.56	0.59
1:D:261:SER:OG	1:D:267:GLU:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:ARG:O	1:E:78:ARG:NH1	2.35	0.59
1:E:414:ASN:ND2	1:E:466:MET:HA	2.17	0.59
1:E:573:SER:HA	1:E:578:MET:HE2	1.84	0.59
1:A:57:MET:O	1:A:60:LEU:HB3	2.03	0.59
1:A:178:GLU:HG3	1:A:178:GLU:O	2.02	0.59
1:A:641:ASN:HD22	1:A:641:ASN:N	2.00	0.59
1:B:487:ASP:CB	1:B:491:ILE:HG13	2.32	0.59
1:B:555:LEU:O	1:B:557:ALA:N	2.36	0.59
1:C:169:SER:O	1:C:170:PHE:HB2	2.02	0.59
1:C:368:MET:HE1	1:C:380:PHE:CD1	2.37	0.59
1:D:69:ARG:N	1:D:112:GLU:OE2	2.32	0.59
1:D:89:VAL:O	1:D:92:GLN:N	2.35	0.59
1:F:191:ASN:O	1:F:195:VAL:HG13	2.01	0.59
1:B:177:ARG:HH11	1:B:179:GLN:HG3	1.67	0.59
1:C:155:TYR:O	1:C:159:MET:HG3	2.02	0.59
1:C:330:SER:HB2	1:C:342:SER:OG	2.02	0.59
1:D:423:ILE:CD1	1:D:652:HIS:CE1	2.85	0.59
1:D:493:LEU:HA	1:D:497:GLU:OE1	2.03	0.59
1:F:89:VAL:O	1:F:92:GLN:N	2.35	0.59
1:B:185:GLY:O	1:B:375:THR:CG2	2.44	0.59
1:B:418:ILE:HD11	1:B:462:TYR:CE1	2.37	0.59
1:D:8:ALA:HB2	1:D:553:LEU:HB2	1.83	0.59
1:D:56:LEU:CD1	1:D:110:MET:HE3	2.29	0.59
1:D:72:TYR:CD2	1:D:79:GLN:HB3	2.38	0.59
1:D:177:ARG:CD	1:E:360:LYS:HB3	2.33	0.59
1:D:482:LEU:HB2	1:D:505:LEU:HD22	1.84	0.59
1:F:25:THR:HG23	1:F:107:ARG:CZ	2.33	0.59
1:F:48:ASP:HB3	1:F:92:GLN:HE21	1.65	0.59
1:B:305:ILE:CD1	1:B:315:ILE:HG21	2.31	0.59
1:B:380:PHE:CE1	1:B:384:HIS:CE1	2.91	0.59
1:C:89:VAL:O	1:C:92:GLN:N	2.35	0.59
1:F:410:GLY:HA3	1:F:470:ASN:ND2	2.17	0.59
1:A:21:ILE:O	1:A:21:ILE:CG1	2.45	0.59
1:A:67:GLU:O	1:A:111:ASN:HB2	2.02	0.59
1:A:454:ARG:HG3	1:A:567:ARG:NH1	2.18	0.59
1:B:25:THR:HG23	1:B:107:ARG:CZ	2.32	0.59
1:B:107:ARG:HD3	1:B:108:GLU:OE1	2.03	0.59
1:B:632:ASP:OD1	1:B:635:VAL:HG23	2.03	0.59
1:C:255:GLY:HA2	1:C:271:ARG:HH12	1.68	0.59
1:C:366:GLY:H	1:C:369:GLU:HG3	1.68	0.59
1:D:508:PHE:CD2	1:D:521:ARG:HD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:458:ASN:O	1:E:459:GLU:C	2.46	0.59
1:E:482:LEU:HB2	1:E:505:LEU:HD22	1.85	0.59
1:F:56:LEU:CD1	1:F:110:MET:HE3	2.29	0.59
1:D:169:SER:O	1:D:170:PHE:HB2	2.02	0.59
1:D:222:TRP:CZ2	1:D:226:GLN:NE2	2.71	0.59
1:D:399:PRO:O	1:D:628:ARG:HD3	2.01	0.59
1:E:61:ASN:C	1:E:63:HIS:N	2.61	0.59
1:E:69:ARG:N	1:E:112:GLU:OE2	2.32	0.59
1:F:57:MET:HE3	1:F:61:ASN:HD21	1.68	0.59
1:F:281:ASP:OD2	1:F:358:HIS:HA	2.03	0.59
1:B:148:SER:CB	1:B:259:LEU:O	2.51	0.58
1:B:515:GLY:O	1:B:516:PRO:C	2.46	0.58
1:C:43:THR:CG2	1:C:49:HIS:C	2.75	0.58
1:E:135:PRO:HB2	1:E:140:ILE:HD11	1.84	0.58
1:C:479:ARG:NH1	1:C:587:THR:OG1	2.36	0.58
1:D:11:GLN:HE22	1:D:133:VAL:H	1.48	0.58
1:D:46:TYR:CE1	1:D:53:VAL:HG21	2.37	0.58
1:D:86:LEU:CD2	1:D:90:LEU:HD22	2.33	0.58
1:D:159:MET:HE1	1:E:155:TYR:CG	2.37	0.58
1:D:177:ARG:NH1	1:E:361:PHE:HE1	2.01	0.58
1:D:555:LEU:O	1:D:557:ALA:N	2.36	0.58
1:D:611:VAL:HG12	1:D:612:HIS:HD2	1.67	0.58
1:F:203:PHE:HB3	1:F:329:GLU:OE2	2.03	0.58
1:F:632:ASP:OD1	1:F:635:VAL:HG23	2.03	0.58
1:C:368:MET:CE	1:C:380:PHE:HD1	2.17	0.58
1:F:74:LEU:HG	1:F:74:LEU:O	2.03	0.58
1:F:86:LEU:HD22	1:F:90:LEU:HD22	1.86	0.58
1:F:482:LEU:HB2	1:F:505:LEU:HD22	1.85	0.58
1:A:18:LEU:HD21	1:A:119:LEU:HD23	1.85	0.58
1:A:155:TYR:CG	1:B:159:MET:CE	2.82	0.58
1:A:158:LYS:HD3	1:A:446:VAL:CG1	2.32	0.58
1:A:414:ASN:HD21	1:A:467:SER:H	1.51	0.58
1:A:495:LEU:HD13	1:A:583:TYR:CZ	2.38	0.58
1:A:568:MET:O	1:A:569:LEU:C	2.44	0.58
1:B:60:LEU:HD22	1:B:106:PHE:HE1	1.68	0.58
1:C:8:ALA:HA	1:C:553:LEU:HD12	1.86	0.58
1:D:22:TYR:C	1:D:69:ARG:HH21	2.11	0.58
1:E:281:ASP:OD2	1:E:358:HIS:HA	2.03	0.58
1:A:353:ARG:C	1:A:355:GLY:H	2.11	0.58
1:A:610:GLY:O	1:A:612:HIS:N	2.36	0.58
1:B:533:MET:HB3	1:B:534:PRO:CD	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:LEU:HD11	1:F:110:MET:CE	2.28	0.58
1:F:374:ALA:C	1:F:376:ARG:H	2.11	0.58
1:A:48:ASP:CG	1:A:52:ALA:H	2.10	0.58
1:A:491:ILE:CD1	1:F:175:LYS:HB2	2.34	0.58
1:B:57:MET:O	1:B:61:ASN:ND2	2.37	0.58
1:B:547:VAL:C	1:B:549:GLY:N	2.62	0.58
1:C:11:GLN:HG3	1:C:15:ASN:ND2	2.19	0.58
1:C:632:ASP:OD1	1:C:635:VAL:HG23	2.03	0.58
1:D:52:ALA:O	1:D:89:VAL:HG22	2.03	0.58
1:D:53:VAL:HG22	1:D:89:VAL:CG1	2.32	0.58
1:A:86:LEU:CD2	1:A:90:LEU:CD2	2.81	0.58
1:A:465:THR:O	1:A:466:MET:HB3	2.03	0.58
1:A:499:ARG:NE	1:A:628:ARG:O	2.36	0.58
1:B:158:LYS:HG2	1:B:437:VAL:HG23	1.82	0.58
1:C:611:VAL:HG12	1:C:612:HIS:CD2	2.39	0.58
1:D:374:ALA:C	1:D:376:ARG:H	2.11	0.58
1:D:421:GLU:HG2	1:D:422:LEU:N	2.10	0.58
1:E:243:VAL:HG23	1:E:385:LYS:HD2	1.86	0.58
1:F:18:LEU:CD2	1:F:119:LEU:HD23	2.31	0.58
1:F:243:VAL:HG23	1:F:385:LYS:HD2	1.86	0.58
1:E:201:PHE:HB3	1:E:216:LYS:CD	2.34	0.58
1:F:64:ARG:O	1:F:78:ARG:NH1	2.37	0.58
1:A:485:ILE:HG22	1:A:486:GLU:HG2	1.86	0.58
1:B:188:ILE:O	1:B:192:ILE:CG1	2.51	0.58
1:B:342:SER:O	1:B:343:LEU:C	2.45	0.58
1:C:61:ASN:C	1:C:63:HIS:N	2.61	0.58
1:D:293:GLU:HG3	3:D:861:HOH:O	2.02	0.58
1:E:632:ASP:OD1	1:E:635:VAL:HG23	2.03	0.58
1:F:414:ASN:ND2	1:F:466:MET:HA	2.17	0.58
1:F:611:VAL:HG12	1:F:612:HIS:CD2	2.39	0.58
1:A:226:GLN:CD	1:A:504:GLU:H	2.11	0.58
1:A:368:MET:CE	1:A:380:PHE:HD2	2.16	0.58
1:B:158:LYS:HD3	1:B:446:VAL:CG1	2.34	0.58
1:C:64:ARG:O	1:C:78:ARG:NH1	2.36	0.58
1:E:317:GLN:HB2	1:E:318:PRO:CD	2.30	0.58
1:F:177:ARG:HD3	1:F:179:GLN:HG3	1.86	0.58
1:A:78:ARG:C	1:A:80:ARG:N	2.59	0.57
1:A:305:ILE:HG23	1:A:340:TYR:CE2	2.39	0.57
1:C:411:MET:HE1	1:C:474:ARG:HB2	1.86	0.57
1:D:57:MET:HE3	1:D:61:ASN:HD21	1.68	0.57
1:D:462:TYR:HB3	1:D:464:ILE:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:573:SER:HA	1:D:578:MET:CE	2.34	0.57
1:D:574:LYS:HG3	1:D:578:MET:HE2	1.86	0.57
1:E:565:PRO:HB2	1:E:568:MET:HG2	1.86	0.57
1:A:486:GLU:HA	1:A:492:THR:HA	1.85	0.57
1:A:522:SER:O	1:A:524:LYS:N	2.37	0.57
1:D:8:ALA:HB1	1:D:546:ALA:HB3	1.84	0.57
1:D:185:GLY:HA2	1:D:375:THR:HG23	1.85	0.57
1:D:565:PRO:HB2	1:D:568:MET:HG2	1.86	0.57
1:E:165:THR:CG2	1:E:449:ASN:HB2	2.27	0.57
1:E:177:ARG:HD3	1:E:179:GLN:HG3	1.86	0.57
1:E:422:LEU:HD22	1:E:570:LEU:HD21	1.85	0.57
1:F:185:GLY:HA2	1:F:375:THR:HG23	1.86	0.57
1:B:299:ALA:O	1:B:300:ILE:C	2.42	0.57
1:B:474:ARG:NH1	3:B:851:HOH:O	2.36	0.57
1:B:482:LEU:HD11	1:B:580:PHE:HB2	1.85	0.57
1:B:560:ARG:HG2	1:B:609:CYS:HB3	1.86	0.57
1:D:25:THR:HG23	1:D:107:ARG:CZ	2.34	0.57
1:D:538:SER:O	1:D:542:GLN:HG3	2.03	0.57
1:E:573:SER:HA	1:E:578:MET:CE	2.34	0.57
1:A:215:ARG:O	1:A:216:LYS:C	2.45	0.57
1:A:280:VAL:O	1:A:280:VAL:HG22	2.03	0.57
1:E:185:GLY:HA2	1:E:375:THR:HG23	1.87	0.57
1:B:247:HIS:HB2	1:B:250:ARG:CG	2.34	0.57
1:B:411:MET:HE3	1:B:512:VAL:HB	1.86	0.57
1:B:593:THR:C	1:B:595:GLY:N	2.61	0.57
1:B:620:ARG:HG3	1:B:624:TYR:CD2	2.39	0.57
1:C:201:PHE:HB3	1:C:216:LYS:CD	2.35	0.57
1:D:554:ASP:CG	1:D:554:ASP:O	2.47	0.57
1:E:609:CYS:C	1:E:611:VAL:H	2.12	0.57
1:F:61:ASN:C	1:F:63:HIS:N	2.60	0.57
1:F:317:GLN:HB2	1:F:318:PRO:CD	2.30	0.57
1:F:477:THR:HB	1:F:479:ARG:NH1	2.20	0.57
1:A:74:LEU:O	1:A:74:LEU:CG	2.52	0.57
1:A:641:ASN:ND2	1:A:641:ASN:C	2.61	0.57
1:B:564:ILE:HB	1:B:565:PRO:HD2	1.87	0.57
1:B:591:LYS:NZ	1:B:591:LYS:CB	2.68	0.57
1:C:177:ARG:HD3	1:C:179:GLN:HG3	1.87	0.57
1:E:46:TYR:CZ	1:E:53:VAL:HG21	2.40	0.57
1:E:411:MET:HE1	1:E:468:ASN:ND2	2.19	0.57
1:F:222:TRP:CZ2	1:F:226:GLN:NE2	2.73	0.57
1:F:239:TRP:HH2	1:F:574:LYS:HD3	1.66	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:543:ALA:HA	1:F:553:LEU:CD1	2.33	0.57
1:A:135:PRO:HB3	1:A:536:PHE:CD1	2.38	0.57
1:B:423:ILE:CD1	1:B:652:HIS:CE1	2.87	0.57
1:B:571:PRO:HB2	3:B:857:HOH:O	2.03	0.57
1:D:611:VAL:HG12	1:D:612:HIS:CD2	2.39	0.57
1:E:8:ALA:O	1:E:547:VAL:CG2	2.53	0.57
1:E:89:VAL:O	1:E:92:GLN:N	2.37	0.57
1:F:43:THR:CG2	1:F:49:HIS:C	2.76	0.57
1:F:466:MET:HE1	1:F:586:VAL:HG11	1.87	0.57
1:A:61:ASN:C	1:A:63:HIS:H	2.12	0.57
1:B:96:TRP:O	1:B:97:TYR:C	2.47	0.57
1:B:139:GLN:HE21	1:B:431:TYR:HB2	1.70	0.57
1:B:147:ASN:ND2	1:B:149:GLU:H	2.03	0.57
1:B:156:SER:O	1:B:157:ALA:C	2.47	0.57
1:B:305:ILE:HD12	1:B:315:ILE:CG2	2.34	0.57
1:B:353:ARG:C	1:B:355:GLY:H	2.12	0.57
1:C:11:GLN:HE22	1:C:133:VAL:H	1.50	0.57
1:C:281:ASP:OD2	1:C:358:HIS:HA	2.04	0.57
1:C:576:GLU:HG2	3:D:687:HOH:O	2.04	0.57
1:D:520:GLU:CG	1:D:521:ARG:N	2.67	0.57
1:E:25:THR:HG23	1:E:107:ARG:CZ	2.35	0.57
1:F:565:PRO:HB2	1:F:568:MET:HG2	1.87	0.57
1:A:79:GLN:NE2	3:A:859:HOH:O	2.37	0.57
1:A:256:PHE:CE2	1:A:377:ASP:HA	2.40	0.57
1:B:158:LYS:HD2	1:B:158:LYS:O	2.04	0.57
1:B:280:VAL:HG21	1:B:353:ARG:HG3	1.85	0.57
1:C:222:TRP:CZ2	1:C:226:GLN:NE2	2.73	0.57
1:A:13:ASP:OD1	1:A:100:ARG:NE	2.33	0.57
1:A:177:ARG:HH11	1:A:179:GLN:HG3	1.70	0.57
1:A:629:ARG:HH11	1:A:629:ARG:HG3	1.70	0.57
1:B:46:TYR:CZ	1:B:53:VAL:HG11	2.40	0.57
1:B:140:ILE:O	1:B:140:ILE:HG22	2.03	0.57
1:C:48:ASP:CB	1:C:92:GLN:HE21	2.18	0.57
1:C:611:VAL:HG12	1:C:612:HIS:HD2	1.67	0.57
1:D:591:LYS:HB2	1:D:591:LYS:NZ	2.20	0.57
1:E:512:VAL:HG11	3:E:834:HOH:O	2.03	0.57
1:F:201:PHE:HB3	1:F:216:LYS:CD	2.35	0.57
1:B:42:ASP:O	1:B:44:SER:N	2.38	0.56
1:B:69:ARG:HA	1:B:264:TYR:CD2	2.39	0.56
1:C:256:PHE:CD2	1:C:378:PRO:HD3	2.40	0.56
1:C:395:THR:HG23	1:C:627:GLU:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:THR:HG23	1:D:627:GLU:O	2.05	0.56
1:E:66:LEU:HD22	1:E:67:GLU:O	2.05	0.56
1:F:283:VAL:HG11	1:F:349:VAL:HB	1.87	0.56
1:C:185:GLY:HA2	1:C:375:THR:HG23	1.86	0.56
1:C:243:VAL:HG23	1:C:385:LYS:HD2	1.87	0.56
1:B:102:ASN:C	1:B:104:ALA:H	2.13	0.56
1:B:197:TRP:CD1	1:B:223:VAL:HG21	2.40	0.56
1:B:390:ILE:HD11	3:B:861:HOH:O	2.04	0.56
1:B:433:LEU:HB2	1:B:448:ILE:HG22	1.88	0.56
1:B:620:ARG:C	1:B:621:PRO:O	2.47	0.56
1:C:160:THR:O	1:C:161:GLN:HB2	2.03	0.56
1:C:477:THR:HB	1:C:479:ARG:NH1	2.20	0.56
1:D:479:ARG:NH1	1:D:587:THR:OG1	2.38	0.56
1:E:72:TYR:CD2	1:E:79:GLN:HB3	2.40	0.56
1:E:76:ASN:HB3	1:E:79:GLN:HB2	1.88	0.56
1:E:86:LEU:HD22	1:E:90:LEU:HD22	1.87	0.56
1:E:155:TYR:O	1:E:159:MET:HG3	2.04	0.56
1:E:260:THR:HG22	1:E:268:PHE:CE1	2.40	0.56
1:F:353:ARG:C	1:F:355:GLY:N	2.63	0.56
1:F:475:LEU:HD23	1:F:476:ALA:H	1.68	0.56
1:A:533:MET:CE	1:A:533:MET:N	2.67	0.56
1:B:457:HIS:HE1	1:B:523:SER:OG	1.89	0.56
1:D:281:ASP:OD2	1:D:358:HIS:HA	2.05	0.56
1:D:591:LYS:HA	1:D:594:GLU:HB2	1.88	0.56
1:E:22:TYR:C	1:E:69:ARG:HH21	2.13	0.56
1:F:48:ASP:CB	1:F:92:GLN:HE21	2.18	0.56
1:A:190:MET:O	1:A:193:HIS:HB3	2.06	0.56
1:A:368:MET:SD	1:A:380:PHE:HB2	2.46	0.56
1:B:352:GLY:C	1:B:354:GLN:H	2.11	0.56
1:C:354:GLN:HA	1:C:354:GLN:NE2	2.19	0.56
1:C:565:PRO:HB2	1:C:568:MET:HG2	1.87	0.56
1:D:522:SER:HB3	1:D:525:ASP:OD1	2.05	0.56
1:E:74:LEU:HG	1:E:74:LEU:O	2.04	0.56
1:E:374:ALA:C	1:E:376:ARG:H	2.12	0.56
1:A:353:ARG:O	1:A:356:ASP:N	2.34	0.56
1:A:459:GLU:OE1	1:A:524:LYS:HD2	2.05	0.56
1:A:489:ASN:HB3	1:A:491:ILE:CD1	2.35	0.56
1:B:65:LEU:HD12	1:B:82:GLU:CG	2.32	0.56
1:C:591:LYS:HA	1:C:594:GLU:HB2	1.87	0.56
1:D:74:LEU:O	1:D:74:LEU:HG	2.06	0.56
1:D:76:ASN:HB3	1:D:79:GLN:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:395:THR:HG23	1:E:627:GLU:O	2.06	0.56
1:A:495:LEU:HD23	1:A:630:ILE:HG21	1.87	0.56
1:B:56:LEU:HD11	1:B:110:MET:HE3	1.87	0.56
1:B:229:ALA:O	1:B:230:ARG:C	2.48	0.56
1:B:322:GLU:O	1:B:323:LEU:C	2.49	0.56
1:C:261:SER:OG	1:C:267:GLU:HG2	2.06	0.56
1:C:482:LEU:HB2	1:C:505:LEU:HD22	1.86	0.56
1:D:31:LYS:O	1:D:35:GLU:HG3	2.06	0.56
1:D:135:PRO:HB3	1:D:536:PHE:CD1	2.41	0.56
1:E:201:PHE:HB3	1:E:216:LYS:HD2	1.88	0.56
1:E:222:TRP:CZ2	1:E:226:GLN:NE2	2.73	0.56
1:F:158:LYS:HD3	1:F:446:VAL:CG1	2.36	0.56
1:F:160:THR:O	1:F:161:GLN:HB2	2.05	0.56
1:F:260:THR:HG22	1:F:268:PHE:CE1	2.40	0.56
1:F:353:ARG:C	1:F:355:GLY:H	2.12	0.56
1:A:89:VAL:C	1:A:91:ASN:N	2.62	0.56
1:A:533:MET:H	1:A:533:MET:HE2	1.68	0.56
1:B:76:ASN:O	1:B:77:THR:C	2.47	0.56
1:C:156:SER:O	1:C:157:ALA:C	2.49	0.56
1:E:42:ASP:O	1:E:45:ILE:HG12	2.05	0.56
1:F:317:GLN:CB	1:F:318:PRO:HD2	2.28	0.56
1:F:395:THR:HG23	1:F:627:GLU:O	2.05	0.56
1:F:591:LYS:HA	1:F:594:GLU:HB2	1.88	0.56
1:A:222:TRP:CG	1:A:622:LEU:HD23	2.40	0.56
1:D:477:THR:HG23	1:D:509:PHE:CD1	2.41	0.56
1:E:353:ARG:NE	1:E:369:GLU:OE2	2.39	0.56
1:E:411:MET:HE1	1:E:474:ARG:HB2	1.88	0.56
1:A:71:TRP:CZ3	1:A:365:PRO:HG2	2.41	0.56
1:A:211:TYR:CE1	1:A:612:HIS:HA	2.41	0.56
1:A:421:GLU:O	1:A:423:ILE:N	2.39	0.56
1:C:69:ARG:N	1:C:112:GLU:OE2	2.32	0.56
1:C:408:PHE:CD1	1:C:588:ASP:HB2	2.41	0.56
1:D:374:ALA:C	1:D:376:ARG:N	2.64	0.56
1:D:521:ARG:NH2	1:D:525:ASP:O	2.38	0.56
1:E:261:SER:OG	1:E:267:GLU:HG2	2.06	0.56
1:F:374:ALA:C	1:F:376:ARG:N	2.64	0.56
1:F:411:MET:HE3	1:F:512:VAL:HB	1.88	0.56
1:A:253:ARG:HH11	1:A:253:ARG:HG3	1.70	0.55
1:B:69:ARG:HG2	1:B:264:TYR:CE2	2.42	0.55
1:B:470:ASN:ND2	1:B:474:ARG:HG3	2.21	0.55
1:C:25:THR:HG23	1:C:107:ARG:CZ	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:MET:HE3	1:C:61:ASN:HD21	1.70	0.55
1:C:560:ARG:NH1	1:C:606:HIS:N	2.54	0.55
1:D:52:ALA:O	1:D:89:VAL:CG2	2.54	0.55
1:D:256:PHE:CD2	1:D:378:PRO:HD3	2.41	0.55
1:E:256:PHE:CD2	1:E:378:PRO:HD3	2.42	0.55
1:A:135:PRO:HG3	1:A:536:PHE:CE1	2.41	0.55
1:A:540:LYS:O	1:A:541:GLU:C	2.49	0.55
1:B:14:ILE:O	1:B:15:ASN:C	2.48	0.55
1:B:95:GLU:CA	1:B:128:LEU:HD21	2.20	0.55
1:B:235:ARG:O	1:B:240:LEU:HB2	2.06	0.55
1:B:248:TRP:CH2	1:B:289:LEU:CD1	2.87	0.55
1:E:11:GLN:HG3	1:E:15:ASN:ND2	2.20	0.55
1:E:62:ASP:HB2	1:E:64:ARG:HG2	1.88	0.55
1:F:188:ILE:O	1:F:192:ILE:HG12	2.05	0.55
1:F:354:GLN:HA	1:F:354:GLN:NE2	2.19	0.55
1:A:187:ASP:OD1	1:A:189:GLY:N	2.35	0.55
1:B:293:GLU:HG2	1:B:297:HIS:HD2	1.72	0.55
1:B:553:LEU:HD13	3:B:867:HOH:O	2.05	0.55
1:D:11:GLN:HG3	1:D:15:ASN:ND2	2.19	0.55
1:E:188:ILE:O	1:E:192:ILE:HG12	2.07	0.55
1:E:278:GLU:H	1:E:354:GLN:HE22	1.54	0.55
1:A:7:ASN:O	1:A:11:GLN:CB	2.54	0.55
1:A:66:LEU:HD13	1:A:111:ASN:ND2	2.22	0.55
1:B:485:ILE:HG13	1:B:581:ASN:ND2	2.22	0.55
1:C:72:TYR:CD2	1:C:79:GLN:HB3	2.41	0.55
1:D:575:PRO:HD2	1:D:576:GLU:HG3	1.89	0.55
1:E:591:LYS:HB2	1:E:591:LYS:NZ	2.21	0.55
1:F:593:THR:C	1:F:595:GLY:H	2.15	0.55
1:A:269:PRO:HB3	1:A:363:LEU:CD2	2.36	0.55
1:B:45:ILE:O	1:B:94:LYS:HG3	2.06	0.55
1:B:57:MET:C	1:B:61:ASN:HD22	2.13	0.55
1:D:201:PHE:HB3	1:D:216:LYS:CD	2.36	0.55
1:E:411:MET:HE3	1:E:512:VAL:HB	1.87	0.55
1:E:574:LYS:HG3	1:E:578:MET:HE2	1.88	0.55
1:F:278:GLU:H	1:F:354:GLN:HE22	1.55	0.55
1:F:609:CYS:C	1:F:611:VAL:H	2.14	0.55
1:A:105:TYR:CD1	1:A:105:TYR:C	2.85	0.55
1:A:468:ASN:HB2	1:A:512:VAL:CG1	2.36	0.55
1:B:100:ARG:O	1:B:104:ALA:HB2	2.06	0.55
1:B:479:ARG:HH21	1:B:618:ASP:CG	2.14	0.55
1:B:609:CYS:C	1:B:611:VAL:H	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:ASN:HB3	1:C:79:GLN:HB2	1.89	0.55
1:C:374:ALA:C	1:C:376:ARG:H	2.13	0.55
1:D:609:CYS:C	1:D:611:VAL:H	2.15	0.55
1:F:76:ASN:HB3	1:F:79:GLN:HB2	1.87	0.55
1:F:324:LEU:HD23	1:F:327:ILE:HD11	1.89	0.55
1:A:287:HIS:HA	1:A:290:GLU:HB2	1.88	0.55
1:B:178:GLU:O	1:B:178:GLU:CG	2.36	0.55
1:B:316:ARG:HD3	3:B:829:HOH:O	2.07	0.55
1:B:377:ASP:OD1	1:B:378:PRO:HD2	2.07	0.55
1:C:56:LEU:CD1	1:C:110:MET:HE3	2.29	0.55
1:C:62:ASP:HB2	1:C:64:ARG:HG2	1.88	0.55
1:C:317:GLN:HB2	1:C:318:PRO:CD	2.30	0.55
1:C:517:GLU:HG2	1:C:518:THR:H	1.71	0.55
1:D:62:ASP:HB2	1:D:64:ARG:HG2	1.88	0.55
1:D:87:PHE:CD1	1:D:121:VAL:HG12	2.42	0.55
1:D:177:ARG:CZ	1:E:361:PHE:HE1	2.20	0.55
1:E:508:PHE:CE2	1:E:521:ARG:CD	2.89	0.55
1:B:13:ASP:CG	1:B:100:ARG:HD2	2.32	0.55
1:B:564:ILE:HB	1:B:565:PRO:CD	2.37	0.55
1:C:8:ALA:CB	1:C:546:ALA:CB	2.85	0.55
1:C:220:PHE:CE2	1:C:329:GLU:HB2	2.42	0.55
1:C:324:LEU:HD23	1:C:327:ILE:HD11	1.89	0.55
1:C:374:ALA:C	1:C:376:ARG:N	2.64	0.55
1:D:61:ASN:C	1:D:63:HIS:N	2.61	0.55
1:D:156:SER:O	1:D:157:ALA:C	2.48	0.55
1:A:273:ASP:OD2	1:B:360:LYS:HE3	2.06	0.55
1:B:145:PHE:CZ	1:B:192:ILE:HD11	2.42	0.55
1:B:258:PRO:HG2	1:B:259:LEU:N	2.22	0.55
1:B:411:MET:HE3	3:B:834:HOH:O	2.06	0.55
1:D:89:VAL:O	1:D:91:ASN:N	2.40	0.55
1:F:62:ASP:HB2	1:F:64:ARG:HG2	1.88	0.55
1:A:195:VAL:HG11	1:A:372:GLU:HB3	1.88	0.55
1:A:235:ARG:O	1:A:240:LEU:HB2	2.07	0.55
1:A:471:ASP:CG	1:A:472:GLY:H	2.15	0.55
1:A:573:SER:HA	1:A:578:MET:HE3	1.89	0.55
1:B:313:ILE:HD12	1:B:314:ASP:N	2.21	0.55
1:C:86:LEU:HD22	1:C:90:LEU:HD22	1.88	0.55
1:C:283:VAL:HG11	1:C:349:VAL:HB	1.87	0.55
1:E:239:TRP:HH2	1:E:574:LYS:HD3	1.62	0.55
1:F:574:LYS:HG3	1:F:578:MET:HE2	1.87	0.55
1:B:5:THR:HG22	1:B:10:LYS:HE3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:GLU:OE1	1:B:386:TYR:OH	2.15	0.54
1:B:373:THR:HG23	1:B:373:THR:O	2.06	0.54
1:C:609:CYS:C	1:C:611:VAL:H	2.14	0.54
1:D:356:ASP:CG	1:D:359:GLY:HA2	2.33	0.54
1:D:573:SER:HA	1:D:578:MET:HE2	1.87	0.54
1:E:639:VAL:HG23	1:E:641:ASN:ND2	2.22	0.54
1:A:185:GLY:CA	1:A:375:THR:HG23	2.37	0.54
1:C:634:ARG:HE	1:E:64:ARG:NE	2.05	0.54
1:E:477:THR:HB	1:E:479:ARG:NH1	2.22	0.54
1:F:155:TYR:O	1:F:159:MET:HG3	2.07	0.54
1:F:408:PHE:CD1	1:F:588:ASP:HB2	2.41	0.54
1:A:87:PHE:CD1	1:A:121:VAL:HG12	2.42	0.54
1:A:300:ILE:HG12	1:A:324:LEU:CD1	2.37	0.54
1:A:330:SER:CB	1:A:342:SER:OG	2.55	0.54
1:A:628:ARG:O	1:A:629:ARG:C	2.49	0.54
1:A:633:GLU:O	1:A:634:ARG:C	2.50	0.54
1:B:256:PHE:CD2	1:B:378:PRO:HD3	2.42	0.54
1:C:76:ASN:HD22	1:C:79:GLN:H	1.56	0.54
1:D:47:ASN:C	1:D:92:GLN:NE2	2.65	0.54
1:D:76:ASN:HD22	1:D:79:GLN:H	1.55	0.54
1:E:43:THR:CG2	1:E:49:HIS:C	2.77	0.54
1:F:89:VAL:O	1:F:91:ASN:N	2.41	0.54
1:F:201:PHE:HB3	1:F:216:LYS:HD2	1.89	0.54
1:F:201:PHE:HA	1:F:213:LEU:HD23	1.89	0.54
1:A:154:ALA:HB2	1:A:433:LEU:HD12	1.90	0.54
1:A:356:ASP:OD1	1:A:359:GLY:HA2	2.06	0.54
1:A:463:LYS:HE3	1:A:520:GLU:OE2	2.08	0.54
1:B:5:THR:HG22	1:B:10:LYS:CE	2.38	0.54
1:B:18:LEU:CD2	1:B:119:LEU:HD23	2.29	0.54
1:B:260:THR:HG22	1:B:268:PHE:CD2	2.42	0.54
1:B:338:GLN:NE2	1:F:316:ARG:HH21	2.05	0.54
1:A:475:LEU:HB3	1:A:589:GLY:HA3	1.90	0.54
1:A:586:VAL:O	1:A:641:ASN:HB2	2.06	0.54
1:B:195:VAL:CG2	1:B:196:THR:N	2.67	0.54
1:B:415:GLY:N	1:B:465:THR:O	2.38	0.54
1:B:424:THR:HA	1:B:457:HIS:HA	1.90	0.54
1:B:592:ASP:C	1:B:594:GLU:N	2.62	0.54
1:C:7:ASN:C	1:C:9:GLN:N	2.50	0.54
1:C:19:ASP:O	1:C:20:LYS:C	2.51	0.54
1:C:87:PHE:CD1	1:C:121:VAL:HG12	2.43	0.54
1:D:384:HIS:O	1:D:388:ASP:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:477:THR:HB	1:D:479:ARG:NH1	2.22	0.54
1:E:5:THR:CG2	1:E:6:GLY:H	2.01	0.54
1:E:354:GLN:NE2	1:E:354:GLN:HA	2.23	0.54
1:E:402:THR:O	1:E:405:ASN:HB2	2.08	0.54
1:F:462:TYR:O	1:F:520:GLU:HA	2.07	0.54
1:F:592:ASP:C	1:F:594:GLU:N	2.66	0.54
1:A:244:ASP:O	1:A:382:ARG:HG3	2.08	0.54
1:A:367:VAL:O	1:A:373:THR:HG22	2.07	0.54
1:A:428:GLU:OE2	1:A:451:ARG:HD2	2.08	0.54
1:A:529:THR:HG23	1:A:566:ASP:HA	1.90	0.54
1:A:574:LYS:CD	1:A:578:MET:HE2	2.38	0.54
1:B:151:ILE:CD1	1:B:433:LEU:HD22	2.37	0.54
1:B:243:VAL:O	1:B:385:LYS:HD3	2.08	0.54
1:C:593:THR:C	1:C:595:GLY:H	2.15	0.54
1:D:44:SER:O	1:D:94:LYS:HD2	2.08	0.54
1:E:591:LYS:HA	1:E:594:GLU:HB2	1.88	0.54
1:F:66:LEU:HD12	1:F:79:GLN:HG2	1.90	0.54
1:F:69:ARG:N	1:F:112:GLU:OE2	2.32	0.54
1:A:40:LEU:CD2	1:A:54:GLU:HG3	2.36	0.54
1:A:433:LEU:HG	1:A:450:ALA:HB2	1.89	0.54
1:A:487:ASP:HB3	1:A:491:ILE:H	1.71	0.54
1:A:574:LYS:HE3	1:A:578:MET:HE2	1.88	0.54
1:B:130:ASP:O	1:B:559:GLU:OE1	2.25	0.54
1:B:345:ASN:O	1:B:348:HIS:HB2	2.08	0.54
1:B:366:GLY:H	1:B:369:GLU:HG3	1.72	0.54
1:B:411:MET:HG3	3:B:834:HOH:O	2.08	0.54
1:B:533:MET:N	1:B:533:MET:CE	2.68	0.54
1:E:53:VAL:HG22	1:E:89:VAL:HG13	1.90	0.54
1:E:89:VAL:O	1:E:91:ASN:N	2.39	0.54
1:E:201:PHE:HA	1:E:213:LEU:HD23	1.89	0.54
1:F:261:SER:OG	1:F:267:GLU:HG2	2.07	0.54
1:A:609:CYS:C	1:A:611:VAL:H	2.16	0.54
1:C:382:ARG:HD2	3:C:712:HOH:O	2.08	0.54
1:E:283:VAL:HG11	1:E:349:VAL:HB	1.89	0.54
1:E:353:ARG:C	1:E:355:GLY:H	2.14	0.54
1:B:489:ASN:HB3	1:B:491:ILE:CD1	2.36	0.54
1:C:37:PHE:CE2	1:C:101:SER:CB	2.90	0.54
1:D:187:ASP:OD1	1:D:189:GLY:N	2.36	0.54
1:E:29:ASP:O	1:E:33:ILE:HG13	2.07	0.54
1:E:37:PHE:CE2	1:E:101:SER:CB	2.91	0.54
1:F:87:PHE:CD1	1:F:121:VAL:HG12	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:HIS:CE1	1:B:407:GLU:HG2	2.43	0.54
1:B:479:ARG:HD2	1:B:587:THR:HG23	1.90	0.54
1:D:66:LEU:HD12	1:D:79:GLN:HG2	1.90	0.54
1:D:226:GLN:HE22	1:D:504:GLU:HB2	1.74	0.54
1:D:324:LEU:HD23	1:D:327:ILE:HD11	1.90	0.54
1:E:226:GLN:HE22	1:E:504:GLU:HB2	1.73	0.54
1:E:353:ARG:C	1:E:355:GLY:N	2.65	0.54
1:F:356:ASP:CG	1:F:359:GLY:HA2	2.32	0.54
1:F:406:LEU:HB2	1:F:639:VAL:HG11	1.90	0.54
1:B:197:TRP:CE2	1:B:223:VAL:HG21	2.43	0.53
1:C:269:PRO:HB3	1:C:363:LEU:CD2	2.38	0.53
1:C:278:GLU:H	1:C:354:GLN:HE22	1.56	0.53
1:D:29:ASP:O	1:D:33:ILE:HG13	2.08	0.53
1:D:56:LEU:HD11	1:D:110:MET:CE	2.31	0.53
1:F:37:PHE:CE2	1:F:101:SER:CB	2.90	0.53
1:A:526:SER:OG	1:A:527:SER:N	2.40	0.53
1:C:201:PHE:HA	1:C:213:LEU:HD23	1.89	0.53
1:C:226:GLN:HE22	1:C:504:GLU:HB2	1.73	0.53
1:C:356:ASP:CG	1:C:359:GLY:HA2	2.33	0.53
1:E:76:ASN:HD22	1:E:79:GLN:H	1.55	0.53
1:F:40:LEU:HD13	1:F:57:MET:HG3	1.90	0.53
1:F:42:ASP:O	1:F:45:ILE:HG12	2.08	0.53
1:F:76:ASN:HD22	1:F:79:GLN:H	1.57	0.53
1:F:256:PHE:CD2	1:F:378:PRO:HD3	2.43	0.53
1:A:120:TYR:CE2	1:A:134:LEU:HD13	2.43	0.53
1:A:149:GLU:O	1:A:150:VAL:C	2.49	0.53
1:A:382:ARG:HD2	3:A:712:HOH:O	2.08	0.53
1:A:540:LYS:O	1:A:544:ASP:HB2	2.07	0.53
1:A:630:ILE:HD13	1:A:636:ILE:CG1	2.39	0.53
1:B:356:ASP:OD1	1:B:359:GLY:HA2	2.08	0.53
1:B:414:ASN:ND2	1:B:467:SER:OG	2.42	0.53
1:B:538:SER:O	1:B:542:GLN:HG3	2.09	0.53
1:C:74:LEU:HG	1:C:74:LEU:O	2.06	0.53
1:C:508:PHE:CE2	1:C:521:ARG:CD	2.92	0.53
1:F:66:LEU:HD22	1:F:67:GLU:O	2.09	0.53
1:A:414:ASN:ND2	1:A:467:SER:H	2.05	0.53
1:B:150:VAL:HG21	1:B:168:VAL:HG12	1.90	0.53
1:C:89:VAL:O	1:C:91:ASN:N	2.41	0.53
1:C:406:LEU:HB2	1:C:639:VAL:HG11	1.89	0.53
1:D:260:THR:HG22	1:D:268:PHE:HE1	1.73	0.53
1:D:353:ARG:O	1:D:355:GLY:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:MET:HE3	1:D:468:ASN:ND2	2.23	0.53
1:E:156:SER:O	1:E:157:ALA:C	2.51	0.53
1:A:201:PHE:HA	1:A:213:LEU:HD23	1.91	0.53
1:B:48:ASP:N	1:B:92:GLN:HE21	2.06	0.53
1:B:301:ASP:CB	1:D:295:ARG:HH22	2.22	0.53
1:C:56:LEU:HD11	1:C:110:MET:CE	2.28	0.53
1:D:201:PHE:HA	1:D:213:LEU:HD23	1.88	0.53
1:E:591:LYS:HB2	1:E:591:LYS:HZ2	1.74	0.53
1:E:620:ARG:HG3	1:E:624:TYR:CD2	2.44	0.53
1:A:185:GLY:HA2	1:A:375:THR:HG23	1.90	0.53
1:A:455:LEU:HG	1:A:456:ASN:N	2.22	0.53
1:B:487:ASP:HB3	1:B:491:ILE:HG13	1.90	0.53
1:B:544:ASP:O	1:B:548:ASN:ND2	2.36	0.53
1:E:324:LEU:HD23	1:E:327:ILE:HD11	1.90	0.53
1:B:165:THR:HA	1:B:449:ASN:O	2.09	0.53
1:B:379:SER:HA	1:B:382:ARG:HB2	1.90	0.53
1:D:47:ASN:HB2	1:D:92:GLN:HB2	1.90	0.53
1:E:220:PHE:CE2	1:E:329:GLU:HB2	2.43	0.53
1:B:43:THR:CG2	1:B:49:HIS:O	2.56	0.53
1:B:573:SER:OG	1:B:574:LYS:N	2.41	0.53
1:F:156:SER:O	1:F:157:ALA:C	2.51	0.53
1:F:639:VAL:HG23	1:F:641:ASN:ND2	2.23	0.53
1:A:53:VAL:C	1:A:55:THR:H	2.16	0.53
1:A:185:GLY:HA2	1:A:375:THR:CG2	2.39	0.53
1:A:580:PHE:HE2	1:A:649:ILE:HB	1.73	0.53
1:B:72:TYR:CD2	1:B:114:GLU:HG2	2.44	0.53
1:D:201:PHE:HB3	1:D:216:LYS:HD2	1.90	0.53
1:D:367:VAL:HG23	1:D:373:THR:O	2.09	0.53
1:D:395:THR:HG21	1:D:500:TRP:CZ3	2.43	0.53
1:D:479:ARG:NH2	1:D:618:ASP:OD2	2.41	0.53
1:D:639:VAL:HG23	1:D:641:ASN:ND2	2.24	0.53
1:E:66:LEU:HD12	1:E:79:GLN:HG2	1.91	0.53
1:E:317:GLN:CB	1:E:318:PRO:HD2	2.27	0.53
1:E:477:THR:HG23	1:E:509:PHE:CD1	2.44	0.53
1:E:578:MET:HE3	1:E:580:PHE:HZ	1.73	0.53
1:B:330:SER:HB2	1:B:342:SER:CB	2.39	0.53
1:C:477:THR:HG23	1:C:509:PHE:CD1	2.44	0.53
1:D:593:THR:C	1:D:595:GLY:H	2.17	0.53
1:E:239:TRP:CH2	1:E:574:LYS:CD	2.83	0.53
1:E:408:PHE:CD1	1:E:588:ASP:HB2	2.44	0.53
1:E:422:LEU:HB3	1:E:649:ILE:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ASN:O	1:A:348:HIS:HB2	2.09	0.52
1:A:508:PHE:CD2	1:A:521:ARG:NE	2.78	0.52
1:A:533:MET:CB	1:A:534:PRO:CD	2.70	0.52
1:B:79:GLN:NE2	3:B:859:HOH:O	2.41	0.52
1:C:639:VAL:HG23	1:C:641:ASN:ND2	2.24	0.52
1:D:188:ILE:O	1:D:192:ILE:HG12	2.09	0.52
1:D:464:ILE:HG21	1:D:478:PHE:CE1	2.43	0.52
1:D:560:ARG:HD3	1:D:611:VAL:HB	1.90	0.52
1:E:255:GLY:HA2	1:E:271:ARG:HH12	1.74	0.52
1:F:255:GLY:HA2	1:F:271:ARG:HH12	1.73	0.52
1:A:78:ARG:O	1:A:79:GLN:C	2.50	0.52
1:A:378:PRO:C	1:A:380:PHE:H	2.16	0.52
1:B:203:PHE:C	1:B:203:PHE:CD1	2.88	0.52
1:C:188:ILE:O	1:C:192:ILE:HG12	2.09	0.52
1:C:592:ASP:C	1:C:594:GLU:N	2.66	0.52
1:F:384:HIS:O	1:F:388:ASP:HB2	2.08	0.52
1:A:508:PHE:CE2	3:A:864:HOH:O	2.54	0.52
1:C:201:PHE:HB3	1:C:216:LYS:HD2	1.90	0.52
1:C:307:ASP:OD2	1:C:311:HIS:HB2	2.09	0.52
1:E:356:ASP:CG	1:E:359:GLY:HA2	2.34	0.52
1:F:226:GLN:HE22	1:F:504:GLU:HB2	1.73	0.52
1:A:199:MET:HE1	3:A:774:HOH:O	2.08	0.52
1:C:395:THR:HG21	1:C:500:TRP:CZ3	2.44	0.52
1:F:307:ASP:HA	1:F:336:ASN:HB2	1.91	0.52
1:F:477:THR:HG23	1:F:509:PHE:CD1	2.44	0.52
1:F:578:MET:HE3	1:F:580:PHE:HZ	1.73	0.52
1:A:40:LEU:HD12	1:A:57:MET:HG3	1.91	0.52
1:A:69:ARG:HG3	1:A:69:ARG:NH1	2.24	0.52
1:A:618:ASP:OD1	1:A:620:ARG:HB2	2.10	0.52
1:B:56:LEU:O	1:B:59:GLU:N	2.42	0.52
1:B:78:ARG:NH1	1:B:82:GLU:CD	2.68	0.52
1:D:491:ILE:O	1:D:492:THR:CG2	2.57	0.52
1:E:395:THR:HG21	1:E:500:TRP:CZ3	2.45	0.52
1:F:8:ALA:CA	1:F:553:LEU:HD12	2.35	0.52
1:F:395:THR:HG21	1:F:500:TRP:CZ3	2.45	0.52
1:A:45:ILE:HD12	1:A:46:TYR:CE1	2.45	0.52
1:B:508:PHE:CE2	1:B:521:ARG:HD3	2.44	0.52
1:C:42:ASP:O	1:C:45:ILE:HG12	2.09	0.52
1:E:307:ASP:HA	1:E:336:ASN:HB2	1.92	0.52
1:F:307:ASP:C	1:F:336:ASN:HD22	2.17	0.52
1:F:478:PHE:CZ	1:F:519:ILE:HD12	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:PHE:HB2	1:A:641:ASN:OD1	2.08	0.52
1:B:20:LYS:H	1:B:435:ASN:HD21	1.54	0.52
1:B:48:ASP:CB	1:B:92:GLN:HE21	2.14	0.52
1:C:159:MET:HE1	1:F:155:TYR:CD1	2.45	0.52
1:C:197:TRP:CE2	1:C:223:VAL:HG21	2.45	0.52
1:C:384:HIS:O	1:C:388:ASP:HB2	2.10	0.52
1:E:575:PRO:HD2	1:E:576:GLU:HG3	1.91	0.52
1:A:574:LYS:HE3	1:A:578:MET:CE	2.39	0.52
1:F:145:PHE:CZ	1:F:372:GLU:HB2	2.45	0.52
1:F:408:PHE:CE2	1:F:411:MET:HG2	2.45	0.52
1:A:48:ASP:OD1	1:A:51:ALA:N	2.43	0.52
1:A:207:ASP:OD1	1:A:333:TYR:OH	2.13	0.52
1:A:248:TRP:CZ3	1:A:289:LEU:CD1	2.92	0.52
1:A:293:GLU:HG3	3:A:861:HOH:O	2.10	0.52
1:B:402:THR:N	1:B:405:ASN:HB2	2.25	0.52
1:B:495:LEU:CD2	1:B:630:ILE:HG21	2.38	0.52
1:B:540:LYS:O	1:B:541:GLU:C	2.48	0.52
1:B:639:VAL:HG23	1:B:641:ASN:ND2	2.25	0.52
1:D:165:THR:HA	1:D:449:ASN:O	2.10	0.52
1:F:89:VAL:C	1:F:91:ASN:N	2.67	0.52
1:A:135:PRO:CG	1:A:140:ILE:HD11	2.38	0.52
1:A:572:LYS:O	1:A:572:LYS:CG	2.56	0.52
1:B:8:ALA:CB	1:B:546:ALA:HB3	2.39	0.52
1:B:68:GLN:HB3	1:B:69:ARG:HH12	1.75	0.52
1:B:251:ILE:HG23	1:B:276:HIS:CE1	2.44	0.52
1:B:316:ARG:HH21	1:D:338:GLN:HE22	1.56	0.52
1:B:487:ASP:CB	1:B:491:ILE:N	2.60	0.52
1:C:130:ASP:O	1:C:559:GLU:CD	2.53	0.52
1:C:494:THR:H	1:C:497:GLU:HB2	1.75	0.52
1:E:87:PHE:CD1	1:E:121:VAL:HG12	2.43	0.52
1:F:414:ASN:ND2	1:F:467:SER:H	2.07	0.52
1:F:620:ARG:HG3	1:F:624:TYR:CD2	2.45	0.52
1:A:150:VAL:HG12	1:A:433:LEU:HD11	1.91	0.51
1:A:411:MET:C	1:A:412:VAL:HG12	2.25	0.51
1:A:522:SER:C	1:A:524:LYS:N	2.64	0.51
1:A:632:ASP:OD1	1:A:634:ARG:HB3	2.09	0.51
1:B:207:ASP:OD2	1:B:212:HIS:CB	2.57	0.51
1:B:508:PHE:CE2	1:B:521:ARG:CD	2.93	0.51
1:B:533:MET:HB3	1:B:534:PRO:HD2	1.91	0.51
1:D:243:VAL:HG23	1:D:385:LYS:HD2	1.92	0.51
1:E:607:ALA:HB1	1:E:617:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:GLN:HG3	1:F:15:ASN:ND2	2.21	0.51
1:F:72:TYR:HD2	1:F:79:GLN:HB3	1.73	0.51
1:A:180:ARG:O	1:A:180:ARG:CG	2.58	0.51
1:A:304:TYR:CD1	1:A:304:TYR:C	2.88	0.51
1:A:455:LEU:O	1:A:567:ARG:HB2	2.10	0.51
1:B:16:HIS:CD2	1:B:27:TYR:CE2	2.99	0.51
1:C:175:LYS:HB2	1:D:491:ILE:CD1	2.39	0.51
1:C:307:ASP:HA	1:C:336:ASN:HB2	1.92	0.51
1:C:454:ARG:CZ	1:C:567:ARG:HD2	2.40	0.51
1:C:620:ARG:HG3	1:C:624:TYR:CD2	2.45	0.51
1:D:283:VAL:HG11	1:D:349:VAL:HB	1.92	0.51
1:D:382:ARG:HD2	3:D:712:HOH:O	2.10	0.51
1:E:46:TYR:HA	1:E:92:GLN:O	2.10	0.51
1:E:177:ARG:NH1	1:E:179:GLN:HG3	2.25	0.51
1:F:517:GLU:HG2	1:F:518:THR:N	2.24	0.51
1:A:225:HIS:HE1	3:A:788:HOH:O	1.91	0.51
1:B:247:HIS:ND1	1:B:250:ARG:HG3	2.25	0.51
1:B:494:THR:O	1:B:495:LEU:C	2.52	0.51
1:B:517:GLU:CG	1:B:518:THR:H	2.23	0.51
1:C:560:ARG:HG2	1:C:609:CYS:SG	2.50	0.51
1:D:278:GLU:H	1:D:354:GLN:HE22	1.58	0.51
1:D:592:ASP:O	1:D:619:ASN:ND2	2.36	0.51
1:E:56:LEU:CD1	1:E:110:MET:HE3	2.29	0.51
1:F:409:SER:O	1:F:470:ASN:ND2	2.39	0.51
1:F:493:LEU:HA	1:F:497:GLU:OE1	2.09	0.51
1:A:165:THR:HB	1:A:449:ASN:HB3	1.91	0.51
1:B:578:MET:HE3	1:B:580:PHE:HZ	1.74	0.51
1:D:197:TRP:CE2	1:D:223:VAL:HG21	2.46	0.51
1:D:307:ASP:HA	1:D:336:ASN:HB2	1.92	0.51
1:D:307:ASP:C	1:D:336:ASN:HD22	2.18	0.51
1:D:462:TYR:O	1:D:520:GLU:HA	2.10	0.51
1:D:586:VAL:O	1:D:641:ASN:HB2	2.10	0.51
1:E:374:ALA:C	1:E:376:ARG:N	2.64	0.51
1:E:479:ARG:NH2	1:E:618:ASP:OD2	2.44	0.51
1:E:591:LYS:C	1:E:594:GLU:HB2	2.35	0.51
1:F:220:PHE:CZ	1:F:329:GLU:HB2	2.46	0.51
1:B:12:GLN:OE1	1:B:547:VAL:HG21	2.10	0.51
1:C:16:HIS:CD2	1:C:27:TYR:CE2	2.98	0.51
1:C:289:LEU:O	1:C:290:GLU:C	2.53	0.51
1:C:301:ASP:CG	1:C:393:LYS:HZ1	2.19	0.51
1:C:414:ASN:ND2	1:C:467:SER:H	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:ASP:C	1:E:336:ASN:HD22	2.18	0.51
1:F:382:ARG:HD2	3:F:712:HOH:O	2.10	0.51
1:F:423:ILE:HD11	1:F:652:HIS:CD2	2.44	0.51
1:A:573:SER:N	3:A:857:HOH:O	2.42	0.51
1:B:187:ASP:OD1	1:B:187:ASP:C	2.52	0.51
1:B:214:ASP:OD2	1:B:615:ALA:HA	2.10	0.51
1:B:239:TRP:CZ3	1:B:574:LYS:CE	2.93	0.51
1:C:307:ASP:C	1:C:336:ASN:HD22	2.19	0.51
1:C:367:VAL:HG23	1:C:373:THR:O	2.10	0.51
1:D:159:MET:CE	1:E:155:TYR:CG	2.93	0.51
1:E:157:ALA:CB	1:E:448:ILE:HG12	2.41	0.51
1:A:630:ILE:HD13	1:A:636:ILE:CD1	2.41	0.51
1:B:499:ARG:HH21	1:B:627:GLU:C	2.19	0.51
1:C:46:TYR:HA	1:C:92:GLN:O	2.11	0.51
1:D:7:ASN:O	1:D:11:GLN:N	2.37	0.51
1:D:289:LEU:O	1:D:290:GLU:C	2.54	0.51
1:F:211:TYR:CE2	1:F:612:HIS:HA	2.46	0.51
1:A:25:THR:HB	1:A:27:TYR:H	1.76	0.51
1:A:179:GLN:NE2	3:A:710:HOH:O	2.31	0.51
1:A:238:ASN:C	1:A:240:LEU:N	2.68	0.51
1:A:313:ILE:CD1	1:A:323:LEU:CD1	2.76	0.51
1:A:620:ARG:HG3	1:A:624:TYR:CD1	2.45	0.51
1:B:441:GLU:HB3	1:B:442:ASN:HD22	1.76	0.51
1:C:211:TYR:CE2	1:C:612:HIS:HA	2.46	0.51
1:D:19:ASP:O	1:D:20:LYS:C	2.53	0.51
1:D:454:ARG:CZ	1:D:567:ARG:HD2	2.41	0.51
1:E:46:TYR:CE1	1:E:98:CYS:SG	3.03	0.51
1:F:220:PHE:CE2	1:F:329:GLU:HB2	2.46	0.51
1:B:293:GLU:HG3	3:B:861:HOH:O	2.10	0.51
1:D:421:GLU:CG	1:D:422:LEU:N	2.70	0.51
1:E:165:THR:HA	1:E:449:ASN:O	2.10	0.51
1:F:491:ILE:O	1:F:492:THR:CG2	2.59	0.51
1:F:508:PHE:CE2	1:F:521:ARG:CD	2.94	0.51
1:A:289:LEU:O	1:A:293:GLU:N	2.32	0.51
1:A:414:ASN:ND2	1:A:466:MET:HA	2.22	0.51
1:B:57:MET:HE3	1:B:61:ASN:HD21	1.76	0.51
1:C:133:VAL:CG2	1:C:555:LEU:HD23	2.41	0.51
1:D:86:LEU:HD22	1:D:90:LEU:HD22	1.93	0.51
1:E:89:VAL:O	1:E:90:LEU:C	2.54	0.51
1:E:211:TYR:CE2	1:E:612:HIS:HA	2.46	0.51
1:A:572:LYS:O	1:A:572:LYS:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ASN:C	1:B:104:ALA:N	2.70	0.50
1:B:183:TYR:CD1	1:B:183:TYR:C	2.88	0.50
1:B:218:GLU:H	1:B:322:GLU:HB3	1.75	0.50
1:B:269:PRO:HB3	1:B:363:LEU:HD23	1.93	0.50
1:B:518:THR:O	1:B:518:THR:HG22	2.11	0.50
1:C:377:ASP:OD1	1:C:378:PRO:HD2	2.11	0.50
1:D:17:LEU:CD2	1:D:103:ALA:O	2.59	0.50
1:D:177:ARG:HD2	1:E:360:LYS:HB3	1.92	0.50
1:D:259:LEU:HD11	1:E:363:LEU:HD12	1.93	0.50
1:D:592:ASP:C	1:D:594:GLU:N	2.67	0.50
1:E:220:PHE:CZ	1:E:329:GLU:HB2	2.46	0.50
1:E:408:PHE:CB	1:E:641:ASN:OD1	2.58	0.50
1:F:269:PRO:CB	1:F:363:LEU:HD23	2.39	0.50
1:F:307:ASP:OD2	1:F:311:HIS:HB2	2.10	0.50
1:A:407:GLU:OE2	1:A:639:VAL:HA	2.11	0.50
1:A:410:GLY:O	1:A:412:VAL:HG12	2.10	0.50
1:A:440:GLY:C	1:A:441:GLU:CD	2.80	0.50
1:B:42:ASP:O	1:B:45:ILE:HG12	2.11	0.50
1:D:411:MET:HE1	1:D:512:VAL:CG1	2.41	0.50
1:D:412:VAL:HB	1:D:640:SER:HB2	1.93	0.50
1:E:382:ARG:HD2	3:E:712:HOH:O	2.11	0.50
1:E:384:HIS:O	1:E:388:ASP:HB2	2.11	0.50
1:A:611:VAL:HG12	1:A:612:HIS:HD2	1.77	0.50
1:B:13:ASP:O	1:B:14:ILE:C	2.54	0.50
1:B:69:ARG:HG3	1:B:69:ARG:HH11	1.75	0.50
1:B:239:TRP:HH2	1:B:574:LYS:HD3	1.68	0.50
1:C:317:GLN:CB	1:C:318:PRO:HD2	2.27	0.50
1:D:211:TYR:CE2	1:D:612:HIS:HA	2.46	0.50
1:D:231:PHE:HE2	1:D:243:VAL:HG11	1.77	0.50
1:E:84:LEU:HD11	1:E:204:TRP:CZ2	2.46	0.50
1:F:46:TYR:HA	1:F:92:GLN:O	2.11	0.50
1:A:178:GLU:C	1:A:180:ARG:H	2.19	0.50
1:A:286:VAL:O	1:A:289:LEU:HB2	2.12	0.50
1:A:531:PRO:O	1:A:531:PRO:HG2	2.12	0.50
1:B:352:GLY:C	1:B:354:GLN:N	2.68	0.50
1:C:423:ILE:HD11	1:C:652:HIS:CD2	2.44	0.50
1:C:586:VAL:O	1:C:641:ASN:HB2	2.12	0.50
1:D:464:ILE:HG21	1:D:478:PHE:HE1	1.74	0.50
1:E:215:ARG:O	1:E:216:LYS:C	2.55	0.50
1:F:594:GLU:O	1:F:594:GLU:HG2	2.10	0.50
1:A:241:ASP:O	1:A:242:PRO:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ALA:O	1:A:375:THR:C	2.53	0.50
1:A:632:ASP:OD1	1:A:634:ARG:CB	2.60	0.50
1:B:158:LYS:HD3	1:B:446:VAL:HG12	1.94	0.50
1:B:479:ARG:NH1	1:B:587:THR:OG1	2.45	0.50
1:C:479:ARG:NH2	1:C:618:ASP:OD2	2.43	0.50
1:C:575:PRO:HB2	3:D:687:HOH:O	2.10	0.50
1:C:607:ALA:HB1	1:C:617:PRO:HD3	1.92	0.50
1:F:53:VAL:HG22	1:F:89:VAL:HG13	1.92	0.50
1:F:289:LEU:O	1:F:290:GLU:C	2.53	0.50
1:A:140:ILE:HG22	1:A:141:THR:HG23	1.94	0.50
1:A:395:THR:HG23	1:A:627:GLU:O	2.12	0.50
1:C:150:VAL:CG1	1:C:433:LEU:HD11	2.36	0.50
1:D:220:PHE:CE2	1:D:329:GLU:HB2	2.46	0.50
1:E:187:ASP:OD1	1:E:189:GLY:N	2.37	0.50
1:E:353:ARG:O	1:E:356:ASP:N	2.36	0.50
1:E:377:ASP:OD1	1:E:378:PRO:HD2	2.12	0.50
1:F:367:VAL:HG23	1:F:373:THR:O	2.11	0.50
1:A:23:GLU:O	1:A:24:PRO:C	2.55	0.50
1:A:439:SER:O	1:A:443:ILE:HG21	2.11	0.50
1:B:477:THR:HG23	1:B:509:PHE:CE1	2.46	0.50
1:B:491:ILE:O	1:B:492:THR:CG2	2.59	0.50
1:C:473:GLU:HA	1:C:512:VAL:O	2.12	0.50
1:D:47:ASN:C	1:D:92:GLN:HE21	2.20	0.50
1:D:68:GLN:HB3	1:D:69:ARG:HH11	1.75	0.50
1:D:255:GLY:HA2	1:D:271:ARG:HH12	1.75	0.50
1:F:353:ARG:O	1:F:356:ASP:N	2.35	0.50
1:F:411:MET:CE	1:F:512:VAL:HB	2.42	0.50
1:A:491:ILE:HG12	1:F:175:LYS:HG3	1.94	0.50
1:A:557:ALA:HB3	1:A:558:TYR:CG	2.47	0.50
1:B:363:LEU:C	1:B:364:PRO:O	2.49	0.50
1:B:488:ASN:H	1:B:490:GLY:H	1.60	0.50
1:B:496:ASP:OD1	1:B:499:ARG:HD3	2.12	0.50
1:C:89:VAL:O	1:C:90:LEU:C	2.55	0.50
1:D:269:PRO:HB3	1:D:363:LEU:CD2	2.41	0.50
1:D:272:PRO:CG	1:E:272:PRO:CG	2.87	0.50
1:E:289:LEU:O	1:E:290:GLU:C	2.54	0.50
1:F:454:ARG:CZ	1:F:567:ARG:HD2	2.42	0.50
1:A:254:GLU:OE2	1:B:360:LYS:NZ	2.45	0.50
1:A:318:PRO:C	1:A:320:GLY:H	2.20	0.50
1:A:530:VAL:CG2	1:A:561:SER:HB3	2.42	0.50
1:B:33:ILE:CD1	1:B:100:ARG:HH22	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:SER:O	1:B:170:PHE:HB2	2.12	0.50
1:B:211:TYR:N	1:B:211:TYR:CD1	2.80	0.50
1:B:506:ASP:OD1	1:B:507:LYS:N	2.45	0.50
1:C:84:LEU:HD11	1:C:204:TRP:CZ2	2.47	0.50
1:C:402:THR:O	1:C:405:ASN:HB2	2.12	0.50
1:D:295:ARG:HG2	1:D:339:TYR:CZ	2.47	0.50
1:E:158:LYS:HD3	1:E:446:VAL:HG12	1.93	0.50
1:E:591:LYS:HG3	1:E:594:GLU:OE2	2.12	0.50
1:F:592:ASP:O	1:F:619:ASN:ND2	2.36	0.50
1:A:392:LYS:NZ	1:A:396:ASP:OD2	2.44	0.49
1:A:565:PRO:HB2	1:A:568:MET:HG2	1.94	0.49
1:A:592:ASP:C	1:A:594:GLU:N	2.70	0.49
1:B:40:LEU:HD22	1:B:57:MET:HG3	1.95	0.49
1:B:461:THR:HG1	1:B:462:TYR:H	1.60	0.49
1:B:575:PRO:HD2	1:B:576:GLU:CG	2.40	0.49
1:C:101:SER:O	1:C:104:ALA:HB3	2.12	0.49
1:C:177:ARG:HG2	1:F:360:LYS:HB3	1.93	0.49
1:C:187:ASP:OD1	1:C:189:GLY:N	2.36	0.49
1:C:487:ASP:HB3	1:C:491:ILE:H	1.77	0.49
1:D:239:TRP:HH2	1:D:574:LYS:HD3	1.69	0.49
1:E:231:PHE:HE2	1:E:243:VAL:HG11	1.77	0.49
1:F:377:ASP:OD1	1:F:378:PRO:HD2	2.12	0.49
1:A:5:THR:O	1:A:5:THR:CG2	2.60	0.49
1:A:620:ARG:HG3	1:A:624:TYR:CD2	2.47	0.49
1:B:38:ASN:C	1:B:40:LEU:H	2.20	0.49
1:C:177:ARG:NH1	1:C:179:GLN:HG3	2.27	0.49
1:E:145:PHE:CZ	1:E:372:GLU:HB2	2.47	0.49
1:F:586:VAL:O	1:F:641:ASN:HB2	2.12	0.49
1:F:591:LYS:HB2	1:F:591:LYS:HZ2	1.75	0.49
1:A:5:THR:O	1:A:6:GLY:O	2.30	0.49
1:A:188:ILE:HG12	3:A:720:HOH:O	2.11	0.49
1:A:330:SER:HB3	1:A:342:SER:OG	2.11	0.49
1:B:122:SER:O	1:B:126:SER:HB3	2.13	0.49
1:B:147:ASN:HD22	1:B:149:GLU:H	1.59	0.49
1:C:89:VAL:C	1:C:91:ASN:N	2.67	0.49
1:C:220:PHE:CZ	1:C:329:GLU:HB2	2.47	0.49
1:C:353:ARG:O	1:C:355:GLY:N	2.45	0.49
1:C:594:GLU:O	1:C:594:GLU:HG2	2.11	0.49
1:D:307:ASP:OD2	1:D:311:HIS:HB2	2.12	0.49
1:E:592:ASP:O	1:E:619:ASN:ND2	2.40	0.49
1:E:641:ASN:ND2	1:E:641:ASN:H	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:226:GLN:O	1:F:227:LEU:C	2.56	0.49
1:F:485:ILE:O	1:F:492:THR:HA	2.11	0.49
1:F:549:GLY:O	1:F:550:GLY:C	2.55	0.49
1:A:159:MET:CE	1:B:155:TYR:CG	2.91	0.49
1:A:308:SER:HA	1:A:336:ASN:ND2	2.28	0.49
1:A:529:THR:HG23	1:A:566:ASP:CA	2.43	0.49
1:B:149:GLU:O	1:B:152:ASP:N	2.45	0.49
1:B:641:ASN:ND2	1:B:641:ASN:H	2.10	0.49
1:C:17:LEU:CD2	1:C:103:ALA:O	2.60	0.49
1:C:560:ARG:CD	1:C:609:CYS:HB3	2.42	0.49
1:D:112:GLU:O	1:D:116:VAL:HG23	2.12	0.49
1:D:392:LYS:NZ	1:D:396:ASP:OD2	2.45	0.49
1:E:295:ARG:HG2	1:E:339:TYR:CZ	2.48	0.49
1:F:607:ALA:HB1	1:F:617:PRO:HD3	1.92	0.49
1:A:165:THR:HG21	1:A:449:ASN:HB2	1.83	0.49
1:B:7:ASN:C	1:B:9:GLN:N	2.62	0.49
1:B:46:TYR:HA	1:B:92:GLN:O	2.13	0.49
1:B:190:MET:C	1:B:192:ILE:N	2.67	0.49
1:B:252:ILE:HD11	1:B:277:PHE:CE1	2.48	0.49
1:C:68:GLN:HB3	1:C:69:ARG:HH11	1.75	0.49
1:C:231:PHE:HE2	1:C:243:VAL:HG11	1.77	0.49
1:C:568:MET:O	1:C:569:LEU:C	2.55	0.49
1:D:66:LEU:HD22	1:D:67:GLU:O	2.11	0.49
1:D:235:ARG:O	1:D:240:LEU:HB2	2.12	0.49
1:D:377:ASP:OD1	1:D:378:PRO:HD2	2.12	0.49
1:D:568:MET:O	1:D:569:LEU:C	2.54	0.49
1:E:494:THR:H	1:E:497:GLU:HB2	1.78	0.49
1:F:177:ARG:NH1	1:F:179:GLN:HG3	2.28	0.49
1:F:487:ASP:HB3	1:F:491:ILE:H	1.77	0.49
1:A:78:ARG:O	1:A:81:LYS:N	2.45	0.49
1:A:222:TRP:CH2	1:A:623:GLY:HA2	2.48	0.49
1:A:226:GLN:O	1:A:227:LEU:O	2.31	0.49
1:A:314:ASP:C	1:A:314:ASP:OD1	2.56	0.49
1:C:574:LYS:HG3	1:C:578:MET:HE2	1.94	0.49
1:D:89:VAL:O	1:D:90:LEU:C	2.55	0.49
1:D:594:GLU:O	1:D:594:GLU:HG2	2.12	0.49
1:E:7:ASN:O	1:E:9:GLN:N	2.44	0.49
1:E:39:PRO:O	1:E:53:VAL:HG11	2.13	0.49
1:E:89:VAL:C	1:E:91:ASN:N	2.66	0.49
1:E:307:ASP:OD2	1:E:311:HIS:HB2	2.12	0.49
1:E:396:ASP:O	1:E:629:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:408:PHE:CE2	1:E:411:MET:HG2	2.47	0.49
1:E:593:THR:C	1:E:595:GLY:H	2.20	0.49
1:F:7:ASN:O	1:F:9:GLN:N	2.46	0.49
1:F:16:HIS:CD2	1:F:27:TYR:CE2	3.00	0.49
1:F:17:LEU:CD2	1:F:103:ALA:O	2.61	0.49
1:A:147:ASN:HB3	1:A:150:VAL:H	1.77	0.49
1:B:301:ASP:CG	1:B:393:LYS:HZ2	2.21	0.49
1:D:5:THR:CG2	1:D:10:LYS:HE3	2.42	0.49
1:D:84:LEU:HD11	1:D:204:TRP:CZ2	2.48	0.49
1:D:89:VAL:C	1:D:91:ASN:N	2.66	0.49
1:D:607:ALA:HB1	1:D:617:PRO:HD3	1.94	0.49
1:E:8:ALA:O	1:E:547:VAL:HG22	2.12	0.49
1:E:222:TRP:CD1	1:E:622:LEU:HD23	2.48	0.49
1:E:367:VAL:HG23	1:E:373:THR:O	2.12	0.49
1:E:411:MET:SD	1:E:468:ASN:ND2	2.85	0.49
1:E:586:VAL:O	1:E:641:ASN:HB2	2.13	0.49
1:F:231:PHE:HE2	1:F:243:VAL:HG11	1.77	0.49
1:F:284:ALA:O	1:F:350:MET:HE1	2.12	0.49
1:F:479:ARG:NH2	1:F:618:ASP:OD2	2.44	0.49
1:A:354:GLN:HA	1:A:354:GLN:HE21	1.77	0.49
1:B:596:HIS:ND1	1:B:596:HIS:N	2.58	0.49
1:D:177:ARG:NH1	1:D:179:GLN:HG3	2.28	0.49
1:D:620:ARG:C	1:D:621:PRO:O	2.55	0.49
1:E:592:ASP:C	1:E:594:GLU:N	2.71	0.49
1:A:521:ARG:NH2	1:A:525:ASP:O	2.46	0.49
1:E:39:PRO:HB2	1:E:53:VAL:HG12	1.95	0.49
1:E:101:SER:O	1:E:104:ALA:HB3	2.13	0.49
1:E:554:ASP:C	1:E:556:SER:N	2.71	0.49
1:F:84:LEU:HD11	1:F:204:TRP:CZ2	2.47	0.49
1:F:89:VAL:O	1:F:90:LEU:C	2.55	0.49
1:F:295:ARG:HG2	1:F:339:TYR:CZ	2.47	0.49
1:B:150:VAL:CG1	1:B:433:LEU:HD11	2.40	0.49
1:B:272:PRO:HD2	1:B:275:ILE:HD12	1.94	0.49
1:B:448:ILE:HG22	1:B:448:ILE:O	2.10	0.49
1:D:101:SER:O	1:D:104:ALA:HB3	2.13	0.49
1:D:468:ASN:HB3	1:D:514:SER:HA	1.94	0.49
1:E:471:ASP:OD1	1:E:471:ASP:C	2.56	0.49
1:F:101:SER:O	1:F:104:ALA:HB3	2.12	0.49
1:F:568:MET:O	1:F:569:LEU:C	2.56	0.49
1:A:403:HIS:C	1:A:405:ASN:N	2.67	0.48
1:B:157:ALA:CB	1:B:448:ILE:HG12	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:SER:HB3	3:B:719:HOH:O	2.13	0.48
1:D:620:ARG:HG3	1:D:624:TYR:CD2	2.48	0.48
1:A:86:LEU:HD23	1:A:86:LEU:O	2.13	0.48
1:A:491:ILE:HD11	1:F:175:LYS:O	2.12	0.48
1:B:303:GLY:O	1:B:315:ILE:HG12	2.11	0.48
1:B:477:THR:O	1:B:586:VAL:HA	2.13	0.48
1:C:66:LEU:HD12	1:C:79:GLN:HG2	1.95	0.48
1:C:226:GLN:O	1:C:227:LEU:C	2.56	0.48
1:D:150:VAL:CG1	1:D:433:LEU:HD11	2.36	0.48
1:D:206:GLU:C	1:D:208:SER:H	2.21	0.48
1:D:330:SER:HB2	1:D:342:SER:CB	2.43	0.48
1:E:559:GLU:O	1:E:560:ARG:HG3	2.13	0.48
1:F:68:GLN:HB3	1:F:69:ARG:HH11	1.74	0.48
1:F:197:TRP:CE2	1:F:223:VAL:HG21	2.48	0.48
1:F:392:LYS:NZ	1:F:396:ASP:OD2	2.46	0.48
1:A:487:ASP:O	1:A:488:ASN:HB3	2.12	0.48
1:B:454:ARG:CZ	1:B:567:ARG:HD2	2.43	0.48
1:C:40:LEU:HD13	1:C:57:MET:HG3	1.95	0.48
1:D:506:ASP:OD2	1:D:521:ARG:NE	2.46	0.48
1:E:411:MET:CE	1:E:468:ASN:ND2	2.69	0.48
1:A:214:ASP:OD2	1:A:616:TYR:N	2.43	0.48
1:A:408:PHE:CA	1:A:641:ASN:OD1	2.61	0.48
1:A:529:THR:HG21	1:A:566:ASP:OD1	2.13	0.48
1:B:214:ASP:OD2	1:B:616:TYR:N	2.40	0.48
1:C:392:LYS:NZ	1:C:396:ASP:OD2	2.46	0.48
3:C:687:HOH:O	1:D:576:GLU:HG2	2.13	0.48
1:D:158:LYS:HD3	1:D:446:VAL:CG1	2.44	0.48
1:E:17:LEU:CD2	1:E:103:ALA:O	2.62	0.48
1:E:66:LEU:CD2	1:E:67:GLU:N	2.77	0.48
1:E:68:GLN:HB3	1:E:69:ARG:HH11	1.76	0.48
1:E:423:ILE:HD11	1:E:652:HIS:CD2	2.47	0.48
1:E:641:ASN:C	1:E:641:ASN:HD22	2.20	0.48
1:F:475:LEU:HD23	1:F:476:ALA:N	2.28	0.48
1:F:559:GLU:O	1:F:560:ARG:HG3	2.13	0.48
1:A:120:TYR:OH	1:A:135:PRO:O	2.31	0.48
1:A:307:ASP:C	1:A:307:ASP:OD1	2.55	0.48
1:A:396:ASP:O	1:A:629:ARG:NH1	2.47	0.48
1:C:37:PHE:CZ	1:C:101:SER:HB3	2.49	0.48
1:C:284:ALA:O	1:C:350:MET:HE1	2.13	0.48
1:E:226:GLN:O	1:E:227:LEU:C	2.55	0.48
1:F:343:LEU:HD11	3:F:861:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:434:ILE:HD11	1:F:447:GLU:HA	1.96	0.48
1:A:7:ASN:O	1:A:11:GLN:HB3	2.14	0.48
1:A:77:THR:HG22	1:A:80:ARG:HH12	1.78	0.48
1:A:90:LEU:HA	1:A:90:LEU:HD12	1.45	0.48
1:C:235:ARG:O	1:C:240:LEU:HB2	2.13	0.48
1:C:259:LEU:HD11	1:F:363:LEU:HD12	1.94	0.48
1:C:592:ASP:O	1:C:619:ASN:ND2	2.36	0.48
1:E:40:LEU:HD13	1:E:57:MET:HG3	1.94	0.48
1:E:424:THR:HA	1:E:457:HIS:HA	1.95	0.48
1:A:48:ASP:OD2	1:A:52:ALA:N	2.46	0.48
1:A:512:VAL:HA	1:A:513:PRO:HD3	1.83	0.48
1:B:201:PHE:HB3	1:B:216:LYS:CD	2.44	0.48
1:C:7:ASN:O	1:C:9:GLN:N	2.46	0.48
1:D:7:ASN:O	1:D:9:GLN:N	2.45	0.48
1:D:48:ASP:HB3	1:D:92:GLN:NE2	2.28	0.48
1:D:380:PHE:CE1	1:D:384:HIS:CE1	3.02	0.48
1:E:7:ASN:O	1:E:11:GLN:N	2.39	0.48
1:F:215:ARG:O	1:F:216:LYS:C	2.55	0.48
1:F:235:ARG:O	1:F:240:LEU:HB2	2.14	0.48
1:A:190:MET:HE2	1:A:565:PRO:HD2	1.94	0.48
1:A:464:ILE:O	1:A:464:ILE:CG2	2.62	0.48
1:B:20:LYS:H	1:B:435:ASN:ND2	2.11	0.48
1:B:59:GLU:HG3	1:B:85:MET:CE	2.43	0.48
1:B:256:PHE:C	1:B:256:PHE:HD1	2.17	0.48
1:C:222:TRP:CD1	1:C:622:LEU:HD23	2.49	0.48
1:D:420:GLY:C	1:D:421:GLU:OE1	2.57	0.48
1:E:150:VAL:CG1	1:E:433:LEU:HD11	2.41	0.48
1:E:284:ALA:O	1:E:350:MET:HE1	2.14	0.48
1:A:139:GLN:HE21	1:A:431:TYR:HB2	1.79	0.48
1:A:305:ILE:HG13	1:A:315:ILE:CG2	2.37	0.48
1:A:316:ARG:HG3	1:A:398:PHE:HE1	1.79	0.48
1:A:430:GLN:HA	1:A:450:ALA:O	2.14	0.48
1:B:68:GLN:HA	1:B:111:ASN:HA	1.95	0.48
1:B:280:VAL:HG22	1:B:283:VAL:HG23	1.96	0.48
1:C:7:ASN:O	1:C:11:GLN:N	2.37	0.48
1:C:434:ILE:HD11	1:C:447:GLU:HA	1.96	0.48
1:D:66:LEU:HD23	1:D:67:GLU:H	1.78	0.48
1:D:215:ARG:O	1:D:216:LYS:C	2.56	0.48
1:E:493:LEU:HA	1:E:497:GLU:OE1	2.13	0.48
1:A:614:GLU:H	1:A:614:GLU:HG3	1.23	0.48
1:B:239:TRP:CH2	1:B:574:LYS:CE	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:GLU:H	1:B:354:GLN:NE2	2.10	0.48
1:B:300:ILE:CG1	1:B:324:LEU:HD11	2.42	0.48
1:B:526:SER:OG	1:B:527:SER:N	2.46	0.48
1:C:53:VAL:HG22	1:C:89:VAL:HG13	1.95	0.48
1:C:71:TRP:CZ3	1:C:365:PRO:HG2	2.49	0.48
1:C:460:PHE:HE2	1:C:462:TYR:CZ	2.32	0.48
1:D:27:TYR:HA	1:D:28:PRO:HD2	1.60	0.48
1:D:641:ASN:ND2	1:D:641:ASN:H	2.12	0.48
1:E:66:LEU:HD23	1:E:67:GLU:H	1.79	0.48
1:F:112:GLU:O	1:F:116:VAL:HG23	2.14	0.48
1:A:53:VAL:C	1:A:55:THR:N	2.70	0.47
1:A:295:ARG:NE	1:A:339:TYR:CE1	2.82	0.47
1:A:564:ILE:HB	1:A:565:PRO:CD	2.44	0.47
1:A:593:THR:O	1:A:595:GLY:N	2.47	0.47
1:C:69:ARG:HG3	1:C:69:ARG:HH11	1.78	0.47
1:C:458:ASN:O	1:C:459:GLU:C	2.57	0.47
1:C:543:ALA:HA	1:C:553:LEU:HD11	1.96	0.47
3:C:687:HOH:O	1:D:575:PRO:HB2	2.13	0.47
1:D:69:ARG:HG3	1:D:69:ARG:HH11	1.79	0.47
1:D:251:ILE:HG23	1:D:276:HIS:NE2	2.28	0.47
1:D:494:THR:O	1:D:495:LEU:C	2.56	0.47
1:F:402:THR:O	1:F:405:ASN:HB2	2.14	0.47
1:A:115:PHE:CZ	1:A:119:LEU:HD22	2.49	0.47
1:A:158:LYS:HD2	1:A:158:LYS:O	2.14	0.47
1:A:588:ASP:O	1:A:589:GLY:C	2.56	0.47
1:B:269:PRO:CB	1:B:363:LEU:HD23	2.44	0.47
1:B:300:ILE:HG12	1:B:324:LEU:CD1	2.44	0.47
1:B:367:VAL:HA	1:B:373:THR:CG2	2.44	0.47
1:D:494:THR:H	1:D:497:GLU:HB2	1.79	0.47
1:D:537:GLN:O	1:D:540:LYS:N	2.44	0.47
1:E:271:ARG:HA	1:E:272:PRO:HD3	1.67	0.47
1:E:343:LEU:HD11	3:E:861:HOH:O	2.14	0.47
1:F:330:SER:HB2	1:F:342:SER:CB	2.44	0.47
1:A:248:TRP:CH2	1:A:289:LEU:CD1	2.91	0.47
1:A:403:HIS:C	1:A:405:ASN:H	2.22	0.47
1:A:593:THR:C	1:A:595:GLY:H	2.22	0.47
1:B:95:GLU:O	1:B:96:TRP:C	2.55	0.47
1:B:226:GLN:O	1:B:227:LEU:C	2.56	0.47
1:C:641:ASN:ND2	1:C:641:ASN:H	2.12	0.47
1:F:301:ASP:OD2	1:F:393:LYS:NZ	2.47	0.47
1:F:573:SER:HA	1:F:578:MET:CE	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:SER:O	1:A:123:VAL:C	2.57	0.47
1:A:201:PHE:N	1:A:201:PHE:CD1	2.82	0.47
1:A:351:LEU:HD13	1:A:379:SER:OG	2.14	0.47
1:A:366:GLY:H	1:A:369:GLU:HG3	1.79	0.47
1:A:424:THR:HA	1:A:457:HIS:HA	1.95	0.47
1:A:496:ASP:OD1	1:A:499:ARG:HD3	2.13	0.47
1:B:628:ARG:O	1:B:630:ILE:HG13	2.15	0.47
1:D:343:LEU:C	1:D:343:LEU:CD2	2.87	0.47
1:E:37:PHE:CZ	1:E:101:SER:HB3	2.48	0.47
1:E:485:ILE:O	1:E:492:THR:HA	2.15	0.47
1:F:37:PHE:CZ	1:F:101:SER:HB3	2.49	0.47
1:F:39:PRO:O	1:F:53:VAL:HG11	2.14	0.47
1:F:239:TRP:CH2	1:F:574:LYS:CD	2.87	0.47
1:A:237:SER:OG	1:A:578:MET:CE	2.61	0.47
1:A:422:LEU:HD23	1:A:422:LEU:HA	1.47	0.47
1:E:34:ALA:O	1:E:109:ARG:NH2	2.48	0.47
1:E:454:ARG:CZ	1:E:567:ARG:HD2	2.43	0.47
1:E:573:SER:OG	1:E:574:LYS:N	2.45	0.47
1:A:12:GLN:OE1	1:A:547:VAL:HG21	2.15	0.47
1:A:256:PHE:CD2	1:A:378:PRO:HD3	2.50	0.47
1:A:378:PRO:C	1:A:380:PHE:N	2.71	0.47
1:A:508:PHE:CZ	3:A:864:HOH:O	2.67	0.47
1:B:491:ILE:O	1:B:492:THR:HG23	2.14	0.47
1:C:215:ARG:O	1:C:216:LYS:C	2.55	0.47
1:D:48:ASP:CA	1:D:92:GLN:HE21	2.27	0.47
1:D:66:LEU:CD2	1:D:67:GLU:N	2.77	0.47
1:E:235:ARG:O	1:E:240:LEU:HB2	2.14	0.47
1:F:458:ASN:O	1:F:459:GLU:C	2.56	0.47
1:A:27:TYR:HA	1:A:28:PRO:HD2	1.66	0.47
1:A:65:LEU:HD12	1:A:65:LEU:HA	1.65	0.47
1:A:105:TYR:OH	1:A:109:ARG:NH1	2.47	0.47
1:A:151:ILE:HA	1:A:151:ILE:HD13	1.43	0.47
1:A:275:ILE:CG2	1:A:275:ILE:O	2.57	0.47
1:A:482:LEU:HB2	1:A:505:LEU:HD22	1.96	0.47
1:A:630:ILE:HD13	1:A:636:ILE:HD11	1.97	0.47
1:A:634:ARG:NH1	1:A:634:ARG:CG	2.41	0.47
1:B:21:ILE:HG13	1:B:21:ILE:O	2.14	0.47
1:B:126:SER:O	1:B:127:LYS:C	2.56	0.47
1:B:132:ILE:CG2	1:B:133:VAL:N	2.76	0.47
1:B:205:TRP:NE1	1:B:213:LEU:HD13	2.30	0.47
1:B:218:GLU:N	1:B:322:GLU:HB3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ASP:CG	1:B:393:LYS:NZ	2.71	0.47
1:B:385:LYS:HE2	3:B:750:HOH:O	2.14	0.47
1:B:403:HIS:C	1:B:405:ASN:N	2.70	0.47
1:B:423:ILE:HA	1:B:650:VAL:O	2.15	0.47
1:C:112:GLU:O	1:C:116:VAL:HG23	2.14	0.47
1:C:494:THR:O	1:C:495:LEU:C	2.57	0.47
1:C:573:SER:OG	1:C:574:LYS:N	2.47	0.47
1:D:37:PHE:CZ	1:D:101:SER:HB3	2.50	0.47
1:D:56:LEU:HD11	1:D:65:LEU:HD21	1.96	0.47
1:D:159:MET:HE2	1:E:155:TYR:HB3	1.96	0.47
1:D:255:GLY:H	1:D:273:ASP:HB3	1.79	0.47
1:D:301:ASP:OD2	1:D:393:LYS:NZ	2.48	0.47
1:D:413:VAL:HA	1:D:466:MET:HB2	1.93	0.47
1:D:491:ILE:O	1:D:492:THR:HG23	2.15	0.47
1:D:521:ARG:HB3	3:D:864:HOH:O	2.14	0.47
1:E:31:LYS:O	1:E:35:GLU:HG3	2.15	0.47
1:E:521:ARG:NH2	1:E:525:ASP:O	2.48	0.47
1:E:554:ASP:C	1:E:556:SER:H	2.23	0.47
1:E:568:MET:O	1:E:569:LEU:C	2.57	0.47
1:F:19:ASP:O	1:F:20:LYS:C	2.57	0.47
1:F:620:ARG:C	1:F:621:PRO:O	2.55	0.47
1:F:641:ASN:C	1:F:641:ASN:HD22	2.23	0.47
1:A:43:THR:HG23	1:A:49:HIS:C	2.40	0.47
1:A:89:VAL:O	1:A:90:LEU:C	2.58	0.47
1:A:364:PRO:HB2	1:A:365:PRO:CD	2.45	0.47
1:C:177:ARG:CG	1:F:360:LYS:HB3	2.45	0.47
1:C:301:ASP:OD2	1:C:393:LYS:NZ	2.48	0.47
1:C:543:ALA:O	1:C:547:VAL:HG12	2.15	0.47
1:C:620:ARG:C	1:C:621:PRO:O	2.55	0.47
1:D:43:THR:HG23	1:D:49:HIS:C	2.40	0.47
1:A:226:GLN:OE1	1:A:504:GLU:N	2.28	0.47
1:A:411:MET:CE	1:A:512:VAL:HG11	2.35	0.47
1:A:487:ASP:CB	1:A:491:ILE:H	2.28	0.47
1:A:533:MET:HE3	1:A:533:MET:N	2.25	0.47
1:B:160:THR:O	1:B:161:GLN:HB2	2.15	0.47
1:B:353:ARG:HE	1:B:369:GLU:CD	2.21	0.47
1:B:399:PRO:O	1:B:628:ARG:HD3	2.15	0.47
1:B:517:GLU:CG	1:B:518:THR:N	2.76	0.47
1:C:323:LEU:HD11	3:C:849:HOH:O	2.15	0.47
1:C:493:LEU:HA	1:C:497:GLU:OE1	2.14	0.47
1:F:66:LEU:CD2	1:F:67:GLU:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:486:GLU:HA	1:F:492:THR:HA	1.97	0.47
1:A:34:ALA:O	1:A:109:ARG:NH2	2.48	0.47
1:A:368:MET:CE	1:A:380:PHE:HA	2.40	0.47
1:B:121:VAL:CG2	1:B:199:MET:HG2	2.35	0.47
1:B:219:LEU:HD12	1:B:219:LEU:HA	1.59	0.47
1:B:488:ASN:H	1:B:490:GLY:N	2.13	0.47
1:C:408:PHE:CE2	1:C:411:MET:HG2	2.50	0.47
1:E:43:THR:HG23	1:E:49:HIS:O	2.15	0.47
1:A:338:GLN:HG2	1:A:338:GLN:O	2.15	0.46
1:B:66:LEU:N	1:B:82:GLU:OE1	2.33	0.46
1:B:287:HIS:C	1:B:289:LEU:N	2.73	0.46
1:B:521:ARG:HG2	1:B:522:SER:N	2.30	0.46
1:C:39:PRO:O	1:C:53:VAL:HG11	2.15	0.46
1:C:237:SER:HA	1:C:574:LYS:CE	2.42	0.46
1:C:280:VAL:HG21	1:C:353:ARG:HG3	1.97	0.46
1:D:8:ALA:O	1:D:547:VAL:HG22	2.14	0.46
1:D:139:GLN:NE2	1:D:432:SER:H	2.13	0.46
1:E:69:ARG:HG3	1:E:69:ARG:HH11	1.80	0.46
1:F:641:ASN:ND2	1:F:641:ASN:H	2.12	0.46
1:A:321:ILE:O	1:A:321:ILE:CG1	2.63	0.46
1:A:632:ASP:CG	1:A:634:ARG:HB2	2.40	0.46
1:A:633:GLU:C	1:A:635:VAL:H	2.20	0.46
1:B:127:LYS:HD3	3:B:869:HOH:O	2.15	0.46
1:B:233:PHE:HE1	1:B:580:PHE:CE1	2.32	0.46
1:B:367:VAL:CG2	1:B:377:ASP:HB2	2.46	0.46
1:B:634:ARG:HG2	1:B:634:ARG:NH1	2.19	0.46
1:C:5:THR:CG2	1:C:6:GLY:H	2.22	0.46
1:C:34:ALA:O	1:C:109:ARG:NH2	2.48	0.46
1:C:60:LEU:HD11	1:C:109:ARG:HG3	1.97	0.46
1:D:69:ARG:HA	1:D:264:TYR:CD2	2.50	0.46
1:D:143:HIS:CE1	1:D:151:ILE:HG21	2.51	0.46
1:D:226:GLN:O	1:D:227:LEU:C	2.56	0.46
1:D:477:THR:HG23	1:D:509:PHE:CE1	2.50	0.46
1:A:418:ILE:CD1	1:A:462:TYR:HD1	2.26	0.46
1:A:479:ARG:NH1	1:A:587:THR:HG21	2.31	0.46
1:B:180:ARG:NH2	1:B:238:ASN:O	2.47	0.46
1:B:280:VAL:HG21	1:B:353:ARG:CG	2.45	0.46
1:B:438:ASP:HA	3:B:727:HOH:O	2.15	0.46
1:C:343:LEU:HD11	3:C:861:HOH:O	2.14	0.46
1:C:375:THR:HA	1:C:380:PHE:CD2	2.49	0.46
1:D:423:ILE:HD11	1:D:652:HIS:CD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:PRO:HB2	1:E:53:VAL:CG1	2.46	0.46
1:F:60:LEU:HD11	1:F:109:ARG:HG3	1.98	0.46
1:A:40:LEU:HD21	1:A:54:GLU:CG	2.43	0.46
1:B:14:ILE:HG12	1:B:132:ILE:HD13	1.97	0.46
1:B:255:GLY:CA	1:B:271:ARG:NH1	2.71	0.46
1:B:441:GLU:O	1:B:443:ILE:HG22	2.16	0.46
1:D:5:THR:HG22	1:D:6:GLY:N	2.26	0.46
1:D:213:LEU:N	1:D:213:LEU:CD1	2.78	0.46
1:D:462:TYR:N	1:D:521:ARG:O	2.44	0.46
1:F:7:ASN:O	1:F:11:GLN:N	2.39	0.46
1:F:573:SER:HA	1:F:578:MET:HE2	1.96	0.46
1:A:466:MET:CE	3:A:834:HOH:O	2.64	0.46
1:A:532:ASP:HB3	3:A:748:HOH:O	2.16	0.46
1:B:5:THR:O	1:B:5:THR:OG1	2.34	0.46
1:B:184:PHE:CD1	1:B:184:PHE:C	2.94	0.46
1:C:9:GLN:O	1:C:10:LYS:C	2.59	0.46
1:C:396:ASP:O	1:C:629:ARG:NH1	2.47	0.46
1:C:641:ASN:C	1:C:641:ASN:HD22	2.23	0.46
1:D:468:ASN:HB3	1:D:514:SER:CA	2.46	0.46
1:D:493:LEU:HB2	1:D:497:GLU:HB2	1.97	0.46
1:E:256:PHE:C	1:E:256:PHE:HD1	2.20	0.46
1:E:475:LEU:HD23	1:E:476:ALA:H	1.80	0.46
1:F:69:ARG:HG3	1:F:69:ARG:HH11	1.79	0.46
1:F:213:LEU:N	1:F:213:LEU:CD1	2.78	0.46
1:F:573:SER:OG	1:F:574:LYS:N	2.45	0.46
1:A:14:ILE:HD13	1:A:96:TRP:HZ2	1.81	0.46
1:A:185:GLY:CA	1:A:375:THR:CG2	2.94	0.46
1:B:322:GLU:C	1:B:324:LEU:N	2.72	0.46
1:B:522:SER:O	1:B:525:ASP:N	2.48	0.46
1:B:532:ASP:N	1:B:532:ASP:OD1	2.49	0.46
1:B:610:GLY:O	1:B:612:HIS:N	2.49	0.46
1:C:213:LEU:N	1:C:213:LEU:CD1	2.78	0.46
1:D:284:ALA:O	1:D:350:MET:HE1	2.16	0.46
1:E:197:TRP:CE2	1:E:223:VAL:HG21	2.50	0.46
1:E:330:SER:HB2	1:E:342:SER:CB	2.46	0.46
1:F:56:LEU:HD11	1:F:65:LEU:HD21	1.97	0.46
1:F:143:HIS:CE1	1:F:151:ILE:HG21	2.51	0.46
1:F:477:THR:HG23	1:F:509:PHE:CE1	2.51	0.46
1:F:494:THR:O	1:F:495:LEU:C	2.58	0.46
1:A:296:ILE:HD12	1:A:296:ILE:HG23	1.69	0.46
1:A:402:THR:O	1:A:405:ASN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:GLN:O	1:C:15:ASN:ND2	2.48	0.46
1:C:195:VAL:CG2	1:C:196:THR:N	2.78	0.46
1:C:316:ARG:HH21	1:E:338:GLN:HE22	1.63	0.46
1:E:620:ARG:C	1:E:621:PRO:O	2.57	0.46
1:F:411:MET:CE	1:F:474:ARG:HB2	2.45	0.46
1:F:493:LEU:HB2	1:F:497:GLU:HB2	1.98	0.46
1:A:19:ASP:O	1:A:107:ARG:NH2	2.48	0.46
1:A:535:SER:O	1:A:539:LEU:HG	2.16	0.46
1:A:557:ALA:HB3	1:A:558:TYR:CE2	2.51	0.46
1:A:653:LEU:HD12	1:A:653:LEU:HA	1.64	0.46
1:B:434:ILE:CG2	1:B:434:ILE:O	2.62	0.46
1:C:69:ARG:HA	1:C:264:TYR:CD2	2.51	0.46
1:C:192:ILE:HD13	1:C:192:ILE:HA	1.87	0.46
1:D:448:ILE:O	1:D:449:ASN:ND2	2.38	0.46
1:A:132:ILE:HG22	1:A:133:VAL:N	2.29	0.46
1:A:281:ASP:CG	1:A:358:HIS:HA	2.40	0.46
1:A:466:MET:HE3	1:A:466:MET:HB2	1.84	0.46
1:B:39:PRO:HB2	1:B:53:VAL:HG12	1.98	0.46
1:B:82:GLU:O	1:B:83:ALA:C	2.59	0.46
1:B:285:HIS:O	1:B:288:ASP:HB2	2.16	0.46
1:B:413:VAL:HG23	1:B:466:MET:HE3	1.97	0.46
1:B:512:VAL:HA	1:B:513:PRO:HD2	1.54	0.46
1:B:624:TYR:CD1	1:B:625:PRO:HB3	2.51	0.46
1:C:468:ASN:OD1	1:C:470:ASN:HB2	2.16	0.46
1:D:106:PHE:O	1:D:107:ARG:C	2.59	0.46
1:D:301:ASP:CB	1:F:295:ARG:HH22	2.29	0.46
1:E:43:THR:CG2	1:E:49:HIS:O	2.64	0.46
1:E:628:ARG:O	1:E:630:ILE:HG13	2.16	0.46
1:F:34:ALA:O	1:F:109:ARG:NH2	2.48	0.46
1:A:177:ARG:HB2	1:A:178:GLU:H	1.26	0.46
1:A:406:LEU:HB2	1:A:639:VAL:HG11	1.98	0.46
1:A:574:LYS:CG	1:A:578:MET:HE2	2.46	0.46
1:B:40:LEU:N	1:B:40:LEU:HD13	2.31	0.46
1:C:39:PRO:HB3	1:C:102:ASN:HD21	1.81	0.46
1:C:66:LEU:HD22	1:C:67:GLU:O	2.16	0.46
1:D:11:GLN:O	1:D:15:ASN:ND2	2.48	0.46
1:D:256:PHE:C	1:D:256:PHE:HD1	2.24	0.46
1:D:421:GLU:O	1:D:422:LEU:HB2	2.16	0.46
1:E:127:LYS:HD3	3:E:869:HOH:O	2.16	0.46
1:E:494:THR:O	1:E:495:LEU:C	2.58	0.46
1:F:150:VAL:CG1	1:F:433:LEU:HD11	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:187:ASP:OD1	1:F:189:GLY:N	2.36	0.46
1:F:219:LEU:HD12	1:F:219:LEU:HA	1.78	0.46
1:F:396:ASP:O	1:F:629:ARG:NH1	2.47	0.46
1:B:343:LEU:HD21	1:B:386:TYR:HE2	1.80	0.45
1:B:403:HIS:C	1:B:405:ASN:H	2.24	0.45
1:C:512:VAL:HG11	3:C:834:HOH:O	2.15	0.45
1:D:151:ILE:HD13	1:D:151:ILE:HA	1.80	0.45
1:D:413:VAL:HG12	1:D:643:LYS:HG2	1.97	0.45
1:D:633:GLU:C	1:D:635:VAL:N	2.74	0.45
1:E:410:GLY:O	1:E:411:MET:C	2.59	0.45
1:E:411:MET:CE	1:E:474:ARG:HB2	2.46	0.45
1:A:23:GLU:HA	1:A:24:PRO:HD2	1.67	0.45
1:A:53:VAL:O	1:A:55:THR:N	2.49	0.45
1:A:125:HIS:CG	1:A:211:TYR:HH	2.30	0.45
1:A:275:ILE:HD13	1:A:275:ILE:HG21	1.69	0.45
1:A:307:ASP:N	1:A:311:HIS:O	2.47	0.45
1:B:46:TYR:CE2	1:B:53:VAL:HG21	2.51	0.45
1:B:418:ILE:HG21	1:B:422:LEU:HD21	1.98	0.45
1:B:443:ILE:HD12	1:B:443:ILE:HA	1.87	0.45
1:C:295:ARG:HG2	1:C:339:TYR:CZ	2.50	0.45
1:C:506:ASP:OD2	1:C:521:ARG:NE	2.48	0.45
1:D:140:ILE:HG22	1:D:141:THR:HG23	1.98	0.45
1:D:239:TRP:CH2	1:D:574:LYS:CD	2.89	0.45
1:E:143:HIS:CE1	1:E:151:ILE:HG21	2.51	0.45
1:E:177:ARG:HH11	1:E:179:GLN:HG3	1.81	0.45
1:E:408:PHE:CA	1:E:641:ASN:OD1	2.64	0.45
1:E:594:GLU:HG2	1:E:594:GLU:O	2.16	0.45
1:F:69:ARG:HA	1:F:264:TYR:CD2	2.51	0.45
1:A:380:PHE:CD1	1:A:380:PHE:C	2.94	0.45
1:A:477:THR:CG2	1:A:509:PHE:CE1	2.99	0.45
1:A:560:ARG:HB2	3:A:819:HOH:O	2.15	0.45
1:A:578:MET:O	1:A:648:LYS:HA	2.16	0.45
1:B:374:ALA:O	1:B:376:ARG:N	2.49	0.45
1:B:510:GLN:HG2	1:B:519:ILE:HD13	1.97	0.45
1:E:480:ILE:HA	1:E:583:TYR:O	2.17	0.45
1:F:72:TYR:CD1	1:F:72:TYR:C	2.95	0.45
1:A:51:ALA:O	1:A:52:ALA:O	2.35	0.45
1:A:213:LEU:CD1	1:A:213:LEU:N	2.79	0.45
1:A:236:LEU:C	1:A:238:ASN:N	2.74	0.45
1:A:291:ILE:HG23	1:A:291:ILE:HD13	1.55	0.45
1:A:368:MET:HE1	1:A:380:PHE:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:HIS:NE2	1:B:27:TYR:CE2	2.84	0.45
1:B:45:ILE:O	1:B:94:LYS:CG	2.65	0.45
1:D:9:GLN:O	1:D:10:LYS:C	2.59	0.45
1:E:106:PHE:O	1:E:107:ARG:C	2.59	0.45
1:E:343:LEU:C	1:E:343:LEU:CD2	2.90	0.45
1:F:66:LEU:HD23	1:F:67:GLU:H	1.81	0.45
1:A:16:HIS:NE2	1:A:27:TYR:CE2	2.85	0.45
1:A:135:PRO:CG	1:A:536:PHE:CE1	3.00	0.45
1:A:574:LYS:HG3	1:A:578:MET:HE2	1.98	0.45
1:A:588:ASP:O	1:A:588:ASP:OD1	2.35	0.45
1:B:366:GLY:O	1:B:367:VAL:C	2.58	0.45
1:C:206:GLU:C	1:C:208:SER:H	2.25	0.45
1:C:475:LEU:HD23	1:C:476:ALA:N	2.31	0.45
1:C:591:LYS:HB2	1:C:591:LYS:HZ2	1.82	0.45
1:E:27:TYR:HA	1:E:28:PRO:HD2	1.66	0.45
1:E:69:ARG:HA	1:E:264:TYR:CD2	2.52	0.45
1:E:419:ASP:HB3	1:E:461:THR:HG23	1.99	0.45
1:E:477:THR:HG23	1:E:509:PHE:CE1	2.51	0.45
1:F:125:HIS:HB3	1:F:211:TYR:OH	2.16	0.45
1:F:639:VAL:HG21	1:F:642:ILE:HD12	1.99	0.45
1:A:22:TYR:C	1:A:69:ARG:HH21	2.25	0.45
1:A:195:VAL:CG1	1:A:372:GLU:HB3	2.46	0.45
1:A:255:GLY:CA	1:A:271:ARG:NH1	2.73	0.45
1:A:493:LEU:CB	1:A:497:GLU:HB2	2.43	0.45
1:B:5:THR:HB	1:B:10:LYS:HE3	1.99	0.45
1:B:275:ILE:HG23	1:B:276:HIS:N	2.31	0.45
1:B:405:ASN:HD22	1:B:405:ASN:HA	1.20	0.45
1:B:582:LEU:HD23	1:B:582:LEU:C	2.42	0.45
1:C:106:PHE:O	1:C:107:ARG:C	2.59	0.45
1:C:466:MET:HE1	1:C:586:VAL:HG11	1.98	0.45
1:D:285:HIS:O	1:D:288:ASP:HB2	2.16	0.45
1:E:285:HIS:O	1:E:288:ASP:HB2	2.17	0.45
1:E:405:ASN:HD22	1:E:405:ASN:HA	1.56	0.45
1:F:78:ARG:NH1	1:F:82:GLU:OE2	2.49	0.45
1:A:260:THR:O	1:A:268:PHE:HD1	1.99	0.45
1:A:589:GLY:O	1:A:593:THR:OG1	2.33	0.45
1:B:572:LYS:O	1:B:573:SER:CB	2.60	0.45
1:C:139:GLN:NE2	1:C:432:SER:H	2.15	0.45
1:C:633:GLU:C	1:C:635:VAL:N	2.74	0.45
1:E:305:ILE:HG23	1:E:340:TYR:CE2	2.52	0.45
1:E:392:LYS:NZ	1:E:396:ASP:OD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:357:PRO:HB2	1:F:358:HIS:CE1	2.52	0.45
1:F:380:PHE:CE1	1:F:384:HIS:CE1	3.05	0.45
1:F:480:ILE:HA	1:F:583:TYR:O	2.17	0.45
1:A:253:ARG:NH1	1:A:253:ARG:HG3	2.30	0.45
1:A:330:SER:HB2	1:A:342:SER:OG	2.16	0.45
1:B:11:GLN:O	1:B:12:GLN:C	2.57	0.45
1:B:40:LEU:HD12	1:B:40:LEU:HA	1.55	0.45
1:B:149:GLU:O	1:B:150:VAL:C	2.58	0.45
1:B:158:LYS:CG	1:B:437:VAL:HG21	2.46	0.45
1:B:371:PHE:C	1:B:373:THR:H	2.25	0.45
1:C:215:ARG:O	1:C:217:GLY:N	2.50	0.45
1:C:636:ILE:HG23	1:C:642:ILE:HG21	1.98	0.45
1:C:639:VAL:HG21	1:C:642:ILE:HD12	1.98	0.45
1:D:628:ARG:O	1:D:630:ILE:HG13	2.16	0.45
1:E:56:LEU:HD11	1:E:65:LEU:HD21	1.99	0.45
1:E:215:ARG:O	1:E:217:GLY:N	2.50	0.45
1:E:256:PHE:CE2	1:E:377:ASP:HA	2.52	0.45
1:F:185:GLY:CA	1:F:375:THR:CG2	2.94	0.45
1:F:197:TRP:HZ2	1:F:219:LEU:HB3	1.81	0.45
1:F:207:ASP:OD2	1:F:212:HIS:CB	2.65	0.45
1:F:377:ASP:HA	1:F:378:PRO:HD3	1.90	0.45
1:A:489:ASN:HB3	1:A:491:ILE:HD11	1.97	0.45
1:A:491:ILE:HG12	1:F:175:LYS:HB2	1.98	0.45
1:B:147:ASN:ND2	1:B:149:GLU:HB3	2.26	0.45
1:C:285:HIS:O	1:C:288:ASP:HB2	2.17	0.45
1:C:413:VAL:HG12	1:C:643:LYS:HG3	1.99	0.45
1:C:573:SER:CB	1:C:649:ILE:HG22	2.47	0.45
1:D:305:ILE:HG23	1:D:340:TYR:CE2	2.51	0.45
1:E:197:TRP:HZ2	1:E:219:LEU:HB3	1.82	0.45
1:E:280:VAL:HG21	1:E:353:ARG:HG3	1.99	0.45
1:E:478:PHE:CZ	1:E:519:ILE:HD12	2.52	0.45
1:F:322:GLU:O	1:F:323:LEU:C	2.60	0.45
1:A:66:LEU:HD21	1:A:70:HIS:ND1	2.32	0.45
1:A:135:PRO:HG2	1:A:140:ILE:HD11	1.99	0.45
1:A:305:ILE:HB	1:A:313:ILE:HG13	1.99	0.45
1:A:349:VAL:HG13	1:A:369:GLU:CD	2.42	0.45
1:A:620:ARG:C	1:A:621:PRO:O	2.60	0.45
1:A:631:PRO:HD2	3:A:818:HOH:O	2.17	0.45
1:B:272:PRO:CD	1:B:272:PRO:O	2.62	0.45
1:B:574:LYS:HA	1:B:575:PRO:HD3	1.87	0.45
1:C:31:LYS:HA	1:C:34:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:THR:CG2	1:C:49:HIS:O	2.64	0.45
1:C:477:THR:HG23	1:C:509:PHE:CE1	2.52	0.45
1:D:147:ASN:HD22	1:D:149:GLU:HB3	1.82	0.45
1:E:56:LEU:HD11	1:E:110:MET:CE	2.32	0.45
1:E:112:GLU:O	1:E:116:VAL:HG23	2.18	0.45
1:E:125:HIS:HB3	1:E:211:TYR:OH	2.16	0.45
1:E:213:LEU:N	1:E:213:LEU:CD1	2.80	0.45
1:E:410:GLY:O	1:E:412:VAL:HG12	2.17	0.45
1:E:475:LEU:HD23	1:E:476:ALA:N	2.32	0.45
1:F:9:GLN:O	1:F:10:LYS:C	2.59	0.45
1:F:84:LEU:HD11	1:F:204:TRP:CE2	2.52	0.45
1:F:222:TRP:CD1	1:F:622:LEU:HD23	2.52	0.45
1:A:538:SER:O	1:A:542:GLN:HG3	2.18	0.44
1:B:14:ILE:CD1	1:B:96:TRP:CZ2	3.00	0.44
1:B:42:ASP:OD1	1:B:44:SER:HB3	2.16	0.44
1:B:56:LEU:O	1:B:57:MET:C	2.60	0.44
1:B:473:GLU:O	1:B:474:ARG:HG2	2.17	0.44
1:B:610:GLY:O	1:B:611:VAL:C	2.60	0.44
1:B:633:GLU:C	1:B:635:VAL:N	2.74	0.44
1:C:125:HIS:HB3	1:C:211:TYR:OH	2.17	0.44
1:C:151:ILE:HD13	1:C:151:ILE:HA	1.76	0.44
1:C:573:SER:HB2	1:C:649:ILE:CG2	2.47	0.44
1:C:628:ARG:O	1:C:630:ILE:HG13	2.17	0.44
1:E:72:TYR:CD1	1:E:72:TYR:C	2.95	0.44
1:F:628:ARG:O	1:F:630:ILE:HG13	2.17	0.44
1:B:13:ASP:OD2	1:B:100:ARG:HD2	2.17	0.44
1:B:222:TRP:CD1	1:B:622:LEU:CD2	3.00	0.44
1:B:517:GLU:HG2	1:B:518:THR:H	1.81	0.44
1:B:555:LEU:C	1:B:557:ALA:N	2.73	0.44
1:C:143:HIS:CE1	1:C:151:ILE:HG21	2.52	0.44
1:C:185:GLY:C	1:C:375:THR:HG22	2.41	0.44
1:C:305:ILE:HG23	1:C:340:TYR:CE2	2.53	0.44
1:C:433:LEU:HG	1:C:450:ALA:HB2	1.99	0.44
1:C:573:SER:HB2	1:C:649:ILE:HG22	1.98	0.44
1:D:37:PHE:CE1	1:D:101:SER:HB3	2.52	0.44
1:D:433:LEU:HG	1:D:450:ALA:HB2	2.00	0.44
1:D:462:TYR:HB3	1:D:464:ILE:CD1	2.47	0.44
1:E:60:LEU:HD11	1:E:109:ARG:HG3	2.00	0.44
1:E:380:PHE:CD2	1:E:380:PHE:C	2.95	0.44
1:F:285:HIS:O	1:F:288:ASP:HB2	2.17	0.44
1:A:304:TYR:CD1	1:A:312:THR:HB	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ILE:HG21	1:A:305:ILE:HD13	1.68	0.44
1:A:466:MET:HE1	3:A:834:HOH:O	2.18	0.44
1:A:521:ARG:HG2	1:A:522:SER:N	2.33	0.44
1:B:82:GLU:C	1:B:85:MET:H	2.24	0.44
1:B:130:ASP:O	1:B:559:GLU:CD	2.61	0.44
1:B:304:TYR:HD1	1:B:306:THR:HG22	1.82	0.44
1:C:197:TRP:HZ2	1:C:219:LEU:HB3	1.82	0.44
1:C:271:ARG:HA	1:C:272:PRO:HD3	1.81	0.44
1:C:408:PHE:CB	1:C:641:ASN:OD1	2.65	0.44
1:D:197:TRP:HZ2	1:D:219:LEU:HB3	1.82	0.44
1:D:480:ILE:HA	1:D:583:TYR:O	2.17	0.44
1:E:357:PRO:HB2	1:E:358:HIS:CE1	2.53	0.44
1:F:106:PHE:O	1:F:107:ARG:C	2.60	0.44
1:F:127:LYS:H	1:F:127:LYS:HG2	1.46	0.44
1:A:57:MET:C	1:A:61:ASN:HD22	2.25	0.44
1:A:559:GLU:H	1:A:559:GLU:HG2	1.70	0.44
1:B:47:ASN:N	1:B:92:GLN:O	2.49	0.44
1:B:48:ASP:OD2	1:B:52:ALA:N	2.49	0.44
1:B:496:ASP:H	1:B:498:ALA:H	1.66	0.44
1:C:300:ILE:HD11	1:C:390:ILE:HG22	2.00	0.44
1:C:316:ARG:HH21	1:E:338:GLN:NE2	2.16	0.44
1:C:330:SER:HB2	1:C:342:SER:CB	2.47	0.44
1:D:420:GLY:HA2	1:D:421:GLU:OE1	2.18	0.44
1:E:230:ARG:NH2	1:E:569:LEU:O	2.50	0.44
1:F:11:GLN:O	1:F:15:ASN:ND2	2.50	0.44
1:A:192:ILE:HD13	1:A:192:ILE:HA	1.93	0.44
1:A:199:MET:CE	3:A:774:HOH:O	2.65	0.44
1:B:34:ALA:O	1:B:109:ARG:NH2	2.50	0.44
1:B:84:LEU:HD21	1:B:204:TRP:CD2	2.53	0.44
1:B:319:LYS:HD3	1:B:319:LYS:HA	1.94	0.44
1:C:66:LEU:CD2	1:C:67:GLU:N	2.80	0.44
1:C:256:PHE:C	1:C:256:PHE:HD1	2.23	0.44
1:C:271:ARG:NH2	1:C:377:ASP:OD1	2.51	0.44
1:C:414:ASN:HD21	1:C:467:SER:H	1.64	0.44
1:C:480:ILE:HA	1:C:583:TYR:O	2.17	0.44
1:D:193:HIS:O	1:D:194:HIS:C	2.60	0.44
1:D:207:ASP:OD2	1:D:212:HIS:CB	2.65	0.44
1:D:220:PHE:CZ	1:D:329:GLU:HB2	2.52	0.44
1:D:256:PHE:HA	1:E:361:PHE:CE1	2.53	0.44
1:D:418:ILE:HD13	1:D:422:LEU:HD11	2.00	0.44
1:D:639:VAL:HG23	1:D:641:ASN:HD22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:LYS:HA	1:E:96:TRP:NE1	2.32	0.44
1:E:323:LEU:HD11	3:E:849:HOH:O	2.17	0.44
1:F:39:PRO:HB3	1:F:102:ASN:HD21	1.82	0.44
1:A:56:LEU:HD11	1:A:65:LEU:HD21	2.00	0.44
1:A:85:MET:CE	3:A:808:HOH:O	2.53	0.44
1:A:461:THR:OG1	1:A:520:GLU:CG	2.65	0.44
1:A:509:PHE:CE1	1:A:593:THR:HG23	2.53	0.44
1:B:37:PHE:CE2	1:B:101:SER:CB	2.99	0.44
1:B:298:GLU:HG2	1:B:302:HIS:HD2	1.82	0.44
1:C:56:LEU:HD11	1:C:65:LEU:HD21	1.99	0.44
1:C:302:HIS:ND1	1:C:304:TYR:CZ	2.85	0.44
1:D:591:LYS:C	1:D:594:GLU:HB2	2.43	0.44
1:E:66:LEU:HD23	1:E:67:GLU:N	2.32	0.44
1:E:84:LEU:HD11	1:E:204:TRP:CE2	2.52	0.44
1:E:322:GLU:O	1:E:323:LEU:C	2.61	0.44
1:A:629:ARG:C	1:A:631:PRO:HD3	2.42	0.44
1:B:296:ILE:HG21	1:B:390:ILE:HG21	1.98	0.44
1:B:484:PRO:HD2	1:B:498:ALA:HB1	2.00	0.44
1:C:84:LEU:HD11	1:C:204:TRP:CE2	2.52	0.44
1:D:40:LEU:HD12	1:D:53:VAL:CG1	2.42	0.44
1:D:71:TRP:CZ3	1:D:365:PRO:HG2	2.53	0.44
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.64	0.44
1:A:473:GLU:O	1:A:512:VAL:O	2.36	0.44
1:A:615:ALA:O	1:A:616:TYR:C	2.61	0.44
1:B:631:PRO:HD2	3:B:818:HOH:O	2.17	0.44
1:C:39:PRO:HB2	1:C:53:VAL:CG1	2.48	0.44
1:C:207:ASP:OD2	1:C:212:HIS:CB	2.65	0.44
1:D:46:TYR:CE2	1:D:53:VAL:HG21	2.51	0.44
1:E:157:ALA:HB3	1:E:448:ILE:CD1	2.47	0.44
1:E:301:ASP:OD2	1:E:393:LYS:NZ	2.50	0.44
1:E:641:ASN:ND2	1:E:641:ASN:N	2.62	0.44
1:F:215:ARG:O	1:F:217:GLY:N	2.51	0.44
1:A:553:LEU:HD23	1:A:553:LEU:HA	1.81	0.44
1:B:295:ARG:NE	1:B:339:TYR:CE1	2.86	0.44
1:B:442:ASN:N	1:B:442:ASN:ND2	2.66	0.44
1:C:56:LEU:HD21	1:C:110:MET:CE	2.48	0.44
1:D:259:LEU:HD11	1:E:363:LEU:CD1	2.48	0.44
1:D:317:GLN:CB	1:D:318:PRO:HD2	2.28	0.44
1:D:385:LYS:HE2	3:D:750:HOH:O	2.17	0.44
1:D:393:LYS:HE3	1:D:393:LYS:HB3	1.82	0.44
1:E:639:VAL:HG21	1:E:642:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:LEU:HD21	1:F:110:MET:CE	2.48	0.44
1:F:125:HIS:CE1	1:F:200:ASP:O	2.71	0.44
1:A:82:GLU:OE1	1:A:114:GLU:OE2	2.36	0.43
1:A:146:THR:O	1:A:147:ASN:O	2.35	0.43
1:A:470:ASN:O	1:A:471:ASP:C	2.61	0.43
1:A:508:PHE:HE2	3:A:864:HOH:O	1.94	0.43
1:B:367:VAL:O	1:B:373:THR:HG22	2.18	0.43
1:B:624:TYR:HA	1:B:625:PRO:HA	1.85	0.43
1:C:405:ASN:HD22	1:C:405:ASN:HA	1.53	0.43
1:D:165:THR:HG22	1:D:449:ASN:CB	2.25	0.43
1:D:195:VAL:CG2	1:D:196:THR:N	2.81	0.43
1:D:222:TRP:CH2	1:D:226:GLN:NE2	2.86	0.43
1:E:168:VAL:HG22	1:E:452:VAL:HA	2.00	0.43
1:E:178:GLU:HG3	1:E:178:GLU:O	2.18	0.43
1:E:464:ILE:O	1:E:519:ILE:N	2.51	0.43
1:F:43:THR:CG2	1:F:49:HIS:O	2.66	0.43
1:F:158:LYS:NZ	1:F:439:SER:HB2	2.33	0.43
1:F:305:ILE:HG23	1:F:340:TYR:CE2	2.53	0.43
1:F:424:THR:O	1:F:651:HIS:ND1	2.37	0.43
1:A:126:SER:O	1:A:128:LEU:N	2.51	0.43
1:A:296:ILE:HD11	1:A:340:TYR:HB3	2.00	0.43
1:A:416:VAL:CG1	1:A:643:LYS:HG3	2.48	0.43
1:A:424:THR:O	1:A:651:HIS:HA	2.18	0.43
1:A:574:LYS:CE	1:A:578:MET:HE2	2.48	0.43
1:A:618:ASP:OD1	1:A:620:ARG:N	2.51	0.43
1:B:158:LYS:HD3	1:B:446:VAL:HG11	1.99	0.43
1:B:177:ARG:NH1	1:B:179:GLN:CG	2.80	0.43
1:B:639:VAL:HG21	1:B:642:ILE:HD12	2.00	0.43
1:C:43:THR:HG23	1:C:49:HIS:O	2.16	0.43
1:C:125:HIS:CE1	1:C:200:ASP:O	2.71	0.43
1:C:614:GLU:H	1:C:614:GLU:HG3	1.40	0.43
1:D:60:LEU:HD11	1:D:109:ARG:HG3	2.00	0.43
1:D:396:ASP:O	1:D:629:ARG:NH1	2.49	0.43
1:D:641:ASN:ND2	1:D:641:ASN:N	2.64	0.43
1:E:125:HIS:CE1	1:E:200:ASP:O	2.71	0.43
1:E:441:GLU:C	1:E:443:ILE:H	2.26	0.43
1:F:39:PRO:HB2	1:F:53:VAL:CG1	2.49	0.43
1:F:177:ARG:HH11	1:F:179:GLN:HG3	1.84	0.43
1:A:230:ARG:CZ	1:A:503:ILE:HD12	2.48	0.43
1:B:18:LEU:CD1	1:B:135:PRO:HG2	2.47	0.43
1:B:241:ASP:HA	1:B:242:PRO:HD3	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ILE:HG22	1:C:141:THR:HG23	2.00	0.43
1:C:168:VAL:HG22	1:C:452:VAL:HA	1.99	0.43
1:C:322:GLU:O	1:C:323:LEU:C	2.60	0.43
1:C:411:MET:CE	1:C:512:VAL:HB	2.47	0.43
1:D:34:ALA:O	1:D:109:ARG:NH2	2.51	0.43
1:D:81:LYS:O	1:D:85:MET:HG2	2.18	0.43
1:D:270:VAL:HG13	1:E:270:VAL:HG13	2.00	0.43
1:D:419:ASP:CB	1:D:463:LYS:HD2	2.47	0.43
1:E:207:ASP:OD2	1:E:212:HIS:CB	2.66	0.43
1:E:522:SER:C	1:E:524:LYS:N	2.74	0.43
1:F:280:VAL:HG21	1:F:353:ARG:HG3	2.00	0.43
1:F:380:PHE:CD2	1:F:380:PHE:C	2.96	0.43
1:F:494:THR:H	1:F:497:GLU:HB2	1.83	0.43
1:F:591:LYS:NZ	1:F:591:LYS:CB	2.81	0.43
1:A:237:SER:OG	1:A:578:MET:HE3	2.18	0.43
1:A:258:PRO:HG2	1:A:259:LEU:N	2.32	0.43
1:A:287:HIS:O	1:A:291:ILE:N	2.40	0.43
1:A:391:PHE:O	1:A:392:LYS:C	2.57	0.43
1:A:406:LEU:HA	1:A:406:LEU:HD23	1.69	0.43
1:A:475:LEU:HA	1:A:511:LYS:HA	2.00	0.43
1:A:495:LEU:HD13	1:A:583:TYR:OH	2.19	0.43
1:B:162:LYS:HA	1:B:163:PRO:HD3	1.77	0.43
1:B:195:VAL:HG11	1:B:372:GLU:HB3	1.99	0.43
1:B:433:LEU:HB2	1:B:448:ILE:CG2	2.48	0.43
1:B:639:VAL:HG23	1:B:641:ASN:HD22	1.83	0.43
1:C:219:LEU:HD12	1:C:219:LEU:HA	1.79	0.43
1:D:5:THR:CG2	1:D:6:GLY:H	2.18	0.43
1:D:86:LEU:HD23	1:D:86:LEU:O	2.19	0.43
1:D:150:VAL:HG21	1:D:168:VAL:CG1	2.30	0.43
1:D:200:ASP:OD2	1:D:609:CYS:SG	2.77	0.43
1:D:343:LEU:HD11	3:D:861:HOH:O	2.18	0.43
1:D:465:THR:HG23	1:D:518:THR:OG1	2.18	0.43
1:E:239:TRP:CZ3	1:E:574:LYS:NZ	2.82	0.43
1:F:10:LYS:HA	1:F:96:TRP:NE1	2.34	0.43
1:F:127:LYS:HD3	3:F:869:HOH:O	2.18	0.43
1:A:60:LEU:HD22	1:A:106:PHE:CE1	2.50	0.43
1:A:124:ILE:HG22	1:A:611:VAL:HG11	2.00	0.43
1:A:441:GLU:CG	1:A:441:GLU:O	2.63	0.43
1:B:255:GLY:H	1:B:273:ASP:CB	2.29	0.43
1:B:271:ARG:HA	1:B:272:PRO:HD3	1.64	0.43
1:C:591:LYS:C	1:C:594:GLU:HB2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:HIS:CE1	1:D:200:ASP:O	2.72	0.43
1:D:125:HIS:HB3	1:D:211:TYR:OH	2.19	0.43
1:D:271:ARG:HA	1:D:272:PRO:HD3	1.81	0.43
1:E:19:ASP:O	1:E:20:LYS:C	2.60	0.43
1:E:578:MET:HG3	1:E:580:PHE:CZ	2.53	0.43
1:F:323:LEU:HD11	3:F:849:HOH:O	2.19	0.43
1:F:324:LEU:HD23	1:F:324:LEU:HA	1.80	0.43
1:A:256:PHE:CZ	1:A:377:ASP:HA	2.53	0.43
1:B:26:LYS:O	1:B:28:PRO:HD2	2.19	0.43
1:B:391:PHE:O	1:B:392:LYS:C	2.61	0.43
1:B:615:ALA:O	1:B:616:TYR:C	2.61	0.43
1:C:127:LYS:HD3	3:C:869:HOH:O	2.19	0.43
1:C:185:GLY:CA	1:C:375:THR:CG2	2.94	0.43
1:C:239:TRP:HH2	1:C:574:LYS:HD3	1.71	0.43
1:C:248:TRP:CZ3	1:C:289:LEU:HD13	2.54	0.43
1:C:256:PHE:CE2	1:C:377:ASP:HA	2.53	0.43
1:C:283:VAL:O	1:C:284:ALA:HB2	2.19	0.43
1:D:322:GLU:O	1:D:323:LEU:C	2.60	0.43
1:D:591:LYS:HB2	1:D:591:LYS:HZ2	1.84	0.43
1:D:614:GLU:H	1:D:614:GLU:HG3	1.42	0.43
1:E:11:GLN:O	1:E:15:ASN:ND2	2.51	0.43
1:E:162:LYS:C	1:E:446:VAL:HG21	2.43	0.43
1:E:428:GLU:OE2	1:E:451:ARG:HD2	2.18	0.43
1:F:185:GLY:C	1:F:375:THR:HG22	2.42	0.43
1:F:230:ARG:NH2	1:F:569:LEU:O	2.50	0.43
1:F:243:VAL:HG23	1:F:385:LYS:CD	2.48	0.43
1:F:300:ILE:HD11	1:F:390:ILE:HG22	2.00	0.43
1:F:442:ASN:HD22	1:F:442:ASN:N	2.17	0.43
1:A:11:GLN:HG3	1:A:15:ASN:ND2	2.26	0.43
1:A:69:ARG:HA	1:A:264:TYR:CD2	2.54	0.43
1:A:328:ILE:O	1:A:328:ILE:CG2	2.60	0.43
1:A:588:ASP:O	1:A:590:ASP:N	2.50	0.43
1:B:313:ILE:HD12	1:B:314:ASP:O	2.18	0.43
1:B:440:GLY:O	1:B:441:GLU:HG3	2.19	0.43
1:C:177:ARG:HH11	1:C:179:GLN:HG3	1.84	0.43
1:D:215:ARG:O	1:D:217:GLY:N	2.51	0.43
1:D:219:LEU:HD12	1:D:219:LEU:HA	1.79	0.43
1:D:364:PRO:HB2	1:D:365:PRO:CD	2.49	0.43
1:E:60:LEU:HD22	1:E:106:PHE:HE1	1.84	0.43
1:E:413:VAL:HG12	1:E:643:LYS:HG3	2.00	0.43
1:F:27:TYR:HA	1:F:28:PRO:HD2	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:178:GLU:O	1:F:178:GLU:HG3	2.18	0.43
1:F:403:HIS:C	1:F:405:ASN:N	2.76	0.43
1:F:591:LYS:C	1:F:594:GLU:HB2	2.44	0.43
1:A:177:ARG:HD3	1:A:179:GLN:HB2	2.00	0.43
1:A:191:ASN:O	1:A:192:ILE:C	2.59	0.43
1:A:275:ILE:HG12	1:A:276:HIS:N	2.34	0.43
1:A:610:GLY:O	1:A:611:VAL:C	2.61	0.43
1:A:642:ILE:HD13	1:A:642:ILE:HG21	1.83	0.43
1:B:489:ASN:HB3	1:B:491:ILE:CG1	2.49	0.43
1:B:530:VAL:HA	1:B:531:PRO:HD2	1.90	0.43
1:C:364:PRO:HB2	1:C:365:PRO:CD	2.49	0.43
1:D:185:GLY:C	1:D:375:THR:HG22	2.41	0.43
1:D:343:LEU:C	1:D:343:LEU:HD23	2.44	0.43
1:E:185:GLY:CA	1:E:375:THR:CG2	2.93	0.43
1:E:633:GLU:C	1:E:635:VAL:N	2.75	0.43
1:F:43:THR:HG23	1:F:49:HIS:O	2.17	0.43
1:F:256:PHE:C	1:F:256:PHE:HD1	2.21	0.43
1:A:424:THR:HA	1:A:456:ASN:O	2.19	0.43
1:A:593:THR:C	1:A:595:GLY:N	2.77	0.43
1:B:27:TYR:O	1:B:30:LEU:N	2.52	0.43
1:B:39:PRO:O	1:B:46:TYR:HE2	2.01	0.43
1:B:68:GLN:HG2	1:B:110:MET:O	2.18	0.43
1:C:259:LEU:HD11	1:F:363:LEU:CD1	2.49	0.43
1:C:260:THR:HG22	1:C:268:PHE:HE1	1.80	0.43
1:C:295:ARG:NE	1:C:339:TYR:CE1	2.87	0.43
1:C:403:HIS:C	1:C:405:ASN:N	2.73	0.43
1:D:155:TYR:CD1	1:E:159:MET:HE1	2.53	0.43
1:D:553:LEU:HD22	1:D:555:LEU:HG	2.00	0.43
1:E:154:ALA:HB2	1:E:433:LEU:HD13	2.01	0.43
1:E:169:SER:O	1:E:170:PHE:CB	2.67	0.43
1:E:398:PHE:HB3	1:E:399:PRO:HD2	2.01	0.43
1:F:31:LYS:HA	1:F:34:ALA:HB3	2.00	0.43
1:F:256:PHE:CE2	1:F:377:ASP:HA	2.54	0.43
1:F:433:LEU:HG	1:F:450:ALA:HB2	2.01	0.43
1:F:639:VAL:HG23	1:F:641:ASN:HD22	1.84	0.43
1:A:48:ASP:OD1	1:A:50:GLY:CA	2.66	0.43
1:A:230:ARG:NH2	1:A:569:LEU:O	2.52	0.43
1:B:14:ILE:HD13	1:B:96:TRP:CZ2	2.53	0.43
1:B:279:ASP:OD1	1:B:286:VAL:N	2.44	0.43
1:B:403:HIS:HE1	1:B:407:GLU:HG2	1.82	0.43
1:C:248:TRP:CZ2	1:C:289:LEU:HD13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:ASP:C	1:C:307:ASP:OD1	2.61	0.43
1:C:540:LYS:O	1:C:541:GLU:C	2.62	0.43
1:D:56:LEU:HD21	1:D:110:MET:CE	2.49	0.43
1:D:510:GLN:OE1	1:D:519:ILE:CG2	2.66	0.43
1:D:520:GLU:HG2	1:D:521:ARG:N	2.32	0.43
1:E:591:LYS:CA	1:E:594:GLU:HB2	2.48	0.43
1:A:133:VAL:HG22	1:A:558:TYR:HB2	2.01	0.42
1:A:190:MET:HE1	1:A:564:ILE:HG21	2.01	0.42
1:B:90:LEU:O	1:B:91:ASN:C	2.60	0.42
1:B:168:VAL:HG22	1:B:452:VAL:HA	2.01	0.42
1:B:570:LEU:HG	1:B:649:ILE:HD11	2.00	0.42
1:B:609:CYS:C	1:B:611:VAL:N	2.77	0.42
1:D:66:LEU:HD23	1:D:67:GLU:N	2.33	0.42
1:D:84:LEU:HD11	1:D:204:TRP:CE2	2.54	0.42
1:D:639:VAL:HG21	1:D:642:ILE:HD12	2.01	0.42
1:E:9:GLN:O	1:E:10:LYS:C	2.61	0.42
1:E:466:MET:O	1:E:466:MET:HG3	2.18	0.42
1:E:468:ASN:HD21	1:E:474:ARG:CG	2.30	0.42
1:F:168:VAL:HG22	1:F:452:VAL:HA	2.00	0.42
1:A:37:PHE:CE2	1:A:101:SER:HB3	2.54	0.42
1:A:86:LEU:HB3	1:A:118:ALA:CB	2.50	0.42
1:A:219:LEU:HD12	1:A:219:LEU:HA	1.91	0.42
1:A:461:THR:OG1	1:A:520:GLU:HG2	2.18	0.42
1:A:479:ARG:NH1	1:A:587:THR:CG2	2.82	0.42
1:A:480:ILE:HD13	1:A:480:ILE:HG21	1.47	0.42
1:B:23:GLU:OE2	1:B:439:SER:O	2.37	0.42
1:B:151:ILE:HD13	1:B:151:ILE:HA	1.88	0.42
1:B:151:ILE:HD13	1:B:433:LEU:HD22	2.00	0.42
1:B:262:TYR:OH	1:B:370:HIS:NE2	2.39	0.42
1:C:135:PRO:CB	1:C:140:ILE:HD11	2.48	0.42
1:C:177:ARG:HD2	1:F:360:LYS:HB3	2.01	0.42
1:C:239:TRP:CH2	1:C:574:LYS:CD	2.90	0.42
1:C:538:SER:O	1:C:542:GLN:HG3	2.18	0.42
1:D:233:PHE:O	1:D:236:LEU:HB3	2.19	0.42
1:D:554:ASP:OD1	1:D:554:ASP:C	2.58	0.42
1:E:45:ILE:HB	1:E:98:CYS:HB2	2.01	0.42
1:F:46:TYR:CD2	1:F:53:VAL:HG21	2.53	0.42
1:F:271:ARG:NH2	1:F:377:ASP:OD1	2.52	0.42
1:F:283:VAL:O	1:F:284:ALA:HB2	2.19	0.42
1:F:414:ASN:HD21	1:F:467:SER:H	1.66	0.42
1:A:100:ARG:O	1:A:101:SER:C	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:MET:HE1	1:A:564:ILE:CG2	2.49	0.42
1:A:427:ASP:CB	1:A:567:ARG:NH1	2.78	0.42
1:A:508:PHE:CD2	1:A:521:ARG:CD	3.01	0.42
1:B:192:ILE:HD12	1:B:192:ILE:HG23	1.82	0.42
1:B:197:TRP:HZ2	1:B:219:LEU:HB3	1.85	0.42
1:B:479:ARG:HD2	1:B:587:THR:CG2	2.49	0.42
1:B:570:LEU:HG	1:B:649:ILE:CD1	2.49	0.42
1:C:515:GLY:O	1:C:516:PRO:C	2.63	0.42
1:D:323:LEU:HD11	3:D:849:HOH:O	2.20	0.42
1:D:408:PHE:CE2	1:D:411:MET:SD	3.12	0.42
1:F:12:GLN:OE1	1:F:547:VAL:HG11	2.19	0.42
1:F:428:GLU:OE2	1:F:451:ARG:HD2	2.19	0.42
1:F:636:ILE:HG23	1:F:642:ILE:HG21	2.01	0.42
1:A:169:SER:O	1:A:170:PHE:CB	2.65	0.42
1:A:411:MET:HE1	1:A:474:ARG:CB	2.50	0.42
1:A:454:ARG:NH1	1:A:567:ARG:CD	2.82	0.42
1:A:529:THR:CG2	1:A:566:ASP:HA	2.48	0.42
1:B:194:HIS:C	1:B:194:HIS:CD2	2.93	0.42
1:B:201:PHE:CD1	1:B:201:PHE:N	2.88	0.42
1:B:295:ARG:HH11	1:B:295:ARG:HD2	1.34	0.42
1:B:296:ILE:HA	1:B:296:ILE:HD13	1.65	0.42
1:B:517:GLU:HG2	1:B:518:THR:N	2.34	0.42
1:C:46:TYR:CD2	1:C:53:VAL:HG21	2.54	0.42
1:C:146:THR:HG21	1:C:433:LEU:HD21	2.00	0.42
1:D:283:VAL:O	1:D:284:ALA:HB2	2.19	0.42
1:D:300:ILE:HD11	1:D:390:ILE:HG22	2.01	0.42
1:D:317:GLN:CB	1:D:318:PRO:CD	2.96	0.42
1:D:485:ILE:O	1:D:492:THR:HA	2.18	0.42
1:D:636:ILE:HG23	1:D:642:ILE:HG21	2.01	0.42
1:F:5:THR:HG22	1:F:6:GLY:N	2.28	0.42
1:F:86:LEU:O	1:F:86:LEU:HD23	2.20	0.42
1:B:26:LYS:O	1:B:28:PRO:CD	2.68	0.42
1:B:350:MET:O	1:B:354:GLN:HG2	2.19	0.42
1:C:159:MET:HE1	1:F:155:TYR:CG	2.55	0.42
1:C:178:GLU:O	1:C:178:GLU:HG3	2.20	0.42
1:C:517:GLU:HG2	1:C:518:THR:N	2.33	0.42
1:E:185:GLY:CA	1:E:375:THR:HG22	2.49	0.42
1:E:639:VAL:HG23	1:E:641:ASN:HD22	1.83	0.42
1:F:66:LEU:HD23	1:F:67:GLU:N	2.34	0.42
1:F:403:HIS:C	1:F:405:ASN:H	2.27	0.42
1:F:408:PHE:CB	1:F:641:ASN:OD1	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:593:THR:C	1:F:595:GLY:N	2.78	0.42
1:A:177:ARG:HH12	1:A:256:PHE:HB2	1.84	0.42
1:A:222:TRP:CZ3	1:A:623:GLY:HA3	2.55	0.42
1:A:271:ARG:HA	1:A:272:PRO:HD3	1.83	0.42
1:A:292:THR:O	1:A:296:ILE:HG12	2.19	0.42
1:A:578:MET:O	1:A:648:LYS:HG3	2.20	0.42
1:A:628:ARG:O	1:A:630:ILE:HG13	2.20	0.42
1:B:428:GLU:OE2	1:B:451:ARG:HD2	2.20	0.42
1:C:398:PHE:HB3	1:C:399:PRO:HD2	2.01	0.42
1:D:155:TYR:HB3	1:E:159:MET:HE2	2.00	0.42
1:D:482:LEU:HD11	1:D:580:PHE:HB2	2.02	0.42
1:D:573:SER:OG	1:D:574:LYS:N	2.48	0.42
1:F:135:PRO:CB	1:F:140:ILE:HD11	2.50	0.42
1:F:634:ARG:HH11	1:F:634:ARG:CG	2.25	0.42
1:A:197:TRP:HZ2	1:A:219:LEU:HB3	1.85	0.42
1:A:591:LYS:CA	1:A:594:GLU:HB2	2.40	0.42
1:A:606:HIS:HB3	1:A:608:GLN:H	1.83	0.42
1:C:5:THR:HG22	1:C:6:GLY:N	2.29	0.42
1:C:302:HIS:ND1	1:C:304:TYR:OH	2.53	0.42
1:C:591:LYS:NZ	1:C:591:LYS:CB	2.82	0.42
1:D:256:PHE:CE2	1:D:377:ASP:HA	2.54	0.42
1:E:634:ARG:HG2	1:E:634:ARG:NH1	2.20	0.42
1:A:619:ASN:C	1:A:620:ARG:O	2.59	0.42
1:B:419:ASP:CB	1:B:463:LYS:HD3	2.50	0.42
1:B:479:ARG:HH11	1:B:587:THR:CG2	2.33	0.42
1:B:625:PRO:C	1:B:626:LEU:HD23	2.45	0.42
1:C:78:ARG:NH1	1:C:82:GLU:OE2	2.49	0.42
1:C:127:LYS:H	1:C:127:LYS:HG2	1.48	0.42
1:C:493:LEU:HB2	1:C:497:GLU:HB2	2.02	0.42
1:E:151:ILE:HD13	1:E:151:ILE:HA	1.77	0.42
1:E:185:GLY:C	1:E:375:THR:HG22	2.41	0.42
1:E:283:VAL:O	1:E:284:ALA:HB2	2.20	0.42
1:E:364:PRO:HB2	1:E:365:PRO:CD	2.50	0.42
1:E:624:TYR:HA	1:E:625:PRO:HA	1.82	0.42
1:A:20:LYS:O	1:A:21:ILE:C	2.63	0.42
1:A:64:ARG:O	1:A:78:ARG:NH1	2.53	0.42
1:A:244:ASP:OD1	1:A:382:ARG:HD3	2.20	0.42
1:A:313:ILE:HG13	1:A:313:ILE:O	2.19	0.42
1:A:406:LEU:HD23	1:A:406:LEU:N	2.32	0.42
3:A:678:HOH:O	1:B:266:GLY:CA	2.66	0.42
1:B:14:ILE:HD13	1:B:96:TRP:HZ2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:ILE:HD11	1:B:462:TYR:HE1	1.83	0.42
1:B:485:ILE:HG13	1:B:581:ASN:HD22	1.83	0.42
1:B:533:MET:O	1:B:534:PRO:C	2.63	0.42
1:B:577:GLY:HA2	1:B:649:ILE:O	2.20	0.42
1:C:233:PHE:O	1:C:236:LEU:HB3	2.20	0.42
1:C:593:THR:C	1:C:595:GLY:N	2.78	0.42
1:D:39:PRO:HB2	1:D:53:VAL:CG1	2.50	0.42
1:D:177:ARG:HH11	1:D:179:GLN:HG3	1.83	0.42
1:E:295:ARG:NE	1:E:339:TYR:CE1	2.88	0.42
1:E:300:ILE:HD11	1:E:390:ILE:HG22	2.00	0.42
1:E:385:LYS:HE2	3:E:750:HOH:O	2.20	0.42
1:E:610:GLY:HA2	1:E:614:GLU:HB2	2.01	0.42
1:F:222:TRP:CH2	1:F:226:GLN:NE2	2.88	0.42
1:B:425:PHE:C	1:B:425:PHE:CD1	2.98	0.42
1:B:489:ASN:CB	1:B:491:ILE:HD11	2.42	0.42
1:B:553:LEU:O	1:B:554:ASP:CB	2.58	0.42
1:C:185:GLY:CA	1:C:375:THR:HG22	2.49	0.42
1:D:41:GLY:O	1:D:42:ASP:HB2	2.19	0.42
1:D:72:TYR:HD2	1:D:79:GLN:HB3	1.83	0.42
1:D:237:SER:HA	1:D:574:LYS:CE	2.47	0.42
1:D:295:ARG:NE	1:D:339:TYR:CE1	2.88	0.42
1:D:380:PHE:CD2	1:D:380:PHE:C	2.96	0.42
1:D:553:LEU:CD2	1:D:555:LEU:HG	2.50	0.42
1:D:591:LYS:CA	1:D:594:GLU:HB2	2.50	0.42
1:E:148:SER:HB2	1:E:259:LEU:O	2.19	0.42
1:F:60:LEU:HD22	1:F:106:PHE:HE1	1.85	0.42
1:F:139:GLN:NE2	1:F:432:SER:H	2.17	0.42
1:F:364:PRO:HB2	1:F:365:PRO:CD	2.50	0.42
1:F:582:LEU:CD2	1:F:584:VAL:HG23	2.49	0.42
1:A:197:TRP:NE1	1:A:223:VAL:HG21	2.35	0.41
1:A:246:LEU:HD11	1:A:277:PHE:CE2	2.54	0.41
1:A:632:ASP:C	1:A:634:ARG:N	2.73	0.41
1:B:301:ASP:CB	1:D:295:ARG:NH2	2.82	0.41
1:B:399:PRO:HA	1:B:400:PRO:HD3	1.94	0.41
1:B:474:ARG:HH11	1:B:474:ARG:HD2	1.44	0.41
1:B:498:ALA:O	1:B:499:ARG:C	2.60	0.41
1:C:222:TRP:CH2	1:C:226:GLN:NE2	2.88	0.41
1:D:78:ARG:NH1	1:D:82:GLU:OE2	2.51	0.41
1:D:368:MET:HE1	1:D:380:PHE:CD1	2.54	0.41
1:E:78:ARG:NH1	1:E:82:GLU:OE2	2.49	0.41
1:E:305:ILE:HB	1:E:313:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:151:ILE:HD13	1:F:151:ILE:HA	1.76	0.41
1:F:398:PHE:HB3	1:F:399:PRO:HD2	2.02	0.41
1:F:578:MET:HG3	1:F:580:PHE:CZ	2.55	0.41
1:F:610:GLY:HA2	1:F:614:GLU:HB2	2.02	0.41
1:F:624:TYR:HA	1:F:625:PRO:HA	1.82	0.41
1:A:89:VAL:C	1:A:91:ASN:H	2.28	0.41
1:A:222:TRP:CH2	1:A:623:GLY:CA	3.03	0.41
1:A:222:TRP:CD1	1:A:622:LEU:HD23	2.55	0.41
1:A:247:HIS:HB2	1:A:250:ARG:CG	2.50	0.41
1:A:353:ARG:NE	1:A:369:GLU:OE2	2.53	0.41
1:A:366:GLY:O	1:A:367:VAL:C	2.63	0.41
1:A:630:ILE:HD13	1:A:630:ILE:HG21	1.70	0.41
1:B:45:ILE:HB	1:B:98:CYS:HB2	2.02	0.41
1:C:56:LEU:HD21	1:C:110:MET:HE3	2.02	0.41
1:C:86:LEU:O	1:C:86:LEU:HD23	2.20	0.41
1:C:522:SER:C	1:C:524:LYS:N	2.78	0.41
1:C:589:GLY:O	1:C:593:THR:OG1	2.35	0.41
1:D:168:VAL:HG22	1:D:452:VAL:HA	2.02	0.41
1:D:222:TRP:CD1	1:D:622:LEU:HD23	2.55	0.41
1:D:248:TRP:CZ2	1:D:289:LEU:HD13	2.54	0.41
1:D:499:ARG:NE	1:D:628:ARG:O	2.53	0.41
1:D:541:GLU:O	1:D:545:ASN:HB2	2.20	0.41
1:E:56:LEU:HD21	1:E:110:MET:CE	2.50	0.41
1:E:175:LYS:O	1:E:176:ASN:HB2	2.20	0.41
1:E:206:GLU:C	1:E:208:SER:H	2.28	0.41
1:E:248:TRP:CZ3	1:E:289:LEU:HD13	2.55	0.41
1:E:411:MET:CE	1:E:512:VAL:HB	2.51	0.41
1:E:466:MET:HE3	1:E:466:MET:HB2	1.87	0.41
1:E:522:SER:O	1:E:523:SER:C	2.62	0.41
1:E:636:ILE:HG23	1:E:642:ILE:HG21	2.00	0.41
1:F:143:HIS:CE1	1:F:151:ILE:CG2	3.04	0.41
1:F:295:ARG:NE	1:F:339:TYR:CE1	2.88	0.41
1:A:377:ASP:OD1	1:A:378:PRO:HD2	2.20	0.41
1:A:413:VAL:HA	1:A:466:MET:HB2	2.02	0.41
1:B:13:ASP:OD1	1:B:100:ARG:NE	2.51	0.41
1:B:43:THR:CG2	1:B:49:HIS:C	2.92	0.41
1:B:66:LEU:HD22	1:B:111:ASN:HD22	1.85	0.41
1:B:157:ALA:HB3	1:B:448:ILE:HG12	2.02	0.41
1:B:206:GLU:C	1:B:208:SER:H	2.28	0.41
1:C:573:SER:N	3:C:857:HOH:O	2.53	0.41
1:C:634:ARG:HH11	1:C:634:ARG:CG	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:LYS:HD3	3:D:869:HOH:O	2.20	0.41
1:D:195:VAL:HG22	1:D:196:THR:N	2.36	0.41
1:D:255:GLY:O	1:E:361:PHE:HZ	2.02	0.41
1:D:307:ASP:C	1:D:307:ASP:OD1	2.63	0.41
1:E:139:GLN:NE2	1:E:432:SER:H	2.18	0.41
1:E:195:VAL:CG2	1:E:196:THR:N	2.82	0.41
1:E:200:ASP:OD2	1:E:609:CYS:SG	2.79	0.41
1:E:322:GLU:O	1:E:325:GLY:N	2.53	0.41
1:F:200:ASP:OD2	1:F:609:CYS:SG	2.79	0.41
1:A:18:LEU:CD2	1:A:119:LEU:HD23	2.48	0.41
1:A:76:ASN:HD22	1:A:79:GLN:H	1.66	0.41
1:A:190:MET:CG	1:A:568:MET:HE2	2.45	0.41
1:A:215:ARG:O	1:A:217:GLY:N	2.53	0.41
1:A:350:MET:O	1:A:350:MET:HG3	2.19	0.41
1:A:465:THR:O	1:A:466:MET:CB	2.68	0.41
1:A:549:GLY:O	1:A:550:GLY:C	2.63	0.41
1:A:639:VAL:O	1:A:639:VAL:HG22	2.20	0.41
1:B:594:GLU:CG	1:B:594:GLU:O	2.68	0.41
1:D:178:GLU:O	1:D:178:GLU:HG3	2.19	0.41
1:D:185:GLY:HA2	1:D:375:THR:HG22	2.01	0.41
1:D:246:LEU:HD11	1:D:277:PHE:HE2	1.85	0.41
1:D:300:ILE:HD13	1:D:390:ILE:O	2.20	0.41
1:D:305:ILE:HB	1:D:313:ILE:HG13	2.03	0.41
1:D:641:ASN:HD22	1:D:641:ASN:C	2.26	0.41
1:E:278:GLU:H	1:E:354:GLN:NE2	2.16	0.41
1:E:317:GLN:CB	1:E:318:PRO:CD	2.96	0.41
1:E:456:ASN:ND2	1:E:457:HIS:N	2.43	0.41
1:F:37:PHE:CD2	1:F:101:SER:HB3	2.55	0.41
1:F:135:PRO:HB3	1:F:536:PHE:CD1	2.56	0.41
1:F:533:MET:HB3	1:F:534:PRO:CD	2.49	0.41
1:F:633:GLU:C	1:F:635:VAL:N	2.74	0.41
1:A:95:GLU:CG	1:A:96:TRP:N	2.82	0.41
1:A:291:ILE:HD12	1:A:291:ILE:HG21	1.53	0.41
1:A:295:ARG:CZ	1:A:339:TYR:CE1	3.04	0.41
1:A:305:ILE:HG22	1:A:306:THR:N	2.35	0.41
1:A:307:ASP:C	1:A:336:ASN:HD22	2.28	0.41
1:A:338:GLN:NE2	1:E:316:ARG:HH21	2.18	0.41
1:A:465:THR:HG23	1:A:518:THR:OG1	2.20	0.41
1:B:38:ASN:C	1:B:40:LEU:N	2.77	0.41
1:B:258:PRO:CG	1:B:259:LEU:N	2.82	0.41
1:B:432:SER:O	1:B:434:ILE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:ILE:HG21	1:B:503:ILE:HD13	1.40	0.41
1:B:591:LYS:HA	1:B:594:GLU:HB2	2.03	0.41
1:B:634:ARG:HH11	1:B:634:ARG:CG	2.24	0.41
1:C:66:LEU:HD23	1:C:67:GLU:H	1.85	0.41
1:C:226:GLN:CD	1:C:504:GLU:H	2.29	0.41
1:C:305:ILE:CG1	1:C:315:ILE:HG21	2.48	0.41
1:C:373:THR:O	1:C:373:THR:HG23	2.21	0.41
1:C:392:LYS:HZ3	1:C:396:ASP:CG	2.28	0.41
1:C:424:THR:HA	1:C:457:HIS:HA	2.01	0.41
1:C:499:ARG:NE	1:C:628:ARG:O	2.54	0.41
1:C:591:LYS:CA	1:C:594:GLU:HB2	2.50	0.41
1:D:185:GLY:CA	1:D:375:THR:CG2	2.94	0.41
1:D:271:ARG:NH2	1:D:377:ASP:OD1	2.53	0.41
1:D:303:GLY:O	1:D:315:ILE:HG12	2.20	0.41
1:D:624:TYR:HA	1:D:625:PRO:HA	1.83	0.41
1:E:469:ASN:HD22	1:E:469:ASN:HA	1.67	0.41
1:E:591:LYS:O	1:E:594:GLU:HB2	2.20	0.41
1:F:353:ARG:NE	1:F:369:GLU:OE2	2.54	0.41
1:A:14:ILE:HG23	1:A:18:LEU:HD11	2.02	0.41
1:A:15:ASN:O	1:A:16:HIS:C	2.60	0.41
1:A:43:THR:O	1:A:43:THR:CG2	2.67	0.41
1:B:344:HIS:O	1:B:345:ASN:C	2.62	0.41
1:B:398:PHE:HB3	1:B:399:PRO:CD	2.46	0.41
1:B:433:LEU:HG	1:B:450:ALA:HB2	2.01	0.41
1:D:133:VAL:HG22	1:D:558:TYR:HB2	2.03	0.41
1:D:589:GLY:O	1:D:593:THR:OG1	2.35	0.41
1:E:16:HIS:HB3	1:E:30:LEU:CD1	2.49	0.41
1:E:313:ILE:HD12	1:E:314:ASP:O	2.21	0.41
1:F:343:LEU:C	1:F:343:LEU:CD2	2.93	0.41
1:A:251:ILE:HD11	3:A:700:HOH:O	2.20	0.41
1:A:295:ARG:HH22	1:E:301:ASP:CB	2.34	0.41
1:A:422:LEU:HD22	1:A:570:LEU:CG	2.50	0.41
1:A:533:MET:C	1:A:534:PRO:O	2.59	0.41
1:B:66:LEU:HD13	1:B:111:ASN:CG	2.45	0.41
1:B:80:ARG:O	1:B:81:LYS:C	2.63	0.41
1:B:392:LYS:HZ3	1:B:396:ASP:CG	2.29	0.41
1:C:413:VAL:HG12	1:C:643:LYS:CG	2.51	0.41
1:D:226:GLN:CD	1:D:504:GLU:H	2.28	0.41
1:D:248:TRP:CZ3	1:D:289:LEU:HD13	2.54	0.41
1:D:322:GLU:O	1:D:325:GLY:N	2.54	0.41
1:D:533:MET:CE	1:D:533:MET:N	2.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:PHE:O	1:E:236:LEU:HB3	2.20	0.41
1:F:154:ALA:HB2	1:F:433:LEU:HD13	2.03	0.41
1:F:248:TRP:CZ2	1:F:289:LEU:HD13	2.55	0.41
1:F:313:ILE:HD12	1:F:314:ASP:O	2.20	0.41
1:F:345:ASN:O	1:F:348:HIS:HB2	2.21	0.41
1:F:423:ILE:HA	1:F:650:VAL:O	2.19	0.41
1:F:641:ASN:ND2	1:F:641:ASN:N	2.64	0.41
1:A:80:ARG:O	1:A:80:ARG:HG2	2.19	0.41
1:A:351:LEU:HD23	1:A:351:LEU:HA	1.58	0.41
1:A:399:PRO:HA	1:A:400:PRO:HD3	1.78	0.41
1:A:564:ILE:CB	1:A:565:PRO:CD	2.99	0.41
1:A:619:ASN:O	1:A:620:ARG:C	2.62	0.41
1:A:629:ARG:HH11	1:A:629:ARG:CG	2.31	0.41
1:B:120:TYR:CE2	1:B:134:LEU:HD13	2.52	0.41
1:B:353:ARG:HH11	1:B:353:ARG:HD2	1.16	0.41
1:B:636:ILE:HG23	1:B:642:ILE:HG21	2.02	0.41
1:B:641:ASN:ND2	1:B:641:ASN:N	2.63	0.41
1:C:71:TRP:CZ3	1:C:365:PRO:CG	3.04	0.41
1:C:357:PRO:HB2	1:C:358:HIS:CE1	2.56	0.41
1:C:610:GLY:HA2	1:C:614:GLU:HB2	2.03	0.41
1:E:158:LYS:NZ	1:E:439:SER:HB2	2.35	0.41
1:E:345:ASN:O	1:E:348:HIS:HB2	2.21	0.41
1:F:148:SER:HB2	1:F:259:LEU:O	2.20	0.41
1:A:100:ARG:HH11	1:A:100:ARG:HD3	1.69	0.41
1:A:112:GLU:CD	1:A:112:GLU:H	2.27	0.41
1:A:322:GLU:O	1:A:323:LEU:C	2.64	0.41
1:A:403:HIS:O	1:A:405:ASN:N	2.53	0.41
1:A:483:CYS:CB	3:A:763:HOH:O	2.69	0.41
1:A:536:PHE:O	1:A:540:LYS:N	2.54	0.41
1:B:9:GLN:O	1:B:10:LYS:O	2.38	0.41
1:B:14:ILE:HD11	1:B:96:TRP:HH2	1.86	0.41
1:B:31:LYS:O	1:B:34:ALA:HB3	2.21	0.41
1:B:83:ALA:HA	1:B:114:GLU:HB3	2.02	0.41
1:B:221:PHE:C	1:B:221:PHE:CD1	2.97	0.41
1:B:222:TRP:CG	1:B:622:LEU:HD23	2.55	0.41
1:B:224:HIS:O	1:B:225:HIS:C	2.59	0.41
1:B:300:ILE:CD1	1:B:390:ILE:HG22	2.47	0.41
1:B:479:ARG:NH2	1:B:618:ASP:CG	2.78	0.41
1:B:641:ASN:HD22	1:B:641:ASN:C	2.27	0.41
1:C:158:LYS:HD3	1:C:446:VAL:HG12	2.03	0.41
1:C:200:ASP:OD2	1:C:609:CYS:SG	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:ILE:HD13	1:C:390:ILE:O	2.19	0.41
1:D:16:HIS:HB3	1:D:30:LEU:CD1	2.51	0.41
1:D:185:GLY:CA	1:D:375:THR:HG22	2.51	0.41
1:D:241:ASP:O	1:D:242:PRO:C	2.64	0.41
1:D:540:LYS:O	1:D:541:GLU:C	2.64	0.41
1:D:610:GLY:HA2	1:D:614:GLU:HB2	2.03	0.41
1:E:8:ALA:O	1:E:547:VAL:HG21	2.20	0.41
1:E:197:TRP:CE3	1:E:197:TRP:O	2.73	0.41
1:E:222:TRP:CH2	1:E:226:GLN:NE2	2.88	0.41
1:E:248:TRP:CZ2	1:E:289:LEU:HD13	2.54	0.41
1:E:493:LEU:HB2	1:E:497:GLU:HB2	2.03	0.41
1:E:509:PHE:CZ	1:E:593:THR:CG2	3.04	0.41
1:F:16:HIS:HB3	1:F:30:LEU:CD1	2.50	0.41
1:F:300:ILE:HD13	1:F:390:ILE:O	2.20	0.41
1:F:303:GLY:O	1:F:315:ILE:HG12	2.21	0.41
1:F:322:GLU:O	1:F:325:GLY:N	2.54	0.41
1:F:410:GLY:O	1:F:411:MET:C	2.64	0.41
1:F:411:MET:HE1	1:F:474:ARG:HB2	2.02	0.41
1:F:522:SER:O	1:F:523:SER:C	2.64	0.41
1:F:632:ASP:C	1:F:634:ARG:N	2.79	0.41
1:A:284:ALA:HB1	1:A:285:HIS:H	1.70	0.41
1:A:287:HIS:O	1:A:290:GLU:HB2	2.21	0.41
1:A:367:VAL:O	1:A:373:THR:CG2	2.68	0.41
1:A:468:ASN:ND2	1:A:514:SER:HA	2.31	0.41
1:A:591:LYS:HB2	1:A:591:LYS:NZ	2.36	0.41
1:A:610:GLY:C	1:A:612:HIS:N	2.79	0.41
1:A:630:ILE:CD1	1:A:636:ILE:HD11	2.51	0.41
1:B:45:ILE:HG12	1:B:45:ILE:H	1.17	0.41
1:B:46:TYR:CZ	1:B:53:VAL:HG21	2.56	0.41
1:B:285:HIS:HB2	1:B:288:ASP:OD2	2.20	0.41
1:B:301:ASP:HB3	1:D:295:ARG:NH2	2.37	0.41
1:B:400:PRO:HB3	1:B:629:ARG:O	2.21	0.41
1:B:493:LEU:HA	1:B:497:GLU:OE1	2.21	0.41
1:B:614:GLU:H	1:B:614:GLU:HG3	1.35	0.41
1:B:620:ARG:HG3	1:B:624:TYR:CD1	2.54	0.41
1:C:252:ILE:HB	1:C:275:ILE:HG22	2.02	0.41
1:D:40:LEU:CD1	1:D:57:MET:HG3	2.49	0.41
1:D:246:LEU:HD11	1:D:277:PHE:CE2	2.56	0.41
1:D:357:PRO:HB2	1:D:358:HIS:CE1	2.55	0.41
1:D:533:MET:HB3	1:D:534:PRO:CD	2.50	0.41
1:E:86:LEU:O	1:E:86:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:THR:CG2	1:F:10:LYS:HE3	2.51	0.41
1:F:195:VAL:CG2	1:F:196:THR:N	2.82	0.41
1:F:443:ILE:HD12	1:F:443:ILE:HA	1.97	0.41
1:F:533:MET:HE3	1:F:533:MET:N	2.30	0.41
1:A:59:GLU:OE1	1:A:64:ARG:CD	2.67	0.40
1:A:393:LYS:HB3	1:A:393:LYS:HE3	1.69	0.40
1:A:491:ILE:HG22	1:A:491:ILE:O	2.21	0.40
1:B:86:LEU:HD22	1:B:90:LEU:CD2	2.50	0.40
1:B:222:TRP:CH2	1:B:623:GLY:HA2	2.56	0.40
1:B:371:PHE:C	1:B:373:THR:N	2.80	0.40
1:B:533:MET:HB3	1:B:534:PRO:HG2	2.02	0.40
1:C:133:VAL:HG21	1:C:555:LEU:HD23	2.02	0.40
1:C:639:VAL:HG23	1:C:641:ASN:HD22	1.84	0.40
1:D:48:ASP:CB	1:D:92:GLN:HE21	2.34	0.40
1:D:56:LEU:HD21	1:D:110:MET:HE3	2.03	0.40
1:E:57:MET:HE3	1:E:61:ASN:ND2	2.35	0.40
1:E:256:PHE:HD1	1:E:256:PHE:O	2.04	0.40
1:F:192:ILE:HD13	1:F:192:ILE:HA	1.89	0.40
1:F:197:TRP:CE3	1:F:197:TRP:O	2.74	0.40
1:F:373:THR:O	1:F:373:THR:HG23	2.22	0.40
1:F:456:ASN:ND2	1:F:457:HIS:N	2.42	0.40
1:F:499:ARG:NE	1:F:628:ARG:O	2.54	0.40
1:A:76:ASN:C	1:A:76:ASN:ND2	2.79	0.40
1:A:626:LEU:N	1:A:626:LEU:HD23	2.35	0.40
1:B:56:LEU:CD1	1:B:110:MET:HE3	2.51	0.40
1:B:316:ARG:HH21	1:D:338:GLN:NE2	2.17	0.40
1:B:568:MET:O	1:B:569:LEU:C	2.65	0.40
1:B:630:ILE:HG23	1:B:636:ILE:HD13	2.03	0.40
1:C:16:HIS:HB3	1:C:30:LEU:CD1	2.50	0.40
1:C:154:ALA:HB2	1:C:433:LEU:HD13	2.04	0.40
1:C:190:MET:HE2	1:C:565:PRO:HD2	2.03	0.40
1:C:205:TRP:NE1	1:C:213:LEU:HD13	2.36	0.40
1:C:322:GLU:O	1:C:325:GLY:N	2.54	0.40
1:D:387:MET:HB3	1:D:387:MET:HE3	1.86	0.40
1:D:441:GLU:C	1:D:443:ILE:H	2.29	0.40
1:D:487:ASP:OD1	1:D:487:ASP:O	2.40	0.40
1:E:121:VAL:HG23	1:E:199:MET:HG2	2.04	0.40
1:E:631:PRO:HD2	3:E:818:HOH:O	2.21	0.40
1:F:134:LEU:HA	1:F:135:PRO:HD3	1.95	0.40
1:F:140:ILE:HG22	1:F:141:THR:HG23	2.02	0.40
1:F:385:LYS:HE2	3:F:750:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:HIS:HB2	1:A:288:ASP:CG	2.47	0.40
1:B:17:LEU:HD23	1:B:17:LEU:HA	1.86	0.40
1:B:30:LEU:HD23	1:B:30:LEU:HA	1.74	0.40
1:B:48:ASP:CA	1:B:92:GLN:HE21	2.33	0.40
1:B:528:VAL:O	1:B:528:VAL:HG23	2.20	0.40
1:C:5:THR:CG2	1:C:10:LYS:HE3	2.51	0.40
1:C:41:GLY:O	1:C:42:ASP:HB2	2.22	0.40
1:D:76:ASN:ND2	1:D:79:GLN:HG3	2.36	0.40
1:D:278:GLU:H	1:D:354:GLN:NE2	2.20	0.40
1:D:408:PHE:CZ	1:D:411:MET:SD	3.15	0.40
1:D:525:ASP:O	1:D:526:SER:C	2.64	0.40
1:E:39:PRO:CB	1:E:53:VAL:CG1	2.99	0.40
1:E:143:HIS:CE1	1:E:151:ILE:CG2	3.04	0.40
1:E:269:PRO:CB	1:E:363:LEU:HD23	2.40	0.40
1:E:540:LYS:O	1:E:541:GLU:C	2.65	0.40
1:E:634:ARG:HH11	1:E:634:ARG:CG	2.24	0.40
1:F:226:GLN:CD	1:F:504:GLU:H	2.28	0.40
1:A:13:ASP:CG	1:A:100:ARG:HD2	2.46	0.40
1:A:395:THR:HG21	1:A:500:TRP:CZ3	2.56	0.40
1:B:206:GLU:C	1:B:208:SER:N	2.77	0.40
1:B:375:THR:HB	3:B:747:HOH:O	2.21	0.40
1:B:594:GLU:O	1:B:594:GLU:HG2	2.22	0.40
1:D:60:LEU:HD22	1:D:106:PHE:HE1	1.87	0.40
1:D:84:LEU:HD12	1:D:84:LEU:HA	1.93	0.40
1:D:211:TYR:CD1	1:D:211:TYR:N	2.89	0.40
1:D:485:ILE:HG12	1:D:581:ASN:ND2	2.36	0.40
1:E:23:GLU:O	1:E:24:PRO:C	2.65	0.40
1:E:30:LEU:HD23	1:E:30:LEU:HA	1.94	0.40
1:E:324:LEU:HD23	1:E:324:LEU:HA	1.80	0.40
1:E:588:ASP:OD1	1:E:588:ASP:O	2.39	0.40
1:F:5:THR:CG2	1:F:6:GLY:H	2.20	0.40
1:F:8:ALA:CB	1:F:553:LEU:HD12	2.51	0.40
1:F:248:TRP:CZ3	1:F:289:LEU:HD13	2.56	0.40
1:A:60:LEU:HA	1:A:65:LEU:HD22	2.04	0.40
1:A:124:ILE:HG22	1:A:611:VAL:CG1	2.51	0.40
1:A:307:ASP:OD1	1:A:310:GLY:N	2.54	0.40
1:A:471:ASP:O	1:A:514:SER:HB2	2.21	0.40
1:A:560:ARG:CB	3:A:819:HOH:O	2.70	0.40
1:B:14:ILE:HD11	1:B:96:TRP:CH2	2.56	0.40
1:B:222:TRP:CG	1:B:622:LEU:CD2	3.04	0.40
1:C:385:LYS:HE2	3:C:750:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:PRO:HA	1:C:400:PRO:HD3	1.91	0.40
1:D:176:ASN:HD22	1:D:176:ASN:HA	1.79	0.40
1:D:205:TRP:NE1	1:D:213:LEU:HD13	2.37	0.40
1:D:230:ARG:NH2	1:D:503:ILE:HD12	2.37	0.40
1:D:377:ASP:HA	1:D:378:PRO:HD3	1.88	0.40
1:E:241:ASP:O	1:E:242:PRO:C	2.65	0.40
1:E:427:ASP:HB3	1:E:567:ARG:HH12	1.86	0.40
1:E:632:ASP:C	1:E:634:ARG:N	2.78	0.40
1:F:56:LEU:HD21	1:F:110:MET:HE3	2.03	0.40
1:F:478:PHE:CZ	1:F:519:ILE:CD1	3.05	0.40
1:F:540:LYS:O	1:F:541:GLU:C	2.65	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ASP:OD1	1:C:49:HIS:CD2[2_647]	1.85	0.35
1:C:594:GLU:OE1	1:F:471:ASP:CB[2_657]	2.13	0.07
1:C:474:ARG:NH2	1:D:41:GLY:O[2_656]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	626/657 (95%)	501 (80%)	97 (16%)	28 (4%)	2	15
1	B	626/657 (95%)	506 (81%)	89 (14%)	31 (5%)	1	13
1	C	626/657 (95%)	517 (83%)	95 (15%)	14 (2%)	5	29
1	D	626/657 (95%)	516 (82%)	91 (14%)	19 (3%)	3	23
1	E	626/657 (95%)	512 (82%)	95 (15%)	19 (3%)	3	23
1	F	626/657 (95%)	503 (80%)	102 (16%)	21 (3%)	3	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3756/3942 (95%)	3055 (81%)	569 (15%)	132 (4%)	3	20

All (132) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	147	ASN
1	A	176	ASN
1	A	441	GLU
1	A	471	ASP
1	B	176	ASN
1	B	472	GLY
1	B	514	SER
1	B	556	SER
1	C	176	ASN
1	D	176	ASN
1	E	176	ASN
1	F	176	ASN
1	A	6	GLY
1	A	7	ASN
1	A	90	LEU
1	A	104	ALA
1	A	242	PRO
1	A	472	GLY
1	A	488	ASN
1	A	555	LEU
1	A	557	ALA
1	A	560	ARG
1	A	589	GLY
1	A	611	VAL
1	B	7	ASN
1	B	147	ASN
1	B	427	ASP
1	B	488	ASN
1	B	489	ASN
1	B	569	LEU
1	B	594	GLU
1	B	611	VAL
1	C	7	ASN
1	C	42	ASP
1	D	7	ASN
1	D	42	ASP

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Mol	Chain	Res	Type
1	D	557	ALA
1	E	7	ASN
1	E	44	SER
1	E	492	THR
1	F	7	ASN
1	F	42	ASP
1	F	557	ALA
1	A	54	GLU
1	A	427	ASP
1	A	569	LEU
1	A	634	ARG
1	B	8	ALA
1	B	42	ASP
1	B	44	SER
1	B	90	LEU
1	B	523	SER
1	B	593	THR
1	B	595	GLY
1	C	44	SER
1	C	90	LEU
1	C	104	ALA
1	C	320	GLY
1	C	569	LEU
1	C	595	GLY
1	D	44	SER
1	D	90	LEU
1	D	104	ALA
1	D	320	GLY
1	D	489	ASN
1	D	514	SER
1	D	569	LEU
1	D	595	GLY
1	E	42	ASP
1	E	90	LEU
1	E	104	ALA
1	E	320	GLY
1	E	489	ASN
1	E	557	ALA
1	E	569	LEU
1	F	44	SER
1	F	90	LEU
1	F	104	ALA

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Mol	Chain	Res	Type
1	F	320	GLY
1	F	489	ASN
1	F	569	LEU
1	F	595	GLY
1	A	24	PRO
1	A	474	ARG
1	A	523	SER
1	A	556	SER
1	A	595	GLY
1	B	101	SER
1	B	411	MET
1	B	433	LEU
1	B	492	THR
1	B	496	ASP
1	B	516	PRO
1	B	589	GLY
1	B	592	ASP
1	C	496	ASP
1	D	427	ASP
1	D	496	ASP
1	D	561	SER
1	E	496	ASP
1	E	595	GLY
1	F	473	GLU
1	F	492	THR
1	F	496	ASP
1	A	473	GLU
1	B	43	THR
1	B	320	GLY
1	C	242	PRO
1	C	427	ASP
1	D	242	PRO
1	D	354	GLN
1	E	242	PRO
1	E	427	ASP
1	E	554	ASP
1	F	242	PRO
1	F	427	ASP
1	A	489	ASN
1	B	192	ILE
1	C	593	THR
1	C	594	GLU

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Mol	Chain	Res	Type
1	D	593	THR
1	E	516	PRO
1	E	592	ASP
1	F	592	ASP
1	F	593	THR
1	F	594	GLU
1	F	472	GLY
1	F	563	GLY
1	B	242	PRO
1	D	28	PRO
1	E	611	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	564/580 (97%)	416 (74%)	148 (26%)	0	3
1	B	564/580 (97%)	424 (75%)	140 (25%)	1	3
1	C	564/580 (97%)	485 (86%)	79 (14%)	3	17
1	D	564/580 (97%)	475 (84%)	89 (16%)	2	13
1	E	564/580 (97%)	491 (87%)	73 (13%)	4	20
1	F	564/580 (97%)	490 (87%)	74 (13%)	4	19
All	All	3384/3480 (97%)	2781 (82%)	603 (18%)	2	10

All (603) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	10	LYS
1	A	12	GLN
1	A	14	ILE
1	A	15	ASN
1	A	23	GLU
1	A	25	THR

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Mol	Chain	Res	Type
1	A	26	LYS
1	A	31	LYS
1	A	32	ASP
1	A	45	ILE
1	A	53	VAL
1	A	56	LEU
1	A	63	HIS
1	A	64	ARG
1	A	66	LEU
1	A	69	ARG
1	A	72	TYR
1	A	77	THR
1	A	85	MET
1	A	90	LEU
1	A	108	GLU
1	A	110	MET
1	A	111	ASN
1	A	112	GLU
1	A	121	VAL
1	A	127	LYS
1	A	139	GLN
1	A	151	ILE
1	A	153	LYS
1	A	156	SER
1	A	159	MET
1	A	162	LYS
1	A	163	PRO
1	A	165	THR
1	A	175	LYS
1	A	176	ASN
1	A	179	GLN
1	A	180	ARG
1	A	195	VAL
1	A	199	MET
1	A	208	SER
1	A	216	LYS
1	A	219	LEU
1	A	235	ARG
1	A	242	PRO
1	A	243	VAL
1	A	244	ASP
1	A	251	ILE

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Mol	Chain	Res	Type
1	A	252	ILE
1	A	256	PHE
1	A	258	PRO
1	A	259	LEU
1	A	263	LYS
1	A	270	VAL
1	A	280	VAL
1	A	281	ASP
1	A	291	ILE
1	A	292	THR
1	A	295	ARG
1	A	297	HIS
1	A	306	THR
1	A	308	SER
1	A	313	ILE
1	A	315	ILE
1	A	316	ARG
1	A	322	GLU
1	A	329	GLU
1	A	330	SER
1	A	335	SER
1	A	343	LEU
1	A	349	VAL
1	A	363	LEU
1	A	365	PRO
1	A	367	VAL
1	A	372	GLU
1	A	373	THR
1	A	375	THR
1	A	382	ARG
1	A	395	THR
1	A	407	GLU
1	A	409	SER
1	A	412	VAL
1	A	416	VAL
1	A	418	ILE
1	A	423	ILE
1	A	427	ASP
1	A	433	LEU
1	A	434	ILE
1	A	438	ASP
1	A	441	GLU

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Mol	Chain	Res	Type
1	A	442	ASN
1	A	444	GLU
1	A	446	VAL
1	A	447	GLU
1	A	453	HIS
1	A	456	ASN
1	A	461	THR
1	A	464	ILE
1	A	465	THR
1	A	466	MET
1	A	467	SER
1	A	474	ARG
1	A	475	LEU
1	A	477	THR
1	A	482	LEU
1	A	491	ILE
1	A	492	THR
1	A	493	LEU
1	A	495	LEU
1	A	501	PHE
1	A	511	LYS
1	A	512	VAL
1	A	513	PRO
1	A	517	GLU
1	A	518	THR
1	A	519	ILE
1	A	523	SER
1	A	530	VAL
1	A	532	ASP
1	A	533	MET
1	A	535	SER
1	A	544	ASP
1	A	547	VAL
1	A	556	SER
1	A	559	GLU
1	A	560	ARG
1	A	567	ARG
1	A	574	LYS
1	A	576	GLU
1	A	578	MET
1	A	579	GLU
1	A	586	VAL

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Mol	Chain	Res	Type
1	A	587	THR
1	A	591	LYS
1	A	596	HIS
1	A	606	HIS
1	A	609	CYS
1	A	614	GLU
1	A	620	ARG
1	A	626	LEU
1	A	634	ARG
1	A	636	ILE
1	A	639	VAL
1	A	641	ASN
1	A	643	LYS
1	A	646	VAL
1	A	650	VAL
1	B	10	LYS
1	B	11	GLN
1	B	18	LEU
1	B	23	GLU
1	B	29	ASP
1	B	31	LYS
1	B	33	ILE
1	B	40	LEU
1	B	45	ILE
1	B	53	VAL
1	B	56	LEU
1	B	63	HIS
1	B	64	ARG
1	B	66	LEU
1	B	67	GLU
1	B	69	ARG
1	B	72	TYR
1	B	77	THR
1	B	81	LYS
1	B	85	MET
1	B	86	LEU
1	B	90	LEU
1	B	108	GLU
1	B	112	GLU
1	B	121	VAL
1	B	151	ILE
1	B	153	LYS

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Mol	Chain	Res	Type
1	B	156	SER
1	B	159	MET
1	B	161	GLN
1	B	162	LYS
1	B	165	THR
1	B	175	LYS
1	B	176	ASN
1	B	179	GLN
1	B	193	HIS
1	B	195	VAL
1	B	199	MET
1	B	208	SER
1	B	211	TYR
1	B	213	LEU
1	B	216	LYS
1	B	219	LEU
1	B	242	PRO
1	B	244	ASP
1	B	251	ILE
1	B	253	ARG
1	B	256	PHE
1	B	258	PRO
1	B	259	LEU
1	B	261	SER
1	B	263	LYS
1	B	270	VAL
1	B	275	ILE
1	B	279	ASP
1	B	280	VAL
1	B	281	ASP
1	B	291	ILE
1	B	297	HIS
1	B	306	THR
1	B	309	ASP
1	B	313	ILE
1	B	316	ARG
1	B	322	GLU
1	B	330	SER
1	B	343	LEU
1	B	349	VAL
1	B	351	LEU
1	B	362	ASN

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Mol	Chain	Res	Type
1	B	363	LEU
1	B	364	PRO
1	B	365	PRO
1	B	367	VAL
1	B	369	GLU
1	B	372	GLU
1	B	373	THR
1	B	375	THR
1	B	382	ARG
1	B	395	THR
1	B	405	ASN
1	B	409	SER
1	B	411	MET
1	B	412	VAL
1	B	413	VAL
1	B	416	VAL
1	B	418	ILE
1	B	423	ILE
1	B	427	ASP
1	B	430	GLN
1	B	437	VAL
1	B	438	ASP
1	B	448	ILE
1	B	453	HIS
1	B	454	ARG
1	B	456	ASN
1	B	463	LYS
1	B	464	ILE
1	B	467	SER
1	B	469	ASN
1	B	473	GLU
1	B	475	LEU
1	B	485	ILE
1	B	487	ASP
1	B	491	ILE
1	B	493	LEU
1	B	501	PHE
1	B	510	GLN
1	B	511	LYS
1	B	514	SER
1	B	516	PRO
1	B	518	THR

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Mol	Chain	Res	Type
1	B	519	ILE
1	B	523	SER
1	B	529	THR
1	B	532	ASP
1	B	533	MET
1	B	535	SER
1	B	544	ASP
1	B	548	ASN
1	B	553	LEU
1	B	554	ASP
1	B	555	LEU
1	B	556	SER
1	B	559	GLU
1	B	560	ARG
1	B	561	SER
1	B	567	ARG
1	B	570	LEU
1	B	576	GLU
1	B	578	MET
1	B	586	VAL
1	B	591	LYS
1	B	596	HIS
1	B	606	HIS
1	B	609	CYS
1	B	620	ARG
1	B	634	ARG
1	B	641	ASN
1	B	643	LYS
1	B	646	VAL
1	C	23	GLU
1	C	56	LEU
1	C	63	HIS
1	C	64	ARG
1	C	66	LEU
1	C	67	GLU
1	C	72	TYR
1	C	77	THR
1	C	85	MET
1	C	92	GLN
1	C	108	GLU
1	C	112	GLU
1	C	121	VAL

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Mol	Chain	Res	Type
1	C	151	ILE
1	C	153	LYS
1	C	165	THR
1	C	175	LYS
1	C	176	ASN
1	C	179	GLN
1	C	195	VAL
1	C	199	MET
1	C	216	LYS
1	C	219	LEU
1	C	233	PHE
1	C	242	PRO
1	C	244	ASP
1	C	246	LEU
1	C	256	PHE
1	C	259	LEU
1	C	270	VAL
1	C	273	ASP
1	C	275	ILE
1	C	279	ASP
1	C	280	VAL
1	C	281	ASP
1	C	297	HIS
1	C	306	THR
1	C	313	ILE
1	C	316	ARG
1	C	322	GLU
1	C	330	SER
1	C	343	LEU
1	C	351	LEU
1	C	363	LEU
1	C	367	VAL
1	C	372	GLU
1	C	373	THR
1	C	375	THR
1	C	382	ARG
1	C	395	THR
1	C	405	ASN
1	C	412	VAL
1	C	416	VAL
1	C	438	ASP
1	C	453	HIS

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Mol	Chain	Res	Type
1	C	456	ASN
1	C	461	THR
1	C	475	LEU
1	C	491	ILE
1	C	492	THR
1	C	493	LEU
1	C	501	PHE
1	C	519	ILE
1	C	532	ASP
1	C	533	MET
1	C	547	VAL
1	C	548	ASN
1	C	555	LEU
1	C	579	GLU
1	C	586	VAL
1	C	591	LYS
1	C	596	HIS
1	C	606	HIS
1	C	609	CYS
1	C	620	ARG
1	C	634	ARG
1	C	641	ASN
1	C	643	LYS
1	C	646	VAL
1	D	29	ASP
1	D	56	LEU
1	D	63	HIS
1	D	64	ARG
1	D	66	LEU
1	D	67	GLU
1	D	72	TYR
1	D	77	THR
1	D	85	MET
1	D	92	GLN
1	D	108	GLU
1	D	112	GLU
1	D	121	VAL
1	D	151	ILE
1	D	153	LYS
1	D	162	LYS
1	D	175	LYS
1	D	176	ASN

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Mol	Chain	Res	Type
1	D	179	GLN
1	D	195	VAL
1	D	199	MET
1	D	216	LYS
1	D	219	LEU
1	D	233	PHE
1	D	242	PRO
1	D	244	ASP
1	D	246	LEU
1	D	256	PHE
1	D	259	LEU
1	D	270	VAL
1	D	273	ASP
1	D	275	ILE
1	D	279	ASP
1	D	280	VAL
1	D	281	ASP
1	D	297	HIS
1	D	306	THR
1	D	313	ILE
1	D	316	ARG
1	D	322	GLU
1	D	330	SER
1	D	343	LEU
1	D	351	LEU
1	D	363	LEU
1	D	367	VAL
1	D	372	GLU
1	D	373	THR
1	D	375	THR
1	D	382	ARG
1	D	395	THR
1	D	405	ASN
1	D	411	MET
1	D	412	VAL
1	D	413	VAL
1	D	416	VAL
1	D	418	ILE
1	D	419	ASP
1	D	438	ASP
1	D	453	HIS
1	D	456	ASN

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Mol	Chain	Res	Type
1	D	461	THR
1	D	464	ILE
1	D	465	THR
1	D	470	ASN
1	D	477	THR
1	D	493	LEU
1	D	501	PHE
1	D	519	ILE
1	D	523	SER
1	D	532	ASP
1	D	533	MET
1	D	545	ASN
1	D	547	VAL
1	D	553	LEU
1	D	554	ASP
1	D	558	TYR
1	D	559	GLU
1	D	579	GLU
1	D	586	VAL
1	D	591	LYS
1	D	596	HIS
1	D	606	HIS
1	D	609	CYS
1	D	620	ARG
1	D	634	ARG
1	D	641	ASN
1	D	643	LYS
1	D	646	VAL
1	D	650	VAL
1	E	53	VAL
1	E	56	LEU
1	E	63	HIS
1	E	64	ARG
1	E	66	LEU
1	E	67	GLU
1	E	72	TYR
1	E	77	THR
1	E	85	MET
1	E	92	GLN
1	E	108	GLU
1	E	112	GLU
1	E	121	VAL

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Mol	Chain	Res	Type
1	E	151	ILE
1	E	153	LYS
1	E	175	LYS
1	E	176	ASN
1	E	179	GLN
1	E	195	VAL
1	E	199	MET
1	E	216	LYS
1	E	219	LEU
1	E	233	PHE
1	E	242	PRO
1	E	244	ASP
1	E	246	LEU
1	E	251	ILE
1	E	256	PHE
1	E	259	LEU
1	E	270	VAL
1	E	273	ASP
1	E	275	ILE
1	E	279	ASP
1	E	280	VAL
1	E	281	ASP
1	E	297	HIS
1	E	306	THR
1	E	313	ILE
1	E	316	ARG
1	E	322	GLU
1	E	330	SER
1	E	343	LEU
1	E	351	LEU
1	E	363	LEU
1	E	367	VAL
1	E	372	GLU
1	E	373	THR
1	E	375	THR
1	E	382	ARG
1	E	395	THR
1	E	405	ASN
1	E	412	VAL
1	E	416	VAL
1	E	438	ASP
1	E	453	HIS

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Mol	Chain	Res	Type
1	E	456	ASN
1	E	461	THR
1	E	493	LEU
1	E	501	PHE
1	E	519	ILE
1	E	532	ASP
1	E	533	MET
1	E	559	GLU
1	E	586	VAL
1	E	591	LYS
1	E	596	HIS
1	E	606	HIS
1	E	609	CYS
1	E	620	ARG
1	E	634	ARG
1	E	641	ASN
1	E	643	LYS
1	E	646	VAL
1	F	56	LEU
1	F	63	HIS
1	F	64	ARG
1	F	66	LEU
1	F	67	GLU
1	F	72	TYR
1	F	77	THR
1	F	85	MET
1	F	92	GLN
1	F	108	GLU
1	F	112	GLU
1	F	121	VAL
1	F	151	ILE
1	F	153	LYS
1	F	175	LYS
1	F	176	ASN
1	F	179	GLN
1	F	195	VAL
1	F	199	MET
1	F	216	LYS
1	F	219	LEU
1	F	233	PHE
1	F	242	PRO
1	F	244	ASP

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Mol	Chain	Res	Type
1	F	246	LEU
1	F	251	ILE
1	F	256	PHE
1	F	259	LEU
1	F	270	VAL
1	F	273	ASP
1	F	275	ILE
1	F	279	ASP
1	F	280	VAL
1	F	281	ASP
1	F	291	ILE
1	F	297	HIS
1	F	306	THR
1	F	313	ILE
1	F	316	ARG
1	F	322	GLU
1	F	330	SER
1	F	343	LEU
1	F	351	LEU
1	F	363	LEU
1	F	367	VAL
1	F	372	GLU
1	F	373	THR
1	F	375	THR
1	F	382	ARG
1	F	395	THR
1	F	405	ASN
1	F	412	VAL
1	F	416	VAL
1	F	438	ASP
1	F	453	HIS
1	F	456	ASN
1	F	461	THR
1	F	463	LYS
1	F	493	LEU
1	F	501	PHE
1	F	519	ILE
1	F	532	ASP
1	F	533	MET
1	F	547	VAL
1	F	586	VAL
1	F	591	LYS

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Mol	Chain	Res	Type
1	F	596	HIS
1	F	606	HIS
1	F	609	CYS
1	F	620	ARG
1	F	634	ARG
1	F	641	ASN
1	F	643	LYS
1	F	646	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (174) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	47	ASN
1	A	61	ASN
1	A	76	ASN
1	A	91	ASN
1	A	92	GLN
1	A	102	ASN
1	A	143	HIS
1	A	147	ASN
1	A	212	HIS
1	A	225	HIS
1	A	276	HIS
1	A	287	HIS
1	A	336	ASN
1	A	338	GLN
1	A	354	GLN
1	A	389	ASN
1	A	394	HIS
1	A	405	ASN
1	A	414	ASN
1	A	430	GLN
1	A	449	ASN
1	A	453	HIS
1	A	456	ASN
1	A	468	ASN
1	A	545	ASN
1	A	548	ASN
1	A	581	ASN
1	A	606	HIS
1	A	608	GLN

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Mol	Chain	Res	Type
1	A	612	HIS
1	B	11	GLN
1	B	47	ASN
1	B	49	HIS
1	B	61	ASN
1	B	63	HIS
1	B	76	ASN
1	B	91	ASN
1	B	92	GLN
1	B	102	ASN
1	B	143	HIS
1	B	147	ASN
1	B	176	ASN
1	B	191	ASN
1	B	225	HIS
1	B	274	ASN
1	B	311	HIS
1	B	338	GLN
1	B	354	GLN
1	B	403	HIS
1	B	405	ASN
1	B	430	GLN
1	B	435	ASN
1	B	442	ASN
1	B	449	ASN
1	B	453	HIS
1	B	456	ASN
1	B	457	HIS
1	B	470	ASN
1	B	488	ASN
1	B	548	ASN
1	B	606	HIS
1	B	612	HIS
1	C	11	GLN
1	C	15	ASN
1	C	61	ASN
1	C	63	HIS
1	C	76	ASN
1	C	92	GLN
1	C	102	ASN
1	C	143	HIS
1	C	147	ASN

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Mol	Chain	Res	Type
1	C	161	GLN
1	C	176	ASN
1	C	191	ASN
1	C	274	ASN
1	C	287	HIS
1	C	336	ASN
1	C	338	GLN
1	C	354	GLN
1	C	389	ASN
1	C	405	ASN
1	C	414	ASN
1	C	430	GLN
1	C	435	ASN
1	C	442	ASN
1	C	449	ASN
1	C	453	HIS
1	C	456	ASN
1	C	469	ASN
1	C	542	GLN
1	C	548	ASN
1	C	606	HIS
1	C	612	HIS
1	D	11	GLN
1	D	15	ASN
1	D	61	ASN
1	D	63	HIS
1	D	76	ASN
1	D	92	GLN
1	D	143	HIS
1	D	147	ASN
1	D	176	ASN
1	D	191	ASN
1	D	274	ASN
1	D	287	HIS
1	D	336	ASN
1	D	338	GLN
1	D	354	GLN
1	D	389	ASN
1	D	414	ASN
1	D	435	ASN
1	D	442	ASN
1	D	449	ASN

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Mol	Chain	Res	Type
1	D	453	HIS
1	D	456	ASN
1	D	606	HIS
1	D	612	HIS
1	E	9	GLN
1	E	11	GLN
1	E	15	ASN
1	E	61	ASN
1	E	63	HIS
1	E	76	ASN
1	E	92	GLN
1	E	102	ASN
1	E	143	HIS
1	E	147	ASN
1	E	161	GLN
1	E	176	ASN
1	E	191	ASN
1	E	274	ASN
1	E	336	ASN
1	E	338	GLN
1	E	354	GLN
1	E	394	HIS
1	E	405	ASN
1	E	414	ASN
1	E	430	GLN
1	E	435	ASN
1	E	442	ASN
1	E	449	ASN
1	E	453	HIS
1	E	456	ASN
1	E	468	ASN
1	E	469	ASN
1	E	606	HIS
1	E	612	HIS
1	F	11	GLN
1	F	15	ASN
1	F	61	ASN
1	F	63	HIS
1	F	76	ASN
1	F	92	GLN
1	F	102	ASN
1	F	143	HIS

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Mol	Chain	Res	Type
1	F	147	ASN
1	F	176	ASN
1	F	191	ASN
1	F	274	ASN
1	F	336	ASN
1	F	338	GLN
1	F	354	GLN
1	F	389	ASN
1	F	405	ASN
1	F	414	ASN
1	F	435	ASN
1	F	442	ASN
1	F	449	ASN
1	F	453	HIS
1	F	456	ASN
1	F	469	ASN
1	F	606	HIS
1	F	612	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.