



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1QXP / pdb_00001qxp
Title : Crystal Structure of a mu-like calpain
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Deposited on : 2003-09-08
Resolution : 2.80 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

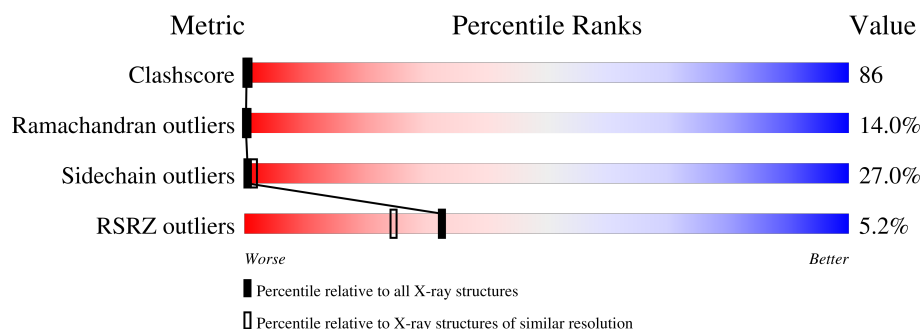
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

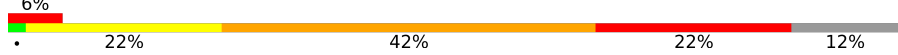
The reported resolution of this entry is 2.80 Å.

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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	900	
1	B	900	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12368 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 mu-like calpain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	783	Total	C	N	O	S	0	0	0
			6053	3846	1037	1143	27			
1	B	788	Total	C	N	O	S	0	0	0
			6003	3830	1015	1129	29			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	SER	CYS	engineered mutation	UNP P97571
B	105	SER	CYS	engineered mutation	UNP P97571
A	702A	GLY	-	cloning artifact	UNP Q07009
A	702B	LYS	-	cloning artifact	UNP Q07009
A	702C	LEU	-	cloning artifact	UNP Q07009
A	702D	ALA	-	cloning artifact	UNP Q07009
A	702E	ALA	-	cloning artifact	UNP Q07009
A	702F	ALA	-	cloning artifact	UNP Q07009
A	702G	ILE	-	cloning artifact	UNP Q07009
A	702H	GLU	-	cloning artifact	UNP Q07009
A	702I	HIS	-	expression tag	UNP Q07009
A	702J	HIS	-	expression tag	UNP Q07009
A	702K	HIS	-	expression tag	UNP Q07009
A	702L	HIS	-	expression tag	UNP Q07009
A	702M	HIS	-	expression tag	UNP Q07009
A	702N	HIS	-	expression tag	UNP Q07009
B	702A	GLY	-	cloning artifact	UNP Q07009
B	702B	LYS	-	cloning artifact	UNP Q07009
B	702C	LEU	-	cloning artifact	UNP Q07009
B	702D	ALA	-	cloning artifact	UNP Q07009
B	702E	ALA	-	cloning artifact	UNP Q07009
B	702F	ALA	-	cloning artifact	UNP Q07009
B	702G	ILE	-	cloning artifact	UNP Q07009
B	702H	GLU	-	cloning artifact	UNP Q07009
B	702I	HIS	-	expression tag	UNP Q07009

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Chain	Residue	Modelled	Actual	Comment	Reference
B	702J	HIS	-	expression tag	UNP Q07009
B	702K	HIS	-	expression tag	UNP Q07009
B	702L	HIS	-	expression tag	UNP Q07009
B	702M	HIS	-	expression tag	UNP Q07009
B	702N	HIS	-	expression tag	UNP Q07009

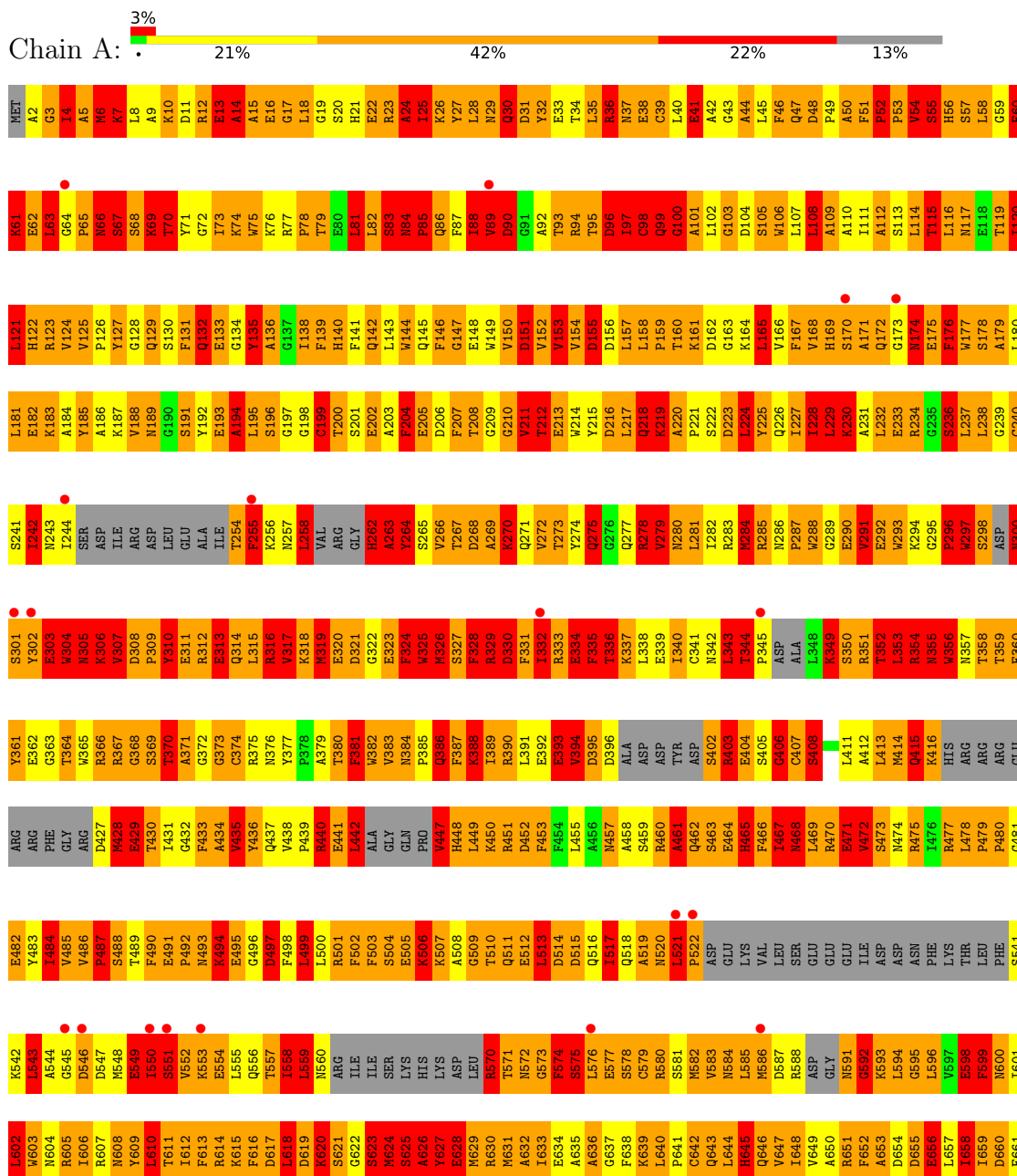
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	172	Total	O	0	0
			172	172		
2	B	140	Total	O	0	0
			140	140		

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: mu-like calpain





I834	Y835	S836	M837	I838	I839	R840	ARG	TYR	S843	D844	E845	T846	Q847	M848	M849	D850	F851	D852	M853	F854	I855	S856	C857	L858	V859	R860	L861	D862	A863	M864	F865	R866	A867	F868	R869	S870	L871	D872	R873	N874	G875	T876	G877	Q878	I879	V881	N882	I883	Q884	E885	W886	L887	Q888	L889	T890	M891	Y892	S893	
A774	V775	M776	D777	S778	D779	T780	T781	G782	K783	L784	G785	F786	E787	F788	F789	K790	Y791	L792	L793	N794	N795	I796	K797	K798	W799	Q800	G801	I802	TYR	LYS	R805	F806	E807	T808	D809	R810	S811	G812	THR	ILE	GLY	SER	ASN	GLU	LEU	P820	G821	A822	F823	E824	A825	A826	G827	F828	H829	L830	M831	Q832	H833
W714	ILE	GLU	ALA	N718	E719	S720	EO	GLU	E723	R724	Q725	F726	R727	K728	L729	F730	F731	Q732	L733	ALA	GLY	ASP	ASP	M738	E739	V740	S741	A742	T743	E744	L745	M746	ASN	ILE	LEU	ASN	LYS	VAL	VAL	THR	ARG	HIS	PRO	ASP	LEU	LYS	THR	ASP	GLY	F764	G765	I766	D767	T768	C769	R770	S771	M772	V773
F661	D662	N663	F664	V665	R666	C667	L668	V669	R670	L671	E672	L673	L674	F675	K676	L677	F678	K679	Q680	L681	D682	F683	E684	M685	T686	G687	T688	I689	Q690	L691	D692	L693	I694	V695	L697	S698	F699	S700	V701	L702	GLY	LYS	LEU	ALA	ALA	ILE	ILE	GLU	HIS	HIS	HIS	HIS	M710	H711	Y712	S713			
I601	L602	M603	M604	R605	I606	R607	M608	Y609	L610	T611	I612	F613	R614	K615	F616	D617	L618	D619	K620	S621	G622	S623	M624	S625	A626	Y627	E628	M629	R630	M631	A632	I633	E634	A635	A636	G637	F638	K639	L640	F641	C642	Q643	L644	H645	Q646	V647	I648	V649	A650	R651	F652	A653	D654	D655	E656	L657	I658	L659	D660

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.74Å 184.60Å 86.37Å 90.00° 100.74° 90.00°	Depositor
Resolution (Å)	91.29 – 2.80 91.29 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.6 (91.29-2.80) 89.7 (91.29-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.229 , 0.311 0.232 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 106.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12368	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	4.56	1459/6177 (23.6%)	3.06	804/8354 (9.6%)
1	B	4.50	1422/6128 (23.2%)	3.05	799/8288 (9.6%)
All	All	4.53	2881/12305 (23.4%)	3.05	1603/16642 (9.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	45
1	B	0	39
All	All	0	84

All (2881) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	869	ARG	CA-CB	26.29	1.92	1.53
1	B	67	SER	CA-CB	25.20	1.96	1.53
1	A	631	MET	SD-CE	24.79	2.41	1.79
1	A	789	PHE	CA-C	-23.95	1.32	1.52
1	B	316	ARG	CA-CB	23.69	1.93	1.53
1	B	883	ILE	CA-CB	23.12	1.81	1.54
1	B	291	VAL	CA-CB	-22.98	1.23	1.54
1	A	680	GLN	CA-CB	22.85	1.92	1.53
1	A	671	LEU	CA-CB	22.48	1.89	1.53
1	A	463	SER	C-O	-22.32	0.97	1.23
1	A	317	VAL	CA-CB	21.80	1.84	1.54
1	A	594	LEU	CA-C	-21.52	1.37	1.52
1	B	824	GLU	CA-CB	21.34	1.86	1.53
1	B	772	MET	SD-CE	20.99	2.32	1.79
1	B	669	VAL	CA-CB	20.77	1.82	1.54
1	B	694	ILE	CA-CB	20.43	1.78	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	624	MET	SD-CE	-20.29	1.28	1.79
1	B	572	ASN	CA-C	20.07	1.77	1.52
1	A	110	ALA	CA-CB	-19.88	1.22	1.53
1	A	434	ALA	C-O	-19.47	1.00	1.23
1	B	6	MET	CG-SD	18.41	2.26	1.80
1	A	796	ILE	CA-CB	17.95	1.74	1.54
1	B	52	PRO	CA-C	-17.90	1.35	1.52
1	A	479	PRO	CA-C	-17.86	1.35	1.52
1	A	392	GLU	C-O	17.75	1.46	1.24
1	A	608	ASN	C-O	-17.45	1.04	1.24
1	B	6	MET	SD-CE	17.40	2.23	1.79
1	B	68	SER	C-O	-17.27	1.01	1.24
1	A	428	MET	CG-SD	17.13	2.23	1.80
1	B	89	VAL	CA-CB	17.05	1.77	1.53
1	B	389	ILE	C-O	16.88	1.41	1.24
1	A	471	GLU	C-O	-16.68	1.02	1.24
1	A	218	GLN	CA-CB	16.67	1.75	1.52
1	A	811	SER	CA-CB	-16.61	1.25	1.53
1	B	640	LEU	N-CA	16.56	1.59	1.45
1	A	200	THR	CA-CB	16.54	1.79	1.53
1	B	479	PRO	CA-CB	-16.48	1.39	1.54
1	A	6	MET	CG-SD	16.46	2.21	1.80
1	B	88	ILE	CA-C	-16.39	1.31	1.52
1	B	74	LYS	CA-C	16.36	1.72	1.52
1	A	770	ARG	C-O	-16.30	1.04	1.24
1	B	456	ALA	CA-C	16.21	1.74	1.52
1	B	441	GLU	CA-CB	-16.09	1.26	1.53
1	B	324	PHE	N-CA	-16.04	1.27	1.46
1	B	30	GLN	C-O	-16.02	1.04	1.23
1	A	833	HIS	CA-C	15.97	1.74	1.52
1	B	210	GLY	C-O	-15.97	1.07	1.24
1	A	389	ILE	CA-CB	-15.89	1.34	1.54
1	A	133	GLU	CA-C	15.81	1.74	1.52
1	B	34	THR	N-CA	15.76	1.66	1.46
1	B	9	ALA	CA-CB	-15.75	1.26	1.53
1	B	349	LYS	CA-C	-15.66	1.31	1.53
1	A	826	ALA	CA-CB	15.64	1.76	1.54
1	B	508	ALA	CA-CB	15.34	1.68	1.53
1	A	502	PHE	C-O	-15.32	1.06	1.24
1	A	379	ALA	CA-CB	-15.24	1.28	1.53
1	B	385	PRO	C-O	15.23	1.40	1.23
1	A	350	SER	CA-C	-15.22	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	579	CYS	CA-CB	15.13	1.78	1.53
1	A	550	ILE	CA-CB	15.10	1.75	1.54
1	A	318	LYS	N-CA	15.03	1.65	1.46
1	B	777	ASP	CA-CB	15.03	1.76	1.53
1	B	394	VAL	C-O	14.90	1.39	1.23
1	A	278	ARG	CA-C	-14.86	1.32	1.52
1	B	631	MET	SD-CE	14.78	2.16	1.79
1	A	217	LEU	CA-C	-14.78	1.32	1.52
1	B	504	SER	N-CA	14.77	1.64	1.46
1	B	193	GLU	CA-C	-14.77	1.38	1.53
1	B	837	MET	CA-C	14.76	1.72	1.52
1	A	112	ALA	CA-CB	-14.75	1.30	1.53
1	B	366	ARG	NE-CZ	-14.67	1.17	1.33
1	A	377	TYR	C-O	-14.63	1.08	1.24
1	A	471	GLU	N-CA	14.62	1.65	1.46
1	B	95	THR	C-O	14.62	1.41	1.23
1	B	647	VAL	C-O	-14.62	1.06	1.24
1	B	403	ARG	CA-C	14.62	1.72	1.52
1	B	39	CYS	C-O	-14.61	1.07	1.24
1	B	338	LEU	CA-CB	-14.59	1.30	1.53
1	A	370	THR	C-O	-14.59	1.04	1.24
1	B	175	GLU	C-O	-14.58	1.05	1.24
1	B	398	ASP	C-N	14.58	1.52	1.33
1	A	99	GLN	CA-CB	14.56	1.78	1.53
1	B	152	VAL	C-O	-14.54	1.08	1.24
1	A	460	ARG	CZ-NH2	14.44	1.52	1.33
1	A	135	TYR	N-CA	-14.41	1.27	1.46
1	A	281	LEU	CA-C	-14.40	1.35	1.52
1	A	211	VAL	CA-C	-14.37	1.34	1.52
1	A	550	ILE	CA-C	14.32	1.71	1.52
1	A	174	ASN	CA-C	14.31	1.72	1.52
1	B	362	GLU	C-O	14.31	1.41	1.24
1	B	502	PHE	CA-C	-14.21	1.35	1.52
1	B	772	MET	C-O	14.21	1.39	1.24
1	B	742	ALA	N-CA	14.20	1.64	1.46
1	A	891	MET	C-O	-14.19	1.07	1.24
1	A	278	ARG	C-O	-14.15	1.06	1.24
1	B	656	GLU	C-O	14.08	1.38	1.23
1	A	385	PRO	CA-C	-14.06	1.37	1.52
1	A	871	LEU	CA-C	-14.05	1.35	1.52
1	B	201	SER	C-O	-14.05	1.07	1.24
1	A	96	ASP	CA-C	-14.04	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	332	ILE	CB-CG2	14.04	1.98	1.52
1	B	865	PHE	CA-C	-14.00	1.40	1.53
1	B	363	GLY	N-CA	13.99	1.58	1.45
1	A	412	ALA	CA-C	-13.99	1.34	1.52
1	B	642	CYS	C-O	-13.96	1.07	1.24
1	B	885	GLU	C-O	-13.94	1.04	1.23
1	A	459	SER	C-O	-13.94	1.07	1.24
1	A	448	HIS	N-CA	13.93	1.64	1.46
1	A	799	TRP	C-O	-13.90	1.06	1.24
1	A	341	CYS	CA-C	13.88	1.71	1.52
1	B	539	LEU	CA-C	13.86	1.71	1.52
1	A	339	GLU	CD-OE1	13.86	1.51	1.25
1	B	113	SER	C-O	13.76	1.40	1.24
1	A	279	VAL	C-O	-13.71	1.07	1.24
1	B	397	ALA	CA-C	13.70	1.69	1.52
1	A	696	TRP	C-O	-13.68	1.06	1.24
1	B	143	LEU	C-O	-13.68	1.07	1.23
1	B	811	SER	CA-C	13.68	1.71	1.52
1	A	518	GLN	CA-C	13.60	1.68	1.52
1	B	553	LYS	CA-CB	13.59	1.76	1.53
1	A	858	LEU	CA-CB	13.56	1.74	1.53
1	B	96	ASP	CA-C	-13.52	1.34	1.52
1	B	83	SER	C-O	13.46	1.41	1.24
1	A	485	VAL	C-O	-13.45	1.10	1.24
1	B	154	VAL	CA-CB	-13.46	1.41	1.55
1	A	492	PRO	C-O	-13.45	1.06	1.23
1	A	383	VAL	C-O	-13.43	1.09	1.24
1	B	786	PHE	CA-CB	13.42	1.74	1.53
1	A	415	GLN	N-CA	13.41	1.62	1.46
1	B	348	LEU	CA-CB	13.38	1.74	1.53
1	A	315	LEU	C-O	-13.35	1.07	1.24
1	A	580	ARG	N-CA	-13.33	1.29	1.46
1	B	329	ARG	CA-C	13.31	1.70	1.52
1	A	10	LYS	N-CA	13.31	1.62	1.46
1	B	465	HIS	C-O	-13.30	1.07	1.24
1	B	150	VAL	CA-C	13.29	1.68	1.52
1	A	382	TRP	C-O	13.25	1.41	1.24
1	A	649	VAL	CA-CB	13.19	1.71	1.54
1	B	324	PHE	CA-C	-13.17	1.35	1.52
1	B	227	ILE	CA-CB	-13.17	1.39	1.54
1	B	796	ILE	CA-C	13.15	1.68	1.52
1	A	461	ALA	N-CA	13.13	1.63	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	GLN	CA-CB	-13.08	1.33	1.53
1	A	670	ARG	C-O	13.07	1.39	1.24
1	A	517	ILE	CA-C	13.05	1.69	1.52
1	B	198	GLY	C-O	13.04	1.41	1.23
1	A	366	ARG	N-CA	13.03	1.61	1.46
1	A	203	ALA	CA-CB	-13.02	1.31	1.53
1	A	242	ILE	C-O	-13.01	1.08	1.24
1	A	429	GLU	N-CA	-12.99	1.30	1.45
1	B	74	LYS	C-O	12.98	1.38	1.23
1	B	334	GLU	N-CA	12.98	1.62	1.46
1	B	38	GLU	C-O	-12.98	1.08	1.24
1	A	864	MET	CA-CB	12.97	1.75	1.53
1	A	831	ASN	CG-OD1	12.94	1.48	1.23
1	A	122	HIS	C-O	12.91	1.40	1.24
1	A	413	LEU	C-O	-12.91	1.08	1.24
1	B	788	GLU	CA-CB	12.90	1.71	1.53
1	A	492	PRO	CA-C	-12.86	1.40	1.53
1	A	106	TRP	C-O	-12.85	1.07	1.24
1	B	265	SER	C-O	-12.84	1.07	1.23
1	A	144	TRP	N-CA	12.83	1.62	1.46
1	A	891	MET	CA-CB	-12.82	1.33	1.53
1	B	11	ASP	CA-C	12.82	1.70	1.52
1	B	162	ASP	CA-C	12.80	1.70	1.52
1	A	290	GLU	C-O	12.80	1.39	1.24
1	B	403	ARG	N-CA	12.80	1.62	1.46
1	A	280	ASN	CG-OD1	-12.79	0.99	1.23
1	A	800	GLN	N-CA	-12.76	1.29	1.46
1	A	329	ARG	N-CA	12.76	1.62	1.46
1	B	139	PHE	N-CA	-12.72	1.29	1.45
1	A	367	ARG	C-O	-12.72	1.07	1.24
1	A	12	ARG	CA-C	12.69	1.71	1.52
1	A	328	PHE	C-O	-12.68	1.07	1.24
1	A	462	GLN	CA-CB	-12.65	1.31	1.53
1	B	73	ILE	C-O	-12.64	1.08	1.24
1	A	119	THR	N-CA	-12.63	1.30	1.46
1	B	808	THR	CA-C	12.62	1.69	1.52
1	B	839	ILE	C-O	12.61	1.39	1.24
1	A	558	ILE	CA-CB	-12.59	1.41	1.54
1	B	503	PHE	C-O	-12.57	1.09	1.24
1	B	399	ASP	C-O	12.56	1.38	1.23
1	B	237	LEU	C-O	-12.54	1.07	1.23
1	A	623	SER	C-O	-12.53	1.08	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	312	ARG	CG-CD	12.52	1.90	1.52
1	A	153	VAL	CA-C	-12.52	1.42	1.52
1	A	483	TYR	CA-CB	-12.52	1.33	1.53
1	A	166	VAL	N-CA	12.51	1.66	1.46
1	A	459	SER	CA-C	-12.51	1.36	1.52
1	A	635	ALA	N-CA	12.50	1.61	1.46
1	A	860	ARG	CZ-NH2	12.50	1.49	1.33
1	A	376	ASN	N-CA	-12.50	1.29	1.46
1	B	806	PHE	CB-CG	12.50	1.79	1.50
1	B	835	TYR	CA-CB	12.43	1.72	1.53
1	A	694	ILE	CA-CB	12.43	1.70	1.54
1	A	320	GLU	CA-CB	12.42	1.74	1.53
1	A	450	LYS	CA-C	-12.41	1.36	1.53
1	B	120	ILE	C-O	-12.41	1.08	1.24
1	B	208	THR	C-O	12.40	1.43	1.23
1	B	159	PRO	C-O	-12.39	1.07	1.24
1	B	582	MET	SD-CE	12.36	2.10	1.79
1	A	452	ASP	CB-CG	12.33	1.82	1.52
1	A	764	PHE	N-CA	12.33	1.61	1.46
1	A	370	THR	CA-CB	-12.28	1.37	1.54
1	B	182	GLU	N-CA	12.28	1.61	1.46
1	A	62	GLU	CA-C	-12.27	1.36	1.52
1	B	597	VAL	CA-C	12.26	1.68	1.52
1	A	120	ILE	C-O	-12.26	1.09	1.24
1	B	673	ILE	CA-C	12.26	1.68	1.52
1	B	54	VAL	CA-CB	-12.21	1.37	1.54
1	B	200	THR	N-CA	12.19	1.62	1.46
1	A	353	LEU	C-O	12.18	1.39	1.24
1	A	386	GLN	C-O	-12.18	1.08	1.23
1	A	89	VAL	CA-CB	12.18	1.71	1.54
1	A	583	VAL	CA-CB	12.14	1.75	1.54
1	A	44	ALA	N-CA	12.12	1.61	1.46
1	A	873	LYS	C-O	12.12	1.38	1.24
1	B	472	VAL	C-O	12.11	1.37	1.24
1	B	412	ALA	C-O	12.11	1.37	1.23
1	B	677	ILE	C-O	12.09	1.39	1.24
1	A	757	PRO	CA-C	12.08	1.69	1.52
1	B	417	HIS	CA-CB	12.06	1.71	1.53
1	B	645	HIS	CA-C	-12.05	1.36	1.52
1	B	89	VAL	CA-C	-12.01	1.38	1.52
1	A	891	MET	SD-CE	11.99	2.09	1.79
1	A	600	ASN	CA-CB	11.98	1.72	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	52	PRO	C-O	-11.98	1.11	1.24
1	A	124	VAL	CA-C	-11.97	1.37	1.52
1	B	136	ALA	N-CA	11.97	1.67	1.46
1	A	673	ILE	CA-CB	11.96	1.71	1.54
1	A	777	ASP	C-O	-11.96	1.09	1.24
1	A	337	LYS	CE-NZ	11.95	1.85	1.49
1	B	266	VAL	CA-CB	11.93	1.68	1.54
1	B	851	PHE	C-O	11.93	1.39	1.24
1	A	802	ILE	CA-CB	-11.93	1.38	1.54
1	B	129	GLN	C-O	-11.93	1.09	1.24
1	B	521	LEU	CA-C	11.88	1.64	1.52
1	A	109	ALA	CA-C	11.88	1.68	1.52
1	A	329	ARG	CZ-NH1	11.87	1.49	1.32
1	B	680	GLN	CA-CB	11.87	1.72	1.53
1	A	584	ASN	CB-CG	-11.86	1.22	1.52
1	A	696	TRP	CA-C	-11.85	1.36	1.52
1	B	295	GLY	N-CA	11.85	1.60	1.44
1	B	396	ASP	C-O	11.83	1.38	1.24
1	A	775	VAL	CA-CB	-11.80	1.37	1.54
1	A	119	THR	CA-CB	-11.80	1.34	1.53
1	A	218	GLN	CB-CG	11.79	1.87	1.52
1	B	94	ARG	CA-CB	11.78	1.72	1.53
1	A	320	GLU	CD-OE2	11.77	1.47	1.25
1	B	69	LYS	C-O	11.77	1.38	1.24
1	A	385	PRO	C-O	-11.72	1.08	1.23
1	A	598	GLU	C-O	-11.71	1.09	1.23
1	A	871	LEU	C-O	-11.70	1.10	1.24
1	B	443	ALA	CA-CB	11.70	1.73	1.53
1	A	65	PRO	CA-C	11.70	1.65	1.52
1	A	99	GLN	CA-C	-11.66	1.37	1.52
1	B	519	ALA	C-O	-11.66	1.10	1.24
1	A	375	ARG	C-O	-11.64	1.09	1.24
1	A	70	THR	CA-CB	11.64	1.68	1.52
1	A	460	ARG	CA-C	-11.64	1.38	1.52
1	A	436	TYR	C-O	11.62	1.38	1.23
1	A	219	LYS	CG-CD	11.62	1.87	1.52
1	A	110	ALA	N-CA	11.61	1.60	1.46
1	A	342	ASN	C-O	-11.61	1.09	1.23
1	B	69	LYS	CB-CG	11.61	1.87	1.52
1	B	203	ALA	CA-CB	11.61	1.72	1.53
1	B	369	SER	C-O	-11.59	1.09	1.24
1	A	867	ALA	CA-CB	11.54	1.71	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	629	MET	SD-CE	-11.52	1.50	1.79
1	B	777	ASP	N-CA	11.51	1.60	1.46
1	B	84	ASN	CG-OD1	11.50	1.45	1.23
1	A	364	THR	CA-C	11.50	1.67	1.52
1	A	255	PHE	N-CA	11.47	1.60	1.46
1	B	429	GLU	CD-OE1	11.47	1.47	1.25
1	A	659	ILE	CA-CB	-11.47	1.38	1.54
1	B	283	ARG	CA-C	-11.47	1.39	1.52
1	B	874	ASN	N-CA	11.46	1.63	1.46
1	A	65	PRO	C-O	11.45	1.35	1.23
1	A	390	ARG	CA-C	11.45	1.67	1.53
1	B	440	ARG	CG-CD	11.45	1.86	1.52
1	B	473	SER	C-O	-11.43	1.09	1.24
1	A	684	GLU	CA-C	-11.42	1.40	1.53
1	A	380	THR	CA-CB	-11.35	1.35	1.53
1	B	729	LEU	C-O	11.35	1.38	1.24
1	A	45	LEU	C-O	11.34	1.37	1.23
1	A	546	ASP	CA-CB	11.33	1.72	1.53
1	B	341	CYS	C-O	-11.33	1.10	1.24
1	B	583	VAL	CA-CB	11.33	1.71	1.55
1	A	511	GLN	C-O	-11.32	1.11	1.23
1	A	40	LEU	C-O	-11.32	1.10	1.24
1	A	516	GLN	N-CA	11.32	1.60	1.46
1	B	487	PRO	C-O	11.31	1.34	1.23
1	B	277	GLN	CA-C	-11.27	1.38	1.52
1	A	41	GLU	CA-CB	11.26	1.72	1.53
1	A	167	PHE	C-O	11.25	1.38	1.24
1	A	833	HIS	C-O	11.22	1.38	1.24
1	B	237	LEU	N-CA	11.22	1.60	1.46
1	B	312	ARG	C-O	-11.21	1.09	1.24
1	B	96	ASP	C-O	-11.21	1.09	1.24
1	A	183	LYS	N-CA	11.21	1.60	1.46
1	B	498	PHE	C-O	11.21	1.36	1.24
1	B	160	THR	N-CA	-11.20	1.31	1.46
1	A	440	ARG	C-O	11.20	1.38	1.24
1	B	226	GLN	CG-CD	11.19	1.80	1.52
1	A	99	GLN	N-CA	11.19	1.60	1.46
1	A	358	THR	CA-C	11.18	1.66	1.52
1	A	332	ILE	CB-CG1	11.18	1.75	1.53
1	B	713	SER	CA-C	11.18	1.67	1.52
1	A	713	SER	CA-C	11.17	1.68	1.52
1	B	56	HIS	CA-C	11.17	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	20	SER	N-CA	11.16	1.58	1.45
1	A	282	ILE	C-O	11.16	1.35	1.24
1	A	479	PRO	C-O	-11.16	1.11	1.24
1	A	186	ALA	CA-CB	-11.11	1.34	1.53
1	A	306	LYS	C-O	-11.10	1.09	1.23
1	A	734	ALA	CA-CB	11.10	1.72	1.53
1	B	640	LEU	C-O	-11.10	1.12	1.24
1	A	271	GLN	CA-C	11.09	1.67	1.52
1	A	380	THR	N-CA	-11.09	1.31	1.46
1	A	790	LYS	CA-C	11.08	1.67	1.52
1	B	624	MET	CA-C	11.07	1.67	1.52
1	B	182	GLU	CA-CB	-11.06	1.35	1.53
1	A	833	HIS	N-CA	11.06	1.60	1.46
1	B	373	GLY	C-O	-11.06	1.13	1.23
1	B	6	MET	CA-C	-11.05	1.39	1.53
1	A	114	LEU	CA-C	-11.04	1.41	1.52
1	B	388	LYS	CA-C	-11.04	1.39	1.52
1	A	243	ASN	CA-C	11.04	1.67	1.52
1	A	685	ASN	CA-C	11.02	1.67	1.52
1	B	267	THR	N-CA	-11.02	1.32	1.46
1	A	738	MET	CA-CB	-11.01	1.34	1.53
1	A	847	GLY	C-O	10.98	1.38	1.23
1	A	780	THR	CA-CB	-10.98	1.35	1.53
1	B	231	ALA	N-CA	10.97	1.59	1.46
1	B	570	ARG	N-CA	10.97	1.67	1.46
1	A	630	ARG	NE-CZ	10.97	1.45	1.33
1	A	414	MET	SD-CE	10.96	2.06	1.79
1	A	434	ALA	CA-C	-10.96	1.39	1.52
1	A	831	ASN	CA-C	-10.95	1.38	1.52
1	B	769	CYS	CA-C	-10.95	1.39	1.52
1	B	380	THR	C-O	10.94	1.38	1.24
1	A	543	LEU	C-O	10.93	1.37	1.24
1	A	169	HIS	CA-C	10.93	1.65	1.52
1	B	384	ASN	CA-CB	-10.91	1.36	1.53
1	A	800	GLN	C-O	10.90	1.37	1.24
1	B	125	VAL	C-O	10.89	1.38	1.24
1	A	437	GLN	C-O	10.87	1.37	1.24
1	B	524	GLU	CA-C	10.85	1.67	1.52
1	A	273	THR	CA-CB	-10.83	1.38	1.53
1	B	0	GLU	CA-CB	10.82	1.75	1.53
1	A	882	ASN	C-O	10.82	1.38	1.23
1	B	225	TYR	CA-C	-10.81	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	663	ASN	CA-C	-10.80	1.38	1.52
1	B	61	LYS	CA-CB	10.79	1.71	1.53
1	B	780	THR	C-O	-10.78	1.10	1.24
1	A	611	THR	CA-CB	-10.78	1.34	1.53
1	A	332	ILE	CA-CB	10.74	1.70	1.54
1	A	142	GLN	CA-C	10.73	1.65	1.52
1	B	643	GLN	CG-CD	10.73	1.78	1.52
1	A	385	PRO	N-CA	-10.73	1.35	1.47
1	B	41	GLU	N-CA	-10.73	1.33	1.46
1	B	344	THR	N-CA	10.73	1.61	1.46
1	B	345	PRO	CA-CB	10.71	1.69	1.53
1	A	174	ASN	CB-CG	10.70	1.78	1.52
1	A	492	PRO	N-CA	-10.69	1.36	1.46
1	A	23	ARG	CA-C	10.69	1.67	1.52
1	B	8	LEU	N-CA	-10.69	1.33	1.46
1	B	839	ILE	CA-C	10.69	1.66	1.52
1	A	661	PHE	CA-C	10.67	1.67	1.52
1	B	865	PHE	C-O	-10.67	1.15	1.23
1	B	377	TYR	N-CA	-10.66	1.35	1.46
1	B	690	GLN	CB-CG	10.66	1.84	1.52
1	A	115	THR	CB-CG2	10.66	1.87	1.52
1	B	243	ASN	N-CA	10.65	1.66	1.46
1	A	406	GLY	C-O	-10.63	1.09	1.23
1	B	142	GLN	CB-CG	10.63	1.84	1.52
1	B	402	SER	C-N	10.63	1.48	1.33
1	B	572	ASN	C-O	10.62	1.37	1.24
1	A	740	VAL	CA-CB	-10.62	1.41	1.54
1	B	876	THR	CA-C	-10.61	1.37	1.52
1	B	219	LYS	CA-C	10.61	1.67	1.52
1	B	400	TYR	CA-C	10.61	1.67	1.52
1	B	680	GLN	C-O	-10.59	1.11	1.24
1	B	425	GLY	N-CA	10.55	1.54	1.45
1	A	361	TYR	CA-C	-10.55	1.39	1.52
1	B	50	ALA	C-O	10.54	1.37	1.24
1	A	275	GLN	N-CA	-10.52	1.31	1.46
1	A	790	LYS	CA-CB	10.52	1.71	1.53
1	B	584	ASN	CA-C	10.51	1.66	1.52
1	B	499	LEU	N-CA	-10.51	1.33	1.46
1	B	344	THR	C-O	-10.50	1.10	1.24
1	B	666	ARG	C-O	-10.49	1.10	1.24
1	A	810	ARG	NE-CZ	10.48	1.44	1.33
1	A	630	ARG	CZ-NH2	10.47	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	499	LEU	C-O	10.46	1.36	1.23
1	A	452	ASP	C-O	10.46	1.36	1.24
1	A	809	ASP	CA-C	10.46	1.66	1.52
1	B	505	GLU	C-O	-10.45	1.10	1.24
1	B	181	LEU	CA-C	-10.45	1.39	1.52
1	B	518	GLN	N-CA	10.45	1.59	1.46
1	A	873	LYS	CA-C	10.44	1.66	1.52
1	B	131	PHE	C-O	-10.44	1.10	1.24
1	A	681	LEU	C-N	-10.43	1.25	1.33
1	B	837	MET	SD-CE	10.43	2.05	1.79
1	A	734	ALA	C-O	10.40	1.37	1.24
1	B	231	ALA	C-O	-10.39	1.11	1.24
1	B	157	LEU	CA-CB	10.38	1.66	1.53
1	B	346	ASP	CB-CG	10.36	1.77	1.52
1	A	600	ASN	CA-C	10.36	1.65	1.52
1	A	892	TYR	CA-CB	10.35	1.65	1.52
1	A	674	LEU	CA-CB	-10.34	1.37	1.53
1	A	89	VAL	C-O	-10.32	1.11	1.24
1	A	428	MET	CB-CG	10.32	1.83	1.52
1	B	241	SER	CA-C	-10.30	1.39	1.52
1	B	296	PRO	CA-C	10.30	1.67	1.52
1	A	686	THR	N-CA	10.30	1.59	1.46
1	B	767	ASP	CA-CB	10.30	1.70	1.53
1	A	477	ARG	NE-CZ	10.29	1.44	1.33
1	A	777	ASP	CA-C	-10.28	1.40	1.52
1	B	304	TRP	C-O	-10.28	1.11	1.24
1	B	61	LYS	N-CA	10.28	1.59	1.46
1	A	301	SER	CA-CB	10.27	1.67	1.53
1	B	112	ALA	CA-C	10.27	1.66	1.52
1	B	167	PHE	C-O	10.27	1.36	1.24
1	A	238	LEU	N-CA	-10.27	1.33	1.46
1	A	293	TRP	CA-C	-10.26	1.39	1.52
1	A	374	CYS	C-O	-10.26	1.10	1.23
1	A	513	LEU	C-O	10.26	1.35	1.23
1	A	553	LYS	CA-CB	10.26	1.70	1.53
1	B	90	ASP	CB-CG	10.25	1.77	1.52
1	A	120	ILE	CA-CB	10.24	1.67	1.54
1	A	648	ILE	CA-CB	-10.24	1.42	1.54
1	A	366	ARG	CA-C	10.23	1.64	1.52
1	B	601	ILE	CA-CB	10.23	1.68	1.54
1	B	682	ASP	CA-C	10.23	1.65	1.52
1	B	54	VAL	C-O	-10.23	1.11	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	382	TRP	C-O	10.21	1.36	1.24
1	A	877	GLY	CA-C	10.21	1.66	1.51
1	A	61	LYS	CA-CB	10.20	1.70	1.53
1	A	500	LEU	C-O	10.20	1.35	1.23
1	A	164	LYS	C-O	10.19	1.36	1.24
1	B	335	PHE	CA-CB	10.18	1.74	1.54
1	B	341	CYS	CA-C	-10.18	1.39	1.52
1	B	281	LEU	C-O	10.17	1.36	1.23
1	A	175	GLU	N-CA	10.15	1.57	1.45
1	A	867	ALA	C-N	-10.15	1.21	1.33
1	B	618	LEU	CA-C	10.14	1.66	1.52
1	B	310	TYR	CA-C	-10.13	1.38	1.52
1	A	465	HIS	N-CA	10.13	1.59	1.46
1	A	440	ARG	C-N	10.12	1.47	1.33
1	A	772	MET	N-CA	-10.11	1.34	1.46
1	B	101	ALA	CA-CB	10.08	1.68	1.53
1	B	315	LEU	CA-C	-10.08	1.39	1.52
1	A	26	LYS	C-O	-10.07	1.12	1.23
1	A	165	LEU	CA-CB	10.07	1.67	1.53
1	A	243	ASN	N-CA	10.07	1.59	1.46
1	A	570	ARG	NE-CZ	10.07	1.44	1.33
1	A	520	ASN	CA-CB	-10.05	1.36	1.53
1	A	889	LEU	C-O	-10.05	1.12	1.24
1	A	608	ASN	C-N	-10.04	1.21	1.33
1	A	859	VAL	CA-CB	-10.04	1.40	1.54
1	A	31	ASP	CA-C	10.04	1.64	1.52
1	A	795	ASN	C-O	-10.04	1.10	1.24
1	B	153	VAL	CA-CB	-10.04	1.40	1.54
1	B	59	GLY	N-CA	10.03	1.56	1.45
1	A	756	HIS	ND1-CE1	10.02	1.42	1.32
1	A	316	ARG	CA-CB	10.02	1.70	1.53
1	B	396	ASP	C-N	10.01	1.46	1.33
1	A	5	ALA	C-O	-10.00	1.11	1.24
1	A	367	ARG	N-CA	-9.99	1.33	1.46
1	B	319	MET	SD-CE	9.98	2.04	1.79
1	A	269	ALA	CA-C	-9.98	1.40	1.52
1	B	123	ARG	CZ-NH1	9.98	1.46	1.32
1	A	310	TYR	CG-CD2	9.98	1.60	1.39
1	B	427	ASP	CA-C	9.97	1.66	1.52
1	A	760	LYS	CA-C	9.97	1.73	1.52
1	B	447	VAL	C-O	-9.97	1.12	1.24
1	B	226	GLN	CA-C	9.97	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	470	ARG	CA-C	-9.96	1.40	1.52
1	A	877	GLY	N-CA	9.95	1.58	1.45
1	B	380	THR	CA-C	9.94	1.65	1.52
1	B	746	MET	SD-CE	9.93	2.04	1.79
1	B	342	ASN	CA-CB	-9.93	1.37	1.53
1	A	474	ASN	N-CA	-9.91	1.33	1.45
1	A	466	PHE	CA-C	-9.91	1.41	1.52
1	A	6	MET	SD-CE	9.90	2.04	1.79
1	B	621	SER	CA-CB	9.90	1.67	1.54
1	B	39	CYS	CA-C	-9.90	1.40	1.52
1	A	18	LEU	CA-C	-9.88	1.39	1.53
1	A	636	ALA	CA-CB	-9.88	1.36	1.53
1	B	608	ASN	CA-C	9.88	1.67	1.52
1	B	727	ARG	C-O	9.87	1.36	1.24
1	A	95	THR	CA-CB	-9.85	1.36	1.53
1	A	867	ALA	CA-C	-9.85	1.40	1.52
1	A	97	ILE	C-O	-9.84	1.12	1.24
1	B	811	SER	CA-CB	9.83	1.70	1.53
1	A	125	VAL	N-CA	9.82	1.58	1.46
1	A	434	ALA	CA-CB	-9.82	1.37	1.53
1	B	57	SER	CA-C	-9.82	1.39	1.52
1	A	336	THR	CA-C	-9.81	1.39	1.53
1	A	797	LYS	C-O	-9.79	1.11	1.24
1	A	81	LEU	C-O	-9.79	1.11	1.24
1	A	105	SER	CA-C	9.78	1.66	1.52
1	A	830	LEU	N-CA	9.78	1.57	1.45
1	B	137	GLY	C-O	-9.78	1.13	1.24
1	A	671	LEU	C-O	-9.78	1.12	1.24
1	A	129	GLN	C-O	-9.77	1.11	1.23
1	A	570	ARG	CB-CG	9.75	1.81	1.52
1	A	92	ALA	C-O	9.75	1.36	1.23
1	B	371	ALA	CA-C	-9.74	1.41	1.53
1	A	519	ALA	C-O	9.73	1.35	1.23
1	A	712	TYR	CA-CB	9.73	1.70	1.53
1	B	110	ALA	CA-C	-9.72	1.40	1.52
1	B	88	ILE	CB-CG2	-9.72	1.20	1.52
1	A	439	PRO	C-O	9.71	1.37	1.24
1	B	53	PRO	CA-C	-9.71	1.41	1.53
1	A	291	VAL	C-O	9.71	1.35	1.24
1	A	123	ARG	NE-CZ	9.69	1.43	1.33
1	A	663	ASN	CA-CB	-9.69	1.36	1.53
1	B	304	TRP	N-CA	9.69	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	856	SER	C-O	-9.69	1.11	1.24
1	A	361	TYR	C-O	9.68	1.35	1.23
1	A	355	ASN	CG-ND2	9.68	1.53	1.33
1	B	285	ARG	CZ-NH1	9.68	1.46	1.32
1	A	520	ASN	CA-C	9.67	1.65	1.52
1	A	856	SER	CA-C	-9.67	1.39	1.52
1	A	275	GLN	C-N	-9.67	1.23	1.33
1	B	389	ILE	CB-CG1	-9.66	1.34	1.53
1	B	324	PHE	CD1-CE1	9.66	1.67	1.38
1	A	114	LEU	N-CA	9.66	1.58	1.46
1	A	778	SER	C-O	9.64	1.38	1.24
1	A	178	SER	C-O	9.64	1.36	1.24
1	A	120	ILE	CG1-CD1	9.63	1.89	1.51
1	A	695	SER	N-CA	9.63	1.57	1.46
1	B	21	HIS	C-O	-9.63	1.12	1.24
1	B	473	SER	N-CA	-9.63	1.35	1.46
1	A	257	ASN	C-O	9.62	1.36	1.24
1	A	582	MET	SD-CE	9.62	2.03	1.79
1	B	329	ARG	C-N	9.62	1.47	1.33
1	A	268	ASP	CA-C	-9.59	1.40	1.52
1	A	863	ALA	CA-CB	-9.59	1.38	1.53
1	A	349	LYS	C-O	9.58	1.36	1.24
1	A	669	VAL	C-N	-9.58	1.22	1.33
1	B	521	LEU	N-CA	9.58	1.57	1.45
1	B	207	PHE	CA-C	9.57	1.65	1.52
1	B	259	VAL	CA-C	9.57	1.73	1.52
1	B	386	GLN	CA-C	-9.56	1.41	1.52
1	B	284	MET	SD-CE	9.56	2.03	1.79
1	B	490	PHE	C-O	-9.54	1.11	1.24
1	B	560	ASN	CA-CB	9.54	1.72	1.53
1	A	393	GLU	C-O	9.53	1.35	1.23
1	B	777	ASP	C-O	9.53	1.35	1.23
1	A	831	ASN	CB-CG	9.53	1.75	1.52
1	B	178	SER	N-CA	9.52	1.57	1.46
1	A	788	GLU	C-O	-9.52	1.11	1.24
1	A	390	ARG	CZ-NH1	9.51	1.46	1.32
1	A	266	VAL	C-O	9.51	1.36	1.24
1	A	354	ARG	NE-CZ	9.50	1.43	1.33
1	A	45	LEU	CA-C	-9.50	1.40	1.52
1	A	194	ALA	CA-CB	-9.49	1.37	1.53
1	B	42	ALA	CA-CB	-9.49	1.36	1.53
1	A	750	ASN	CA-CB	9.48	1.69	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	GLY	CA-C	9.48	1.64	1.52
1	B	189	ASN	N-CA	-9.46	1.33	1.46
1	A	331	PHE	C-O	9.46	1.35	1.24
1	A	127	TYR	CA-C	-9.44	1.40	1.53
1	A	109	ALA	CA-CB	9.43	1.68	1.53
1	B	681	LEU	C-O	9.43	1.36	1.24
1	A	578	SER	N-CA	9.43	1.57	1.46
1	A	642	CYS	N-CA	9.43	1.57	1.46
1	B	46	PHE	C-O	-9.41	1.12	1.23
1	B	610	LEU	CG-CD1	9.41	1.83	1.52
1	A	713	SER	N-CA	9.41	1.58	1.46
1	B	517	ILE	CA-C	9.40	1.64	1.52
1	B	443	ALA	N-CA	9.40	1.58	1.46
1	A	665	VAL	N-CA	9.40	1.57	1.46
1	A	359	THR	N-CA	-9.39	1.34	1.46
1	A	120	ILE	CA-C	-9.38	1.40	1.52
1	B	415	GLN	CB-CG	-9.37	1.24	1.52
1	B	263	ALA	CA-C	-9.37	1.40	1.52
1	A	377	TYR	CA-C	-9.35	1.42	1.53
1	A	884	GLN	N-CA	-9.34	1.35	1.46
1	B	643	GLN	C-O	-9.34	1.12	1.24
1	A	845	GLU	CA-C	9.33	1.72	1.52
1	B	24	ALA	CA-CB	-9.33	1.37	1.53
1	A	757	PRO	CG-CD	9.31	1.82	1.50
1	B	164	LYS	CG-CD	9.30	1.80	1.52
1	A	437	GLN	N-CA	-9.30	1.34	1.46
1	A	574	PHE	CA-C	9.30	1.65	1.52
1	A	639	LYS	CE-NZ	9.28	1.77	1.49
1	B	243	ASN	C-O	9.28	1.42	1.23
1	B	415	GLN	N-CA	9.28	1.56	1.45
1	A	150	VAL	CA-C	9.27	1.64	1.52
1	A	756	HIS	CG-CD2	9.26	1.46	1.35
1	A	124	VAL	CA-CB	9.26	1.67	1.54
1	B	665	VAL	C-O	9.26	1.35	1.24
1	B	346	ASP	CG-OD1	9.24	1.43	1.25
1	B	223	ASP	CA-C	-9.24	1.38	1.52
1	B	673	ILE	CG1-CD1	-9.24	1.15	1.51
1	B	636	ALA	C-O	9.23	1.36	1.24
1	B	838	ILE	CA-C	-9.23	1.41	1.52
1	A	888	GLN	C-O	9.23	1.34	1.24
1	A	510	THR	C-O	-9.22	1.12	1.23
1	A	75	TRP	CA-C	-9.21	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	555	LEU	N-CA	9.21	1.57	1.46
1	A	133	GLU	C-O	9.19	1.35	1.24
1	A	296	PRO	N-CA	-9.19	1.40	1.47
1	A	618	LEU	CG-CD2	9.19	1.82	1.52
1	B	470	ARG	CA-C	9.18	1.64	1.52
1	B	126	PRO	C-O	-9.17	1.12	1.24
1	B	855	ILE	N-CA	9.17	1.57	1.46
1	B	436	TYR	CA-CB	-9.16	1.39	1.53
1	B	647	VAL	CA-CB	9.16	1.67	1.54
1	B	323	GLU	CA-C	9.14	1.64	1.52
1	A	394	VAL	C-O	-9.13	1.11	1.23
1	B	690	GLN	C-O	-9.13	1.13	1.24
1	B	47	GLN	C-O	-9.12	1.13	1.24
1	B	789	PHE	C-O	9.12	1.35	1.24
1	A	381	PHE	CA-C	-9.12	1.40	1.52
1	B	98	CYS	C-O	-9.11	1.12	1.23
1	A	93	THR	CA-C	9.09	1.62	1.53
1	A	468	ASN	CG-ND2	9.08	1.52	1.33
1	A	115	THR	CA-C	9.07	1.65	1.52
1	A	129	GLN	N-CA	9.07	1.57	1.45
1	A	821	GLY	C-O	9.07	1.36	1.23
1	A	355	ASN	CG-OD1	9.06	1.40	1.23
1	B	68	SER	CA-C	-9.05	1.40	1.52
1	A	58	LEU	C-O	9.05	1.36	1.24
1	B	636	ALA	CA-CB	-9.05	1.38	1.53
1	A	167	PHE	N-CA	-9.04	1.34	1.46
1	A	616	PHE	C-O	9.04	1.36	1.24
1	A	326	MET	SD-CE	-9.04	1.56	1.79
1	B	269	ALA	N-CA	9.04	1.57	1.46
1	A	593	LYS	CA-CB	9.03	1.69	1.53
1	B	328	PHE	CD1-CE1	-9.03	1.11	1.38
1	A	362	GLU	N-CA	9.03	1.57	1.46
1	A	213	GLU	C-O	-9.02	1.13	1.23
1	A	448	HIS	C-O	-9.01	1.09	1.23
1	B	487	PRO	N-CD	-9.01	1.35	1.47
1	A	88	ILE	C-O	9.00	1.33	1.23
1	A	743	THR	C-O	9.00	1.34	1.24
1	B	456	ALA	N-CA	9.00	1.57	1.46
1	B	115	THR	CA-C	-8.99	1.40	1.52
1	B	153	VAL	C-O	8.99	1.34	1.24
1	B	345	PRO	C-O	-8.99	1.12	1.24
1	B	154	VAL	CB-CG2	-8.98	1.23	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	796	ILE	C-O	-8.98	1.14	1.24
1	A	878	GLN	CD-OE1	8.98	1.40	1.23
1	A	71	TYR	CA-C	-8.97	1.41	1.52
1	A	713	SER	C-O	8.96	1.35	1.24
1	A	30	GLN	CD-NE2	8.95	1.52	1.33
1	A	691	LEU	C-O	-8.95	1.13	1.23
1	B	641	PRO	C-O	-8.94	1.13	1.23
1	A	478	LEU	CG-CD1	8.92	1.81	1.52
1	B	378	PRO	CA-C	-8.92	1.38	1.52
1	B	391	LEU	CA-C	-8.92	1.42	1.52
1	B	176	PHE	CE1-CZ	-8.90	1.11	1.38
1	A	168	VAL	CA-CB	-8.90	1.43	1.54
1	B	858	LEU	CA-C	8.88	1.64	1.52
1	B	360	PHE	CB-CG	-8.88	1.30	1.50
1	B	690	GLN	CG-CD	8.88	1.74	1.52
1	A	94	ARG	C-O	-8.88	1.12	1.24
1	A	637	GLY	C-O	8.88	1.35	1.23
1	A	487	PRO	N-CA	-8.87	1.37	1.46
1	A	619	ASP	N-CA	-8.87	1.35	1.46
1	B	571	THR	CA-C	8.87	1.62	1.52
1	B	583	VAL	N-CA	-8.87	1.35	1.46
1	A	557	THR	C-O	8.86	1.35	1.24
1	A	770	ARG	C-N	-8.85	1.21	1.34
1	B	156	ASP	CA-CB	8.85	1.63	1.53
1	A	631	MET	CG-SD	8.85	2.02	1.80
1	A	86	GLN	CA-C	-8.84	1.41	1.52
1	B	217	LEU	N-CA	8.84	1.57	1.46
1	B	185	TYR	CD1-CE1	-8.84	1.12	1.38
1	B	399	ASP	CG-OD2	8.84	1.42	1.25
1	A	636	ALA	CA-C	-8.83	1.40	1.52
1	A	639	LYS	CA-C	8.82	1.64	1.52
1	A	768	THR	CA-CB	-8.82	1.38	1.53
1	A	319	MET	CG-SD	-8.81	1.58	1.80
1	B	206	ASP	C-O	-8.80	1.13	1.24
1	A	124	VAL	C-O	-8.80	1.13	1.24
1	A	129	GLN	CD-NE2	8.79	1.51	1.33
1	B	95	THR	N-CA	8.79	1.56	1.46
1	A	321	ASP	CA-C	8.78	1.64	1.52
1	A	350	SER	CA-CB	8.78	1.68	1.53
1	A	662	ASP	CA-C	-8.78	1.41	1.52
1	A	83	SER	C-O	-8.78	1.12	1.24
1	A	265	SER	C-O	-8.77	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	447	VAL	N-CA	8.76	1.62	1.46
1	A	310	TYR	CE2-CZ	8.75	1.59	1.38
1	A	212	THR	C-O	8.75	1.35	1.23
1	A	774	ALA	C-O	-8.75	1.13	1.24
1	A	331	PHE	CA-CB	-8.75	1.39	1.53
1	B	17	GLY	CA-C	8.75	1.64	1.51
1	A	629	MET	CA-CB	8.74	1.68	1.53
1	B	687	GLY	CA-C	8.74	1.63	1.51
1	B	181	LEU	CG-CD1	-8.74	1.23	1.52
1	A	850	ASP	N-CA	8.74	1.56	1.45
1	B	643	GLN	CD-OE1	8.73	1.40	1.23
1	A	676	LYS	CA-CB	8.73	1.66	1.53
1	B	133	GLU	N-CA	8.73	1.56	1.46
1	B	658	ILE	CA-C	-8.73	1.41	1.52
1	A	193	GLU	CD-OE2	8.72	1.42	1.25
1	A	196	SER	CA-C	8.72	1.64	1.52
1	B	508	ALA	C-O	-8.72	1.07	1.23
1	A	179	ALA	C-O	-8.72	1.12	1.24
1	A	75	TRP	CB-CG	8.72	1.77	1.50
1	A	739	GLU	CA-C	-8.71	1.41	1.52
1	A	47	GLN	CA-CB	-8.71	1.40	1.53
1	A	349	LYS	CA-C	-8.70	1.41	1.52
1	A	415	GLN	C-O	-8.70	1.13	1.24
1	A	628	GLU	C-O	8.70	1.35	1.24
1	A	737	ASP	C-O	8.70	1.34	1.24
1	B	435	VAL	C-O	-8.69	1.13	1.24
1	A	798	LYS	CA-C	-8.69	1.41	1.52
1	A	125	VAL	CA-C	8.69	1.62	1.52
1	B	138	ILE	N-CA	8.68	1.57	1.46
1	B	729	LEU	CA-C	8.68	1.64	1.52
1	B	333	ARG	CG-CD	8.68	1.78	1.52
1	B	451	ARG	CA-C	-8.67	1.42	1.52
1	B	632	ALA	C-O	8.67	1.34	1.24
1	A	97	ILE	CA-CB	8.67	1.66	1.54
1	A	831	ASN	N-CA	-8.67	1.35	1.46
1	B	357	ASN	CA-C	-8.67	1.42	1.52
1	B	152	VAL	CA-CB	-8.67	1.43	1.54
1	A	117	ASN	CG-ND2	8.63	1.51	1.33
1	A	701	VAL	CA-C	8.63	1.63	1.52
1	B	402	SER	C-O	8.63	1.35	1.23
1	B	514	ASP	C-O	8.63	1.33	1.23
1	B	424	PHE	C-O	8.62	1.40	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	488	SER	C-O	8.62	1.33	1.23
1	B	188	VAL	N-CA	8.62	1.56	1.46
1	A	865	PHE	C-O	-8.62	1.14	1.24
1	A	795	ASN	CA-C	-8.62	1.40	1.52
1	B	396	ASP	CA-C	8.61	1.64	1.52
1	B	57	SER	N-CA	-8.60	1.34	1.46
1	B	826	ALA	CA-CB	8.60	1.67	1.53
1	B	7	LYS	C-O	-8.60	1.13	1.24
1	B	359	THR	CA-C	-8.59	1.41	1.52
1	B	8	LEU	C-O	8.58	1.34	1.24
1	A	663	ASN	N-CA	8.57	1.57	1.46
1	B	23	ARG	C-N	-8.56	1.21	1.33
1	A	13	GLU	N-CA	-8.56	1.35	1.46
1	A	333	ARG	CG-CD	8.56	1.78	1.52
1	A	154	VAL	CA-C	8.55	1.63	1.52
1	B	408	SER	CA-C	-8.55	1.42	1.52
1	A	7	LYS	CD-CE	8.55	1.78	1.52
1	B	400	TYR	N-CA	8.54	1.57	1.46
1	B	502	PHE	CA-CB	8.54	1.67	1.53
1	A	850	ASP	C-O	-8.54	1.12	1.23
1	A	772	MET	CB-CG	8.54	1.78	1.52
1	B	274	TYR	CA-C	8.53	1.62	1.52
1	A	616	PHE	CE1-CZ	-8.53	1.13	1.38
1	B	62	GLU	C-O	8.53	1.34	1.24
1	B	320	GLU	CD-OE2	8.53	1.41	1.25
1	A	123	ARG	CZ-NH1	8.52	1.44	1.32
1	A	388	LYS	C-O	8.52	1.33	1.23
1	B	212	THR	CA-C	-8.52	1.42	1.52
1	B	439	PRO	CA-C	8.52	1.61	1.53
1	A	628	GLU	N-CA	-8.52	1.33	1.45
1	B	776	MET	CA-C	-8.52	1.41	1.52
1	B	871	LEU	CA-CB	-8.51	1.39	1.53
1	A	324	PHE	CA-C	-8.51	1.41	1.52
1	A	615	LYS	CE-NZ	8.51	1.74	1.49
1	A	810	ARG	CA-C	8.50	1.64	1.52
1	A	229	LEU	N-CA	-8.50	1.35	1.46
1	A	624	MET	SD-CE	-8.50	1.58	1.79
1	B	859	VAL	C-O	-8.49	1.11	1.24
1	B	869	ARG	CA-C	-8.49	1.41	1.52
1	A	136	ALA	CA-C	-8.49	1.41	1.52
1	B	26	LYS	CB-CG	8.49	1.77	1.52
1	A	516	GLN	CA-C	-8.48	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	366	ARG	CG-CD	8.48	1.77	1.52
1	B	868	PHE	N-CA	-8.48	1.35	1.46
1	A	331	PHE	CE1-CZ	8.48	1.64	1.38
1	A	36	ARG	CA-C	8.47	1.64	1.52
1	A	66	ASN	C-O	-8.47	1.13	1.24
1	B	329	ARG	NE-CZ	8.47	1.42	1.33
1	A	596	LEU	N-CA	8.47	1.58	1.46
1	B	418	ARG	N-CA	8.47	1.62	1.46
1	A	166	VAL	CA-CB	-8.47	1.43	1.54
1	B	585	LEU	CA-C	-8.47	1.41	1.52
1	B	475	ARG	N-CA	-8.46	1.35	1.46
1	A	107	LEU	CA-C	-8.46	1.41	1.52
1	A	674	LEU	CA-C	-8.46	1.41	1.52
1	A	776	MET	CG-SD	-8.46	1.59	1.80
1	B	477	ARG	CB-CG	8.46	1.77	1.52
1	A	185	TYR	CA-C	-8.45	1.42	1.52
1	B	19	GLY	N-CA	-8.45	1.33	1.45
1	A	571	THR	CA-CB	8.44	1.67	1.53
1	B	9	ALA	C-O	8.44	1.34	1.24
1	B	891	MET	SD-CE	-8.44	1.58	1.79
1	A	167	PHE	CA-CB	-8.44	1.39	1.53
1	B	15	ALA	N-CA	8.44	1.57	1.46
1	B	643	GLN	CA-CB	8.43	1.67	1.53
1	A	84	ASN	C-N	8.43	1.44	1.33
1	A	736	ASP	CA-C	8.42	1.61	1.52
1	A	171	ALA	C-O	-8.42	1.14	1.23
1	A	820	PRO	CA-C	8.41	1.70	1.52
1	B	48	ASP	CB-CG	8.41	1.73	1.52
1	A	783	LYS	C-O	8.41	1.36	1.23
1	B	61	LYS	CA-C	8.41	1.64	1.52
1	B	377	TYR	C-O	8.41	1.33	1.24
1	A	547	ASP	N-CA	8.40	1.56	1.46
1	A	794	ASN	N-CA	-8.40	1.34	1.46
1	B	611	THR	CA-C	8.40	1.64	1.52
1	A	542	LYS	N-CA	8.40	1.58	1.46
1	B	90	ASP	CA-CB	8.40	1.69	1.53
1	A	389	ILE	CA-C	-8.39	1.42	1.52
1	A	477	ARG	CG-CD	8.39	1.77	1.52
1	B	467	ILE	CA-CB	8.39	1.65	1.54
1	A	162	ASP	N-CA	8.38	1.55	1.46
1	B	510	THR	CA-C	-8.38	1.42	1.52
1	B	434	ALA	C-O	-8.38	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	392	GLU	CA-C	8.37	1.64	1.52
1	B	164	LYS	C-O	8.37	1.34	1.23
1	A	238	LEU	CA-CB	-8.36	1.41	1.53
1	B	51	PHE	CA-C	8.36	1.62	1.52
1	A	89	VAL	CB-CG1	8.36	1.80	1.52
1	B	185	TYR	CA-C	-8.35	1.40	1.52
1	B	726	PHE	CE1-CZ	8.35	1.63	1.38
1	A	460	ARG	C-O	-8.35	1.14	1.24
1	A	311	GLU	C-O	8.34	1.33	1.24
1	B	377	TYR	C-N	-8.34	1.25	1.34
1	B	391	LEU	CA-CB	8.33	1.65	1.53
1	A	602	LEU	CG-CD1	8.33	1.80	1.52
1	B	238	LEU	CA-C	8.33	1.63	1.52
1	B	728	LYS	CA-CB	8.33	1.67	1.53
1	B	856	SER	CA-CB	8.32	1.67	1.53
1	A	437	GLN	CD-NE2	8.32	1.50	1.33
1	B	494	LYS	CD-CE	8.32	1.77	1.52
1	B	601	ILE	CA-C	8.32	1.63	1.52
1	A	151	ASP	CG-OD1	8.32	1.41	1.25
1	A	239	GLY	CA-C	8.32	1.58	1.52
1	B	14	ALA	CA-CB	-8.32	1.39	1.53
1	B	351	ARG	CA-CB	8.31	1.70	1.53
1	B	398	ASP	CG-OD1	8.31	1.41	1.25
1	B	161	LYS	N-CA	8.30	1.56	1.46
1	A	150	VAL	N-CA	-8.30	1.36	1.46
1	B	34	THR	CB-CG2	-8.30	1.25	1.52
1	B	780	THR	CB-CG2	8.30	1.79	1.52
1	A	463	SER	CA-CB	-8.29	1.40	1.53
1	A	591	ASN	CB-CG	8.29	1.72	1.52
1	B	18	LEU	N-CA	-8.29	1.35	1.46
1	A	586	MET	C-O	8.29	1.34	1.24
1	A	492	PRO	CA-CB	-8.28	1.40	1.54
1	A	645	HIS	C-N	-8.28	1.21	1.33
1	B	169	HIS	N-CA	-8.28	1.35	1.45
1	A	616	PHE	CG-CD2	-8.27	1.21	1.38
1	A	677	ILE	N-CA	-8.27	1.36	1.46
1	A	9	ALA	CA-C	-8.27	1.42	1.52
1	B	99	GLN	C-O	-8.27	1.12	1.23
1	A	681	LEU	C-O	-8.26	1.13	1.24
1	B	233	GLU	CD-OE1	8.26	1.41	1.25
1	B	829	HIS	C-O	-8.25	1.13	1.24
1	B	297	TRP	CZ3-CH2	-8.25	1.19	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	328	PHE	CE1-CZ	-8.25	1.13	1.38
1	A	294	LYS	C-O	8.24	1.34	1.24
1	A	155	ASP	CG-OD1	8.24	1.41	1.25
1	B	12	ARG	CA-C	-8.22	1.41	1.52
1	A	854	PHE	C-O	8.22	1.34	1.23
1	A	884	GLN	CD-NE2	8.21	1.50	1.33
1	A	746	MET	SD-CE	8.21	2.00	1.79
1	A	240	CYS	N-CA	-8.21	1.35	1.45
1	B	467	ILE	N-CA	8.21	1.56	1.46
1	A	200	THR	CA-C	-8.21	1.41	1.52
1	A	233	GLU	N-CA	-8.20	1.37	1.46
1	A	601	ILE	C-O	8.20	1.34	1.24
1	B	263	ALA	N-CA	8.20	1.56	1.46
1	A	648	ILE	C-N	-8.20	1.24	1.33
1	B	725	GLN	CA-CB	8.20	1.67	1.53
1	A	175	GLU	C-O	8.19	1.34	1.23
1	B	843	SER	CA-C	8.19	1.70	1.52
1	A	4	ILE	CA-CB	8.19	1.65	1.54
1	B	48	ASP	N-CA	-8.19	1.33	1.46
1	B	447	VAL	CA-C	8.18	1.63	1.52
1	B	326	MET	N-CA	-8.18	1.35	1.45
1	B	428	MET	SD-CE	8.18	2.00	1.79
1	B	639	LYS	CA-CB	8.18	1.68	1.53
1	A	787	GLU	C-O	-8.17	1.14	1.24
1	A	485	VAL	CB-CG1	-8.16	1.25	1.52
1	A	623	SER	N-CA	-8.16	1.35	1.46
1	B	322	GLY	CA-C	8.16	1.63	1.51
1	B	323	GLU	CD-OE1	8.16	1.40	1.25
1	B	718	ASN	CA-CB	8.15	1.69	1.53
1	A	601	ILE	N-CA	8.14	1.56	1.46
1	A	473	SER	N-CA	8.14	1.56	1.45
1	B	117	ASN	CA-C	8.14	1.63	1.52
1	A	451	ARG	C-O	8.14	1.34	1.24
1	A	784	LEU	CA-C	-8.13	1.42	1.52
1	B	146	PHE	CB-CG	8.13	1.69	1.50
1	B	450	LYS	C-O	8.13	1.34	1.23
1	B	766	ILE	N-CA	-8.13	1.36	1.46
1	A	39	CYS	CA-C	-8.13	1.43	1.52
1	A	216	ASP	C-O	-8.12	1.14	1.24
1	A	631	MET	C-O	8.12	1.33	1.23
1	B	773	VAL	N-CA	8.11	1.56	1.46
1	A	789	PHE	C-O	-8.11	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	652	PHE	CA-CB	-8.11	1.40	1.53
1	B	339	GLU	N-CA	8.11	1.55	1.46
1	A	767	ASP	CG-OD1	8.10	1.40	1.25
1	B	348	LEU	CB-CG	8.10	1.69	1.53
1	B	447	VAL	C-N	-8.10	1.22	1.33
1	B	418	ARG	CZ-NH2	8.09	1.44	1.33
1	A	514	ASP	CG-OD2	8.09	1.40	1.25
1	A	384	ASN	CG-ND2	8.09	1.50	1.33
1	B	738	MET	SD-CE	8.09	1.99	1.79
1	B	386	GLN	C-O	-8.08	1.14	1.23
1	A	208	THR	C-O	8.08	1.32	1.24
1	A	556	GLN	C-O	8.08	1.34	1.24
1	B	229	LEU	N-CA	8.08	1.56	1.46
1	B	451	ARG	NE-CZ	8.07	1.42	1.33
1	B	277	GLN	CB-CG	8.07	1.76	1.52
1	B	105	SER	N-CA	-8.07	1.34	1.46
1	A	626	ALA	N-CA	-8.06	1.35	1.46
1	A	646	GLN	C-N	8.06	1.43	1.33
1	A	413	LEU	CG-CD1	8.06	1.79	1.52
1	A	784	LEU	C-O	8.06	1.33	1.23
1	B	143	LEU	CA-CB	8.06	1.67	1.53
1	B	240	CYS	CA-C	-8.05	1.43	1.52
1	A	609	TYR	CZ-OH	8.05	1.54	1.38
1	A	110	ALA	CA-C	-8.04	1.42	1.52
1	A	831	ASN	CA-CB	8.04	1.67	1.53
1	A	186	ALA	C-O	8.03	1.34	1.24
1	B	345	PRO	CG-CD	8.03	1.78	1.50
1	B	678	PHE	CD2-CE2	-8.03	1.14	1.38
1	A	629	MET	SD-CE	8.02	1.99	1.79
1	B	230	LYS	CD-CE	8.02	1.76	1.52
1	B	629	MET	CA-C	-8.01	1.42	1.52
1	B	242	ILE	C-O	-8.01	1.15	1.24
1	B	349	LYS	N-CA	8.00	1.56	1.45
1	A	339	GLU	C-O	-8.00	1.14	1.24
1	A	360	PHE	CE1-CZ	7.99	1.62	1.38
1	A	625	SER	N-CA	7.99	1.56	1.46
1	A	217	LEU	CG-CD2	-7.97	1.26	1.52
1	A	684	GLU	CA-CB	7.97	1.62	1.52
1	A	649	VAL	CA-C	-7.96	1.41	1.52
1	B	651	ARG	CA-C	7.96	1.63	1.52
1	A	172	GLN	CA-C	7.96	1.63	1.52
1	A	734	ALA	N-CA	7.95	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	194	ALA	CA-CB	-7.94	1.40	1.53
1	B	49	PRO	N-CA	-7.94	1.37	1.47
1	B	358	THR	CA-C	7.94	1.62	1.52
1	A	688	THR	CB-CG2	7.94	1.78	1.52
1	B	697	LEU	CA-CB	7.93	1.66	1.53
1	A	630	ARG	CZ-NH1	7.93	1.43	1.32
1	A	121	LEU	C-O	-7.93	1.15	1.24
1	A	270	LYS	CE-NZ	7.92	1.73	1.49
1	B	272	VAL	CA-C	-7.92	1.45	1.52
1	B	626	ALA	C-O	-7.92	1.14	1.24
1	A	218	GLN	CA-C	7.92	1.63	1.52
1	B	146	PHE	CD2-CE2	-7.92	1.14	1.38
1	B	366	ARG	CZ-NH1	7.91	1.43	1.32
1	B	855	ILE	CA-CB	7.91	1.65	1.54
1	B	660	ASP	C-O	7.91	1.33	1.23
1	B	405	SER	N-CA	7.91	1.56	1.46
1	A	26	LYS	CE-NZ	7.90	1.73	1.49
1	A	383	VAL	CA-CB	-7.90	1.44	1.54
1	A	189	ASN	C-O	7.90	1.34	1.24
1	A	593	LYS	N-CA	-7.90	1.36	1.45
1	B	267	THR	C-O	-7.90	1.14	1.24
1	B	854	PHE	N-CA	-7.90	1.36	1.46
1	A	474	ASN	CB-CG	7.90	1.71	1.52
1	A	613	PHE	CB-CG	-7.90	1.32	1.50
1	A	820	PRO	N-CA	7.90	1.58	1.47
1	B	311	GLU	C-O	-7.90	1.13	1.24
1	A	407	CYS	CA-C	-7.89	1.42	1.52
1	B	305	ASN	CB-CG	7.89	1.71	1.52
1	B	333	ARG	CA-C	7.89	1.63	1.52
1	B	481	GLY	C-O	7.89	1.34	1.23
1	A	866	ARG	C-O	7.89	1.33	1.24
1	A	660	ASP	CA-CB	-7.88	1.41	1.53
1	A	654	ASP	CA-CB	7.88	1.64	1.53
1	A	698	SER	CA-C	7.87	1.62	1.52
1	A	852	ASP	CA-C	-7.86	1.43	1.52
1	A	429	GLU	CD-OE1	7.86	1.40	1.25
1	B	436	TYR	CD1-CE1	7.86	1.62	1.38
1	A	714	ASN	C-O	7.85	1.33	1.24
1	B	176	PHE	CE2-CZ	-7.85	1.15	1.38
1	B	327	SER	N-CA	7.84	1.55	1.46
1	A	652	PHE	CD1-CE1	7.84	1.62	1.38
1	B	89	VAL	CB-CG1	7.84	1.78	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	467	ILE	CB-CG1	7.84	1.69	1.53
1	B	87	PHE	CA-C	-7.83	1.42	1.52
1	B	849	MET	N-CA	7.83	1.56	1.46
1	A	195	LEU	CA-C	-7.83	1.41	1.52
1	B	48	ASP	CA-C	7.83	1.63	1.52
1	B	394	VAL	N-CA	7.83	1.54	1.46
1	A	603	TRP	CA-C	-7.83	1.42	1.52
1	A	731	VAL	N-CA	7.82	1.56	1.46
1	B	477	ARG	CD-NE	-7.82	1.35	1.46
1	B	609	TYR	CD1-CE1	7.82	1.62	1.38
1	B	744	GLU	CD-OE1	7.82	1.40	1.25
1	A	458	ALA	CA-CB	-7.81	1.41	1.53
1	B	311	GLU	N-CA	7.81	1.56	1.45
1	B	239	GLY	CA-C	7.81	1.58	1.52
1	B	384	ASN	C-O	7.81	1.34	1.24
1	B	784	LEU	C-O	-7.81	1.13	1.23
1	B	284	MET	CB-CG	7.81	1.75	1.52
1	B	881	VAL	CA-C	7.81	1.62	1.52
1	B	596	LEU	C-N	7.80	1.44	1.33
1	A	234	ARG	CG-CD	-7.80	1.29	1.52
1	B	65	PRO	C-O	7.80	1.32	1.23
1	A	230	LYS	N-CA	7.79	1.56	1.46
1	A	310	TYR	CA-C	-7.79	1.42	1.52
1	B	140	HIS	CA-CB	-7.79	1.37	1.54
1	B	291	VAL	CA-C	-7.79	1.42	1.52
1	B	681	LEU	CA-C	7.79	1.63	1.52
1	B	678	PHE	C-O	7.79	1.33	1.24
1	B	390	ARG	CD-NE	-7.78	1.35	1.46
1	B	639	LYS	CA-C	7.78	1.61	1.52
1	B	398	ASP	CG-OD2	7.77	1.40	1.25
1	A	146	PHE	C-O	-7.77	1.13	1.23
1	B	277	GLN	CD-OE1	7.77	1.38	1.23
1	A	390	ARG	N-CA	-7.76	1.36	1.46
1	B	559	LEU	C-N	7.76	1.44	1.33
1	A	656	GLU	CD-OE1	7.76	1.40	1.25
1	A	11	ASP	C-O	-7.76	1.15	1.24
1	B	837	MET	C-O	7.76	1.33	1.24
1	A	17	GLY	C-O	-7.75	1.13	1.24
1	A	339	GLU	N-CA	-7.75	1.36	1.46
1	A	486	VAL	C-N	7.75	1.43	1.33
1	B	130	SER	CA-C	7.75	1.62	1.52
1	B	835	TYR	C-O	7.75	1.34	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	ALA	CA-C	-7.74	1.42	1.52
1	A	427	ASP	N-CA	7.74	1.60	1.46
1	A	520	ASN	C-O	7.74	1.33	1.23
1	B	357	ASN	C-O	-7.74	1.14	1.24
1	B	650	ALA	N-CA	-7.74	1.36	1.46
1	B	665	VAL	CB-CG2	-7.74	1.27	1.52
1	A	665	VAL	CA-CB	7.73	1.62	1.54
1	B	212	THR	C-N	-7.73	1.23	1.33
1	B	478	LEU	CB-CG	7.73	1.69	1.53
1	A	204	PHE	CE2-CZ	7.73	1.61	1.38
1	B	644	LEU	C-O	-7.73	1.14	1.24
1	B	369	SER	CB-OG	-7.73	1.26	1.42
1	A	79	THR	C-O	-7.72	1.14	1.24
1	B	505	GLU	CA-C	7.72	1.63	1.52
1	B	847	GLY	C-O	7.72	1.33	1.23
1	A	199	CYS	N-CA	-7.72	1.36	1.46
1	B	275	GLN	CA-C	-7.72	1.42	1.53
1	B	586	MET	CA-C	7.72	1.63	1.52
1	B	343	LEU	CB-CG	-7.72	1.38	1.53
1	B	638	PHE	CG-CD1	-7.72	1.22	1.38
1	B	328	PHE	CG-CD2	-7.71	1.22	1.38
1	B	873	LYS	CA-CB	7.71	1.66	1.53
1	A	744	GLU	CA-C	7.71	1.63	1.52
1	B	292	GLU	CA-CB	7.71	1.66	1.53
1	A	429	GLU	CA-C	7.70	1.62	1.52
1	B	201	SER	C-N	-7.70	1.23	1.33
1	A	176	PHE	CA-CB	-7.70	1.41	1.53
1	B	493	ASN	CA-C	7.69	1.63	1.52
1	A	881	VAL	CA-CB	-7.69	1.47	1.55
1	B	672	GLU	CD-OE1	7.68	1.40	1.25
1	A	660	ASP	CA-C	-7.68	1.42	1.53
1	B	354	ARG	N-CA	7.68	1.60	1.46
1	B	294	LYS	CG-CD	7.68	1.75	1.52
1	A	130	SER	C-O	7.67	1.32	1.23
1	B	188	VAL	CB-CG2	-7.67	1.27	1.52
1	B	294	LYS	CA-C	7.67	1.62	1.52
1	B	559	LEU	N-CA	7.67	1.55	1.46
1	A	484	ILE	CA-CB	7.66	1.64	1.54
1	A	783	LYS	CA-C	7.66	1.63	1.53
1	B	94	ARG	C-O	-7.66	1.13	1.23
1	B	878	GLN	CA-C	-7.65	1.42	1.52
1	A	193	GLU	CD-OE1	7.65	1.39	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	113	SER	N-CA	-7.65	1.37	1.46
1	A	344	THR	N-CA	-7.64	1.35	1.46
1	B	742	ALA	CA-C	7.64	1.63	1.52
1	B	662	ASP	CA-C	7.64	1.63	1.52
1	B	792	LEU	CA-C	-7.64	1.42	1.52
1	B	319	MET	C-O	7.63	1.33	1.24
1	A	95	THR	C-O	-7.63	1.14	1.24
1	B	495	GLU	CD-OE1	7.63	1.39	1.25
1	B	213	GLU	CA-C	7.62	1.61	1.52
1	B	269	ALA	C-O	-7.62	1.14	1.24
1	A	133	GLU	CD-OE1	7.62	1.39	1.25
1	B	282	ILE	N-CA	-7.62	1.37	1.46
1	A	145	GLN	N-CA	7.61	1.55	1.46
1	B	290	GLU	N-CA	7.61	1.55	1.45
1	B	123	ARG	NE-CZ	7.61	1.41	1.33
1	A	331	PHE	CA-C	-7.60	1.43	1.52
1	A	671	LEU	CA-C	-7.60	1.43	1.52
1	A	521	LEU	CA-C	7.59	1.62	1.52
1	A	799	TRP	N-CA	7.59	1.55	1.46
1	B	267	THR	CA-CB	7.59	1.67	1.53
1	B	314	GLN	CA-C	7.59	1.61	1.53
1	A	756	HIS	CE1-NE2	7.59	1.40	1.32
1	B	78	PRO	CA-CB	-7.59	1.43	1.53
1	B	34	THR	CA-C	-7.58	1.42	1.52
1	B	57	SER	C-O	-7.58	1.14	1.24
1	B	521	LEU	C-O	7.58	1.33	1.24
1	B	648	ILE	CA-CB	7.58	1.64	1.54
1	B	117	ASN	C-O	7.57	1.32	1.24
1	A	803	TYR	CD1-CE1	7.57	1.61	1.38
1	A	309	PRO	CA-C	-7.56	1.43	1.52
1	B	88	ILE	C-N	-7.56	1.24	1.33
1	B	161	LYS	CA-C	7.56	1.61	1.52
1	A	164	LYS	CA-C	7.56	1.61	1.52
1	B	211	VAL	C-N	-7.56	1.23	1.33
1	B	256	LYS	N-CA	7.56	1.60	1.46
1	B	609	TYR	CA-CB	7.56	1.65	1.53
1	B	313	GLU	CB-CG	7.56	1.75	1.52
1	A	468	ASN	CB-CG	7.55	1.71	1.52
1	B	308	ASP	CG-OD2	7.55	1.39	1.25
1	A	165	LEU	C-O	-7.54	1.15	1.24
1	B	657	LEU	CA-C	7.54	1.62	1.52
1	B	806	PHE	N-CA	7.54	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	361	TYR	N-CA	7.54	1.55	1.46
1	A	277	GLN	C-O	7.54	1.33	1.24
1	A	616	PHE	CB-CG	7.53	1.68	1.50
1	A	65	PRO	CB-CG	7.53	1.87	1.49
1	A	836	SER	CA-CB	-7.53	1.38	1.53
1	B	617	ASP	CA-C	-7.53	1.42	1.52
1	B	623	SER	C-O	7.53	1.32	1.23
1	B	586	MET	CG-SD	7.52	1.99	1.80
1	A	145	GLN	CA-CB	-7.52	1.41	1.53
1	A	849	MET	SD-CE	-7.52	1.60	1.79
1	A	149	TRP	CE3-CZ3	-7.51	1.16	1.38
1	B	79	THR	CB-CG2	-7.51	1.27	1.52
1	A	168	VAL	C-O	-7.51	1.14	1.24
1	A	660	ASP	N-CA	-7.51	1.35	1.45
1	B	185	TYR	C-O	-7.51	1.14	1.24
1	A	632	ALA	CA-CB	-7.51	1.40	1.53
1	A	222	SER	C-O	7.51	1.36	1.24
1	A	262	HIS	N-CA	7.50	1.60	1.46
1	A	472	VAL	CA-CB	7.50	1.63	1.54
1	A	81	LEU	N-CA	7.50	1.55	1.46
1	A	773	VAL	CB-CG1	7.50	1.77	1.52
1	B	335	PHE	CD1-CE1	7.50	1.61	1.38
1	A	610	LEU	CG-CD2	7.50	1.77	1.52
1	B	92	ALA	CA-CB	7.50	1.66	1.53
1	B	338	LEU	CA-C	-7.50	1.43	1.52
1	A	756	HIS	CD2-NE2	7.50	1.46	1.37
1	B	442	LEU	N-CA	-7.50	1.36	1.46
1	B	653	ALA	CA-C	7.50	1.61	1.52
1	A	435	VAL	C-O	-7.49	1.16	1.24
1	B	138	ILE	C-O	-7.49	1.15	1.23
1	B	612	ILE	CA-CB	7.49	1.65	1.54
1	B	138	ILE	C-N	-7.49	1.24	1.33
1	A	218	GLN	C-O	-7.49	1.13	1.23
1	B	881	VAL	C-O	7.49	1.32	1.24
1	A	392	GLU	CA-CB	-7.48	1.40	1.53
1	B	231	ALA	CA-C	-7.48	1.43	1.52
1	A	155	ASP	CA-C	-7.47	1.44	1.52
1	B	279	VAL	C-O	-7.47	1.15	1.24
1	B	343	LEU	CG-CD2	7.47	1.77	1.52
1	A	28	LEU	N-CA	7.47	1.56	1.46
1	B	163	GLY	C-O	-7.47	1.14	1.24
1	B	75	TRP	N-CA	-7.47	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	ILE	CA-C	7.46	1.63	1.52
1	B	256	LYS	CB-CG	7.46	1.74	1.52
1	B	730	PHE	C-O	7.46	1.35	1.24
1	A	237	LEU	N-CA	7.46	1.56	1.46
1	B	653	ALA	C-O	7.46	1.32	1.24
1	B	123	ARG	C-O	-7.46	1.14	1.24
1	A	110	ALA	C-O	-7.46	1.15	1.24
1	B	621	SER	CA-C	7.46	1.62	1.52
1	A	485	VAL	N-CA	-7.46	1.37	1.46
1	B	788	GLU	N-CA	7.45	1.55	1.46
1	A	344	THR	CA-CB	-7.45	1.41	1.53
1	B	115	THR	C-N	-7.45	1.24	1.33
1	A	652	PHE	C-O	7.44	1.33	1.24
1	A	868	PHE	CG-CD1	-7.44	1.23	1.38
1	B	15	ALA	CA-C	7.44	1.62	1.52
1	B	211	VAL	C-O	-7.44	1.14	1.23
1	B	392	GLU	C-O	7.44	1.33	1.24
1	A	854	PHE	CA-CB	-7.43	1.41	1.53
1	A	662	ASP	N-CA	7.43	1.55	1.46
1	B	407	CYS	N-CA	7.43	1.54	1.45
1	B	127	TYR	C-O	-7.43	1.14	1.23
1	B	363	GLY	CA-C	7.43	1.59	1.52
1	B	154	VAL	C-O	7.42	1.32	1.23
1	B	284	MET	C-O	7.42	1.33	1.23
1	B	518	GLN	CA-C	-7.42	1.42	1.52
1	A	504	SER	CB-OG	7.41	1.56	1.42
1	B	688	THR	CA-CB	7.41	1.66	1.53
1	B	470	ARG	CB-CG	7.40	1.74	1.52
1	A	667	CYS	C-O	7.40	1.32	1.24
1	A	366	ARG	C-N	-7.40	1.23	1.33
1	A	24	ALA	C-O	-7.39	1.14	1.24
1	A	41	GLU	CG-CD	7.39	1.70	1.52
1	A	495	GLU	CA-CB	-7.39	1.42	1.53
1	A	465	HIS	CA-C	-7.39	1.42	1.52
1	B	468	ASN	C-N	7.39	1.42	1.33
1	A	658	ILE	C-O	-7.39	1.14	1.23
1	A	668	LEU	C-O	7.39	1.33	1.24
1	B	655	ASP	CA-CB	7.39	1.65	1.53
1	A	503	PHE	CE2-CZ	-7.38	1.16	1.38
1	B	582	MET	CA-C	7.38	1.62	1.52
1	B	456	ALA	C-O	7.38	1.33	1.24
1	A	808	THR	CB-CG2	7.38	1.76	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	775	VAL	CA-C	-7.38	1.42	1.52
1	B	630	ARG	C-N	7.37	1.43	1.33
1	A	368	GLY	CA-C	-7.37	1.41	1.51
1	A	56	HIS	C-O	-7.37	1.14	1.24
1	B	118	GLU	N-CA	-7.37	1.37	1.46
1	A	100	GLY	CA-C	7.37	1.62	1.51
1	A	627	TYR	CB-CG	7.37	1.67	1.51
1	A	822	ALA	CA-CB	-7.37	1.42	1.53
1	A	831	ASN	CG-ND2	7.37	1.48	1.33
1	B	84	ASN	CA-CB	-7.37	1.45	1.53
1	A	603	TRP	C-O	-7.36	1.15	1.24
1	B	84	ASN	CA-C	-7.36	1.43	1.52
1	B	426	ARG	C-O	7.36	1.33	1.24
1	B	468	ASN	CA-C	7.36	1.63	1.52
1	A	711	HIS	N-CA	7.36	1.55	1.46
1	B	270	LYS	CA-C	-7.36	1.43	1.52
1	B	451	ARG	CD-NE	7.36	1.56	1.46
1	A	654	ASP	C-O	-7.36	1.16	1.23
1	B	537	LYS	CG-CD	7.36	1.74	1.52
1	B	608	ASN	C-O	7.36	1.32	1.24
1	B	828	PHE	CE2-CZ	7.35	1.60	1.38
1	B	55	SER	CA-CB	7.35	1.66	1.54
1	A	155	ASP	CB-CG	-7.35	1.33	1.52
1	A	203	ALA	C-O	7.35	1.33	1.24
1	A	669	VAL	CB-CG1	7.35	1.76	1.52
1	B	365	TRP	C-O	-7.35	1.13	1.23
1	A	633	ILE	CA-CB	-7.34	1.44	1.54
1	B	60	PHE	CA-CB	-7.34	1.39	1.53
1	A	31	ASP	CG-OD1	7.33	1.39	1.25
1	A	4	ILE	C-N	-7.33	1.23	1.33
1	A	680	GLN	CA-C	-7.33	1.43	1.52
1	A	666	ARG	CZ-NH1	7.33	1.43	1.32
1	A	19	GLY	N-CA	7.33	1.58	1.44
1	A	845	GLU	CA-CB	7.33	1.68	1.53
1	A	11	ASP	N-CA	-7.32	1.37	1.46
1	B	335	PHE	CE2-CZ	7.32	1.60	1.38
1	B	256	LYS	CD-CE	7.32	1.74	1.52
1	B	73	ILE	C-N	-7.31	1.24	1.33
1	A	341	CYS	N-CA	-7.31	1.37	1.46
1	B	394	VAL	CB-CG2	-7.31	1.28	1.52
1	A	167	PHE	CG-CD2	-7.31	1.23	1.38
1	B	426	ARG	N-CA	7.31	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	440	ARG	CA-C	-7.31	1.43	1.52
1	A	145	GLN	CA-C	7.30	1.61	1.52
1	B	392	GLU	CA-C	7.30	1.62	1.52
1	A	68	SER	CA-C	-7.30	1.43	1.52
1	A	314	GLN	CA-C	-7.30	1.42	1.52
1	B	626	ALA	CA-C	-7.30	1.42	1.52
1	A	210	GLY	C-O	7.30	1.30	1.24
1	A	505	GLU	C-O	-7.29	1.14	1.24
1	A	375	ARG	C-N	-7.29	1.22	1.33
1	A	323	GLU	C-O	7.29	1.33	1.24
1	B	670	ARG	CZ-NH2	-7.29	1.24	1.33
1	A	315	LEU	CA-CB	7.29	1.65	1.53
1	B	320	GLU	CA-C	7.29	1.62	1.52
1	B	393	GLU	C-O	-7.29	1.14	1.24
1	A	796	ILE	CA-C	-7.28	1.44	1.52
1	A	883	ILE	CG1-CD1	7.28	1.80	1.51
1	B	479	PRO	C-O	7.28	1.30	1.24
1	A	286	ASN	CA-CB	-7.28	1.39	1.52
1	A	490	PHE	N-CA	-7.28	1.37	1.46
1	A	651	ARG	CA-C	7.28	1.62	1.52
1	A	122	HIS	CB-CG	-7.27	1.40	1.50
1	A	124	VAL	CB-CG2	-7.27	1.28	1.52
1	B	75	TRP	CA-CB	-7.27	1.43	1.53
1	A	257	ASN	CA-C	7.27	1.62	1.52
1	B	304	TRP	CA-CB	7.27	1.65	1.53
1	A	756	HIS	N-CA	7.27	1.60	1.46
1	A	367	ARG	NE-CZ	7.27	1.41	1.33
1	B	2	ALA	N-CA	7.26	1.60	1.46
1	A	800	GLN	CA-CB	-7.26	1.41	1.53
1	A	579	CYS	C-O	7.26	1.32	1.24
1	A	878	GLN	CA-C	7.26	1.61	1.52
1	B	311	GLU	CA-C	7.26	1.62	1.52
1	A	665	VAL	CB-CG2	-7.25	1.28	1.52
1	B	672	GLU	CD-OE2	7.25	1.39	1.25
1	A	141	PHE	CA-CB	-7.25	1.41	1.54
1	A	388	LYS	CG-CD	7.25	1.74	1.52
1	B	283	ARG	C-O	-7.25	1.14	1.23
1	B	738	MET	CG-SD	7.25	1.98	1.80
1	A	797	LYS	CG-CD	7.25	1.74	1.52
1	A	23	ARG	N-CA	7.25	1.55	1.46
1	B	625	SER	N-CA	7.25	1.55	1.46
1	B	892	TYR	C-O	7.24	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	34	THR	CA-CB	-7.24	1.41	1.53
1	A	238	LEU	C-O	7.24	1.32	1.24
1	B	351	ARG	CA-C	7.23	1.68	1.52
1	B	375	ARG	C-O	7.23	1.33	1.24
1	B	319	MET	CG-SD	7.22	1.98	1.80
1	B	362	GLU	CG-CD	7.22	1.70	1.52
1	B	879	ILE	N-CA	7.22	1.54	1.46
1	A	340	ILE	CB-CG2	7.22	1.76	1.52
1	A	437	GLN	C-N	7.22	1.41	1.33
1	B	596	LEU	C-O	7.22	1.33	1.24
1	A	891	MET	N-CA	7.22	1.54	1.46
1	B	31	ASP	N-CA	-7.22	1.37	1.46
1	B	439	PRO	CA-CB	-7.21	1.42	1.54
1	B	691	LEU	CA-C	7.21	1.61	1.52
1	A	339	GLU	CA-C	-7.21	1.44	1.52
1	B	87	PHE	C-N	-7.21	1.23	1.33
1	B	485	VAL	CA-CB	-7.21	1.45	1.54
1	B	24	ALA	C-O	7.21	1.32	1.24
1	B	134	GLY	C-O	-7.21	1.14	1.24
1	B	669	VAL	N-CA	7.20	1.55	1.46
1	B	129	GLN	CA-CB	-7.20	1.42	1.53
1	A	158	LEU	CA-C	-7.20	1.44	1.52
1	B	843	SER	N-CA	7.20	1.59	1.46
1	B	643	GLN	N-CA	7.18	1.54	1.46
1	A	648	ILE	CA-C	-7.18	1.44	1.52
1	A	360	PHE	CA-C	-7.17	1.44	1.52
1	B	273	THR	N-CA	-7.17	1.37	1.46
1	A	108	LEU	CA-C	-7.17	1.43	1.52
1	A	73	ILE	C-O	7.17	1.32	1.24
1	B	674	LEU	C-O	7.17	1.33	1.24
1	A	759	LEU	CA-C	7.16	1.61	1.53
1	A	460	ARG	C-N	-7.16	1.23	1.33
1	A	243	ASN	CA-CB	7.16	1.61	1.52
1	A	43	GLY	C-O	-7.15	1.14	1.24
1	B	199	CYS	CA-C	7.15	1.63	1.53
1	A	388	LYS	N-CA	-7.15	1.37	1.46
1	A	570	ARG	CG-CD	7.15	1.73	1.52
1	B	166	VAL	CA-CB	7.15	1.62	1.54
1	A	697	LEU	CA-C	-7.14	1.43	1.52
1	B	810	ARG	C-O	7.14	1.32	1.24
1	A	113	SER	CA-C	-7.14	1.43	1.52
1	B	151	ASP	N-CA	-7.14	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	602	LEU	C-N	-7.14	1.25	1.33
1	A	227	ILE	CG1-CD1	7.14	1.79	1.51
1	A	473	SER	CA-C	-7.14	1.44	1.52
1	B	462	GLN	C-O	-7.14	1.15	1.24
1	A	275	GLN	C-O	-7.13	1.14	1.23
1	B	386	GLN	CA-CB	-7.13	1.41	1.53
1	A	829	HIS	CA-CB	7.13	1.62	1.53
1	B	480	PRO	N-CD	-7.13	1.37	1.47
1	A	764	PHE	CA-C	-7.12	1.44	1.52
1	A	846	THR	CA-C	-7.12	1.43	1.52
1	A	883	ILE	CB-CG2	7.12	1.76	1.52
1	B	8	LEU	CG-CD2	7.12	1.76	1.52
1	A	653	ALA	C-O	-7.11	1.14	1.23
1	A	611	THR	CA-C	-7.11	1.43	1.52
1	A	407	CYS	CA-CB	-7.11	1.41	1.53
1	B	740	VAL	CB-CG1	7.11	1.76	1.52
1	B	775	VAL	CA-CB	-7.10	1.44	1.54
1	B	343	LEU	CA-C	-7.09	1.43	1.52
1	A	177	TRP	CG-CD1	-7.08	1.19	1.36
1	A	109	ALA	C-O	7.08	1.32	1.24
1	A	891	MET	CA-C	-7.08	1.43	1.52
1	A	371	ALA	N-CA	-7.07	1.38	1.46
1	B	60	PHE	N-CA	7.07	1.57	1.46
1	B	730	PHE	C-N	7.07	1.43	1.33
1	A	433	PHE	N-CA	7.07	1.54	1.46
1	A	812	GLY	N-CA	7.07	1.56	1.45
1	B	519	ALA	N-CA	7.06	1.54	1.46
1	A	280	ASN	CA-C	7.06	1.61	1.52
1	A	862	ASP	CB-CG	-7.05	1.34	1.52
1	B	296	PRO	CB-CG	-7.05	1.14	1.49
1	B	786	PHE	C-O	-7.05	1.16	1.24
1	B	278	ARG	CD-NE	7.05	1.56	1.46
1	A	669	VAL	N-CA	-7.05	1.37	1.46
1	A	702	LEU	N-CA	7.04	1.59	1.46
1	B	651	ARG	NE-CZ	7.04	1.40	1.33
1	B	880	GLN	C-O	-7.04	1.16	1.24
1	B	288	TRP	CD2-CE2	-7.03	1.29	1.41
1	A	573	GLY	C-N	-7.03	1.23	1.33
1	B	194	ALA	C-N	-7.03	1.24	1.33
1	A	74	LYS	N-CA	-7.02	1.38	1.46
1	B	142	GLN	CA-C	-7.02	1.44	1.52
1	B	416	LYS	C-O	-7.02	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	806	PHE	CA-CB	7.01	1.65	1.53
1	A	464	GLU	CA-C	-7.01	1.43	1.52
1	A	767	ASP	CG-OD2	7.01	1.38	1.25
1	A	207	PHE	CD2-CE2	7.01	1.59	1.38
1	A	862	ASP	CG-OD2	-7.00	1.12	1.25
1	A	691	LEU	CA-C	-7.00	1.44	1.52
1	A	863	ALA	C-N	-7.00	1.23	1.33
1	A	264	TYR	C-O	-7.00	1.15	1.24
1	A	368	GLY	C-O	7.00	1.33	1.24
1	B	165	LEU	CA-C	-7.00	1.43	1.52
1	A	157	LEU	N-CA	-7.00	1.36	1.45
1	B	290	GLU	CA-CB	6.99	1.65	1.53
1	B	557	THR	N-CA	-6.99	1.37	1.46
1	A	477	ARG	CD-NE	6.99	1.56	1.46
1	B	87	PHE	CE2-CZ	6.99	1.59	1.38
1	B	464	GLU	CG-CD	6.99	1.69	1.52
1	B	658	ILE	C-O	6.99	1.32	1.24
1	A	11	ASP	C-N	-6.99	1.25	1.33
1	A	220	ALA	C-N	-6.99	1.24	1.33
1	A	892	TYR	C-O	6.99	1.32	1.23
1	B	55	SER	CA-C	6.99	1.62	1.52
1	B	675	PHE	C-O	6.99	1.32	1.24
1	A	581	SER	C-O	6.98	1.32	1.24
1	A	50	ALA	C-O	6.98	1.33	1.24
1	A	466	PHE	C-O	-6.98	1.15	1.24
1	B	648	ILE	CB-CG2	-6.98	1.29	1.52
1	B	727	ARG	CA-C	6.98	1.62	1.52
1	B	831	ASN	C-O	6.98	1.32	1.24
1	B	559	LEU	C-O	6.97	1.32	1.24
1	B	140	HIS	CA-C	-6.97	1.44	1.52
1	B	141	PHE	CE1-CZ	-6.97	1.17	1.38
1	B	346	ASP	N-CA	6.96	1.55	1.46
1	B	881	VAL	CB-CG2	-6.96	1.29	1.52
1	B	572	ASN	C-N	6.95	1.42	1.33
1	B	342	ASN	CG-OD1	6.95	1.36	1.23
1	B	416	LYS	CB-CG	6.95	1.73	1.52
1	B	277	GLN	CG-CD	6.94	1.69	1.52
1	B	84	ASN	C-O	-6.94	1.16	1.24
1	A	777	ASP	CA-CB	6.94	1.65	1.53
1	B	378	PRO	CG-CD	6.93	1.74	1.50
1	A	215	TYR	CA-CB	-6.93	1.40	1.54
1	B	227	ILE	CA-C	6.93	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	57	SER	C-N	-6.93	1.24	1.33
1	B	322	GLY	C-O	6.93	1.33	1.23
1	A	73	ILE	C-N	-6.93	1.24	1.33
1	A	691	LEU	N-CA	6.93	1.54	1.46
1	A	823	PHE	CA-C	6.93	1.60	1.53
1	A	740	VAL	C-O	6.92	1.31	1.24
1	B	285	ARG	CA-C	-6.92	1.44	1.52
1	B	348	LEU	CG-CD1	6.92	1.75	1.52
1	A	23	ARG	C-O	6.91	1.32	1.24
1	B	50	ALA	CA-CB	-6.91	1.42	1.53
1	B	370	THR	C-O	6.91	1.32	1.24
1	B	720	SER	C-O	6.91	1.32	1.24
1	A	477	ARG	CA-C	-6.90	1.44	1.52
1	A	620	LYS	CA-C	6.90	1.62	1.52
1	B	237	LEU	CA-C	6.90	1.61	1.52
1	B	156	ASP	C-O	6.90	1.33	1.23
1	B	404	GLU	N-CA	6.90	1.56	1.47
1	A	350	SER	CB-OG	6.90	1.55	1.42
1	B	470	ARG	CZ-NH1	-6.90	1.23	1.32
1	B	778	SER	CB-OG	6.90	1.55	1.42
1	A	284	MET	C-O	6.89	1.32	1.23
1	A	868	PHE	CA-CB	6.89	1.64	1.53
1	B	455	LEU	N-CA	6.89	1.54	1.46
1	B	467	ILE	C-O	-6.89	1.15	1.24
1	B	519	ALA	C-N	-6.89	1.22	1.33
1	A	360	PHE	CB-CG	-6.89	1.34	1.50
1	A	343	LEU	N-CA	-6.89	1.37	1.46
1	A	826	ALA	C-O	-6.89	1.15	1.24
1	B	427	ASP	CA-CB	6.89	1.64	1.53
1	A	74	LYS	CG-CD	6.88	1.73	1.52
1	B	891	MET	C-O	6.88	1.33	1.24
1	A	148	GLU	C-O	-6.88	1.15	1.23
1	A	666	ARG	CZ-NH2	6.88	1.42	1.33
1	B	770	ARG	CA-C	6.88	1.61	1.52
1	A	860	ARG	CZ-NH1	6.88	1.42	1.32
1	B	28	LEU	C-O	6.88	1.33	1.23
1	A	225	TYR	CD2-CE2	6.87	1.59	1.38
1	B	664	PHE	C-O	6.87	1.32	1.24
1	B	619	ASP	N-CA	6.87	1.54	1.46
1	A	308	ASP	CA-C	-6.87	1.44	1.52
1	B	331	PHE	CA-C	-6.87	1.43	1.52
1	A	205	GLU	CA-C	-6.87	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	ILE	N-CA	-6.87	1.38	1.46
1	B	833	HIS	N-CA	6.87	1.55	1.46
1	A	543	LEU	CA-CB	6.86	1.65	1.53
1	A	744	GLU	C-O	6.86	1.32	1.24
1	A	340	ILE	CA-CB	-6.86	1.45	1.53
1	B	607	ARG	NE-CZ	6.86	1.40	1.33
1	B	692	ASP	CA-C	6.86	1.61	1.52
1	A	511	GLN	CD-OE1	6.85	1.36	1.23
1	A	870	SER	N-CA	6.85	1.55	1.46
1	B	780	THR	N-CA	6.85	1.55	1.46
1	A	314	GLN	C-O	-6.84	1.15	1.24
1	B	361	TYR	C-O	6.84	1.32	1.24
1	A	86	GLN	CD-OE1	6.84	1.36	1.23
1	A	797	LYS	CB-CG	6.84	1.73	1.52
1	A	800	GLN	CB-CG	-6.84	1.31	1.52
1	A	25	ILE	CB-CG2	-6.84	1.29	1.52
1	A	33	GLU	N-CA	6.84	1.54	1.46
1	B	228	ILE	CB-CG2	6.83	1.75	1.52
1	B	743	THR	CA-CB	6.83	1.64	1.53
1	B	27	TYR	CA-CB	-6.83	1.42	1.53
1	A	376	ASN	CA-C	6.83	1.62	1.52
1	B	729	LEU	CG-CD2	6.83	1.75	1.52
1	A	639	LYS	C-O	6.82	1.32	1.24
1	A	200	THR	C-N	-6.82	1.24	1.33
1	B	600	ASN	C-O	6.82	1.32	1.24
1	B	356	TRP	CA-CB	-6.81	1.42	1.53
1	A	701	VAL	C-N	6.81	1.42	1.33
1	B	66	ASN	C-O	-6.80	1.15	1.24
1	A	879	ILE	CA-C	-6.80	1.44	1.52
1	B	146	PHE	C-O	-6.80	1.15	1.23
1	A	387	PHE	CE2-CZ	6.80	1.59	1.38
1	B	120	ILE	CB-CG2	6.80	1.75	1.52
1	A	185	TYR	CZ-OH	-6.79	1.23	1.38
1	A	340	ILE	CG1-CD1	6.79	1.78	1.51
1	A	570	ARG	CA-CB	6.79	1.67	1.53
1	B	266	VAL	N-CA	-6.79	1.38	1.46
1	B	29	ASN	CA-C	-6.78	1.43	1.52
1	B	220	ALA	C-N	-6.78	1.24	1.33
1	B	797	LYS	C-O	6.78	1.32	1.24
1	A	177	TRP	CD2-CE2	-6.78	1.29	1.41
1	B	621	SER	C-O	6.78	1.32	1.24
1	A	828	PHE	C-O	6.78	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	232	LEU	CG-CD1	-6.78	1.30	1.52
1	B	11	ASP	CG-OD2	6.78	1.38	1.25
1	B	259	VAL	CA-CB	6.78	1.72	1.54
1	A	267	THR	CA-CB	-6.77	1.44	1.54
1	B	745	LEU	CA-C	-6.76	1.44	1.52
1	B	745	LEU	C-O	-6.76	1.16	1.24
1	A	200	THR	CB-CG2	6.76	1.74	1.52
1	B	521	LEU	C-N	6.76	1.42	1.33
1	B	372	GLY	C-O	6.76	1.33	1.23
1	A	174	ASN	C-O	6.76	1.32	1.24
1	A	860	ARG	CG-CD	6.76	1.72	1.52
1	B	26	LYS	CG-CD	6.75	1.72	1.52
1	B	883	ILE	CA-C	-6.75	1.44	1.52
1	A	166	VAL	CB-CG2	-6.75	1.30	1.52
1	A	327	SER	CA-C	6.75	1.62	1.53
1	A	545	GLY	CA-C	6.75	1.61	1.51
1	B	452	ASP	CG-OD1	6.75	1.38	1.25
1	B	131	PHE	CD1-CE1	-6.75	1.18	1.38
1	A	738	MET	CA-C	-6.74	1.43	1.52
1	A	572	ASN	CG-OD1	6.74	1.36	1.23
1	B	168	VAL	CA-C	-6.74	1.45	1.52
1	B	460	ARG	N-CA	-6.74	1.37	1.46
1	A	193	GLU	CA-C	-6.74	1.43	1.52
1	B	13	GLU	CD-OE2	6.74	1.38	1.25
1	A	867	ALA	C-O	-6.73	1.16	1.24
1	A	658	ILE	CB-CG2	-6.73	1.30	1.52
1	B	671	LEU	C-O	6.73	1.31	1.24
1	A	170	SER	CA-C	6.73	1.61	1.52
1	A	269	ALA	C-N	6.73	1.42	1.33
1	A	314	GLN	CG-CD	6.73	1.68	1.52
1	B	13	GLU	CD-OE1	6.73	1.38	1.25
1	B	99	GLN	N-CA	-6.73	1.36	1.45
1	B	153	VAL	N-CA	-6.73	1.38	1.46
1	A	596	LEU	CA-CB	6.72	1.63	1.53
1	A	617	ASP	CG-OD1	6.72	1.38	1.25
1	B	701	VAL	CA-C	6.72	1.61	1.52
1	B	828	PHE	CE1-CZ	-6.72	1.18	1.38
1	B	185	TYR	C-N	-6.71	1.25	1.33
1	B	472	VAL	CA-CB	-6.71	1.46	1.54
1	B	626	ALA	CA-CB	-6.71	1.42	1.53
1	B	213	GLU	CA-CB	6.70	1.65	1.53
1	B	263	ALA	C-O	-6.70	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	317	VAL	N-CA	-6.70	1.38	1.46
1	A	12	ARG	CA-CB	6.70	1.64	1.53
1	A	733	LEU	C-N	6.70	1.43	1.33
1	A	488	SER	C-O	-6.70	1.15	1.24
1	B	90	ASP	CG-OD2	6.70	1.38	1.25
1	B	831	ASN	CA-C	6.70	1.61	1.52
1	B	634	GLU	CA-CB	6.69	1.63	1.53
1	A	505	GLU	CA-C	-6.69	1.43	1.52
1	A	241	SER	N-CA	6.69	1.54	1.45
1	A	324	PHE	C-N	-6.69	1.23	1.33
1	A	518	GLN	CA-CB	-6.69	1.42	1.53
1	B	229	LEU	CG-CD1	-6.69	1.30	1.52
1	B	850	ASP	CA-CB	6.69	1.64	1.53
1	B	318	LYS	C-O	6.69	1.33	1.23
1	A	499	LEU	N-CA	6.68	1.54	1.46
1	A	502	PHE	CA-CB	-6.68	1.43	1.53
1	B	872	ASP	C-O	-6.68	1.16	1.23
1	B	284	MET	CG-SD	-6.68	1.64	1.80
1	B	320	GLU	CD-OE1	6.68	1.38	1.25
1	B	659	ILE	CA-C	6.68	1.60	1.52
1	B	887	LEU	CG-CD2	-6.68	1.30	1.52
1	B	292	GLU	C-O	6.68	1.32	1.24
1	B	503	PHE	CA-C	-6.68	1.44	1.52
1	B	387	PHE	CB-CG	-6.67	1.35	1.50
1	B	180	LEU	CA-C	6.67	1.61	1.52
1	A	307	VAL	CA-C	-6.67	1.44	1.52
1	A	285	ARG	CB-CG	6.67	1.72	1.52
1	A	433	PHE	CD1-CE1	6.67	1.58	1.38
1	B	648	ILE	C-O	-6.67	1.16	1.24
1	B	793	TRP	CA-C	-6.67	1.44	1.52
1	B	312	ARG	CB-CG	6.66	1.72	1.52
1	B	513	LEU	CB-CG	6.66	1.66	1.53
1	A	174	ASN	CG-OD1	6.66	1.36	1.23
1	B	415	GLN	CD-NE2	6.66	1.47	1.33
1	B	71	TYR	C-O	6.66	1.31	1.23
1	A	662	ASP	CB-CG	-6.66	1.35	1.52
1	A	627	TYR	CE2-CZ	-6.65	1.22	1.38
1	B	155	ASP	CA-CB	-6.65	1.42	1.53
1	B	264	TYR	C-O	6.65	1.32	1.23
1	B	440	ARG	C-O	-6.65	1.15	1.24
1	B	627	TYR	CA-C	6.65	1.61	1.52
1	B	668	LEU	CG-CD2	6.65	1.74	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	837	MET	N-CA	6.65	1.54	1.46
1	A	313	GLU	CA-CB	-6.64	1.42	1.53
1	A	822	ALA	N-CA	6.64	1.60	1.46
1	A	586	MET	CA-CB	6.64	1.64	1.53
1	B	732	GLN	CA-C	6.64	1.61	1.52
1	A	73	ILE	CG1-CD1	6.64	1.77	1.51
1	B	657	LEU	CB-CG	6.64	1.66	1.53
1	A	134	GLY	CA-C	6.63	1.61	1.51
1	A	317	VAL	N-CA	6.63	1.54	1.46
1	A	512	GLU	CA-CB	6.63	1.63	1.53
1	B	216	ASP	C-O	6.63	1.32	1.24
1	B	781	THR	CA-CB	6.63	1.64	1.53
1	A	746	MET	CG-SD	-6.63	1.64	1.80
1	A	119	THR	C-O	6.62	1.31	1.24
1	A	743	THR	C-N	-6.62	1.25	1.34
1	A	696	TRP	C-N	-6.62	1.25	1.33
1	B	626	ALA	N-CA	-6.62	1.37	1.46
1	B	31	ASP	CG-OD1	6.62	1.38	1.25
1	A	303	GLU	CD-OE2	-6.62	1.12	1.25
1	B	451	ARG	N-CA	-6.62	1.38	1.46
1	A	27	TYR	C-O	-6.62	1.15	1.24
1	B	361	TYR	CD1-CE1	6.62	1.58	1.38
1	B	470	ARG	N-CA	-6.61	1.38	1.46
1	B	827	GLY	C-O	-6.61	1.15	1.24
1	B	849	MET	CA-C	-6.61	1.44	1.52
1	A	263	ALA	CA-CB	-6.61	1.42	1.53
1	A	273	THR	CB-CG2	6.61	1.74	1.52
1	B	321	ASP	C-O	6.61	1.34	1.23
1	B	783	LYS	CA-CB	6.61	1.64	1.53
1	A	82	LEU	CA-CB	6.61	1.64	1.53
1	B	414	MET	SD-CE	6.60	1.96	1.79
1	A	134	GLY	C-O	6.60	1.32	1.23
1	B	598	GLU	C-O	6.60	1.31	1.24
1	A	329	ARG	CB-CG	6.60	1.72	1.52
1	B	156	ASP	CA-C	6.60	1.63	1.52
1	A	749	LEU	C-O	6.60	1.32	1.24
1	B	329	ARG	N-CA	-6.60	1.37	1.46
1	A	33	GLU	C-O	6.60	1.31	1.24
1	A	144	TRP	CA-C	-6.60	1.44	1.52
1	A	458	ALA	C-O	-6.59	1.15	1.23
1	A	702	LEU	CB-CG	6.59	1.66	1.53
1	B	368	GLY	CA-C	6.59	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	581	SER	CA-C	6.59	1.61	1.52
1	A	582	MET	CA-CB	-6.59	1.42	1.53
1	B	15	ALA	CA-CB	6.58	1.64	1.53
1	A	7	LYS	CA-C	-6.58	1.44	1.52
1	A	114	LEU	CB-CG	-6.58	1.40	1.53
1	A	790	LYS	C-O	-6.58	1.15	1.24
1	B	176	PHE	CA-C	6.58	1.61	1.52
1	B	585	LEU	CG-CD1	6.58	1.74	1.52
1	B	426	ARG	CA-C	6.58	1.61	1.52
1	B	539	LEU	N-CA	6.58	1.54	1.46
1	B	574	PHE	CA-CB	6.58	1.64	1.53
1	A	625	SER	C-O	-6.57	1.15	1.24
1	A	585	LEU	CG-CD2	6.57	1.74	1.52
1	B	340	ILE	CA-CB	6.57	1.61	1.54
1	B	740	VAL	CB-CG2	6.57	1.74	1.52
1	A	338	LEU	C-O	-6.57	1.16	1.24
1	A	618	LEU	C-O	6.57	1.32	1.24
1	B	69	LYS	N-CA	-6.57	1.37	1.46
1	B	150	VAL	CA-CB	6.57	1.62	1.54
1	B	15	ALA	C-O	-6.56	1.15	1.24
1	B	603	TRP	CA-CB	6.56	1.64	1.53
1	B	631	MET	CG-SD	6.56	1.97	1.80
1	A	236	SER	CA-CB	-6.56	1.42	1.53
1	B	201	SER	N-CA	-6.56	1.38	1.46
1	B	468	ASN	C-O	6.55	1.31	1.24
1	B	120	ILE	CA-CB	-6.55	1.45	1.54
1	B	220	ALA	CA-C	-6.55	1.45	1.53
1	A	111	ILE	C-O	6.55	1.31	1.24
1	A	679	LYS	CA-CB	-6.55	1.42	1.53
1	B	74	LYS	N-CA	-6.55	1.38	1.46
1	A	301	SER	C-O	-6.55	1.16	1.23
1	B	478	LEU	CG-CD2	-6.55	1.30	1.52
1	A	882	ASN	CB-CG	6.54	1.68	1.52
1	A	307	VAL	C-O	-6.54	1.16	1.24
1	A	18	LEU	N-CA	-6.54	1.37	1.45
1	A	292	GLU	CA-C	6.54	1.62	1.52
1	A	505	GLU	CG-CD	6.53	1.68	1.52
1	A	204	PHE	CG-CD1	6.53	1.52	1.38
1	A	240	CYS	CA-C	-6.53	1.44	1.52
1	A	656	GLU	CA-C	-6.53	1.43	1.52
1	A	99	GLN	C-O	-6.53	1.15	1.24
1	A	766	ILE	CA-CB	6.53	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	329	ARG	CZ-NH2	6.53	1.42	1.33
1	A	36	ARG	NE-CZ	6.52	1.40	1.33
1	A	41	GLU	CD-OE1	6.52	1.37	1.25
1	A	177	TRP	CA-CB	-6.52	1.43	1.53
1	A	12	ARG	NE-CZ	6.52	1.40	1.33
1	A	257	ASN	CA-CB	-6.52	1.42	1.53
1	A	385	PRO	CA-CB	-6.52	1.43	1.53
1	A	403	ARG	CA-C	6.52	1.61	1.52
1	A	576	LEU	C-O	6.52	1.32	1.24
1	A	51	PHE	C-O	6.51	1.32	1.24
1	B	512	GLU	CA-CB	6.51	1.63	1.53
1	B	397	ALA	N-CA	6.51	1.53	1.46
1	A	9	ALA	CA-CB	6.51	1.64	1.53
1	A	379	ALA	CA-C	6.51	1.61	1.52
1	B	93	THR	N-CA	-6.51	1.37	1.46
1	A	192	TYR	C-N	6.51	1.43	1.34
1	A	312	ARG	CZ-NH2	6.51	1.42	1.33
1	A	311	GLU	CA-CB	6.51	1.63	1.53
1	B	161	LYS	C-O	6.51	1.32	1.24
1	B	297	TRP	CA-CB	-6.50	1.42	1.53
1	A	655	ASP	CB-CG	6.50	1.68	1.52
1	B	257	ASN	C-O	6.49	1.32	1.24
1	B	409	PHE	CB-CG	-6.49	1.35	1.50
1	A	739	GLU	CD-OE2	6.49	1.37	1.25
1	B	578	SER	CA-C	-6.49	1.44	1.52
1	B	22	GLU	N-CA	6.49	1.54	1.46
1	B	435	VAL	N-CA	6.48	1.55	1.46
1	A	502	PHE	CB-CG	6.48	1.65	1.50
1	B	598	GLU	CA-CB	6.48	1.63	1.53
1	B	178	SER	C-N	6.48	1.42	1.33
1	B	639	LYS	C-N	6.48	1.41	1.32
1	A	69	LYS	CE-NZ	-6.47	1.29	1.49
1	A	349	LYS	N-CA	6.47	1.54	1.46
1	A	731	VAL	C-O	6.47	1.31	1.24
1	B	730	PHE	CA-CB	6.47	1.64	1.53
1	A	664	PHE	CA-CB	6.47	1.64	1.53
1	A	674	LEU	CG-CD1	-6.47	1.31	1.52
1	A	175	GLU	CG-CD	6.46	1.68	1.52
1	B	278	ARG	CB-CG	6.46	1.71	1.52
1	B	461	ALA	C-O	-6.46	1.15	1.24
1	A	684	GLU	C-O	-6.46	1.15	1.23
1	A	25	ILE	N-CA	-6.46	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	788	GLU	CA-C	6.46	1.61	1.52
1	B	661	PHE	CE2-CZ	6.46	1.58	1.38
1	B	469	LEU	CB-CG	-6.46	1.40	1.53
1	A	860	ARG	NE-CZ	6.45	1.40	1.33
1	B	216	ASP	CA-C	-6.45	1.44	1.52
1	A	236	SER	CA-C	-6.45	1.44	1.52
1	B	597	VAL	CA-CB	6.45	1.63	1.54
1	A	343	LEU	CB-CG	-6.44	1.40	1.53
1	B	39	CYS	CA-CB	6.44	1.63	1.53
1	A	319	MET	CA-CB	6.44	1.64	1.53
1	A	482	GLU	CA-CB	-6.44	1.45	1.53
1	B	231	ALA	C-N	-6.44	1.25	1.34
1	B	7	LYS	N-CA	-6.44	1.38	1.46
1	A	54	VAL	CA-CB	-6.44	1.45	1.54
1	B	742	ALA	CA-CB	6.43	1.63	1.53
1	A	275	GLN	CD-NE2	-6.43	1.19	1.33
1	A	371	ALA	C-N	-6.43	1.24	1.33
1	B	130	SER	CB-OG	6.43	1.55	1.42
1	B	133	GLU	C-O	-6.43	1.16	1.24
1	A	673	ILE	N-CA	6.43	1.54	1.46
1	B	468	ASN	CA-CB	6.42	1.63	1.53
1	B	193	GLU	C-O	-6.42	1.16	1.23
1	A	431	ILE	N-CA	6.42	1.53	1.46
1	B	866	ARG	CA-C	6.42	1.61	1.52
1	A	480	PRO	C-O	-6.41	1.15	1.24
1	B	42	ALA	CA-C	-6.41	1.43	1.52
1	B	775	VAL	CB-CG2	-6.41	1.31	1.52
1	A	325	TRP	CA-CB	6.41	1.62	1.53
1	A	65	PRO	N-CA	6.41	1.54	1.47
1	B	267	THR	C-N	-6.41	1.24	1.33
1	B	503	PHE	CD2-CE2	6.41	1.57	1.38
1	A	828	PHE	CA-CB	6.40	1.62	1.53
1	B	131	PHE	CG-CD1	-6.40	1.25	1.38
1	B	435	VAL	CB-CG2	6.40	1.73	1.52
1	B	439	PRO	N-CA	-6.40	1.40	1.46
1	B	886	TRP	CA-C	-6.40	1.44	1.52
1	A	159	PRO	CA-CB	-6.39	1.45	1.53
1	A	601	ILE	C-N	6.39	1.42	1.33
1	A	772	MET	CA-CB	-6.39	1.43	1.53
1	B	157	LEU	CG-CD1	-6.39	1.31	1.52
1	B	775	VAL	N-CA	-6.39	1.38	1.46
1	B	699	PHE	CG-CD2	6.39	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	ALA	CA-C	6.39	1.61	1.52
1	A	852	ASP	N-CA	6.39	1.54	1.46
1	B	646	GLN	CA-C	6.39	1.61	1.52
1	A	646	GLN	CA-CB	6.39	1.63	1.53
1	B	667	CYS	C-O	6.38	1.32	1.24
1	A	271	GLN	CD-OE1	6.38	1.35	1.23
1	A	617	ASP	CA-C	6.37	1.61	1.53
1	A	381	PHE	CG-CD1	6.37	1.52	1.38
1	A	265	SER	CB-OG	6.37	1.54	1.42
1	B	62	GLU	CD-OE2	6.37	1.37	1.25
1	A	27	TYR	CZ-OH	-6.36	1.24	1.38
1	A	225	TYR	CA-CB	6.36	1.63	1.53
1	A	362	GLU	CG-CD	-6.36	1.36	1.52
1	A	461	ALA	CA-C	-6.36	1.44	1.52
1	B	242	ILE	N-CA	6.36	1.53	1.46
1	A	874	ASN	CB-CG	6.36	1.68	1.52
1	A	76	LYS	CB-CG	6.36	1.71	1.52
1	B	873	LYS	N-CA	-6.36	1.38	1.46
1	B	382	TRP	CA-C	6.35	1.61	1.52
1	B	489	THR	C-O	6.35	1.31	1.24
1	B	583	VAL	C-N	-6.35	1.24	1.33
1	A	468	ASN	C-O	6.35	1.33	1.23
1	A	308	ASP	CG-OD1	6.35	1.37	1.25
1	A	309	PRO	CA-CB	6.35	1.62	1.53
1	A	870	SER	CB-OG	6.35	1.54	1.42
1	B	399	ASP	C-N	6.35	1.42	1.33
1	A	278	ARG	CZ-NH2	6.35	1.41	1.33
1	B	341	CYS	CB-SG	6.35	2.02	1.81
1	B	597	VAL	N-CA	6.35	1.54	1.46
1	B	90	ASP	C-O	-6.35	1.16	1.24
1	A	157	LEU	CA-C	6.34	1.61	1.53
1	B	140	HIS	C-O	6.34	1.31	1.23
1	B	452	ASP	N-CA	6.34	1.53	1.46
1	B	517	ILE	CA-CB	6.34	1.63	1.54
1	B	649	VAL	CA-C	6.34	1.60	1.52
1	A	305	ASN	C-N	-6.34	1.24	1.33
1	A	677	ILE	C-O	-6.34	1.16	1.24
1	B	710	MET	CA-CB	6.34	1.66	1.53
1	A	266	VAL	CA-CB	6.34	1.62	1.54
1	B	27	TYR	C-N	-6.34	1.25	1.33
1	B	450	LYS	CB-CG	6.34	1.71	1.52
1	B	424	PHE	C-N	6.33	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	GLU	N-CA	6.33	1.54	1.46
1	A	334	GLU	CA-C	6.33	1.61	1.52
1	A	824	GLU	CA-CB	6.33	1.63	1.53
1	A	573	GLY	N-CA	6.32	1.51	1.45
1	A	115	THR	C-O	-6.32	1.16	1.24
1	A	854	PHE	N-CA	-6.32	1.38	1.46
1	A	430	THR	N-CA	6.32	1.54	1.46
1	B	493	ASN	C-O	6.31	1.31	1.24
1	A	488	SER	CB-OG	6.31	1.54	1.42
1	B	296	PRO	N-CA	-6.31	1.39	1.47
1	B	478	LEU	CA-C	-6.31	1.46	1.52
1	A	571	THR	N-CA	6.31	1.53	1.46
1	B	175	GLU	CA-CB	6.31	1.64	1.53
1	B	349	LYS	CE-NZ	6.31	1.68	1.49
1	B	550	ILE	CA-CB	-6.30	1.37	1.54
1	A	578	SER	C-O	6.30	1.31	1.24
1	B	885	GLU	C-N	-6.30	1.26	1.33
1	B	283	ARG	NE-CZ	6.30	1.40	1.33
1	B	746	MET	CG-SD	6.30	1.96	1.80
1	A	503	PHE	CG-CD1	-6.30	1.25	1.38
1	B	832	GLN	CA-CB	6.30	1.64	1.53
1	B	23	ARG	CB-CG	6.29	1.71	1.52
1	B	38	GLU	C-N	-6.29	1.26	1.33
1	A	139	PHE	CD2-CE2	6.29	1.57	1.38
1	A	30	GLN	CG-CD	-6.29	1.36	1.52
1	A	282	ILE	N-CA	-6.29	1.38	1.46
1	B	200	THR	CA-CB	-6.29	1.43	1.53
1	A	345	PRO	C-O	-6.29	1.15	1.24
1	A	769	CYS	C-O	6.29	1.31	1.24
1	B	72	GLY	C-O	6.29	1.32	1.23
1	B	140	HIS	N-CA	6.28	1.53	1.45
1	B	655	ASP	CB-CG	6.28	1.67	1.52
1	A	273	THR	N-CA	6.28	1.53	1.46
1	A	242	ILE	CG1-CD1	6.28	1.76	1.51
1	B	354	ARG	C-O	-6.28	1.10	1.23
1	B	869	ARG	C-O	-6.28	1.15	1.23
1	A	494	LYS	CE-NZ	6.28	1.68	1.49
1	B	555	LEU	CA-C	-6.28	1.45	1.52
1	B	620	LYS	C-O	6.27	1.31	1.24
1	B	83	SER	CA-C	6.27	1.61	1.52
1	B	350	SER	CA-C	6.27	1.61	1.53
1	A	218	GLN	CD-OE1	6.27	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	80	GLU	CA-C	6.27	1.61	1.53
1	A	182	GLU	CA-CB	-6.27	1.43	1.53
1	B	262	HIS	N-CA	6.27	1.54	1.46
1	B	162	ASP	N-CA	-6.26	1.38	1.46
1	B	577	GLU	CD-OE1	6.26	1.37	1.25
1	B	346	ASP	C-O	-6.25	1.16	1.24
1	B	170	SER	CB-OG	6.25	1.54	1.42
1	A	736	ASP	CA-CB	6.25	1.63	1.53
1	B	193	GLU	CG-CD	-6.25	1.36	1.52
1	B	738	MET	CB-CG	6.25	1.71	1.52
1	B	230	LYS	CB-CG	-6.25	1.33	1.52
1	B	659	ILE	C-O	-6.25	1.16	1.24
1	A	388	LYS	CE-NZ	6.24	1.68	1.49
1	A	448	HIS	CG-ND1	-6.24	1.31	1.38
1	A	123	ARG	C-O	6.24	1.32	1.24
1	A	520	ASN	CB-CG	-6.24	1.36	1.52
1	B	699	PHE	CE1-CZ	6.24	1.57	1.38
1	B	878	GLN	C-O	-6.24	1.16	1.24
1	A	382	TRP	CA-C	6.23	1.61	1.52
1	A	655	ASP	C-O	-6.23	1.16	1.24
1	B	700	SER	C-O	6.23	1.32	1.23
1	A	385	PRO	CG-CD	-6.23	1.29	1.50
1	A	74	LYS	C-O	6.23	1.31	1.24
1	B	429	GLU	CG-CD	6.23	1.67	1.52
1	A	671	LEU	C-N	-6.23	1.26	1.33
1	A	852	ASP	CA-CB	6.23	1.63	1.53
1	A	889	LEU	N-CA	6.22	1.54	1.46
1	B	399	ASP	N-CA	6.22	1.53	1.46
1	A	439	PRO	CA-C	6.22	1.60	1.52
1	A	758	ASP	N-CA	-6.22	1.38	1.46
1	A	502	PHE	CE2-CZ	-6.22	1.20	1.38
1	A	831	ASN	C-O	-6.22	1.16	1.24
1	B	88	ILE	N-CA	6.22	1.54	1.46
1	B	219	LYS	CA-CB	6.22	1.64	1.53
1	A	133	GLU	CD-OE2	6.22	1.37	1.25
1	A	491	GLU	C-N	-6.22	1.25	1.33
1	B	416	LYS	CD-CE	6.21	1.71	1.52
1	A	852	ASP	C-O	-6.21	1.17	1.24
1	B	183	LYS	CD-CE	6.21	1.71	1.52
1	B	340	ILE	CB-CG2	-6.21	1.32	1.52
1	A	68	SER	C-O	-6.21	1.16	1.24
1	A	323	GLU	N-CA	-6.21	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	122	HIS	CD2-NE2	-6.21	1.31	1.37
1	A	683	PRO	CA-C	6.20	1.61	1.52
1	B	131	PHE	CE1-CZ	6.20	1.57	1.38
1	B	291	VAL	CB-CG2	6.20	1.73	1.52
1	A	35	LEU	N-CA	6.20	1.53	1.46
1	A	394	VAL	CA-CB	-6.20	1.44	1.54
1	B	48	ASP	CG-OD2	6.20	1.37	1.25
1	A	338	LEU	CG-CD2	-6.20	1.32	1.52
1	A	430	THR	CA-CB	6.20	1.61	1.53
1	B	164	LYS	CB-CG	6.20	1.71	1.52
1	A	107	LEU	CG-CD2	-6.19	1.32	1.52
1	A	455	LEU	CA-CB	-6.19	1.43	1.53
1	A	645	HIS	CA-C	-6.19	1.44	1.52
1	B	308	ASP	C-O	6.19	1.35	1.23
1	B	480	PRO	CB-CG	6.19	1.80	1.49
1	B	109	ALA	C-O	6.19	1.31	1.24
1	B	167	PHE	CG-CD1	-6.18	1.25	1.38
1	B	791	TYR	CB-CG	6.18	1.65	1.51
1	A	58	LEU	CA-C	6.18	1.61	1.52
1	A	734	ALA	CA-C	6.18	1.61	1.52
1	B	227	ILE	C-N	-6.18	1.26	1.33
1	B	629	MET	C-O	-6.18	1.16	1.24
1	A	871	LEU	CG-CD1	6.18	1.73	1.52
1	B	451	ARG	CG-CD	6.18	1.71	1.52
1	A	490	PHE	CA-CB	-6.18	1.43	1.53
1	A	670	ARG	NE-CZ	-6.17	1.26	1.33
1	B	197	GLY	CA-C	6.17	1.60	1.51
1	B	328	PHE	CA-C	-6.17	1.44	1.52
1	B	236	SER	N-CA	-6.17	1.38	1.46
1	B	674	LEU	N-CA	-6.17	1.38	1.46
1	A	313	GLU	C-N	6.16	1.42	1.33
1	A	582	MET	CA-C	-6.16	1.44	1.52
1	B	428	MET	CG-SD	-6.16	1.65	1.80
1	B	638	PHE	CA-CB	-6.16	1.44	1.53
1	A	27	TYR	CD1-CE1	6.16	1.57	1.38
1	A	517	ILE	CA-CB	6.16	1.62	1.54
1	B	36	ARG	NE-CZ	6.16	1.39	1.33
1	A	403	ARG	N-CA	6.16	1.54	1.46
1	B	369	SER	CA-C	-6.16	1.44	1.52
1	A	10	LYS	C-O	-6.16	1.16	1.24
1	A	453	PHE	CE2-CZ	6.16	1.57	1.38
1	A	760	LYS	C-O	6.16	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	VAL	C-O	6.16	1.31	1.24
1	A	379	ALA	C-N	6.16	1.42	1.33
1	A	388	LYS	CA-C	6.16	1.60	1.52
1	A	780	THR	CB-CG2	-6.16	1.32	1.52
1	B	278	ARG	CG-CD	6.16	1.71	1.52
1	A	484	ILE	C-O	6.15	1.31	1.24
1	A	664	PHE	C-O	-6.15	1.16	1.24
1	B	146	PHE	N-CA	6.15	1.55	1.46
1	B	440	ARG	C-N	6.15	1.42	1.33
1	B	469	LEU	C-N	-6.15	1.26	1.33
1	A	512	GLU	CG-CD	6.15	1.67	1.52
1	A	763	GLY	C-O	6.15	1.35	1.23
1	A	209	GLY	C-O	-6.15	1.15	1.24
1	A	498	PHE	CB-CG	-6.15	1.36	1.50
1	A	356	TRP	CA-CB	-6.14	1.43	1.53
1	A	450	LYS	CE-NZ	6.14	1.67	1.49
1	A	129	GLN	CA-CB	6.14	1.64	1.53
1	B	510	THR	CB-CG2	6.14	1.72	1.52
1	A	453	PHE	CB-CG	-6.14	1.36	1.50
1	B	135	TYR	CD1-CE1	-6.14	1.20	1.38
1	A	223	ASP	CA-C	6.13	1.60	1.52
1	A	571	THR	CA-C	6.13	1.59	1.52
1	B	34	THR	C-O	-6.13	1.16	1.24
1	B	21	HIS	CD2-NE2	-6.13	1.31	1.37
1	B	343	LEU	CA-CB	-6.13	1.43	1.53
1	A	182	GLU	CA-C	-6.13	1.44	1.52
1	B	872	ASP	N-CA	6.13	1.55	1.46
1	A	440	ARG	CA-CB	-6.13	1.43	1.53
1	A	621	SER	C-O	-6.13	1.16	1.23
1	A	642	CYS	CA-CB	6.13	1.63	1.53
1	B	487	PRO	CA-C	-6.12	1.45	1.52
1	B	630	ARG	N-CA	6.12	1.54	1.46
1	A	11	ASP	CA-C	-6.12	1.45	1.52
1	B	272	VAL	C-O	-6.12	1.16	1.23
1	B	483	TYR	CA-C	-6.11	1.45	1.52
1	A	151	ASP	CA-C	-6.11	1.44	1.52
1	A	786	PHE	CA-CB	6.11	1.63	1.53
1	B	484	ILE	CB-CG1	-6.11	1.41	1.53
1	B	204	PHE	CG-CD1	6.11	1.51	1.38
1	A	149	TRP	C-N	-6.10	1.25	1.33
1	A	654	ASP	N-CA	-6.10	1.39	1.46
1	B	225	TYR	CE1-CZ	-6.10	1.23	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	ALA	C-N	-6.10	1.24	1.33
1	B	811	SER	CB-OG	6.10	1.54	1.42
1	A	459	SER	C-N	-6.10	1.25	1.33
1	B	677	ILE	CG1-CD1	6.10	1.75	1.51
1	A	751	LYS	N-CA	6.10	1.57	1.46
1	B	54	VAL	CA-C	-6.10	1.45	1.52
1	A	543	LEU	C-N	6.09	1.42	1.33
1	A	612	ILE	CA-CB	-6.09	1.46	1.54
1	A	633	ILE	CB-CG2	-6.09	1.32	1.52
1	B	607	ARG	CB-CG	6.09	1.70	1.52
1	B	713	SER	C-N	6.09	1.41	1.33
1	A	265	SER	N-CA	-6.09	1.38	1.45
1	A	482	GLU	CA-C	-6.09	1.45	1.52
1	B	20	SER	CA-C	-6.09	1.45	1.52
1	B	291	VAL	C-O	6.09	1.31	1.24
1	A	238	LEU	CG-CD1	6.09	1.72	1.52
1	B	223	ASP	C-O	-6.09	1.15	1.24
1	B	552	VAL	N-CA	6.09	1.53	1.46
1	A	241	SER	CA-CB	6.08	1.64	1.53
1	A	61	LYS	C-O	-6.08	1.16	1.24
1	A	94	ARG	NE-CZ	6.08	1.39	1.33
1	B	200	THR	CA-C	6.08	1.60	1.52
1	B	823	PHE	N-CA	6.08	1.54	1.46
1	B	204	PHE	CE2-CZ	6.08	1.56	1.38
1	A	702	LEU	CA-CB	6.08	1.65	1.53
1	A	733	LEU	C-O	6.08	1.31	1.24
1	A	511	GLN	CD-NE2	6.08	1.46	1.33
1	A	872	ASP	N-CA	6.08	1.54	1.46
1	B	317	VAL	CA-C	6.07	1.60	1.52
1	B	682	ASP	CA-CB	-6.07	1.43	1.53
1	A	764	PHE	CA-CB	6.07	1.63	1.53
1	A	199	CYS	C-O	-6.07	1.16	1.24
1	A	463	SER	N-CA	-6.07	1.38	1.46
1	B	872	ASP	CB-CG	-6.07	1.36	1.52
1	A	387	PHE	N-CA	-6.06	1.38	1.46
1	A	792	LEU	C-O	6.06	1.31	1.24
1	B	199	CYS	CB-SG	6.06	2.01	1.81
1	A	450	LYS	CD-CE	6.06	1.70	1.52
1	B	169	HIS	ND1-CE1	6.06	1.38	1.32
1	B	290	GLU	CD-OE2	6.06	1.36	1.25
1	B	453	PHE	CA-C	-6.06	1.44	1.52
1	B	879	ILE	C-O	-6.06	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	TYR	CE1-CZ	6.06	1.52	1.38
1	B	88	ILE	CG1-CD1	6.06	1.75	1.51
1	A	570	ARG	CD-NE	6.06	1.54	1.46
1	B	365	TRP	C-N	-6.06	1.25	1.33
1	A	690	GLN	CA-C	6.06	1.59	1.52
1	B	271	GLN	CG-CD	6.06	1.67	1.52
1	B	330	ASP	C-O	-6.06	1.15	1.24
1	B	688	THR	C-O	-6.06	1.17	1.23
1	B	135	TYR	N-CA	-6.06	1.38	1.46
1	A	310	TYR	C-O	-6.05	1.16	1.24
1	A	154	VAL	CB-CG1	6.05	1.72	1.52
1	B	82	LEU	CB-CG	-6.05	1.41	1.53
1	B	340	ILE	CG1-CD1	6.05	1.75	1.51
1	B	150	VAL	CB-CG1	-6.05	1.32	1.52
1	B	336	THR	C-O	6.05	1.31	1.23
1	B	375	ARG	CZ-NH1	6.04	1.41	1.32
1	B	223	ASP	C-N	-6.04	1.25	1.33
1	B	480	PRO	C-O	6.04	1.31	1.23
1	A	491	GLU	CA-CB	-6.04	1.42	1.52
1	A	114	LEU	CG-CD1	6.04	1.72	1.52
1	A	541	SER	N-CA	6.04	1.57	1.46
1	B	376	ASN	CG-ND2	6.03	1.46	1.33
1	B	858	LEU	N-CA	6.03	1.53	1.46
1	B	500	LEU	C-O	-6.03	1.16	1.23
1	A	638	PHE	CA-C	-6.03	1.45	1.52
1	A	339	GLU	CD-OE2	6.03	1.36	1.25
1	B	217	LEU	C-O	-6.03	1.16	1.24
1	A	316	ARG	C-O	-6.02	1.16	1.24
1	A	457	ASN	CG-OD1	6.02	1.34	1.23
1	B	409	PHE	CD2-CE2	6.02	1.56	1.38
1	B	479	PRO	CA-C	-6.02	1.48	1.52
1	A	876	THR	CB-OG1	6.02	1.53	1.43
1	B	444	GLY	C-O	6.02	1.35	1.23
1	A	244	ILE	CA-CB	6.02	1.70	1.54
1	A	112	ALA	N-CA	-6.01	1.39	1.46
1	A	453	PHE	CD2-CE2	-6.01	1.20	1.38
1	B	681	LEU	N-CA	6.01	1.54	1.46
1	A	26	LYS	CD-CE	6.01	1.70	1.52
1	A	151	ASP	C-O	-6.01	1.16	1.24
1	A	793	TRP	CG-CD2	-6.01	1.32	1.43
1	A	480	PRO	C-N	-6.01	1.26	1.33
1	B	371	ALA	CA-CB	6.01	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	685	ASN	C-N	6.01	1.42	1.33
1	B	489	THR	C-N	6.01	1.42	1.33
1	B	163	GLY	CA-C	6.00	1.59	1.51
1	B	679	LYS	C-O	6.00	1.31	1.24
1	B	36	ARG	C-N	-6.00	1.26	1.33
1	B	502	PHE	CD1-CE1	6.00	1.56	1.38
1	A	507	LYS	CD-CE	6.00	1.70	1.52
1	A	609	TYR	N-CA	-6.00	1.39	1.46
1	B	305	ASN	CG-ND2	6.00	1.45	1.33
1	B	454	PHE	CB-CG	5.99	1.64	1.50
1	A	888	GLN	CA-C	-5.99	1.44	1.52
1	B	732	GLN	C-O	5.99	1.31	1.24
1	B	459	SER	CA-C	5.99	1.60	1.52
1	A	682	ASP	N-CA	-5.98	1.41	1.46
1	B	458	ALA	CA-CB	-5.98	1.42	1.53
1	B	509	GLY	CA-C	-5.98	1.43	1.51
1	A	668	LEU	CA-C	5.98	1.61	1.52
1	B	487	PRO	CA-CB	-5.98	1.47	1.54
1	A	229	LEU	CA-C	-5.98	1.44	1.52
1	A	544	ALA	CA-CB	5.98	1.63	1.53
1	B	277	GLN	C-O	-5.98	1.16	1.24
1	A	20	SER	C-O	-5.98	1.15	1.23
1	B	192	TYR	CZ-OH	5.97	1.50	1.38
1	B	486	VAL	CA-C	5.97	1.59	1.52
1	A	558	ILE	CB-CG1	-5.97	1.41	1.53
1	B	28	LEU	C-N	-5.97	1.25	1.33
1	B	833	HIS	C-O	5.97	1.31	1.24
1	B	882	ASN	CA-CB	-5.97	1.45	1.53
1	B	180	LEU	C-N	5.97	1.41	1.33
1	B	408	SER	C-N	5.97	1.41	1.33
1	A	203	ALA	N-CA	5.96	1.53	1.46
1	B	186	ALA	C-O	-5.96	1.17	1.24
1	A	891	MET	C-N	-5.96	1.25	1.33
1	B	47	GLN	CA-CB	-5.96	1.44	1.53
1	B	182	GLU	CD-OE2	5.96	1.36	1.25
1	A	111	ILE	N-CA	-5.96	1.39	1.46
1	A	10	LYS	CE-NZ	5.96	1.67	1.49
1	B	170	SER	N-CA	-5.96	1.38	1.46
1	A	200	THR	CB-OG1	5.95	1.53	1.43
1	A	313	GLU	CD-OE2	5.95	1.36	1.25
1	B	189	ASN	CA-C	-5.95	1.44	1.52
1	B	264	TYR	N-CA	-5.95	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	456	ALA	CA-CB	5.95	1.63	1.53
1	B	728	LYS	N-CA	5.95	1.53	1.46
1	B	417	HIS	CB-CG	5.95	1.58	1.50
1	B	218	GLN	C-N	-5.94	1.25	1.33
1	B	436	TYR	CZ-OH	5.94	1.50	1.38
1	A	464	GLU	CA-CB	5.94	1.63	1.53
1	A	490	PHE	CE2-CZ	-5.94	1.20	1.38
1	B	388	LYS	N-CA	5.94	1.53	1.45
1	B	399	ASP	CB-CG	5.94	1.66	1.52
1	A	874	ASN	CG-ND2	5.94	1.45	1.33
1	B	79	THR	C-O	5.93	1.31	1.24
1	B	777	ASP	CA-C	5.93	1.60	1.52
1	A	144	TRP	CA-CB	-5.93	1.44	1.53
1	A	880	GLN	C-O	-5.93	1.16	1.23
1	B	49	PRO	N-CD	-5.93	1.39	1.47
1	A	351	ARG	NE-CZ	5.93	1.39	1.33
1	B	580	ARG	N-CA	5.93	1.53	1.46
1	A	278	ARG	C-N	-5.93	1.25	1.33
1	B	79	THR	CA-CB	-5.93	1.44	1.53
1	A	498	PHE	CE2-CZ	-5.93	1.20	1.38
1	A	200	THR	C-O	5.92	1.31	1.24
1	B	242	ILE	CB-CG2	-5.92	1.33	1.52
1	B	38	GLU	CA-CB	-5.92	1.44	1.53
1	B	271	GLN	C-O	-5.92	1.16	1.24
1	A	644	LEU	CG-CD1	-5.92	1.33	1.52
1	A	520	ASN	N-CA	5.92	1.53	1.46
1	A	69	LYS	CA-C	5.91	1.60	1.52
1	A	892	TYR	CG-CD2	-5.91	1.26	1.39
1	B	468	ASN	CG-OD1	5.91	1.34	1.23
1	A	340	ILE	CA-C	-5.91	1.46	1.52
1	B	112	ALA	N-CA	5.91	1.53	1.46
1	B	628	GLU	CD-OE2	5.91	1.36	1.25
1	B	665	VAL	CA-CB	5.91	1.62	1.54
1	A	285	ARG	C-O	5.90	1.31	1.24
1	B	857	CYS	CB-SG	5.90	2.00	1.81
1	B	598	GLU	CA-C	5.90	1.60	1.52
1	B	690	GLN	CD-OE1	5.90	1.34	1.23
1	B	613	PHE	N-CA	5.89	1.53	1.46
1	B	179	ALA	C-O	5.89	1.30	1.24
1	A	97	ILE	CA-C	-5.89	1.45	1.52
1	B	204	PHE	CA-C	5.89	1.60	1.52
1	B	123	ARG	CB-CG	5.89	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	ASP	CA-C	5.88	1.61	1.52
1	A	48	ASP	CA-C	5.88	1.60	1.52
1	B	373	GLY	CA-C	-5.88	1.46	1.52
1	A	601	ILE	CA-CB	5.88	1.63	1.54
1	B	304	TRP	CA-C	-5.88	1.44	1.52
1	A	34	THR	CA-C	-5.88	1.45	1.52
1	B	22	GLU	CA-C	5.88	1.60	1.52
1	B	502	PHE	CE2-CZ	-5.88	1.21	1.38
1	A	223	ASP	CG-OD2	5.87	1.36	1.25
1	B	431	ILE	C-O	-5.87	1.18	1.24
1	B	494	LYS	CG-CD	5.87	1.70	1.52
1	B	651	ARG	CD-NE	5.87	1.54	1.46
1	A	53	PRO	C-O	5.87	1.31	1.24
1	A	615	LYS	CB-CG	5.86	1.70	1.52
1	A	848	ASN	C-O	5.86	1.31	1.24
1	B	241	SER	C-O	5.86	1.31	1.23
1	B	335	PHE	CG-CD2	5.86	1.51	1.38
1	A	511	GLN	N-CA	-5.86	1.39	1.46
1	A	861	LEU	CG-CD2	5.86	1.71	1.52
1	A	764	PHE	CE1-CZ	-5.86	1.21	1.38
1	A	777	ASP	CG-OD1	5.86	1.36	1.25
1	A	113	SER	CB-OG	5.86	1.53	1.42
1	A	699	PHE	C-O	5.86	1.31	1.24
1	B	297	TRP	C-O	5.86	1.31	1.24
1	B	351	ARG	C-O	5.86	1.35	1.23
1	B	799	TRP	CB-CG	5.86	1.68	1.50
1	A	330	ASP	C-O	-5.86	1.16	1.24
1	B	472	VAL	N-CA	5.85	1.53	1.46
1	A	749	LEU	CG-CD2	5.85	1.71	1.52
1	B	491	GLU	CD-OE1	5.85	1.36	1.25
1	A	337	LYS	CG-CD	-5.84	1.34	1.52
1	A	620	LYS	C-O	-5.84	1.16	1.24
1	B	360	PHE	CD2-CE2	5.83	1.56	1.38
1	A	9	ALA	N-CA	-5.83	1.39	1.46
1	A	664	PHE	CE1-CZ	5.83	1.56	1.38
1	A	35	LEU	CB-CG	5.83	1.65	1.53
1	B	865	PHE	CB-CG	-5.83	1.37	1.50
1	A	208	THR	CA-CB	-5.83	1.44	1.53
1	A	795	ASN	CB-CG	-5.83	1.37	1.52
1	B	309	PRO	C-O	-5.83	1.16	1.24
1	B	409	PHE	CG-CD2	-5.83	1.26	1.38
1	B	652	PHE	N-CA	-5.83	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	297	TRP	CA-C	5.82	1.60	1.52
1	B	890	THR	C-O	-5.82	1.17	1.23
1	A	7	LYS	CE-NZ	5.82	1.66	1.49
1	B	208	THR	CA-CB	-5.82	1.42	1.54
1	A	892	TYR	CZ-OH	-5.82	1.25	1.38
1	B	464	GLU	CD-OE1	5.82	1.36	1.25
1	A	668	LEU	C-N	5.82	1.40	1.33
1	A	274	TYR	CE1-CZ	-5.81	1.24	1.38
1	A	609	TYR	C-N	-5.81	1.26	1.34
1	A	116	LEU	C-O	-5.81	1.17	1.24
1	A	586	MET	CA-C	5.81	1.60	1.52
1	A	663	ASN	CB-CG	5.81	1.66	1.52
1	B	172	GLN	CG-CD	-5.81	1.37	1.52
1	B	215	TYR	CA-C	5.81	1.59	1.52
1	A	876	THR	CA-C	-5.81	1.44	1.52
1	A	884	GLN	CA-C	5.81	1.60	1.52
1	B	99	GLN	CD-OE1	5.80	1.34	1.23
1	B	381	PHE	CA-CB	-5.80	1.44	1.53
1	A	864	MET	N-CA	5.80	1.53	1.46
1	B	114	LEU	CA-C	-5.80	1.45	1.52
1	B	584	ASN	C-O	5.80	1.31	1.24
1	B	852	ASP	C-O	5.79	1.31	1.23
1	B	434	ALA	CA-CB	-5.79	1.42	1.53
1	A	643	GLN	CG-CD	-5.79	1.37	1.52
1	A	738	MET	C-O	5.79	1.31	1.24
1	B	891	MET	CA-C	5.79	1.60	1.52
1	A	281	LEU	CB-CG	5.79	1.65	1.53
1	B	30	GLN	N-CA	5.78	1.53	1.46
1	B	324	PHE	CB-CG	-5.78	1.37	1.50
1	B	839	ILE	CA-CB	-5.78	1.46	1.54
1	A	152	VAL	CA-C	5.78	1.59	1.52
1	B	12	ARG	CD-NE	5.78	1.54	1.46
1	A	67	SER	CA-CB	5.77	1.63	1.53
1	B	201	SER	CA-C	-5.77	1.45	1.52
1	A	254	THR	C-N	5.77	1.41	1.33
1	A	678	PHE	CD2-CE2	-5.77	1.21	1.38
1	A	464	GLU	N-CA	5.77	1.53	1.46
1	B	17	GLY	N-CA	5.77	1.53	1.45
1	B	357	ASN	CG-OD1	5.77	1.34	1.23
1	A	390	ARG	CB-CG	5.77	1.69	1.52
1	A	438	VAL	CA-C	5.76	1.59	1.52
1	B	631	MET	CA-CB	5.76	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	885	GLU	CD-OE2	5.76	1.36	1.25
1	B	870	SER	C-O	-5.76	1.17	1.24
1	B	68	SER	C-N	-5.76	1.25	1.33
1	B	418	ARG	CZ-NH1	5.76	1.40	1.32
1	A	733	LEU	N-CA	5.76	1.53	1.46
1	A	772	MET	CA-C	-5.76	1.45	1.52
1	B	598	GLU	CD-OE2	5.76	1.36	1.25
1	A	361	TYR	CB-CG	5.76	1.64	1.51
1	A	451	ARG	CZ-NH1	5.76	1.40	1.32
1	A	886	TRP	N-CA	5.75	1.53	1.46
1	B	161	LYS	CG-CD	5.75	1.69	1.52
1	A	157	LEU	CA-CB	-5.75	1.44	1.53
1	A	609	TYR	CG-CD1	-5.75	1.27	1.39
1	B	258	LEU	CA-C	-5.75	1.45	1.52
1	A	846	THR	N-CA	5.75	1.53	1.46
1	B	500	LEU	N-CA	5.75	1.53	1.45
1	A	193	GLU	CA-CB	-5.75	1.43	1.53
1	B	185	TYR	CB-CG	5.75	1.64	1.51
1	A	649	VAL	C-O	-5.75	1.16	1.24
1	A	433	PHE	CG-CD1	-5.74	1.26	1.38
1	B	228	ILE	C-O	-5.74	1.17	1.24
1	A	169	HIS	C-O	-5.74	1.17	1.23
1	A	331	PHE	CB-CG	-5.74	1.37	1.50
1	B	135	TYR	CA-CB	-5.74	1.43	1.53
1	B	67	SER	CA-C	5.74	1.60	1.52
1	B	436	TYR	C-O	-5.74	1.16	1.23
1	B	620	LYS	CA-C	5.74	1.60	1.52
1	B	865	PHE	N-CA	-5.74	1.40	1.47
1	B	130	SER	CA-CB	-5.73	1.43	1.53
1	B	551	SER	CA-C	5.73	1.60	1.52
1	A	474	ASN	CG-OD1	5.73	1.34	1.23
1	B	508	ALA	C-N	-5.73	1.25	1.33
1	B	346	ASP	CG-OD2	5.72	1.36	1.25
1	B	679	LYS	CA-C	5.72	1.60	1.52
1	A	508	ALA	CA-C	-5.72	1.45	1.52
1	B	428	MET	C-O	-5.72	1.16	1.24
1	A	323	GLU	CG-CD	5.72	1.66	1.52
1	A	509	GLY	CA-C	-5.72	1.45	1.52
1	B	143	LEU	N-CA	5.72	1.52	1.45
1	A	188	VAL	CB-CG2	-5.72	1.33	1.52
1	B	333	ARG	N-CA	5.71	1.53	1.46
1	B	463	SER	CB-OG	5.71	1.53	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	452	ASP	CA-C	-5.71	1.45	1.52
1	B	882	ASN	N-CA	-5.71	1.37	1.46
1	B	438	VAL	CA-C	-5.71	1.47	1.52
1	A	146	PHE	N-CA	5.71	1.55	1.46
1	A	414	MET	CA-CB	5.71	1.62	1.53
1	A	453	PHE	C-O	-5.71	1.17	1.24
1	A	736	ASP	CB-CG	5.71	1.66	1.52
1	B	274	TYR	C-N	5.71	1.40	1.33
1	A	515	ASP	C-N	5.70	1.41	1.33
1	A	46	PHE	C-O	-5.70	1.16	1.23
1	B	172	GLN	CB-CG	5.70	1.69	1.52
1	B	516	GLN	CA-C	5.70	1.59	1.52
1	B	883	ILE	C-O	-5.70	1.17	1.24
1	A	745	LEU	CA-CB	5.70	1.63	1.53
1	B	326	MET	C-N	5.70	1.41	1.33
1	B	574	PHE	C-O	-5.70	1.16	1.24
1	B	143	LEU	CG-CD1	-5.70	1.33	1.52
1	A	152	VAL	CA-CB	5.69	1.61	1.54
1	B	313	GLU	CG-CD	5.69	1.66	1.52
1	A	689	ILE	CA-CB	-5.69	1.45	1.55
1	B	328	PHE	CE2-CZ	-5.69	1.21	1.38
1	B	387	PHE	CD1-CE1	5.69	1.55	1.38
1	A	181	LEU	C-O	-5.69	1.17	1.24
1	A	334	GLU	N-CA	5.69	1.53	1.46
1	B	268	ASP	CA-CB	5.69	1.63	1.53
1	A	298	SER	N-CA	5.69	1.57	1.46
1	B	784	LEU	CA-C	-5.69	1.44	1.53
1	B	863	ALA	C-N	-5.69	1.25	1.33
1	A	102	LEU	N-CA	-5.68	1.42	1.47
1	A	879	ILE	C-O	-5.68	1.17	1.24
1	A	30	GLN	C-O	5.68	1.30	1.23
1	A	202	GLU	CD-OE2	5.68	1.36	1.25
1	A	787	GLU	N-CA	5.68	1.52	1.46
1	B	90	ASP	CG-OD1	5.68	1.36	1.25
1	B	641	PRO	CG-CD	5.68	1.70	1.50
1	A	267	THR	CB-OG1	5.68	1.52	1.43
1	A	194	ALA	C-O	5.68	1.31	1.24
1	A	312	ARG	CZ-NH1	5.68	1.40	1.32
1	B	44	ALA	N-CA	-5.68	1.38	1.45
1	B	552	VAL	C-O	5.68	1.30	1.24
1	B	796	ILE	C-O	5.68	1.30	1.24
1	B	166	VAL	CB-CG2	5.67	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	240	CYS	C-O	5.67	1.31	1.23
1	A	690	GLN	CD-NE2	5.67	1.45	1.33
1	A	55	SER	CA-C	-5.67	1.44	1.52
1	A	131	PHE	C-O	5.67	1.31	1.24
1	B	308	ASP	CA-C	5.67	1.64	1.52
1	A	863	ALA	C-O	5.67	1.30	1.24
1	B	719	GLU	CA-C	5.67	1.61	1.53
1	A	176	PHE	CE1-CZ	5.66	1.55	1.38
1	A	730	PHE	N-CA	5.66	1.56	1.46
1	B	86	GLN	CA-CB	-5.66	1.44	1.53
1	B	538	THR	CA-C	-5.66	1.45	1.52
1	B	787	GLU	CA-CB	5.66	1.62	1.53
1	A	10	LYS	CA-C	5.65	1.60	1.52
1	A	469	LEU	C-O	-5.65	1.16	1.23
1	A	317	VAL	CA-C	-5.65	1.45	1.52
1	B	166	VAL	N-CA	5.65	1.53	1.46
1	A	888	GLN	CB-CG	5.64	1.69	1.52
1	B	195	LEU	N-CA	5.64	1.53	1.46
1	A	294	LYS	N-CA	5.64	1.53	1.46
1	A	306	LYS	CE-NZ	5.64	1.66	1.49
1	A	362	GLU	CA-C	5.64	1.60	1.52
1	B	360	PHE	CE2-CZ	5.64	1.55	1.38
1	B	135	TYR	C-O	5.64	1.31	1.24
1	A	351	ARG	CD-NE	5.64	1.54	1.46
1	A	355	ASN	CB-CG	5.64	1.66	1.52
1	A	744	GLU	CD-OE1	5.64	1.36	1.25
1	B	199	CYS	N-CA	5.64	1.53	1.45
1	B	23	ARG	CA-C	-5.64	1.47	1.53
1	A	669	VAL	CA-C	-5.63	1.45	1.52
1	B	652	PHE	C-O	5.63	1.31	1.24
1	A	501	ARG	NE-CZ	-5.63	1.26	1.33
1	A	774	ALA	CA-CB	-5.63	1.44	1.53
1	B	843	SER	CA-CB	5.63	1.64	1.53
1	B	138	ILE	CB-CG2	-5.62	1.33	1.52
1	B	616	PHE	N-CA	5.62	1.51	1.46
1	A	386	GLN	CD-OE1	5.62	1.34	1.23
1	A	636	ALA	C-O	-5.62	1.16	1.24
1	B	150	VAL	C-O	-5.62	1.17	1.24
1	A	650	ALA	CA-CB	5.62	1.62	1.53
1	A	8	LEU	CA-C	5.62	1.60	1.52
1	A	889	LEU	C-N	-5.62	1.25	1.33
1	A	41	GLU	CA-C	5.62	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	222	SER	C-O	-5.62	1.17	1.24
1	A	377	TYR	N-CA	5.62	1.52	1.46
1	A	470	ARG	CZ-NH2	-5.62	1.26	1.33
1	B	317	VAL	CA-CB	5.61	1.62	1.54
1	A	294	LYS	C-N	5.61	1.41	1.33
1	A	303	GLU	CD-OE1	5.61	1.36	1.25
1	B	81	LEU	CG-CD2	5.61	1.71	1.52
1	B	441	GLU	N-CA	5.61	1.53	1.46
1	B	366	ARG	CG-CD	5.61	1.69	1.52
1	A	354	ARG	CG-CD	-5.60	1.35	1.52
1	A	182	GLU	CD-OE1	5.60	1.35	1.25
1	A	482	GLU	C-O	-5.60	1.17	1.24
1	A	666	ARG	C-O	-5.60	1.17	1.24
1	B	441	GLU	CA-C	5.60	1.60	1.52
1	A	404	GLU	N-CA	5.60	1.53	1.46
1	A	436	TYR	CZ-OH	-5.60	1.26	1.38
1	B	190	GLY	N-CA	5.60	1.53	1.45
1	B	480	PRO	CA-CB	5.60	1.60	1.53
1	B	145	GLN	C-N	-5.59	1.26	1.33
1	B	377	TYR	CD1-CE1	5.59	1.55	1.38
1	B	780	THR	CA-CB	5.59	1.62	1.53
1	A	323	GLU	CB-CG	5.59	1.69	1.52
1	A	227	ILE	CA-C	5.59	1.60	1.52
1	A	337	LYS	CA-CB	-5.58	1.44	1.53
1	B	295	GLY	CA-C	5.58	1.59	1.51
1	B	740	VAL	N-CA	5.58	1.53	1.46
1	A	605	ARG	C-O	5.58	1.31	1.24
1	B	452	ASP	CB-CG	5.58	1.66	1.52
1	B	497	ASP	CA-CB	-5.58	1.43	1.53
1	B	115	THR	CB-OG1	5.58	1.52	1.43
1	B	340	ILE	N-CA	-5.58	1.39	1.46
1	B	454	PHE	N-CA	5.58	1.53	1.46
1	B	149	TRP	CG-CD1	-5.57	1.23	1.36
1	B	86	GLN	CD-OE1	-5.57	1.12	1.23
1	A	337	LYS	N-CA	-5.57	1.39	1.46
1	A	599	PHE	CA-C	5.57	1.62	1.52
1	B	578	SER	N-CA	-5.57	1.39	1.46
1	B	701	VAL	C-O	5.57	1.30	1.24
1	B	339	GLU	CA-CB	-5.57	1.44	1.53
1	B	888	GLN	CD-NE2	5.57	1.45	1.33
1	B	852	ASP	C-N	5.56	1.41	1.33
1	B	78	PRO	C-N	5.56	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	349	LYS	CD-CE	5.56	1.69	1.52
1	A	613	PHE	CG-CD2	-5.56	1.27	1.38
1	A	468	ASN	N-CA	5.56	1.53	1.46
1	A	387	PHE	CD1-CE1	5.56	1.55	1.38
1	B	787	GLU	N-CA	-5.56	1.39	1.46
1	A	756	HIS	CG-ND1	5.55	1.44	1.38
1	B	279	VAL	CA-CB	5.55	1.61	1.54
1	B	609	TYR	C-O	5.55	1.31	1.24
1	A	774	ALA	C-N	-5.55	1.27	1.34
1	A	304	TRP	CA-CB	5.54	1.62	1.53
1	A	791	TYR	C-O	-5.54	1.17	1.24
1	B	430	THR	CB-OG1	5.54	1.52	1.43
1	B	587	ASP	CB-CG	5.54	1.66	1.52
1	A	518	GLN	N-CA	-5.54	1.39	1.45
1	B	884	GLN	C-O	5.54	1.31	1.24
1	A	191	SER	C-O	-5.54	1.16	1.24
1	A	114	LEU	CA-CB	-5.54	1.44	1.54
1	B	200	THR	C-O	-5.54	1.16	1.24
1	A	113	SER	N-CA	-5.53	1.39	1.46
1	A	296	PRO	C-O	5.53	1.31	1.24
1	A	511	GLN	CB-CG	5.53	1.69	1.52
1	A	263	ALA	CA-C	5.53	1.60	1.52
1	B	507	LYS	CB-CG	5.52	1.69	1.52
1	A	482	GLU	CD-OE2	5.52	1.35	1.25
1	A	747	ASN	CA-CB	5.52	1.61	1.53
1	B	325	TRP	CZ2-CH2	5.52	1.47	1.37
1	B	572	ASN	CG-ND2	-5.52	1.21	1.33
1	B	470	ARG	CA-CB	5.52	1.61	1.53
1	A	168	VAL	CB-CG1	-5.52	1.34	1.52
1	A	216	ASP	CA-C	-5.52	1.45	1.52
1	B	465	HIS	N-CA	5.52	1.53	1.46
1	B	889	LEU	CA-C	5.51	1.60	1.52
1	A	319	MET	SD-CE	5.51	1.93	1.79
1	B	675	PHE	N-CA	-5.51	1.39	1.46
1	A	773	VAL	N-CA	-5.51	1.40	1.46
1	B	13	GLU	CG-CD	5.51	1.65	1.52
1	B	633	ILE	CA-CB	5.51	1.62	1.54
1	B	694	ILE	CG1-CD1	-5.51	1.30	1.51
1	B	880	GLN	CA-C	-5.51	1.45	1.52
1	A	292	GLU	N-CA	-5.51	1.38	1.46
1	B	475	ARG	CB-CG	5.51	1.69	1.52
1	A	642	CYS	C-O	-5.50	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	288	TRP	CA-CB	5.50	1.63	1.53
1	A	770	ARG	N-CA	5.50	1.52	1.46
1	B	92	ALA	N-CA	5.50	1.53	1.46
1	B	417	HIS	N-CA	5.50	1.53	1.46
1	B	475	ARG	CZ-NH2	-5.50	1.26	1.33
1	A	384	ASN	CG-OD1	-5.50	1.13	1.23
1	B	373	GLY	N-CA	5.50	1.51	1.45
1	A	188	VAL	C-N	5.50	1.41	1.34
1	A	710	MET	C-N	5.50	1.41	1.33
1	B	27	TYR	CA-C	5.50	1.60	1.52
1	A	550	ILE	N-CA	5.49	1.53	1.46
1	B	374	CYS	N-CA	5.49	1.53	1.45
1	A	313	GLU	CD-OE1	5.49	1.35	1.25
1	A	416	LYS	CA-C	-5.49	1.41	1.52
1	B	122	HIS	CB-CG	5.49	1.57	1.50
1	A	33	GLU	CA-CB	-5.49	1.44	1.53
1	B	838	ILE	CA-CB	-5.49	1.47	1.54
1	A	174	ASN	C-N	5.48	1.40	1.33
1	B	580	ARG	NE-CZ	5.48	1.39	1.33
1	A	415	GLN	C-N	-5.48	1.25	1.33
1	A	879	ILE	C-N	-5.48	1.26	1.33
1	B	496	GLY	C-N	5.48	1.40	1.33
1	B	517	ILE	CG1-CD1	5.48	1.73	1.51
1	A	395	ASP	CG-OD2	5.47	1.35	1.25
1	A	45	LEU	CG-CD2	-5.47	1.34	1.52
1	B	613	PHE	CB-CG	-5.47	1.38	1.50
1	A	22	GLU	CA-C	-5.47	1.45	1.52
1	B	198	GLY	C-N	5.47	1.41	1.33
1	A	202	GLU	N-CA	-5.47	1.39	1.46
1	A	149	TRP	CE2-CZ2	-5.47	1.28	1.39
1	A	226	GLN	C-O	5.46	1.31	1.24
1	B	362	GLU	CA-C	-5.46	1.46	1.52
1	B	776	MET	C-O	-5.46	1.16	1.24
1	A	284	MET	CA-C	5.46	1.60	1.53
1	A	308	ASP	N-CA	-5.46	1.38	1.46
1	B	174	ASN	CA-CB	5.46	1.66	1.53
1	A	450	LYS	C-O	-5.46	1.16	1.23
1	A	627	TYR	N-CA	-5.46	1.39	1.46
1	A	747	ASN	C-O	5.46	1.31	1.24
1	A	609	TYR	C-O	5.46	1.30	1.24
1	A	472	VAL	CA-C	-5.45	1.45	1.52
1	A	382	TRP	CD2-CE2	-5.45	1.32	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	TRP	CZ2-CH2	-5.45	1.26	1.37
1	B	627	TYR	CG-CD1	5.45	1.50	1.39
1	A	289	GLY	N-CA	-5.45	1.37	1.45
1	B	211	VAL	CA-C	-5.45	1.45	1.53
1	B	539	LEU	C-N	5.45	1.41	1.33
1	B	646	GLN	CD-OE1	5.45	1.33	1.23
1	A	802	ILE	CA-C	-5.44	1.45	1.52
1	A	610	LEU	CA-C	5.44	1.60	1.52
1	B	883	ILE	CB-CG2	5.44	1.70	1.52
1	B	791	TYR	C-O	-5.44	1.17	1.24
1	B	846	THR	CA-CB	-5.44	1.45	1.53
1	A	490	PHE	CG-CD2	-5.44	1.27	1.38
1	B	436	TYR	CG-CD1	5.43	1.50	1.39
1	A	496	GLY	CA-C	-5.43	1.46	1.51
1	A	511	GLN	CA-C	5.43	1.59	1.52
1	B	597	VAL	C-O	5.43	1.30	1.24
1	A	57	SER	CB-OG	-5.43	1.31	1.42
1	A	355	ASN	CA-C	5.43	1.60	1.52
1	B	324	PHE	C-O	-5.43	1.16	1.23
1	A	52	PRO	CA-C	-5.43	1.47	1.52
1	B	585	LEU	CB-CG	5.43	1.64	1.53
1	B	683	PRO	CG-CD	5.43	1.69	1.50
1	B	481	GLY	CA-C	-5.42	1.46	1.51
1	B	600	ASN	N-CA	5.42	1.52	1.46
1	A	243	ASN	C-N	5.42	1.41	1.33
1	A	510	THR	N-CA	5.42	1.52	1.45
1	A	436	TYR	CE2-CZ	-5.42	1.25	1.38
1	A	451	ARG	N-CA	5.42	1.53	1.46
1	A	811	SER	CA-C	5.42	1.60	1.52
1	B	685	ASN	CB-CG	5.42	1.65	1.52
1	A	239	GLY	C-O	-5.42	1.16	1.23
1	B	63	LEU	N-CA	5.42	1.53	1.46
1	A	141	PHE	CG-CD2	5.42	1.50	1.38
1	A	149	TRP	N-CA	5.42	1.52	1.46
1	B	207	PHE	N-CA	-5.42	1.38	1.46
1	B	576	LEU	CA-CB	5.42	1.62	1.53
1	B	786	PHE	C-N	-5.42	1.26	1.33
1	A	594	LEU	CA-CB	5.41	1.61	1.53
1	A	888	GLN	CD-OE1	-5.41	1.13	1.23
1	A	483	TYR	CB-CG	5.41	1.63	1.51
1	B	643	GLN	CA-C	5.41	1.60	1.52
1	A	333	ARG	C-O	5.41	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	662	ASP	C-O	5.41	1.30	1.24
1	A	758	ASP	CA-CB	5.41	1.62	1.53
1	A	869	ARG	CZ-NH1	5.41	1.40	1.32
1	B	397	ALA	C-N	5.41	1.41	1.33
1	A	553	LYS	C-O	5.41	1.30	1.24
1	A	694	ILE	CG1-CD1	5.41	1.72	1.51
1	B	578	SER	C-O	-5.41	1.17	1.24
1	A	329	ARG	NE-CZ	5.41	1.39	1.33
1	A	359	THR	CB-CG2	-5.41	1.34	1.52
1	B	714	ASN	CA-C	5.41	1.64	1.52
1	B	719	GLU	N-CA	5.41	1.54	1.46
1	A	357	ASN	C-O	-5.40	1.17	1.23
1	A	341	CYS	C-N	5.40	1.40	1.33
1	B	259	VAL	C-O	5.40	1.34	1.23
1	A	124	VAL	C-N	-5.40	1.27	1.33
1	A	177	TRP	CE3-CZ3	-5.40	1.22	1.38
1	B	76	LYS	N-CA	-5.40	1.39	1.45
1	A	467	ILE	C-N	5.39	1.40	1.33
1	A	750	ASN	C-N	5.39	1.41	1.33
1	A	868	PHE	CD2-CE2	-5.39	1.22	1.38
1	B	160	THR	CA-CB	-5.39	1.43	1.53
1	A	559	LEU	C-O	-5.39	1.17	1.24
1	A	808	THR	C-N	5.39	1.41	1.33
1	A	868	PHE	C-N	-5.39	1.26	1.33
1	B	297	TRP	CD2-CE2	-5.39	1.32	1.41
1	A	640	LEU	CA-CB	-5.39	1.46	1.53
1	B	428	MET	CA-C	5.38	1.59	1.52
1	B	649	VAL	N-CA	-5.38	1.39	1.46
1	B	865	PHE	C-N	-5.38	1.26	1.34
1	A	349	LYS	CA-CB	5.38	1.62	1.53
1	A	615	LYS	C-O	-5.38	1.17	1.24
1	B	225	TYR	N-CA	-5.38	1.39	1.46
1	A	288	TRP	CE2-CZ2	-5.38	1.28	1.39
1	B	337	LYS	CA-CB	-5.38	1.43	1.53
1	B	47	GLN	N-CA	5.37	1.52	1.46
1	B	268	ASP	C-O	-5.37	1.17	1.24
1	B	424	PHE	CA-C	5.37	1.64	1.52
1	B	605	ARG	C-O	5.37	1.30	1.24
1	A	647	VAL	CA-CB	-5.37	1.47	1.54
1	B	437	GLN	CD-OE1	5.37	1.33	1.23
1	A	150	VAL	C-O	5.37	1.29	1.24
1	A	859	VAL	CA-C	-5.37	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	742	ALA	C-O	-5.36	1.17	1.24
1	A	53	PRO	C-N	-5.36	1.26	1.33
1	B	179	ALA	CA-CB	-5.36	1.44	1.53
1	A	57	SER	CA-CB	-5.36	1.44	1.53
1	A	296	PRO	CA-C	5.36	1.58	1.52
1	A	616	PHE	CE2-CZ	-5.35	1.22	1.38
1	B	103	GLY	C-O	5.35	1.31	1.23
1	B	368	GLY	C-O	5.35	1.31	1.24
1	B	784	LEU	CG-CD1	5.35	1.70	1.52
1	A	51	PHE	N-CA	5.35	1.53	1.46
1	A	142	GLN	CB-CG	-5.35	1.36	1.52
1	A	738	MET	N-CA	-5.35	1.39	1.46
1	B	640	LEU	CG-CD1	5.35	1.70	1.52
1	A	8	LEU	CG-CD1	-5.35	1.34	1.52
1	A	405	SER	CA-C	5.35	1.59	1.52
1	B	196	SER	N-CA	5.35	1.52	1.46
1	B	390	ARG	CG-CD	-5.35	1.36	1.52
1	B	783	LYS	N-CA	5.35	1.52	1.46
1	A	100	GLY	C-O	5.35	1.31	1.23
1	B	274	TYR	N-CA	-5.34	1.39	1.46
1	B	851	PHE	CA-C	5.34	1.59	1.52
1	A	579	CYS	CA-C	5.34	1.60	1.52
1	A	159	PRO	CA-C	-5.34	1.46	1.52
1	A	448	HIS	CB-CG	5.34	1.57	1.50
1	A	880	GLN	CD-NE2	5.34	1.44	1.33
1	B	471	GLU	C-O	5.34	1.30	1.23
1	B	733	LEU	CA-CB	5.34	1.64	1.53
1	A	715	ILE	CA-C	5.34	1.64	1.52
1	A	140	HIS	C-O	-5.34	1.17	1.23
1	B	226	GLN	C-O	5.34	1.30	1.24
1	B	587	ASP	CA-CB	5.33	1.64	1.53
1	A	354	ARG	CA-CB	5.33	1.61	1.53
1	A	468	ASN	C-N	5.33	1.40	1.33
1	A	776	MET	SD-CE	5.33	1.92	1.79
1	B	605	ARG	CA-CB	5.33	1.62	1.53
1	B	371	ALA	N-CA	-5.33	1.39	1.46
1	A	90	ASP	CG-OD1	5.33	1.35	1.25
1	B	133	GLU	CG-CD	5.33	1.65	1.52
1	A	797	LYS	C-N	-5.32	1.26	1.33
1	A	827	GLY	CA-C	-5.32	1.44	1.51
1	B	189	ASN	C-O	-5.32	1.17	1.24
1	B	624	MET	N-CA	5.32	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	176	PHE	C-N	-5.32	1.27	1.33
1	B	520	ASN	CA-CB	5.32	1.60	1.53
1	A	67	SER	CA-C	5.32	1.59	1.52
1	A	352	THR	N-CA	5.32	1.53	1.46
1	B	714	ASN	C-O	5.32	1.34	1.23
1	B	273	THR	CA-C	5.32	1.59	1.52
1	B	467	ILE	CB-CG2	5.32	1.70	1.52
1	B	558	ILE	CA-C	-5.31	1.46	1.52
1	A	334	GLU	CD-OE2	5.31	1.35	1.25
1	B	271	GLN	CD-NE2	5.31	1.44	1.33
1	B	557	THR	CB-CG2	5.31	1.70	1.52
1	A	14	ALA	C-O	-5.31	1.17	1.24
1	B	39	CYS	C-N	-5.31	1.27	1.33
1	B	280	ASN	CG-ND2	-5.31	1.22	1.33
1	A	467	ILE	CA-CB	-5.31	1.46	1.55
1	A	45	LEU	CA-CB	-5.30	1.45	1.53
1	A	272	VAL	N-CA	-5.30	1.39	1.46
1	A	337	LYS	C-O	-5.30	1.17	1.24
1	B	81	LEU	N-CA	5.30	1.53	1.46
1	A	886	TRP	CA-CB	-5.30	1.45	1.53
1	B	433	PHE	N-CA	-5.30	1.38	1.46
1	B	539	LEU	CG-CD1	5.30	1.70	1.52
1	B	54	VAL	CB-CG2	-5.30	1.35	1.52
1	A	233	GLU	CG-CD	5.30	1.65	1.52
1	B	120	ILE	CG1-CD1	5.29	1.72	1.51
1	B	331	PHE	CB-CG	-5.29	1.38	1.50
1	B	618	LEU	C-O	5.29	1.30	1.24
1	B	628	GLU	CD-OE1	5.29	1.35	1.25
1	A	167	PHE	CA-C	5.29	1.59	1.52
1	A	24	ALA	CA-C	-5.29	1.45	1.52
1	A	674	LEU	C-N	-5.29	1.27	1.33
1	A	745	LEU	C-O	-5.29	1.17	1.24
1	A	756	HIS	CA-CB	5.29	1.64	1.53
1	A	795	ASN	C-N	-5.29	1.27	1.33
1	B	335	PHE	CB-CG	5.29	1.62	1.50
1	A	735	GLY	C-O	5.28	1.31	1.23
1	B	517	ILE	N-CA	5.28	1.52	1.46
1	A	284	MET	N-CA	5.28	1.52	1.45
1	B	583	VAL	CA-C	-5.28	1.46	1.52
1	B	634	GLU	C-O	5.28	1.30	1.24
1	B	305	ASN	CA-CB	5.28	1.64	1.53
1	B	575	SER	CA-CB	-5.28	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	682	ASP	CB-CG	-5.28	1.38	1.52
1	B	606	ILE	CB-CG1	5.28	1.64	1.53
1	A	217	LEU	C-O	-5.28	1.17	1.24
1	A	502	PHE	CD1-CE1	-5.27	1.22	1.38
1	A	857	CYS	C-O	5.27	1.30	1.24
1	B	740	VAL	CA-C	-5.27	1.46	1.52
1	A	511	GLN	CG-CD	5.27	1.65	1.52
1	B	641	PRO	CA-C	-5.27	1.45	1.52
1	A	672	GLU	C-O	-5.27	1.18	1.24
1	B	294	LYS	CE-NZ	5.27	1.65	1.49
1	A	38	GLU	CA-CB	5.27	1.62	1.53
1	A	301	SER	CB-OG	5.27	1.52	1.42
1	A	428	MET	C-O	5.27	1.30	1.23
1	B	204	PHE	C-O	-5.27	1.18	1.24
1	B	264	TYR	CZ-OH	-5.27	1.26	1.38
1	B	355	ASN	CG-OD1	-5.26	1.13	1.23
1	B	784	LEU	CG-CD2	5.26	1.70	1.52
1	B	523	ASP	C-O	5.26	1.30	1.23
1	B	684	GLU	C-N	-5.26	1.26	1.33
1	A	141	PHE	C-N	-5.26	1.26	1.33
1	A	608	ASN	CG-ND2	5.26	1.44	1.33
1	B	349	LYS	CG-CD	-5.26	1.36	1.52
1	B	614	ARG	CA-CB	-5.26	1.44	1.53
1	B	41	GLU	CA-CB	-5.26	1.45	1.53
1	A	760	LYS	N-CA	5.26	1.56	1.46
1	A	652	PHE	CE2-CZ	5.25	1.54	1.38
1	B	482	GLU	CD-OE1	5.25	1.35	1.25
1	B	676	LYS	C-O	-5.25	1.17	1.24
1	B	689	ILE	C-O	-5.25	1.18	1.24
1	A	202	GLU	CA-C	-5.25	1.45	1.52
1	A	357	ASN	CA-CB	-5.25	1.44	1.53
1	B	313	GLU	CA-C	-5.25	1.45	1.52
1	B	398	ASP	CA-C	5.25	1.64	1.52
1	A	507	LYS	CG-CD	5.25	1.68	1.52
1	B	436	TYR	N-CA	-5.25	1.39	1.45
1	B	166	VAL	CB-CG1	-5.25	1.35	1.52
1	A	744	GLU	C-N	5.24	1.41	1.33
1	B	375	ARG	CA-C	-5.24	1.45	1.52
1	B	850	ASP	C-O	5.24	1.30	1.24
1	A	853	ASN	N-CA	5.24	1.52	1.46
1	A	6	MET	CA-CB	-5.24	1.47	1.53
1	A	803	TYR	CE2-CZ	5.24	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	13	GLU	C-O	-5.24	1.17	1.24
1	B	484	ILE	CG1-CD1	5.23	1.72	1.51
1	B	110	ALA	CA-CB	5.23	1.61	1.53
1	A	138	ILE	CB-CG2	5.23	1.69	1.52
1	B	415	GLN	CA-C	-5.23	1.46	1.52
1	B	839	ILE	C-N	5.23	1.40	1.33
1	A	497	ASP	N-CA	5.22	1.52	1.45
1	B	211	VAL	CB-CG1	-5.22	1.35	1.52
1	A	117	ASN	CB-CG	5.22	1.65	1.52
1	A	130	SER	CB-OG	5.22	1.52	1.42
1	A	626	ALA	C-O	5.22	1.30	1.24
1	A	774	ALA	CA-C	-5.22	1.45	1.52
1	B	144	TRP	CG-CD1	-5.22	1.24	1.36
1	B	524	GLU	C-O	5.22	1.30	1.24
1	A	598	GLU	CA-C	-5.21	1.45	1.52
1	A	809	ASP	C-O	5.21	1.30	1.24
1	B	415	GLN	C-N	5.21	1.40	1.33
1	B	767	ASP	N-CA	5.21	1.52	1.46
1	A	103	GLY	C-O	-5.21	1.15	1.23
1	B	429	GLU	N-CA	-5.21	1.39	1.45
1	A	324	PHE	CB-CG	-5.21	1.38	1.50
1	B	370	THR	N-CA	-5.20	1.38	1.45
1	A	675	PHE	N-CA	5.20	1.52	1.46
1	B	493	ASN	N-CA	-5.20	1.39	1.46
1	A	230	LYS	C-O	-5.20	1.17	1.24
1	B	192	TYR	CG-CD1	-5.20	1.28	1.39
1	A	451	ARG	NE-CZ	5.20	1.38	1.33
1	A	297	TRP	CD2-CE2	5.20	1.50	1.41
1	B	85	PRO	CA-C	5.20	1.59	1.52
1	B	846	THR	CA-C	5.20	1.59	1.52
1	B	889	LEU	N-CA	-5.20	1.39	1.46
1	A	466	PHE	CD2-CE2	5.19	1.54	1.38
1	B	483	TYR	CZ-OH	5.19	1.49	1.38
1	A	223	ASP	C-O	5.19	1.31	1.24
1	A	350	SER	C-O	-5.19	1.17	1.24
1	A	650	ALA	N-CA	5.19	1.52	1.46
1	B	406	GLY	C-O	5.19	1.30	1.23
1	A	55	SER	C-N	-5.19	1.26	1.33
1	A	320	GLU	CD-OE1	5.19	1.35	1.25
1	A	215	TYR	CE2-CZ	-5.19	1.25	1.38
1	B	663	ASN	CG-ND2	5.19	1.44	1.33
1	A	79	THR	CB-OG1	5.18	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	801	GLY	C-O	5.18	1.30	1.23
1	B	607	ARG	CZ-NH1	5.18	1.40	1.32
1	A	353	LEU	CA-CB	5.18	1.62	1.53
1	A	549	GLU	CA-CB	5.18	1.60	1.53
1	B	730	PHE	CA-C	5.18	1.62	1.52
1	B	40	LEU	C-O	-5.18	1.18	1.24
1	B	399	ASP	CG-OD1	5.18	1.35	1.25
1	A	521	LEU	N-CA	5.17	1.53	1.46
1	B	834	ILE	CA-C	5.17	1.59	1.52
1	A	4	ILE	N-CA	-5.17	1.39	1.46
1	A	130	SER	CA-C	-5.17	1.46	1.52
1	B	33	GLU	CD-OE1	5.17	1.35	1.25
1	B	93	THR	CA-CB	5.17	1.62	1.53
1	A	16	GLU	C-O	-5.17	1.17	1.24
1	B	127	TYR	CA-CB	5.17	1.60	1.53
1	B	892	TYR	CZ-OH	5.17	1.48	1.38
1	A	47	GLN	C-N	5.16	1.40	1.32
1	B	107	LEU	CG-CD1	5.16	1.69	1.52
1	B	231	ALA	CA-CB	5.16	1.61	1.53
1	B	862	ASP	N-CA	-5.16	1.39	1.46
1	B	386	GLN	CD-NE2	5.16	1.44	1.33
1	B	491	GLU	N-CA	5.16	1.53	1.46
1	A	213	GLU	CB-CG	-5.16	1.36	1.52
1	B	724	ARG	CA-CB	5.16	1.59	1.52
1	A	447	VAL	C-N	-5.16	1.27	1.33
1	A	452	ASP	N-CA	5.16	1.52	1.46
1	A	616	PHE	N-CA	5.16	1.52	1.46
1	B	214	TRP	CG-CD1	-5.16	1.24	1.36
1	B	516	GLN	C-O	5.16	1.29	1.24
1	A	830	LEU	CA-CB	-5.15	1.45	1.53
1	B	162	ASP	CG-OD2	5.15	1.35	1.25
1	A	289	GLY	C-N	-5.15	1.26	1.33
1	B	732	GLN	N-CA	5.15	1.52	1.46
1	B	655	ASP	CG-OD2	5.15	1.35	1.25
1	A	131	PHE	CB-CG	-5.15	1.38	1.50
1	B	330	ASP	CB-CG	5.15	1.65	1.52
1	A	176	PHE	CG-CD2	5.14	1.49	1.38
1	A	584	ASN	CG-ND2	-5.14	1.22	1.33
1	A	870	SER	CA-CB	5.14	1.62	1.53
1	B	30	GLN	CD-OE1	5.14	1.33	1.23
1	B	202	GLU	C-N	-5.14	1.26	1.33
1	A	66	ASN	CG-OD1	-5.14	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	333	ARG	CB-CG	5.14	1.67	1.52
1	B	82	LEU	C-O	-5.14	1.17	1.23
1	B	810	ARG	CA-C	5.14	1.59	1.52
1	A	18	LEU	CA-CB	5.14	1.61	1.53
1	A	18	LEU	CB-CG	5.14	1.63	1.53
1	A	876	THR	CA-CB	-5.14	1.44	1.53
1	B	292	GLU	N-CA	5.14	1.52	1.46
1	B	36	ARG	C-O	-5.14	1.18	1.24
1	A	646	GLN	CB-CG	5.14	1.67	1.52
1	A	505	GLU	CD-OE1	5.13	1.35	1.25
1	A	783	LYS	CA-CB	-5.13	1.46	1.53
1	B	118	GLU	CA-CB	-5.13	1.45	1.53
1	B	684	GLU	CD-OE1	5.13	1.35	1.25
1	A	670	ARG	CZ-NH1	5.13	1.40	1.32
1	B	135	TYR	CD2-CE2	-5.13	1.23	1.38
1	B	635	ALA	CA-C	-5.13	1.46	1.52
1	B	475	ARG	NE-CZ	-5.13	1.27	1.33
1	A	165	LEU	N-CA	5.13	1.52	1.46
1	A	232	LEU	N-CA	-5.13	1.39	1.46
1	B	216	ASP	CG-OD2	5.13	1.35	1.25
1	B	501	ARG	CB-CG	5.13	1.67	1.52
1	B	30	GLN	CG-CD	-5.12	1.39	1.52
1	B	661	PHE	N-CA	5.12	1.52	1.46
1	A	233	GLU	CA-CB	-5.12	1.46	1.53
1	B	85	PRO	C-O	5.12	1.30	1.24
1	B	194	ALA	CA-C	-5.12	1.46	1.52
1	B	335	PHE	CD2-CE2	5.12	1.54	1.38
1	B	491	GLU	CA-C	-5.12	1.46	1.53
1	B	668	LEU	CA-C	5.12	1.59	1.52
1	B	731	VAL	C-O	-5.12	1.18	1.24
1	A	180	LEU	CG-CD2	-5.12	1.35	1.52
1	B	358	THR	CB-OG1	5.12	1.51	1.43
1	A	470	ARG	CD-NE	5.12	1.53	1.46
1	A	127	TYR	C-N	-5.11	1.27	1.33
1	A	257	ASN	C-N	5.11	1.40	1.33
1	A	402	SER	C-N	5.11	1.40	1.33
1	A	514	ASP	C-O	5.11	1.30	1.23
1	B	518	GLN	CG-CD	5.11	1.64	1.52
1	A	35	LEU	C-N	-5.11	1.27	1.34
1	A	739	GLU	CB-CG	5.11	1.67	1.52
1	B	656	GLU	CD-OE1	5.11	1.35	1.25
1	B	879	ILE	CA-CB	-5.11	1.47	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4	ILE	CG1-CD1	5.10	1.71	1.51
1	A	45	LEU	N-CA	5.10	1.52	1.46
1	A	557	THR	N-CA	5.10	1.52	1.46
1	A	475	ARG	CZ-NH1	5.10	1.39	1.32
1	B	578	SER	C-N	-5.10	1.27	1.34
1	A	133	GLU	N-CA	-5.10	1.39	1.46
1	A	106	TRP	N-CA	5.09	1.52	1.46
1	B	501	ARG	CA-C	-5.09	1.46	1.52
1	B	677	ILE	C-N	5.09	1.40	1.33
1	A	784	LEU	N-CA	-5.09	1.39	1.46
1	A	324	PHE	CD2-CE2	-5.09	1.23	1.38
1	A	661	PHE	N-CA	5.09	1.52	1.46
1	B	378	PRO	C-N	-5.09	1.26	1.33
1	A	56	HIS	CA-CB	-5.09	1.44	1.53
1	B	646	GLN	CG-CD	5.09	1.64	1.52
1	B	727	ARG	C-N	5.09	1.40	1.33
1	A	12	ARG	CD-NE	-5.08	1.39	1.46
1	A	731	VAL	CB-CG1	5.08	1.69	1.52
1	B	361	TYR	CA-C	5.08	1.58	1.52
1	B	214	TRP	CB-CG	-5.08	1.34	1.50
1	B	270	LYS	CA-CB	-5.08	1.45	1.53
1	B	42	ALA	C-O	-5.08	1.17	1.24
1	A	558	ILE	CA-C	5.07	1.58	1.52
1	A	656	GLU	CD-OE2	5.07	1.34	1.25
1	B	293	TRP	C-O	5.07	1.30	1.23
1	A	412	ALA	C-O	5.07	1.30	1.23
1	A	202	GLU	C-O	5.07	1.30	1.24
1	A	3	GLY	C-O	-5.07	1.16	1.23
1	B	89	VAL	CB-CG2	5.07	1.69	1.52
1	B	325	TRP	CE3-CZ3	5.07	1.53	1.38
1	A	215	TYR	CA-C	5.07	1.58	1.52
1	A	293	TRP	CA-CB	5.07	1.59	1.53
1	A	763	GLY	N-CA	5.06	1.53	1.45
1	B	3	GLY	CA-C	-5.06	1.45	1.52
1	A	177	TRP	CG-CD2	5.06	1.52	1.43
1	A	618	LEU	N-CA	5.06	1.52	1.46
1	A	834	ILE	C-O	5.06	1.30	1.24
1	B	476	ILE	CA-CB	-5.06	1.46	1.55
1	A	330	ASP	N-CA	-5.06	1.39	1.46
1	A	692	ASP	C-O	5.06	1.30	1.23
1	B	426	ARG	CG-CD	5.06	1.67	1.52
1	B	604	ASN	N-CA	5.06	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	411	LEU	C-O	5.05	1.30	1.24
1	A	265	SER	CA-C	-5.05	1.46	1.52
1	B	369	SER	C-N	-5.05	1.25	1.33
1	B	110	ALA	C-O	-5.05	1.18	1.24
1	B	505	GLU	CD-OE1	5.05	1.34	1.25
1	A	697	LEU	N-CA	-5.05	1.40	1.46
1	B	61	LYS	CE-NZ	5.05	1.64	1.49
1	B	64	GLY	CA-C	5.05	1.59	1.51
1	B	104	ASP	C-N	-5.05	1.26	1.33
1	A	381	PHE	CD2-CE2	5.05	1.53	1.38
1	A	344	THR	C-O	-5.05	1.17	1.24
1	B	384	ASN	CB-CG	-5.05	1.39	1.52
1	A	614	ARG	CZ-NH1	5.04	1.39	1.32
1	A	149	TRP	CA-C	5.04	1.58	1.52
1	B	854	PHE	CG-CD2	5.04	1.49	1.38
1	A	207	PHE	CA-CB	-5.04	1.45	1.53
1	B	328	PHE	N-CA	5.04	1.52	1.46
1	B	607	ARG	CA-C	-5.04	1.46	1.52
1	A	14	ALA	C-N	-5.04	1.26	1.33
1	B	395	ASP	CA-CB	-5.04	1.45	1.53
1	B	330	ASP	CA-C	5.04	1.59	1.52
1	A	624	MET	N-CA	5.03	1.52	1.46
1	A	51	PHE	CG-CD1	5.03	1.49	1.38
1	A	579	CYS	C-N	-5.03	1.27	1.33
1	A	229	LEU	CA-CB	-5.03	1.45	1.53
1	B	633	ILE	CA-C	5.03	1.59	1.52
1	A	560	ASN	CA-C	5.03	1.63	1.52
1	A	500	LEU	CA-C	-5.03	1.46	1.52
1	A	681	LEU	CA-C	-5.03	1.46	1.52
1	B	75	TRP	CG-CD1	-5.03	1.24	1.36
1	B	8	LEU	CG-CD1	5.02	1.69	1.52
1	A	481	GLY	CA-C	5.02	1.57	1.51
1	B	121	LEU	CA-C	-5.01	1.46	1.52
1	B	331	PHE	CD1-CE1	-5.01	1.23	1.38
1	B	771	SER	CA-CB	-5.01	1.45	1.53
1	A	415	GLN	CB-CG	-5.01	1.37	1.52
1	B	70	THR	CA-CB	5.01	1.61	1.53
1	B	649	VAL	C-N	-5.01	1.27	1.34
1	A	71	TYR	CB-CG	5.01	1.62	1.51
1	A	739	GLU	CA-CB	5.01	1.61	1.53
1	B	237	LEU	CG-CD1	5.01	1.69	1.52
1	B	615	LYS	CB-CG	5.01	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	683	PRO	C-O	5.01	1.30	1.24
1	A	263	ALA	C-O	5.01	1.30	1.24
1	A	342	ASN	CG-OD1	5.01	1.33	1.23
1	B	189	ASN	CA-CB	-5.01	1.45	1.53
1	A	500	LEU	CG-CD1	-5.00	1.36	1.52
1	A	366	ARG	CZ-NH2	-5.00	1.26	1.33
1	A	777	ASP	CG-OD2	5.00	1.34	1.25
1	B	114	LEU	N-CA	-5.00	1.39	1.46
1	A	449	LEU	CG-CD1	5.00	1.69	1.52

All (1603) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	742	ALA	N-CA-C	-22.12	86.27	111.71
1	A	303	GLU	N-CA-C	17.00	132.20	108.74
1	B	858	LEU	N-CA-C	16.18	133.35	113.12
1	A	460	ARG	NE-CZ-NH1	-16.09	105.41	121.50
1	B	83	SER	CA-C-N	-15.83	104.00	123.15
1	B	83	SER	C-N-CA	-15.83	104.00	123.15
1	A	96	ASP	N-CA-C	-14.96	92.97	112.41
1	B	865	PHE	N-CA-C	-14.87	81.72	110.56
1	A	789	PHE	N-CA-C	-14.41	92.38	112.13
1	A	305	ASN	N-CA-C	-14.30	95.91	113.50
1	B	882	ASN	N-CA-C	-14.12	90.66	108.45
1	B	583	VAL	N-CA-C	-13.98	88.42	108.42
1	A	852	ASP	N-CA-C	-13.90	96.12	111.14
1	B	402	SER	CA-C-N	13.64	147.60	121.54
1	B	402	SER	C-N-CA	13.64	147.60	121.54
1	B	124	VAL	N-CA-C	-13.21	100.45	111.81
1	A	630	ARG	N-CA-C	-13.15	96.95	111.28
1	A	319	MET	N-CA-C	13.05	128.52	108.42
1	B	188	VAL	N-CA-C	-13.01	96.82	111.00
1	B	402	SER	O-C-N	12.83	137.69	122.68
1	A	37	ASN	N-CA-C	-12.81	96.12	112.90
1	A	312	ARG	N-CA-C	-12.75	93.44	111.81
1	A	159	PRO	CA-C-O	-12.69	107.95	121.27
1	A	184	ALA	N-CA-C	-12.68	96.29	112.90
1	A	861	LEU	N-CA-C	-12.64	96.14	111.69
1	A	211	VAL	CB-CA-C	-12.51	92.12	110.63
1	B	433	PHE	N-CA-C	12.47	124.17	108.45
1	A	303	GLU	CB-CG-CD	-12.39	91.53	112.60
1	A	595	GLY	CA-C-O	-12.38	113.53	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	GLY	N-CA-C	12.32	132.32	115.32
1	B	681	LEU	N-CA-C	12.26	127.67	112.23
1	A	243	ASN	N-CA-C	12.23	128.21	108.63
1	A	329	ARG	NE-CZ-NH2	-12.21	108.22	119.20
1	A	891	MET	N-CA-C	-12.18	98.03	111.07
1	A	448	HIS	N-CA-C	12.15	125.13	110.91
1	B	349	LYS	N-CA-C	-12.15	94.49	110.53
1	A	824	GLU	N-CA-C	-12.02	98.18	111.28
1	A	331	PHE	N-CA-C	11.93	124.37	111.36
1	B	193	GLU	N-CA-C	-11.89	95.19	111.96
1	A	329	ARG	NE-CZ-NH1	11.87	133.37	121.50
1	A	57	SER	N-CA-C	-11.80	98.90	113.18
1	A	601	ILE	O-C-N	11.76	133.78	121.90
1	B	472	VAL	CB-CA-C	-11.62	93.16	110.81
1	A	462	GLN	O-C-N	-11.56	110.07	123.25
1	B	358	THR	N-CA-C	11.49	127.03	110.14
1	B	697	LEU	N-CA-C	-11.43	97.83	112.23
1	A	328	PHE	O-C-N	-11.42	107.40	122.59
1	B	330	ASP	N-CA-C	-11.28	97.75	112.41
1	B	402	SER	N-CA-C	11.28	126.95	110.59
1	B	666	ARG	N-CA-C	-11.22	98.09	112.23
1	B	389	ILE	N-CA-C	-11.20	92.35	108.48
1	A	205	GLU	N-CA-C	-11.20	98.12	112.23
1	A	637	GLY	CA-C-N	-11.19	106.16	122.94
1	A	637	GLY	C-N-CA	-11.19	106.16	122.94
1	A	159	PRO	O-C-N	11.16	135.15	122.98
1	B	400	TYR	N-CA-C	11.12	134.49	110.80
1	B	767	ASP	N-CA-C	-11.07	98.97	111.71
1	B	680	GLN	N-CA-C	-11.01	98.01	111.33
1	A	434	ALA	CA-C-O	-10.95	109.52	121.23
1	A	796	ILE	N-CA-C	-10.93	99.70	110.30
1	A	68	SER	N-CA-C	-10.89	99.49	111.36
1	B	573	GLY	N-CA-C	-10.88	99.16	112.33
1	A	628	GLU	CB-CG-CD	-10.80	94.24	112.60
1	A	803	TYR	CA-C-O	10.80	139.16	120.80
1	A	105	SER	N-CA-C	10.78	124.38	111.33
1	B	711	HIS	N-CA-C	-10.78	99.32	111.82
1	A	319	MET	CA-C-N	-10.73	101.04	121.54
1	A	319	MET	C-N-CA	-10.73	101.04	121.54
1	A	486	VAL	O-C-N	10.67	133.27	121.10
1	B	572	ASN	N-CA-C	10.65	126.40	110.64
1	B	838	ILE	CA-C-O	-10.60	107.53	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	652	PHE	N-CA-C	10.55	125.52	112.23
1	B	521	LEU	N-CA-C	10.51	126.71	109.58
1	B	182	GLU	N-CA-C	10.45	123.98	111.33
1	B	267	THR	O-C-N	-10.37	110.96	123.30
1	B	714	ASN	CA-C-O	10.36	138.41	120.80
1	B	298	SER	CA-CB-OG	-10.35	90.40	111.10
1	B	788	GLU	N-CA-C	-10.29	98.26	112.25
1	B	398	ASP	CA-C-O	-10.23	103.40	120.80
1	B	611	THR	N-CA-C	10.23	124.84	111.75
1	A	828	PHE	CA-C-N	-10.20	109.21	122.77
1	A	828	PHE	C-N-CA	-10.20	109.21	122.77
1	B	89	VAL	CB-CA-C	-10.19	99.78	111.09
1	B	344	THR	OG1-CB-CG2	-10.19	88.92	109.30
1	B	294	LYS	CA-CB-CG	10.17	134.43	114.10
1	A	266	VAL	N-CA-C	-10.15	93.58	108.71
1	B	396	ASP	CA-C-N	10.14	138.87	121.64
1	B	396	ASP	C-N-CA	10.14	138.87	121.64
1	A	702	LEU	CA-C-O	-10.11	103.61	120.80
1	B	727	ARG	N-CA-C	10.11	124.12	111.69
1	A	281	LEU	N-CA-C	-10.10	95.29	110.14
1	B	743	THR	CA-C-N	10.02	134.52	120.29
1	B	743	THR	C-N-CA	10.02	134.52	120.29
1	A	340	ILE	CB-CG1-CD1	10.01	134.82	113.80
1	B	347	ALA	N-CA-C	-9.98	101.24	113.41
1	B	388	LYS	N-CA-C	9.95	125.22	109.50
1	A	85	PRO	CA-C-O	-9.89	110.06	121.34
1	A	189	ASN	N-CA-C	9.88	123.28	111.82
1	B	315	LEU	CA-CB-CG	9.88	150.88	116.30
1	A	102	LEU	N-CA-C	-9.86	99.41	113.21
1	A	520	ASN	N-CA-C	9.86	124.87	110.28
1	A	500	LEU	N-CA-C	-9.84	94.34	110.17
1	A	49	PRO	N-CA-C	-9.82	100.71	113.57
1	B	446	PRO	N-CD-CG	-9.77	88.55	103.20
1	A	477	ARG	NE-CZ-NH2	9.70	127.93	119.20
1	B	449	LEU	O-C-N	9.69	133.79	122.94
1	B	310	TYR	N-CA-C	-9.68	100.97	113.17
1	A	486	VAL	CA-C-O	-9.66	107.00	119.95
1	A	394	VAL	N-CA-C	9.66	122.88	109.45
1	A	460	ARG	NE-CZ-NH2	9.63	127.87	119.20
1	A	296	PRO	CA-C-O	9.61	129.24	118.38
1	A	831	ASN	CB-CA-C	9.60	129.53	110.42
1	A	319	MET	O-C-N	-9.59	113.97	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	ILE	CB-CA-C	-9.54	96.52	110.63
1	A	751	LYS	CA-C-O	-9.51	104.63	120.80
1	A	306	LYS	CA-CB-CG	-9.51	95.08	114.10
1	A	350	SER	O-C-N	9.47	135.19	122.59
1	B	802	ILE	CA-C-O	-9.47	104.69	120.80
1	A	833	HIS	N-CA-C	9.47	130.97	110.80
1	B	0	GLU	CA-C-O	-9.47	104.70	120.80
1	B	205	GLU	N-CA-C	-9.47	100.92	111.14
1	B	4	ILE	N-CA-CB	9.46	121.61	110.55
1	B	374	CYS	N-CA-C	9.43	123.68	109.63
1	A	218	GLN	CA-C-N	9.41	139.51	121.54
1	A	218	GLN	C-N-CA	9.41	139.51	121.54
1	A	114	LEU	CA-C-O	-9.40	107.38	120.07
1	B	377	TYR	CA-C-O	9.40	131.62	121.28
1	B	572	ASN	OD1-CG-ND2	-9.40	113.20	122.60
1	B	339	GLU	N-CA-C	9.39	124.70	109.59
1	A	447	VAL	CA-C-N	-9.38	108.76	122.93
1	A	447	VAL	C-N-CA	-9.38	108.76	122.93
1	A	494	LYS	CA-C-O	-9.38	110.42	120.46
1	B	430	THR	OG1-CB-CG2	-9.37	90.56	109.30
1	A	18	LEU	N-CA-C	-9.36	98.17	110.53
1	B	289	GLY	N-CA-C	9.36	127.38	115.21
1	B	470	ARG	NE-CZ-NH2	9.34	127.61	119.20
1	B	379	ALA	N-CA-C	-9.34	102.02	113.41
1	B	218	GLN	N-CA-C	-9.34	101.58	113.16
1	B	315	LEU	CB-CA-C	-9.34	91.84	110.42
1	A	350	SER	N-CA-C	-9.32	90.95	110.80
1	B	645	HIS	N-CA-C	-9.28	101.96	113.28
1	A	288	TRP	N-CA-C	-9.28	100.92	112.88
1	B	145	GLN	CA-C-O	9.26	130.51	120.32
1	B	862	ASP	N-CA-C	-9.24	91.12	110.80
1	A	286	ASN	CA-C-O	9.24	126.15	119.32
1	B	398	ASP	O-C-N	-9.22	108.24	123.00
1	B	366	ARG	NH1-CZ-NH2	9.22	131.29	119.30
1	B	641	PRO	CA-C-O	-9.22	110.62	121.86
1	B	36	ARG	CG-CD-NE	9.20	132.24	112.00
1	A	311	GLU	O-C-N	9.20	131.92	122.08
1	A	128	GLY	CA-C-O	-9.19	109.12	119.88
1	B	188	VAL	CA-CB-CG1	9.19	126.03	110.40
1	B	241	SER	CA-C-O	-9.19	110.78	120.89
1	B	155	ASP	CA-C-O	-9.19	110.88	121.72
1	A	887	LEU	N-CA-C	9.18	122.12	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	GLY	CA-C-O	-9.15	112.00	121.61
1	B	880	GLN	CA-C-O	-9.14	110.18	120.32
1	A	112	ALA	N-CA-C	9.11	121.21	111.28
1	A	464	GLU	N-CA-C	-9.11	96.52	110.10
1	B	90	ASP	CB-CA-C	9.10	126.17	109.70
1	B	667	CYS	CA-C-N	-9.09	106.74	121.19
1	B	667	CYS	C-N-CA	-9.09	106.74	121.19
1	B	10	LYS	N-CA-C	9.05	120.92	111.14
1	B	640	LEU	O-C-N	-9.04	114.50	121.55
1	B	520	ASN	N-CA-C	9.03	123.98	107.99
1	A	278	ARG	NE-CZ-NH1	-9.02	112.48	121.50
1	B	743	THR	O-C-N	9.00	132.41	122.15
1	B	538	THR	CB-CA-C	-9.00	92.51	110.42
1	A	7	LYS	CB-CG-CD	8.99	131.98	111.30
1	A	763	GLY	CA-C-N	8.99	133.58	120.90
1	A	763	GLY	C-N-CA	8.99	133.58	120.90
1	A	756	HIS	CA-C-N	8.98	131.06	119.84
1	A	756	HIS	C-N-CA	8.98	131.06	119.84
1	A	628	GLU	N-CA-CB	-8.97	98.50	110.88
1	A	550	ILE	CA-C-N	8.96	138.66	121.54
1	A	550	ILE	C-N-CA	8.96	138.66	121.54
1	B	864	MET	N-CA-C	8.96	124.00	112.89
1	B	362	GLU	CB-CG-CD	8.94	127.80	112.60
1	B	415	GLN	CA-C-O	-8.94	111.06	121.16
1	B	123	ARG	N-CA-C	8.93	123.44	112.54
1	A	354	ARG	NE-CZ-NH2	8.91	127.22	119.20
1	A	212	THR	N-CA-C	8.91	124.85	107.57
1	A	572	ASN	CA-C-N	-8.89	112.05	121.48
1	A	572	ASN	C-N-CA	-8.89	112.05	121.48
1	B	407	CYS	N-CA-C	-8.89	95.49	109.72
1	B	433	PHE	N-CA-CB	-8.89	94.93	110.76
1	B	409	PHE	N-CA-C	8.87	122.64	109.24
1	A	598	GLU	N-CA-C	-8.87	101.16	114.64
1	B	54	VAL	CA-C-O	-8.84	109.74	120.78
1	A	759	LEU	CA-C-N	8.83	137.59	121.70
1	A	759	LEU	C-N-CA	8.83	137.59	121.70
1	A	227	ILE	N-CA-C	-8.81	101.82	110.72
1	A	758	ASP	CA-C-N	-8.79	109.42	122.78
1	A	758	ASP	C-N-CA	-8.79	109.42	122.78
1	B	121	LEU	N-CA-C	8.78	120.62	111.14
1	B	850	ASP	OD1-CG-OD2	-8.77	101.85	122.90
1	B	296	PRO	CB-CA-C	8.75	125.99	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	499	LEU	CB-CA-C	-8.73	95.87	110.19
1	B	277	GLN	CB-CG-CD	8.70	127.40	112.60
1	B	386	GLN	N-CA-C	8.70	123.79	109.95
1	A	28	LEU	CA-C-O	8.70	130.58	120.32
1	A	185	TYR	N-CA-C	-8.70	100.79	111.40
1	A	429	GLU	CB-CA-C	8.68	124.12	109.80
1	B	825	ALA	CA-C-N	8.68	136.53	122.65
1	B	825	ALA	C-N-CA	8.68	136.53	122.65
1	A	38	GLU	N-CA-C	-8.67	102.87	113.19
1	A	596	LEU	N-CA-C	8.66	123.17	113.21
1	B	604	ASN	N-CA-C	8.65	120.40	110.97
1	B	100	GLY	N-CA-C	8.62	121.81	112.33
1	B	466	PHE	CB-CA-C	-8.61	96.73	110.94
1	B	311	GLU	CA-C-N	8.60	135.74	122.24
1	B	311	GLU	C-N-CA	8.60	135.74	122.24
1	A	786	PHE	N-CA-C	-8.59	92.50	110.80
1	B	806	PHE	CA-CB-CG	8.59	122.39	113.80
1	A	73	ILE	CA-C-N	-8.58	110.68	122.86
1	A	73	ILE	C-N-CA	-8.58	110.68	122.86
1	B	331	PHE	CB-CA-C	-8.57	93.36	110.42
1	A	273	THR	N-CA-C	8.56	122.34	109.25
1	B	665	VAL	CA-C-O	8.54	128.26	119.20
1	A	710	MET	CA-C-N	8.54	137.86	121.54
1	A	710	MET	C-N-CA	8.54	137.86	121.54
1	A	756	HIS	C-N-CD	-8.54	89.97	125.00
1	B	366	ARG	N-CA-C	8.54	123.34	109.76
1	B	366	ARG	NE-CZ-NH1	-8.54	112.96	121.50
1	B	609	TYR	N-CA-CB	8.53	123.35	110.22
1	A	164	LYS	CA-C-O	8.53	129.75	120.71
1	A	356	TRP	N-CA-C	-8.52	92.66	110.80
1	A	188	VAL	CA-C-O	-8.52	111.36	120.64
1	B	115	THR	CA-C-O	8.51	129.03	119.41
1	B	432	GLY	O-C-N	8.49	133.29	123.44
1	B	786	PHE	CA-C-O	8.46	129.62	120.90
1	B	147	GLY	CA-C-O	-8.45	109.59	119.06
1	B	661	PHE	N-CA-C	8.45	121.25	111.11
1	B	489	THR	CA-C-O	-8.40	111.11	120.69
1	B	177	TRP	N-CA-C	8.39	121.48	111.33
1	A	165	LEU	CB-CA-C	8.39	124.05	110.29
1	A	447	VAL	CB-CA-C	-8.37	95.49	111.40
1	A	339	GLU	CG-CD-OE2	-8.37	99.14	118.40
1	A	791	TYR	N-CA-C	-8.37	101.19	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	GLY	O-C-N	-8.37	113.40	121.77
1	A	136	ALA	N-CA-C	8.35	128.59	110.80
1	B	473	SER	N-CA-C	8.34	121.69	107.93
1	A	733	LEU	CA-C-O	-8.34	111.87	120.54
1	A	830	LEU	N-CA-C	8.34	123.59	110.17
1	A	591	ASN	N-CA-C	-8.34	87.66	111.00
1	B	624	MET	N-CA-CB	-8.33	103.84	111.59
1	B	653	ALA	CA-C-O	8.32	129.55	120.32
1	B	275	GLN	N-CA-C	-8.32	99.99	111.30
1	B	58	LEU	N-CA-C	-8.31	103.27	113.41
1	A	492	PRO	CA-C-N	8.31	134.16	122.36
1	A	492	PRO	C-N-CA	8.31	134.16	122.36
1	A	191	SER	CA-C-O	-8.30	112.19	121.40
1	B	439	PRO	CA-C-O	-8.30	111.75	121.96
1	A	665	VAL	N-CA-CB	8.29	119.72	110.51
1	B	34	THR	CA-CB-OG1	-8.26	97.20	109.60
1	A	467	ILE	N-CA-C	8.24	122.59	108.90
1	B	658	ILE	O-C-N	8.24	132.88	122.57
1	B	891	MET	CA-C-N	-8.22	110.62	123.12
1	B	891	MET	C-N-CA	-8.22	110.62	123.12
1	B	641	PRO	N-CD-CG	-8.20	90.90	103.20
1	B	808	THR	O-C-N	-8.18	111.72	122.59
1	B	404	GLU	CB-CA-C	-8.17	105.11	115.89
1	A	84	ASN	CA-C-N	8.17	128.17	119.76
1	A	84	ASN	C-N-CA	8.17	128.17	119.76
1	A	700	SER	N-CA-C	-8.16	103.35	112.57
1	A	39	CYS	N-CA-C	-8.15	101.84	112.68
1	A	676	LYS	N-CA-C	-8.13	102.36	111.07
1	B	383	VAL	O-C-N	8.12	130.98	121.80
1	A	860	ARG	NE-CZ-NH1	-8.12	113.39	121.50
1	B	495	GLU	CB-CG-CD	8.11	126.39	112.60
1	A	810	ARG	NE-CZ-NH2	8.11	126.50	119.20
1	A	621	SER	N-CA-C	-8.09	103.61	113.97
1	A	812	GLY	CA-C-O	-8.08	103.82	120.80
1	B	859	VAL	N-CA-C	-8.08	102.50	113.00
1	A	645	HIS	N-CA-C	-8.07	103.22	113.23
1	A	160	THR	N-CA-C	8.07	121.42	109.24
1	B	65	PRO	N-CA-C	-8.07	99.31	111.41
1	A	434	ALA	N-CA-C	8.06	121.13	108.79
1	B	888	GLN	N-CA-C	-8.05	101.79	111.69
1	B	116	LEU	CD1-CG-CD2	-8.05	93.09	110.80
1	B	329	ARG	CA-C-N	8.04	135.11	122.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	329	ARG	C-N-CA	8.04	135.11	122.49
1	A	357	ASN	N-CA-C	8.03	121.88	110.23
1	A	889	LEU	O-C-N	-8.03	112.45	122.17
1	A	792	LEU	N-CA-C	8.02	120.93	111.71
1	B	11	ASP	N-CA-C	-8.02	102.59	112.38
1	A	72	GLY	N-CA-C	-8.02	103.61	115.72
1	A	210	GLY	CA-C-O	-8.00	113.74	121.90
1	A	73	ILE	CA-C-O	7.99	130.15	121.04
1	B	634	GLU	O-C-N	7.99	130.59	122.12
1	B	389	ILE	CB-CA-C	-7.98	98.72	110.62
1	B	791	TYR	N-CA-C	-7.95	98.33	111.37
1	B	396	ASP	O-C-N	7.93	133.14	122.59
1	B	398	ASP	N-CA-C	7.93	133.19	111.00
1	A	185	TYR	O-C-N	7.92	131.76	122.17
1	A	670	ARG	CD-NE-CZ	-7.92	113.31	124.40
1	A	633	ILE	O-C-N	7.92	130.75	121.80
1	B	340	ILE	CB-CG1-CD1	7.91	130.42	113.80
1	B	697	LEU	CB-CA-C	7.91	126.52	110.38
1	A	275	GLN	O-C-N	-7.91	113.09	122.58
1	B	336	THR	N-CA-C	-7.91	97.00	109.50
1	A	851	PHE	CA-C-N	7.90	131.19	120.44
1	A	851	PHE	C-N-CA	7.90	131.19	120.44
1	A	89	VAL	CA-CB-CG1	7.89	123.81	110.40
1	B	193	GLU	CA-C-O	-7.89	108.75	120.42
1	B	13	GLU	N-CA-CB	7.86	121.76	110.13
1	A	698	SER	N-CA-C	7.84	119.73	111.03
1	B	368	GLY	CA-C-O	7.83	127.72	119.02
1	B	6	MET	N-CA-CB	7.83	122.36	110.14
1	B	383	VAL	CA-C-O	-7.82	112.02	120.47
1	A	269	ALA	O-C-N	7.82	133.06	123.44
1	B	556	GLN	N-CA-C	-7.82	98.55	111.37
1	B	440	ARG	CB-CA-C	-7.82	94.87	110.42
1	A	768	THR	N-CA-CB	-7.81	97.28	110.49
1	A	255	PHE	CA-C-N	-7.81	111.71	122.95
1	A	255	PHE	C-N-CA	-7.81	111.71	122.95
1	A	175	GLU	CA-CB-CG	7.80	129.70	114.10
1	B	676	LYS	N-CA-C	-7.75	102.91	111.36
1	A	105	SER	CA-C-O	7.75	129.00	120.63
1	A	830	LEU	CA-C-N	-7.75	106.75	121.54
1	A	830	LEU	C-N-CA	-7.75	106.75	121.54
1	B	679	LYS	CA-C-N	7.74	130.99	120.38
1	B	679	LYS	C-N-CA	7.74	130.99	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	576	LEU	N-CA-C	-7.73	102.95	112.38
1	B	242	ILE	N-CA-C	7.73	119.73	108.53
1	A	35	LEU	CA-C-N	-7.72	109.16	120.28
1	A	35	LEU	C-N-CA	-7.72	109.16	120.28
1	B	118	GLU	N-CA-C	7.71	119.37	110.97
1	A	332	ILE	CG1-CB-CG2	7.70	133.80	110.70
1	B	742	ALA	CA-C-O	7.68	128.85	119.79
1	B	559	LEU	O-C-N	7.68	131.49	122.20
1	B	677	ILE	N-CA-C	-7.68	101.50	111.09
1	B	776	MET	CB-CG-SD	-7.68	89.67	112.70
1	A	634	GLU	CA-C-N	7.66	130.88	120.38
1	A	634	GLU	C-N-CA	7.66	130.88	120.38
1	B	470	ARG	NE-CZ-NH1	-7.66	113.84	121.50
1	A	285	ARG	NE-CZ-NH2	-7.65	112.32	119.20
1	B	241	SER	O-C-N	7.65	132.04	123.48
1	B	394	VAL	O-C-N	7.64	131.66	123.02
1	B	119	THR	N-CA-CB	-7.63	98.46	110.28
1	B	616	PHE	CA-C-O	7.62	127.44	119.51
1	B	640	LEU	N-CA-C	7.61	122.34	109.09
1	A	339	GLU	N-CA-CB	-7.61	98.44	110.69
1	A	463	SER	CB-CA-C	-7.61	97.45	109.70
1	B	469	LEU	CB-CA-C	7.58	127.53	111.91
1	B	295	GLY	N-CA-C	7.57	127.79	112.34
1	A	613	PHE	N-CA-C	-7.57	102.18	111.33
1	A	522	PRO	CA-C-O	-7.56	96.31	119.00
1	A	775	VAL	CB-CA-C	-7.56	100.44	112.16
1	A	429	GLU	O-C-N	-7.56	114.49	123.03
1	B	200	THR	OG1-CB-CG2	-7.55	94.19	109.30
1	B	700	SER	O-C-N	7.55	132.30	122.03
1	A	352	THR	N-CA-C	7.55	120.94	109.62
1	A	287	PRO	CA-C-N	-7.54	110.83	122.60
1	A	287	PRO	C-N-CA	-7.54	110.83	122.60
1	B	522	PRO	CA-C-O	-7.54	112.81	121.56
1	A	358	THR	OG1-CB-CG2	-7.53	94.24	109.30
1	A	614	ARG	NE-CZ-NH2	-7.53	112.43	119.20
1	A	269	ALA	CA-C-O	-7.51	110.07	120.21
1	B	291	VAL	CB-CA-C	-7.51	98.98	111.29
1	A	278	ARG	CB-CA-C	-7.50	95.49	110.42
1	A	871	LEU	N-CA-CB	7.49	121.09	110.07
1	A	645	HIS	N-CA-CB	7.49	122.12	110.44
1	B	118	GLU	O-C-N	-7.49	114.24	122.03
1	B	48	ASP	CB-CA-C	7.47	121.95	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	510	THR	CA-C-O	-7.46	112.64	120.70
1	B	447	VAL	O-C-N	-7.46	113.25	122.57
1	B	140	HIS	N-CA-C	7.46	120.79	109.23
1	B	470	ARG	N-CA-CB	-7.46	99.20	110.01
1	B	624	MET	N-CA-C	7.44	119.28	108.34
1	B	501	ARG	NE-CZ-NH2	-7.44	112.50	119.20
1	B	227	ILE	CA-C-N	-7.44	111.40	120.70
1	B	227	ILE	C-N-CA	-7.44	111.40	120.70
1	A	396	ASP	OD1-CG-OD2	-7.43	105.06	122.90
1	B	50	ALA	N-CA-C	-7.43	104.36	113.50
1	A	384	ASN	N-CA-CB	7.42	120.02	109.78
1	A	889	LEU	CA-C-O	7.42	128.49	120.55
1	A	855	ILE	CB-CA-C	-7.42	101.22	112.05
1	A	701	VAL	CA-C-N	7.42	135.05	121.70
1	A	701	VAL	C-N-CA	7.42	135.05	121.70
1	B	665	VAL	N-CA-C	-7.41	104.10	113.22
1	A	808	THR	CA-C-N	7.40	135.68	121.54
1	A	808	THR	C-N-CA	7.40	135.68	121.54
1	A	306	LYS	N-CA-C	7.40	120.55	110.55
1	A	358	THR	CA-CB-CG2	-7.40	97.92	110.50
1	A	640	LEU	CA-C-N	7.39	127.43	119.89
1	A	640	LEU	C-N-CA	7.39	127.43	119.89
1	A	620	LYS	CB-CA-C	7.39	125.13	110.42
1	A	110	ALA	O-C-N	7.39	129.95	122.12
1	B	389	ILE	CA-C-O	7.38	129.31	120.67
1	A	96	ASP	CB-CA-C	-7.38	99.06	111.02
1	A	665	VAL	CA-CB-CG2	-7.38	97.85	110.40
1	A	647	VAL	CA-C-O	7.37	128.21	120.25
1	A	432	GLY	CA-C-O	-7.36	114.41	121.41
1	A	213	GLU	N-CA-C	7.35	120.61	110.24
1	B	44	ALA	N-CA-CB	-7.35	99.39	111.66
1	B	440	ARG	CA-C-O	-7.35	110.00	120.51
1	A	468	ASN	N-CA-CB	7.34	119.70	110.45
1	B	93	THR	CA-CB-CG2	7.34	122.99	110.50
1	A	691	LEU	N-CA-C	-7.34	95.50	108.13
1	B	93	THR	OG1-CB-CG2	-7.34	94.62	109.30
1	B	65	PRO	N-CD-CG	7.33	114.20	103.20
1	A	291	VAL	N-CA-CB	7.33	123.32	111.23
1	B	286	ASN	CA-C-N	7.32	128.99	119.84
1	B	286	ASN	C-N-CA	7.32	128.99	119.84
1	B	878	GLN	CA-C-O	-7.32	113.28	121.40
1	B	130	SER	N-CA-C	7.32	120.19	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	PHE	CA-C-O	-7.31	112.01	120.20
1	A	515	ASP	CA-C-O	-7.31	113.06	121.47
1	A	333	ARG	N-CA-C	-7.31	95.23	108.02
1	B	514	ASP	CB-CG-OD2	-7.31	101.59	118.40
1	A	588	ARG	CA-C-O	7.30	133.21	120.80
1	B	733	LEU	CA-C-O	-7.30	108.39	120.80
1	A	121	LEU	CA-C-O	-7.30	113.16	120.82
1	A	779	ASP	N-CA-C	7.29	122.18	113.28
1	B	106	TRP	N-CA-C	7.29	121.08	111.75
1	A	229	LEU	N-CA-C	-7.27	95.31	110.80
1	B	806	PHE	N-CA-C	-7.27	95.31	110.80
1	B	360	PHE	CA-C-O	-7.27	112.30	120.66
1	A	756	HIS	CB-CA-C	7.26	123.90	110.10
1	A	116	LEU	CA-C-N	-7.26	112.89	123.05
1	A	116	LEU	C-N-CA	-7.26	112.89	123.05
1	A	356	TRP	CA-C-N	-7.26	110.41	120.71
1	A	356	TRP	C-N-CA	-7.26	110.41	120.71
1	B	631	MET	CA-CB-CG	7.26	128.61	114.10
1	B	362	GLU	CA-CB-CG	-7.25	99.59	114.10
1	B	303	GLU	CA-C-N	7.25	135.39	121.54
1	B	303	GLU	C-N-CA	7.25	135.39	121.54
1	B	848	ASN	CA-C-N	7.24	135.36	121.54
1	B	848	ASN	C-N-CA	7.24	135.36	121.54
1	A	163	GLY	O-C-N	7.24	131.45	122.41
1	A	876	THR	N-CA-CB	7.23	121.56	110.14
1	B	94	ARG	CA-C-N	7.22	134.79	122.37
1	B	94	ARG	C-N-CA	7.22	134.79	122.37
1	A	175	GLU	CG-CD-OE2	7.22	135.01	118.40
1	A	40	LEU	CD1-CG-CD2	-7.21	94.94	110.80
1	A	335	PHE	N-CA-C	-7.21	102.43	112.45
1	A	554	GLU	N-CA-C	-7.21	103.55	113.56
1	B	485	VAL	CA-CB-CG2	-7.20	98.16	110.40
1	B	776	MET	N-CA-C	7.20	123.08	113.72
1	B	407	CYS	CA-C-O	-7.19	112.98	121.11
1	A	88	ILE	CG1-CB-CG2	-7.19	89.14	110.70
1	A	795	ASN	N-CA-C	-7.18	104.65	113.41
1	A	339	GLU	CA-C-O	-7.18	113.10	120.71
1	B	285	ARG	NE-CZ-NH2	-7.17	112.74	119.20
1	A	257	ASN	CA-C-N	7.17	134.61	121.70
1	A	257	ASN	C-N-CA	7.17	134.61	121.70
1	B	153	VAL	CA-C-O	7.17	130.50	121.40
1	A	608	ASN	O-C-N	-7.17	114.58	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	780	THR	CA-CB-OG1	-7.17	98.85	109.60
1	A	355	ASN	N-CA-CB	-7.17	98.38	110.49
1	A	573	GLY	N-CA-C	7.16	121.56	111.10
1	A	208	THR	CA-C-O	7.16	126.63	118.47
1	B	499	LEU	N-CA-CB	-7.15	99.14	110.79
1	B	349	LYS	O-C-N	7.14	130.94	122.79
1	A	10	LYS	CA-C-N	-7.14	110.92	120.63
1	A	10	LYS	C-N-CA	-7.14	110.92	120.63
1	B	839	ILE	N-CA-C	7.14	124.19	109.34
1	A	237	LEU	CA-C-O	-7.14	113.13	120.84
1	B	745	LEU	CA-C-O	-7.14	113.51	121.00
1	B	89	VAL	O-C-N	7.12	129.61	122.71
1	A	344	THR	CA-C-O	-7.11	110.42	120.16
1	A	442	LEU	CA-C-O	-7.11	108.71	120.80
1	B	378	PRO	N-CD-CG	-7.11	92.53	103.20
1	B	866	ARG	CA-CB-CG	7.11	128.32	114.10
1	A	120	ILE	N-CA-C	7.11	117.90	110.72
1	A	341	CYS	CA-C-N	7.10	130.96	120.87
1	A	341	CYS	C-N-CA	7.10	130.96	120.87
1	A	886	TRP	N-CA-C	7.10	118.67	111.07
1	A	6	MET	CG-SD-CE	-7.09	85.30	100.90
1	A	831	ASN	N-CA-CB	7.08	122.46	110.49
1	B	890	THR	OG1-CB-CG2	-7.08	95.14	109.30
1	A	75	TRP	CA-C-O	-7.08	112.67	120.81
1	B	891	MET	N-CA-C	-7.08	104.52	113.72
1	B	143	LEU	O-C-N	-7.06	114.26	123.16
1	A	350	SER	N-CA-CB	7.06	122.42	110.49
1	A	169	HIS	N-CA-C	7.06	118.87	108.14
1	B	308	ASP	N-CA-CB	-7.05	98.51	110.50
1	A	831	ASN	N-CA-C	-7.05	95.78	110.80
1	A	665	VAL	CB-CA-C	-7.05	102.86	111.88
1	A	505	GLU	CA-C-O	-7.04	110.57	119.31
1	B	428	MET	CG-SD-CE	7.04	116.40	100.90
1	A	126	PRO	O-C-N	7.04	131.72	123.06
1	A	270	LYS	N-CA-C	7.04	120.23	108.13
1	B	30	GLN	N-CA-C	7.04	120.58	110.10
1	B	360	PHE	N-CA-C	7.03	120.99	109.24
1	A	343	LEU	CD1-CG-CD2	-7.03	95.33	110.80
1	B	617	ASP	CB-CA-C	-7.03	96.43	110.42
1	B	129	GLN	CA-C-O	-7.02	112.63	120.70
1	B	631	MET	N-CA-CB	7.02	120.81	110.49
1	A	105	SER	O-C-N	-7.01	114.69	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	ALA	N-CA-C	7.01	118.72	111.14
1	B	436	TYR	CE1-CZ-OH	7.01	140.94	119.90
1	B	701	VAL	CA-C-N	7.01	134.32	121.70
1	B	701	VAL	C-N-CA	7.01	134.32	121.70
1	A	183	LYS	CA-C-O	7.01	128.02	120.10
1	A	831	ASN	CA-C-O	-7.00	110.50	120.51
1	A	674	LEU	CA-C-N	-7.00	111.10	120.54
1	A	674	LEU	C-N-CA	-7.00	111.10	120.54
1	B	93	THR	N-CA-C	-6.99	95.92	110.80
1	A	803	TYR	OH-CZ-CE2	6.98	140.85	119.90
1	B	485	VAL	N-CA-C	6.98	117.94	107.75
1	A	384	ASN	N-CA-C	-6.98	99.92	110.39
1	A	223	ASP	CA-C-O	6.97	126.94	119.34
1	B	235	GLY	CA-C-O	6.97	126.87	119.06
1	A	16	GLU	N-CA-C	6.96	121.08	112.59
1	B	53	PRO	CA-C-O	6.96	126.46	121.31
1	A	211	VAL	CA-C-N	-6.96	112.47	122.77
1	A	211	VAL	C-N-CA	-6.96	112.47	122.77
1	A	238	LEU	CA-C-N	-6.96	115.59	121.58
1	A	238	LEU	C-N-CA	-6.96	115.59	121.58
1	B	12	ARG	N-CA-C	-6.96	103.47	112.23
1	A	116	LEU	CA-C-O	-6.95	113.12	120.63
1	A	382	TRP	N-CA-C	6.95	121.35	113.01
1	B	135	TYR	CA-C-N	-6.95	112.81	125.66
1	B	135	TYR	C-N-CA	-6.95	112.81	125.66
1	A	49	PRO	CA-C-N	-6.94	108.75	121.52
1	A	49	PRO	C-N-CA	-6.94	108.75	121.52
1	B	451	ARG	NE-CZ-NH2	6.93	125.44	119.20
1	A	243	ASN	CB-CA-C	-6.93	99.79	110.88
1	B	572	ASN	CB-CG-ND2	6.93	126.79	116.40
1	A	429	GLU	CA-C-O	6.93	130.11	121.66
1	B	728	LYS	N-CA-C	-6.92	96.06	110.80
1	B	399	ASP	CA-C-O	-6.92	110.63	120.11
1	B	193	GLU	CB-CG-CD	-6.91	100.85	112.60
1	A	165	LEU	CA-CB-CG	-6.91	92.11	116.30
1	A	110	ALA	CA-C-N	6.91	129.40	120.56
1	A	110	ALA	C-N-CA	6.91	129.40	120.56
1	B	389	ILE	N-CA-CB	6.91	123.41	111.39
1	B	540	PHE	CA-C-O	-6.91	109.06	120.80
1	B	361	TYR	N-CA-C	6.90	120.65	109.40
1	A	115	THR	O-C-N	-6.90	113.41	122.59
1	B	872	ASP	N-CA-C	-6.89	100.21	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	825	ALA	CA-C-O	6.88	127.03	118.43
1	A	594	LEU	O-C-N	6.88	129.67	121.76
1	A	522	PRO	N-CA-C	6.88	129.30	112.10
1	B	159	PRO	N-CD-CG	-6.88	92.88	103.20
1	A	868	PHE	N-CA-C	6.87	118.42	111.07
1	B	51	PHE	O-C-N	-6.87	115.33	121.17
1	B	296	PRO	N-CD-CG	-6.87	92.90	103.20
1	B	598	GLU	CA-CB-CG	6.86	127.82	114.10
1	B	336	THR	OG1-CB-CG2	-6.86	95.58	109.30
1	B	68	SER	N-CA-C	-6.85	102.93	112.45
1	B	181	LEU	N-CA-CB	6.84	120.18	110.12
1	B	847	GLY	N-CA-C	-6.83	102.06	112.51
1	A	46	PHE	N-CA-C	6.83	120.27	110.24
1	B	473	SER	O-C-N	-6.83	114.80	123.26
1	A	499	LEU	CA-C-O	-6.82	112.81	120.32
1	A	166	VAL	N-CA-C	6.82	117.98	111.91
1	B	162	ASP	O-C-N	-6.82	113.52	122.59
1	B	463	SER	N-CA-C	6.81	119.53	108.63
1	A	770	ARG	CA-C-N	6.81	130.66	120.31
1	A	770	ARG	C-N-CA	6.81	130.66	120.31
1	A	502	PHE	N-CA-C	6.81	119.51	108.41
1	A	63	LEU	CA-C-N	-6.81	111.18	121.87
1	A	63	LEU	C-N-CA	-6.81	111.18	121.87
1	B	161	LYS	CA-C-O	6.81	128.05	120.70
1	B	79	THR	CB-CA-C	-6.80	99.50	110.79
1	B	606	ILE	N-CA-C	-6.80	101.79	111.17
1	A	193	GLU	CB-CA-C	-6.79	97.63	110.67
1	A	787	GLU	N-CA-C	6.79	122.50	111.37
1	A	282	ILE	CG1-CB-CG2	-6.78	90.35	110.70
1	A	50	ALA	CA-C-O	6.78	127.53	119.60
1	A	70	THR	CA-C-N	-6.78	112.30	122.74
1	A	70	THR	C-N-CA	-6.78	112.30	122.74
1	A	324	PHE	N-CA-CB	6.78	121.94	110.49
1	A	549	GLU	N-CA-C	6.77	121.54	111.04
1	B	451	ARG	N-CA-C	-6.77	103.83	111.14
1	A	53	PRO	N-CA-CB	-6.77	96.14	103.25
1	A	218	GLN	N-CA-CB	6.77	120.07	110.46
1	A	205	GLU	CA-CB-CG	6.77	127.64	114.10
1	A	370	THR	CA-C-N	6.76	133.34	122.32
1	A	370	THR	C-N-CA	6.76	133.34	122.32
1	A	188	VAL	CB-CA-C	-6.76	102.18	112.05
1	B	340	ILE	CA-CB-CG2	6.75	121.98	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	ARG	NE-CZ-NH1	6.75	128.25	121.50
1	B	832	GLN	N-CA-C	-6.75	104.14	112.38
1	B	61	LYS	CA-CB-CG	6.75	127.59	114.10
1	B	378	PRO	N-CA-CB	6.75	109.94	103.19
1	B	317	VAL	CA-C-O	-6.74	112.35	120.78
1	A	430	THR	CA-CB-CG2	6.74	121.95	110.50
1	B	825	ALA	N-CA-CB	-6.74	100.34	111.06
1	B	633	ILE	CA-C-N	6.74	129.31	120.28
1	B	633	ILE	C-N-CA	6.74	129.31	120.28
1	A	212	THR	CA-C-O	-6.73	113.85	121.39
1	B	218	GLN	CA-C-O	6.73	127.42	119.28
1	A	20	SER	N-CA-C	6.73	119.41	110.53
1	B	76	LYS	N-CA-C	6.73	120.48	109.72
1	B	110	ALA	CA-C-N	-6.72	112.09	120.56
1	B	110	ALA	C-N-CA	-6.72	112.09	120.56
1	B	176	PHE	N-CA-C	6.72	121.31	113.18
1	A	492	PRO	N-CD-CG	-6.72	93.12	103.20
1	B	131	PHE	N-CA-CB	-6.72	100.52	110.53
1	A	591	ASN	CB-CA-C	6.72	122.86	110.10
1	A	448	HIS	N-CA-CB	6.71	122.67	111.53
1	B	630	ARG	CA-C-O	-6.71	110.91	120.51
1	B	388	LYS	CB-CA-C	-6.71	95.35	109.38
1	A	280	ASN	CB-CG-ND2	6.71	126.46	116.40
1	A	447	VAL	O-C-N	-6.71	112.27	123.00
1	B	345	PRO	CA-C-N	6.71	134.35	121.54
1	B	345	PRO	C-N-CA	6.71	134.35	121.54
1	A	434	ALA	N-CA-CB	-6.71	101.17	111.56
1	B	109	ALA	CA-C-O	6.71	127.66	120.55
1	A	93	THR	CA-C-N	6.70	134.33	121.54
1	A	93	THR	C-N-CA	6.70	134.33	121.54
1	A	870	SER	CA-CB-OG	6.69	124.47	111.10
1	B	240	CYS	CA-CB-SG	-6.69	99.02	114.40
1	A	134	GLY	O-C-N	6.69	131.39	122.70
1	B	123	ARG	CD-NE-CZ	-6.69	115.04	124.40
1	A	390	ARG	N-CA-CB	-6.68	99.66	110.69
1	B	375	ARG	NE-CZ-NH2	-6.68	113.19	119.20
1	A	161	LYS	CB-CG-CD	6.67	126.63	111.30
1	B	487	PRO	CA-C-N	-6.67	110.40	121.80
1	B	487	PRO	C-N-CA	-6.67	110.40	121.80
1	A	743	THR	N-CA-C	6.67	118.43	111.03
1	A	165	LEU	N-CA-C	-6.66	99.06	109.25
1	A	408	SER	N-CA-C	6.66	120.02	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	GLU	CA-CB-CG	6.66	127.41	114.10
1	B	222	SER	CA-C-O	-6.65	112.75	120.20
1	B	136	ALA	N-CA-C	6.64	126.58	113.29
1	A	455	LEU	N-CA-C	-6.64	105.25	113.15
1	B	78	PRO	CB-CG-CD	-6.64	84.86	106.10
1	B	654	ASP	CA-C-N	6.64	130.40	120.31
1	B	654	ASP	C-N-CA	6.64	130.40	120.31
1	A	429	GLU	N-CA-CB	-6.64	100.21	110.56
1	A	878	GLN	N-CA-C	6.64	119.72	108.90
1	B	71	TYR	O-C-N	6.64	130.54	123.11
1	B	143	LEU	N-CA-C	6.64	120.50	109.95
1	A	10	LYS	N-CA-C	-6.63	103.30	111.33
1	A	93	THR	N-CA-C	6.63	121.31	111.96
1	B	684	GLU	N-CA-C	6.63	124.92	110.80
1	A	175	GLU	OE1-CD-OE2	-6.63	107.00	122.90
1	A	47	GLN	CA-C-O	-6.62	113.21	120.30
1	A	756	HIS	N-CA-C	-6.62	92.45	111.00
1	B	310	TYR	CA-C-O	-6.62	111.60	119.35
1	B	640	LEU	CA-C-N	-6.62	113.12	120.14
1	B	640	LEU	C-N-CA	-6.62	113.12	120.14
1	A	92	ALA	N-CA-C	-6.61	101.62	110.55
1	B	647	VAL	CG1-CB-CG2	-6.61	96.26	110.80
1	A	780	THR	OG1-CB-CG2	-6.61	96.09	109.30
1	B	174	ASN	O-C-N	6.60	131.78	123.19
1	B	121	LEU	CD1-CG-CD2	-6.60	96.27	110.80
1	B	310	TYR	O-C-N	6.60	130.59	122.34
1	A	167	PHE	N-CA-C	6.60	124.86	110.80
1	B	512	GLU	CB-CG-CD	6.60	123.82	112.60
1	A	646	GLN	CG-CD-NE2	6.59	126.28	116.40
1	B	890	THR	N-CA-C	-6.57	104.66	114.64
1	B	117	ASN	N-CA-C	6.55	119.58	107.99
1	A	326	MET	CG-SD-CE	6.54	115.28	100.90
1	B	208	THR	CA-CB-CG2	-6.54	99.39	110.50
1	A	516	GLN	CB-CA-C	-6.53	98.49	109.53
1	B	451	ARG	CA-CB-CG	6.53	127.16	114.10
1	A	802	ILE	N-CA-C	6.53	122.91	109.34
1	A	614	ARG	CA-C-O	-6.52	113.92	120.90
1	B	125	VAL	CA-C-O	6.52	128.68	119.95
1	B	326	MET	N-CA-C	6.52	118.67	108.96
1	A	285	ARG	N-CA-C	6.51	124.67	110.80
1	B	333	ARG	CA-CB-CG	-6.51	101.08	114.10
1	B	348	LEU	N-CA-CB	6.50	121.90	112.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	120	ILE	CA-C-N	6.49	129.27	120.44
1	B	120	ILE	C-N-CA	6.49	129.27	120.44
1	B	336	THR	CA-CB-OG1	6.49	119.34	109.60
1	B	89	VAL	CA-CB-CG1	6.49	121.43	110.40
1	A	570	ARG	CA-CB-CG	6.48	127.07	114.10
1	B	34	THR	OG1-CB-CG2	-6.48	96.34	109.30
1	B	16	GLU	CB-CG-CD	6.48	123.61	112.60
1	B	476	ILE	CA-CB-CG1	6.47	121.41	110.40
1	B	501	ARG	NE-CZ-NH1	6.47	127.97	121.50
1	A	643	GLN	CB-CA-C	-6.46	100.73	110.88
1	A	820	PRO	N-CD-CG	-6.46	93.50	103.20
1	B	871	LEU	CD1-CG-CD2	-6.46	96.58	110.80
1	A	2	ALA	N-CA-C	-6.46	92.91	111.00
1	A	55	SER	CA-C-N	-6.46	109.93	120.72
1	A	55	SER	C-N-CA	-6.46	109.93	120.72
1	A	335	PHE	CA-CB-CG	-6.46	107.34	113.80
1	B	84	ASN	CB-CG-ND2	-6.46	106.71	116.40
1	B	8	LEU	CA-C-N	-6.46	109.21	121.54
1	B	8	LEU	C-N-CA	-6.46	109.21	121.54
1	A	775	VAL	CA-C-N	-6.45	112.34	122.73
1	A	775	VAL	C-N-CA	-6.45	112.34	122.73
1	B	742	ALA	N-CA-C	6.45	120.36	112.23
1	A	778	SER	N-CA-C	-6.45	103.41	113.02
1	A	310	TYR	CE1-CZ-OH	-6.44	100.57	119.90
1	B	427	ASP	CA-C-O	6.44	127.38	119.97
1	B	375	ARG	NE-CZ-NH1	6.44	127.94	121.50
1	A	242	ILE	CA-CB-CG2	6.44	121.44	110.50
1	A	884	GLN	O-C-N	-6.43	115.08	122.03
1	B	145	GLN	N-CA-CB	-6.43	100.45	110.55
1	B	388	LYS	O-C-N	6.43	131.15	123.24
1	A	123	ARG	N-CA-C	-6.42	104.54	112.38
1	B	657	LEU	CB-CG-CD2	6.42	129.97	110.70
1	B	697	LEU	CA-C-O	6.42	127.37	119.79
1	A	114	LEU	O-C-N	6.42	130.75	122.03
1	B	725	GLN	N-CA-C	-6.42	97.14	110.80
1	B	38	GLU	O-C-N	-6.41	114.74	122.11
1	B	465	HIS	N-CA-C	6.41	124.44	110.80
1	B	631	MET	CB-CA-C	6.40	121.78	112.05
1	B	598	GLU	N-CA-C	-6.40	103.44	111.11
1	B	634	GLU	CA-C-O	-6.39	113.77	120.55
1	A	181	LEU	CB-CA-C	-6.39	100.13	110.74
1	A	100	GLY	N-CA-C	6.38	128.31	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	470	ARG	CA-C-O	6.38	127.52	120.82
1	A	73	ILE	CB-CG1-CD1	6.38	127.19	113.80
1	B	596	LEU	CA-C-N	6.38	133.45	121.97
1	B	596	LEU	C-N-CA	6.38	133.45	121.97
1	B	405	SER	N-CA-C	6.37	118.58	107.49
1	B	811	SER	CB-CA-C	6.37	123.10	110.42
1	B	741	SER	CA-C-O	-6.37	114.58	121.14
1	A	277	GLN	CA-C-O	6.37	128.47	121.40
1	B	199	CYS	O-C-N	-6.37	114.82	122.65
1	A	132	GLN	CB-CA-C	-6.37	102.48	115.28
1	B	76	LYS	N-CA-CB	-6.37	100.19	111.08
1	A	640	LEU	CA-C-O	-6.37	112.71	120.54
1	A	471	GLU	CA-C-N	6.36	131.48	123.14
1	A	471	GLU	C-N-CA	6.36	131.48	123.14
1	A	502	PHE	CA-C-O	-6.36	113.49	120.30
1	A	861	LEU	CA-C-O	6.36	127.30	120.24
1	B	150	VAL	N-CA-C	6.36	117.45	108.36
1	B	883	ILE	N-CA-C	6.36	116.52	110.42
1	A	237	LEU	N-CA-CB	6.35	120.87	110.39
1	A	541	SER	CA-C-N	-6.35	112.96	123.37
1	A	541	SER	C-N-CA	-6.35	112.96	123.37
1	B	58	LEU	CA-CB-CG	6.35	138.51	116.30
1	A	32	TYR	CA-C-O	-6.34	114.34	121.00
1	A	150	VAL	N-CA-CB	-6.34	102.26	111.52
1	A	740	VAL	N-CA-CB	-6.34	102.66	111.41
1	B	36	ARG	NH1-CZ-NH2	-6.34	111.05	119.30
1	B	786	PHE	CA-C-N	6.34	128.78	120.28
1	B	786	PHE	C-N-CA	6.34	128.78	120.28
1	A	792	LEU	CB-CA-C	-6.34	98.91	110.63
1	A	97	ILE	CA-C-O	-6.34	112.86	120.78
1	A	279	VAL	N-CA-C	6.33	122.52	109.34
1	A	331	PHE	CB-CA-C	-6.33	100.08	110.85
1	A	297	TRP	CB-CA-C	6.33	123.02	110.42
1	B	237	LEU	O-C-N	-6.33	114.64	122.68
1	A	389	ILE	CA-CB-CG2	-6.33	99.74	110.50
1	B	312	ARG	CB-CG-CD	6.33	125.85	111.30
1	A	462	GLN	N-CA-C	6.33	118.68	109.07
1	B	645	HIS	N-CA-CB	6.32	120.39	110.46
1	A	350	SER	CA-C-O	-6.32	111.47	120.51
1	B	639	LYS	CA-C-O	-6.32	113.53	120.36
1	A	25	ILE	CA-C-N	6.32	131.96	122.23
1	A	25	ILE	C-N-CA	6.32	131.96	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	GLN	CA-C-N	6.32	132.68	121.75
1	B	129	GLN	C-N-CA	6.32	132.68	121.75
1	A	289	GLY	CA-C-N	-6.32	111.67	121.02
1	A	289	GLY	C-N-CA	-6.32	111.67	121.02
1	A	474	ASN	N-CA-C	6.31	118.78	109.24
1	A	124	VAL	CB-CA-C	-6.31	100.94	111.29
1	A	62	GLU	O-C-N	6.31	130.98	122.59
1	B	41	GLU	CA-CB-CG	6.31	126.72	114.10
1	B	409	PHE	CA-C-N	6.30	130.81	122.30
1	B	409	PHE	C-N-CA	6.30	130.81	122.30
1	B	415	GLN	CA-C-N	6.30	131.87	122.99
1	B	415	GLN	C-N-CA	6.30	131.87	122.99
1	A	94	ARG	N-CA-C	-6.30	97.39	110.80
1	A	639	LYS	CA-C-O	6.29	127.20	120.46
1	B	777	ASP	N-CA-CB	6.29	119.22	109.85
1	A	447	VAL	CA-CB-CG1	6.29	121.09	110.40
1	B	95	THR	OG1-CB-CG2	-6.29	96.73	109.30
1	B	582	MET	CA-C-O	6.28	129.49	120.51
1	B	601	ILE	CB-CA-C	6.28	121.59	111.29
1	A	89	VAL	CA-C-O	-6.28	112.93	120.78
1	B	228	ILE	N-CA-C	6.28	116.39	110.30
1	B	364	THR	N-CA-C	6.28	119.25	109.52
1	B	291	VAL	CG1-CB-CG2	6.27	124.60	110.80
1	B	312	ARG	O-C-N	-6.27	115.44	122.34
1	A	339	GLU	N-CA-C	6.26	119.67	109.59
1	A	743	THR	CA-C-O	6.26	127.35	120.90
1	B	879	ILE	CA-C-O	-6.26	114.74	121.19
1	A	33	GLU	O-C-N	6.25	128.59	122.09
1	A	463	SER	CA-CB-OG	6.25	123.60	111.10
1	A	111	ILE	CA-C-N	-6.25	111.91	120.28
1	A	111	ILE	C-N-CA	-6.25	111.91	120.28
1	A	345	PRO	CB-CG-CD	-6.25	86.11	106.10
1	A	6	MET	CB-CA-C	-6.24	103.48	111.22
1	B	3	GLY	O-C-N	6.24	129.54	122.62
1	A	742	ALA	CA-C-N	-6.23	112.15	120.63
1	A	742	ALA	C-N-CA	-6.23	112.15	120.63
1	B	333	ARG	CB-CA-C	6.23	120.06	109.53
1	B	397	ALA	O-C-N	-6.22	116.33	123.42
1	B	399	ASP	CB-CA-C	-6.22	101.15	110.24
1	B	341	CYS	CA-C-O	-6.22	113.60	120.69
1	A	94	ARG	CA-C-N	6.22	133.41	121.54
1	A	94	ARG	C-N-CA	6.22	133.41	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	486	VAL	CA-C-N	6.21	128.34	120.51
1	A	486	VAL	C-N-CA	6.21	128.34	120.51
1	A	290	GLU	CA-CB-CG	-6.21	101.68	114.10
1	B	783	LYS	CA-C-N	-6.21	113.19	123.37
1	B	783	LYS	C-N-CA	-6.21	113.19	123.37
1	A	110	ALA	CA-C-O	-6.20	113.97	120.55
1	A	366	ARG	CA-C-O	6.20	127.28	120.71
1	B	512	GLU	OE1-CD-OE2	-6.20	108.03	122.90
1	B	221	PRO	N-CA-C	-6.19	101.53	111.38
1	A	279	VAL	CA-C-O	-6.19	113.04	120.78
1	A	223	ASP	N-CA-C	6.18	122.23	113.02
1	A	630	ARG	CB-CA-C	6.18	121.06	110.79
1	A	856	SER	N-CA-C	-6.18	105.89	113.50
1	B	506	LYS	O-C-N	-6.18	115.64	123.24
1	A	627	TYR	N-CA-C	6.18	123.97	110.80
1	A	635	ALA	CB-CA-C	-6.18	100.18	110.68
1	A	834	ILE	N-CA-C	-6.18	96.49	109.34
1	B	789	PHE	O-C-N	6.17	130.79	122.59
1	A	386	GLN	N-CA-C	6.17	119.59	109.85
1	A	428	MET	N-CA-C	-6.16	100.87	110.17
1	B	85	PRO	CB-CA-C	-6.16	101.40	111.56
1	B	91	GLY	CA-C-O	-6.16	109.85	120.57
1	A	374	CYS	O-C-N	-6.16	114.04	122.23
1	A	808	THR	N-CA-CB	6.16	121.97	111.50
1	B	23	ARG	CA-C-O	6.16	126.31	120.09
1	B	156	ASP	CA-C-N	-6.15	114.85	122.84
1	B	156	ASP	C-N-CA	-6.15	114.85	122.84
1	B	448	HIS	N-CA-C	6.14	123.89	110.80
1	A	312	ARG	NE-CZ-NH1	-6.14	115.36	121.50
1	A	608	ASN	CA-C-O	6.14	127.44	121.00
1	B	329	ARG	CB-CG-CD	6.14	125.41	111.30
1	A	342	ASN	N-CA-C	6.13	119.35	110.28
1	B	220	ALA	CA-C-O	6.13	126.48	120.23
1	B	36	ARG	CA-C-N	-6.13	112.47	120.44
1	B	36	ARG	C-N-CA	-6.13	112.47	120.44
1	A	185	TYR	N-CA-CB	6.12	119.19	110.13
1	A	326	MET	N-CA-C	6.12	123.84	110.80
1	A	232	LEU	CB-CG-CD1	-6.12	92.34	110.70
1	A	661	PHE	CA-C-O	6.11	127.00	119.97
1	A	570	ARG	N-CA-C	-6.11	93.89	111.00
1	A	351	ARG	CA-C-N	6.11	131.09	122.05
1	A	351	ARG	C-N-CA	6.11	131.09	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	TYR	CB-CA-C	-6.11	97.43	110.32
1	B	173	GLY	CA-C-N	-6.11	113.22	122.81
1	B	173	GLY	C-N-CA	-6.11	113.22	122.81
1	A	241	SER	CA-CB-OG	-6.10	98.89	111.10
1	A	374	CYS	N-CA-C	6.10	118.77	110.35
1	A	317	VAL	CA-CB-CG2	6.10	120.76	110.40
1	A	332	ILE	CA-C-O	6.10	127.41	119.85
1	B	811	SER	CA-CB-OG	6.10	123.29	111.10
1	B	158	LEU	CB-CA-C	6.09	116.80	109.31
1	B	337	LYS	CA-CB-CG	-6.09	101.92	114.10
1	A	462	GLN	N-CA-CB	-6.09	101.49	111.66
1	A	374	CYS	CA-C-O	6.09	128.76	121.88
1	A	478	LEU	CB-CG-CD2	-6.08	92.45	110.70
1	A	238	LEU	N-CA-CB	-6.08	101.00	110.55
1	A	110	ALA	CB-CA-C	-6.08	100.69	110.79
1	B	84	ASN	CB-CA-C	6.07	120.61	111.14
1	A	618	LEU	CB-CG-CD2	6.07	128.90	110.70
1	B	297	TRP	CA-CB-CG	6.07	125.12	113.60
1	B	381	PHE	N-CA-C	-6.07	104.58	111.07
1	B	432	GLY	CA-C-O	-6.07	115.24	121.61
1	A	323	GLU	CB-CG-CD	6.06	122.90	112.60
1	B	830	LEU	N-CA-C	-6.06	97.90	110.80
1	B	424	PHE	CA-C-N	6.05	133.65	122.70
1	B	424	PHE	C-N-CA	6.05	133.65	122.70
1	B	490	PHE	CB-CA-C	-6.04	98.39	110.42
1	B	724	ARG	CD-NE-CZ	6.04	132.86	124.40
1	B	359	THR	OG1-CB-CG2	-6.04	97.21	109.30
1	A	133	GLU	CB-CG-CD	6.04	122.87	112.60
1	A	330	ASP	CA-C-N	6.04	128.87	120.29
1	A	330	ASP	C-N-CA	6.04	128.87	120.29
1	B	788	GLU	N-CA-CB	6.04	119.72	110.79
1	B	140	HIS	CA-C-O	-6.03	114.06	121.06
1	B	470	ARG	N-CA-C	-6.03	104.62	111.07
1	B	601	ILE	CG1-CB-CG2	-6.03	92.62	110.70
1	A	35	LEU	CA-C-O	6.02	127.14	120.63
1	A	329	ARG	CB-CA-C	-6.02	98.43	110.42
1	A	448	HIS	CA-C-N	6.02	129.31	120.82
1	A	448	HIS	C-N-CA	6.02	129.31	120.82
1	B	221	PRO	N-CD-CG	-6.02	94.18	103.20
1	A	58	LEU	O-C-N	6.01	130.70	122.46
1	A	616	PHE	CA-C-O	6.01	126.59	119.56
1	B	514	ASP	CB-CG-OD1	6.01	132.22	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	868	PHE	O-C-N	-6.01	114.60	122.59
1	A	60	PHE	CA-CB-CG	6.01	119.81	113.80
1	B	28	LEU	CA-C-O	6.00	127.78	120.57
1	B	320	GLU	CA-CB-CG	-6.00	102.11	114.10
1	A	143	LEU	N-CA-CB	-5.99	100.15	111.00
1	B	371	ALA	CA-C-O	-5.99	115.48	122.37
1	B	418	ARG	CA-CB-CG	5.99	126.08	114.10
1	B	740	VAL	CA-C-O	-5.99	113.30	120.78
1	B	890	THR	CA-C-N	-5.99	112.74	122.26
1	B	890	THR	C-N-CA	-5.99	112.74	122.26
1	A	677	ILE	N-CA-C	5.99	121.79	109.34
1	B	792	LEU	CA-CB-CG	-5.99	95.35	116.30
1	A	4	ILE	O-C-N	-5.98	115.10	122.57
1	A	216	ASP	N-CA-C	-5.98	97.98	108.20
1	A	736	ASP	CA-C-N	5.98	129.10	120.79
1	A	736	ASP	C-N-CA	5.98	129.10	120.79
1	B	340	ILE	CA-CB-CG1	-5.97	100.25	110.40
1	A	112	ALA	CB-CA-C	-5.97	100.89	110.79
1	B	200	THR	CA-C-O	5.97	126.25	119.27
1	B	23	ARG	CG-CD-NE	-5.96	98.88	112.00
1	A	217	LEU	N-CA-C	-5.96	98.10	110.80
1	B	461	ALA	N-CA-CB	-5.96	100.42	110.49
1	B	133	GLU	CA-C-N	5.96	133.21	121.06
1	B	133	GLU	C-N-CA	5.96	133.21	121.06
1	A	742	ALA	O-C-N	-5.96	115.25	122.22
1	A	415	GLN	O-C-N	-5.95	116.24	123.27
1	A	776	MET	CB-CG-SD	-5.95	94.86	112.70
1	B	435	VAL	CA-C-O	-5.95	112.96	120.69
1	B	601	ILE	CA-C-N	-5.95	110.41	120.58
1	B	601	ILE	C-N-CA	-5.95	110.41	120.58
1	B	82	LEU	N-CA-C	5.95	119.17	109.06
1	B	90	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	169	HIS	N-CA-CB	-5.94	101.59	111.57
1	A	375	ARG	N-CA-CB	-5.94	101.07	110.22
1	A	786	PHE	N-CA-CB	5.94	120.53	110.49
1	B	159	PRO	CA-CB-CG	-5.94	93.22	104.50
1	A	830	LEU	CB-CG-CD2	5.94	128.51	110.70
1	A	821	GLY	N-CA-C	-5.93	99.12	113.18
1	B	634	GLU	N-CA-CB	5.93	118.84	110.12
1	A	823	PHE	CA-C-N	5.93	128.22	120.28
1	A	823	PHE	C-N-CA	5.93	128.22	120.28
1	A	750	ASN	CA-C-N	5.93	132.37	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	750	ASN	C-N-CA	5.93	132.37	121.70
1	B	682	ASP	N-CA-CB	-5.92	99.83	110.37
1	A	477	ARG	CD-NE-CZ	5.92	132.69	124.40
1	A	506	LYS	CA-CB-CG	5.92	125.93	114.10
1	B	636	ALA	CA-C-O	5.92	126.87	119.12
1	A	268	ASP	N-CA-C	5.91	117.53	108.42
1	B	15	ALA	N-CA-C	5.90	123.37	110.80
1	A	354	ARG	CB-CA-C	5.90	120.86	110.36
1	A	860	ARG	CB-CG-CD	5.90	124.87	111.30
1	B	372	GLY	N-CA-C	5.90	127.16	113.18
1	A	665	VAL	N-CA-C	5.90	116.55	110.36
1	A	78	PRO	CA-C-O	-5.89	109.87	120.60
1	A	459	SER	N-CA-C	-5.89	100.39	109.76
1	A	885	GLU	CA-C-O	5.89	126.75	119.97
1	B	233	GLU	CA-C-O	5.89	125.87	119.15
1	B	95	THR	N-CA-C	5.89	119.07	109.06
1	B	349	LYS	CA-C-O	-5.89	115.04	121.87
1	B	890	THR	CA-CB-OG1	5.89	118.44	109.60
1	B	229	LEU	N-CA-C	5.89	121.08	111.37
1	A	694	ILE	CB-CA-C	5.88	120.08	112.14
1	B	23	ARG	CA-C-N	-5.88	114.40	122.93
1	B	23	ARG	C-N-CA	-5.88	114.40	122.93
1	B	89	VAL	CA-C-O	-5.88	114.33	120.51
1	A	771	SER	CA-CB-OG	-5.88	99.34	111.10
1	A	336	THR	OG1-CB-CG2	-5.88	97.55	109.30
1	A	369	SER	N-CA-C	5.88	123.32	110.80
1	A	889	LEU	N-CA-CB	-5.88	101.43	110.13
1	B	303	GLU	CB-CA-C	-5.88	98.93	110.10
1	B	484	ILE	CB-CA-C	-5.88	102.07	110.83
1	A	237	LEU	CB-CG-CD2	5.88	128.33	110.70
1	B	264	TYR	CA-C-N	-5.87	113.59	122.81
1	B	264	TYR	C-N-CA	-5.87	113.59	122.81
1	A	469	LEU	N-CA-C	5.87	117.44	108.52
1	A	165	LEU	CB-CG-CD2	5.87	128.30	110.70
1	B	233	GLU	CG-CD-OE2	-5.87	104.91	118.40
1	B	649	VAL	O-C-N	-5.87	115.24	122.57
1	A	157	LEU	N-CA-CB	-5.86	101.97	110.36
1	B	53	PRO	CB-CA-C	-5.86	103.67	112.04
1	A	624	MET	N-CA-CB	5.85	120.38	110.49
1	A	258	LEU	CA-C-O	-5.85	110.85	120.80
1	B	199	CYS	N-CA-C	-5.85	102.98	110.53
1	B	349	LYS	CB-CG-CD	-5.85	97.84	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ASP	CB-CG-OD2	-5.84	104.97	118.40
1	B	732	GLN	N-CA-C	5.84	123.24	110.80
1	B	777	ASP	N-CA-C	5.84	118.72	109.96
1	A	809	ASP	OD1-CG-OD2	-5.84	108.89	122.90
1	B	449	LEU	CA-C-O	-5.84	114.83	121.72
1	B	41	GLU	O-C-N	-5.83	115.94	122.12
1	A	147	GLY	N-CA-C	5.83	123.41	115.30
1	A	436	TYR	CA-C-N	-5.83	114.95	123.00
1	A	436	TYR	C-N-CA	-5.83	114.95	123.00
1	B	869	ARG	CB-CA-C	5.83	118.48	109.03
1	A	407	CYS	N-CA-C	-5.83	98.39	110.80
1	B	514	ASP	N-CA-C	5.83	117.00	108.14
1	A	303	GLU	CG-CD-OE2	-5.82	105.01	118.40
1	A	465	HIS	CA-CB-CG	-5.82	107.98	113.80
1	A	491	GLU	CA-C-O	5.82	126.64	120.64
1	B	436	TYR	OH-CZ-CE2	-5.82	102.44	119.90
1	A	355	ASN	O-C-N	-5.82	114.85	122.59
1	A	126	PRO	CA-C-N	5.82	131.99	121.06
1	A	126	PRO	C-N-CA	5.82	131.99	121.06
1	B	724	ARG	NE-CZ-NH2	5.82	124.43	119.20
1	B	779	ASP	CB-CG-OD2	5.82	131.78	118.40
1	A	342	ASN	CA-C-N	5.81	129.12	120.87
1	A	342	ASN	C-N-CA	5.81	129.12	120.87
1	B	314	GLN	CA-C-O	5.81	131.32	122.20
1	B	166	VAL	CA-CB-CG2	5.81	120.27	110.40
1	B	92	ALA	N-CA-CB	5.81	120.31	110.49
1	A	140	HIS	N-CA-C	5.81	119.02	109.85
1	B	328	PHE	O-C-N	5.80	128.82	122.20
1	A	645	HIS	CA-C-O	5.80	126.06	119.27
1	B	658	ILE	N-CA-CB	5.80	120.80	111.23
1	A	146	PHE	CA-C-O	-5.80	115.12	121.84
1	B	13	GLU	N-CA-C	-5.80	104.33	111.40
1	B	441	GLU	CA-C-O	5.80	128.80	120.51
1	B	770	ARG	CA-C-N	-5.79	113.38	122.65
1	B	770	ARG	C-N-CA	-5.79	113.38	122.65
1	A	640	LEU	CB-CG-CD2	5.79	128.07	110.70
1	A	553	LYS	CA-C-N	-5.79	114.64	124.31
1	A	553	LYS	C-N-CA	-5.79	114.64	124.31
1	B	312	ARG	CD-NE-CZ	5.79	132.50	124.40
1	B	729	LEU	CB-CA-C	5.79	121.94	110.42
1	A	808	THR	O-C-N	5.79	132.26	123.00
1	B	263	ALA	CB-CA-C	-5.79	98.91	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	308	ASP	CB-CG-OD1	-5.79	105.09	118.40
1	B	362	GLU	CA-C-N	-5.78	114.63	122.03
1	B	362	GLU	C-N-CA	-5.78	114.63	122.03
1	A	607	ARG	CA-C-N	5.78	128.28	120.65
1	A	607	ARG	C-N-CA	5.78	128.28	120.65
1	A	469	LEU	N-CA-CB	5.78	120.43	111.24
1	A	602	LEU	CA-C-O	5.78	127.53	120.31
1	B	629	MET	CG-SD-CE	5.77	113.60	100.90
1	A	117	ASN	N-CA-C	5.77	117.92	108.52
1	A	570	ARG	NH1-CZ-NH2	-5.77	111.80	119.30
1	A	386	GLN	CA-C-O	-5.77	114.71	121.46
1	A	473	SER	CA-C-O	-5.77	114.37	121.06
1	B	597	VAL	CB-CA-C	5.77	120.75	111.29
1	B	211	VAL	O-C-N	-5.77	116.92	122.97
1	B	462	GLN	N-CA-C	5.76	123.08	110.80
1	B	297	TRP	CA-C-N	-5.76	111.33	121.70
1	B	297	TRP	C-N-CA	-5.76	111.33	121.70
1	B	184	ALA	CB-CA-C	-5.76	101.83	110.88
1	A	115	THR	N-CA-C	5.76	123.06	110.80
1	B	554	GLU	N-CA-C	5.76	118.77	111.69
1	A	102	LEU	N-CA-CB	-5.75	100.83	110.65
1	A	392	GLU	N-CA-CB	-5.75	100.78	110.49
1	A	396	ASP	CB-CG-OD1	5.75	131.62	118.40
1	B	414	MET	O-C-N	-5.75	115.72	123.19
1	B	68	SER	CA-CB-OG	-5.74	99.61	111.10
1	B	364	THR	CA-CB-OG1	5.74	118.22	109.60
1	B	513	LEU	CB-CA-C	-5.74	101.33	110.81
1	B	621	SER	CA-CB-OG	5.74	122.59	111.10
1	B	868	PHE	CA-C-N	-5.74	112.48	122.36
1	B	868	PHE	C-N-CA	-5.74	112.48	122.36
1	B	822	ALA	CA-C-N	5.74	132.50	121.54
1	B	822	ALA	C-N-CA	5.74	132.50	121.54
1	B	95	THR	CA-C-O	5.74	127.48	120.60
1	B	330	ASP	CB-CG-OD2	5.74	131.59	118.40
1	B	521	LEU	O-C-N	5.74	126.73	121.80
1	B	233	GLU	CB-CG-CD	5.73	122.35	112.60
1	A	366	ARG	N-CA-C	5.73	118.82	109.59
1	A	438	VAL	N-CA-C	5.73	115.27	108.96
1	A	513	LEU	CB-CG-CD1	-5.73	93.50	110.70
1	B	145	GLN	O-C-N	-5.73	116.51	123.27
1	A	634	GLU	CG-CD-OE2	5.73	131.58	118.40
1	B	177	TRP	CB-CA-C	-5.73	100.94	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	619	ASP	N-CA-C	5.73	118.05	108.02
1	B	630	ARG	NE-CZ-NH1	-5.73	115.77	121.50
1	A	176	PHE	CA-C-O	-5.72	113.10	119.34
1	A	658	ILE	N-CA-CB	-5.72	102.85	112.47
1	B	414	MET	CA-C-N	-5.72	113.67	122.87
1	B	414	MET	C-N-CA	-5.72	113.67	122.87
1	A	11	ASP	N-CA-C	5.71	117.37	111.03
1	A	610	LEU	CD1-CG-CD2	5.71	123.36	110.80
1	B	579	CYS	CB-CA-C	5.71	121.19	110.63
1	B	172	GLN	CB-CG-CD	-5.71	102.90	112.60
1	A	630	ARG	CB-CG-CD	5.71	124.42	111.30
1	A	867	ALA	CA-C-O	5.70	126.47	120.42
1	B	683	PRO	CA-C-O	-5.70	110.22	120.60
1	A	200	THR	CA-C-N	-5.70	112.69	120.44
1	A	200	THR	C-N-CA	-5.70	112.69	120.44
1	A	324	PHE	CB-CA-C	-5.70	99.08	110.42
1	A	119	THR	N-CA-CB	-5.70	101.73	110.16
1	A	216	ASP	OD1-CG-OD2	-5.70	109.23	122.90
1	B	380	THR	N-CA-CB	-5.70	102.31	110.80
1	B	606	ILE	O-C-N	-5.70	116.15	121.90
1	A	297	TRP	CA-C-N	5.69	131.95	121.70
1	A	297	TRP	C-N-CA	5.69	131.95	121.70
1	A	503	PHE	CB-CA-C	-5.69	99.40	109.70
1	A	757	PRO	N-CD-CG	-5.69	94.67	103.20
1	B	397	ALA	CA-C-N	5.69	131.94	121.70
1	B	397	ALA	C-N-CA	5.69	131.94	121.70
1	A	94	ARG	CA-C-O	-5.69	112.38	120.51
1	A	236	SER	N-CA-C	5.69	118.52	110.50
1	B	183	LYS	CG-CD-CE	-5.69	98.22	111.30
1	A	810	ARG	NH1-CZ-NH2	-5.68	111.91	119.30
1	B	285	ARG	CA-C-O	-5.68	114.46	121.11
1	B	193	GLU	OE1-CD-OE2	5.68	136.53	122.90
1	B	488	SER	N-CA-C	5.68	116.89	108.60
1	A	472	VAL	CB-CA-C	-5.67	102.23	110.63
1	A	29	ASN	CB-CA-C	5.67	120.50	111.48
1	A	390	ARG	NE-CZ-NH2	-5.67	114.10	119.20
1	A	262	HIS	CA-CB-CG	5.67	119.47	113.80
1	B	468	ASN	CA-C-N	5.66	131.50	122.10
1	B	468	ASN	C-N-CA	5.66	131.50	122.10
1	B	720	SER	O-C-N	5.66	130.12	122.59
1	A	359	THR	CA-CB-OG1	5.66	118.09	109.60
1	A	671	LEU	CA-C-O	5.66	126.42	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	325	TRP	CB-CA-C	5.66	118.98	109.48
1	B	869	ARG	N-CA-C	-5.66	106.92	113.88
1	A	362	GLU	CB-CA-C	5.65	119.09	109.53
1	A	501	ARG	N-CA-C	5.65	118.68	109.24
1	B	308	ASP	CB-CA-C	5.65	120.84	110.10
1	A	349	LYS	O-C-N	5.65	130.10	122.59
1	B	151	ASP	OD1-CG-OD2	-5.65	109.35	122.90
1	B	398	ASP	N-CA-CB	-5.65	100.90	110.50
1	A	169	HIS	O-C-N	-5.65	117.64	123.29
1	B	555	LEU	CB-CA-C	-5.64	102.27	110.96
1	A	465	HIS	O-C-N	5.64	130.09	122.59
1	B	181	LEU	N-CA-C	-5.64	105.14	111.28
1	B	388	LYS	CB-CG-CD	-5.64	98.34	111.30
1	B	370	THR	N-CA-CB	-5.63	103.11	110.88
1	A	468	ASN	CA-C-O	-5.63	113.99	122.38
1	B	62	GLU	CA-C-N	5.63	132.30	121.54
1	B	62	GLU	C-N-CA	5.63	132.30	121.54
1	B	319	MET	CG-SD-CE	5.63	113.29	100.90
1	B	108	LEU	N-CA-CB	-5.63	101.55	110.22
1	B	256	LYS	CD-CE-NZ	5.63	129.91	111.90
1	A	393	GLU	N-CA-C	-5.63	102.15	110.48
1	A	57	SER	CA-C-N	-5.62	111.76	121.66
1	A	57	SER	C-N-CA	-5.62	111.76	121.66
1	B	296	PRO	N-CA-C	-5.62	100.89	112.47
1	B	168	VAL	N-CA-C	-5.62	102.28	109.30
1	B	193	GLU	CG-CD-OE1	-5.62	105.48	118.40
1	A	497	ASP	CB-CG-OD1	-5.62	105.48	118.40
1	B	673	ILE	CB-CG1-CD1	-5.62	102.01	113.80
1	B	469	LEU	N-CA-C	-5.61	100.80	108.38
1	B	359	THR	N-CA-C	-5.61	99.99	108.52
1	A	505	GLU	CG-CD-OE1	5.61	131.30	118.40
1	A	592	GLY	CA-C-N	-5.61	111.92	121.85
1	A	592	GLY	C-N-CA	-5.61	111.92	121.85
1	B	876	THR	OG1-CB-CG2	-5.61	98.09	109.30
1	A	643	GLN	O-C-N	5.60	127.84	122.07
1	B	680	GLN	CA-C-O	-5.60	114.58	120.63
1	A	335	PHE	CA-C-N	-5.60	113.21	122.39
1	A	335	PHE	C-N-CA	-5.60	113.21	122.39
1	A	711	HIS	N-CA-CB	5.60	119.95	110.49
1	B	228	ILE	CB-CA-C	-5.59	104.82	111.81
1	A	225	TYR	CB-CA-C	5.59	120.35	110.85
1	B	59	GLY	CA-C-O	-5.59	116.32	121.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	CYS	CA-CB-SG	-5.58	101.56	114.40
1	B	796	ILE	N-CA-C	-5.58	104.50	110.36
1	B	858	LEU	CB-CA-C	-5.58	100.35	109.56
1	B	84	ASN	CA-C-N	5.58	126.81	119.84
1	B	84	ASN	C-N-CA	5.58	126.81	119.84
1	B	345	PRO	CA-N-CD	-5.58	104.19	112.00
1	B	825	ALA	O-C-N	5.58	127.84	121.93
1	B	689	ILE	N-CA-C	5.58	116.61	108.53
1	A	854	PHE	N-CA-C	-5.57	104.01	112.04
1	B	95	THR	CA-CB-CG2	5.57	119.97	110.50
1	B	745	LEU	N-CA-C	-5.57	104.89	110.97
1	B	141	PHE	CA-C-N	-5.57	115.36	122.77
1	B	141	PHE	C-N-CA	-5.57	115.36	122.77
1	A	4	ILE	N-CA-C	5.57	120.93	109.34
1	B	128	GLY	N-CA-C	5.57	122.52	114.67
1	B	644	LEU	CA-CB-CG	-5.57	96.80	116.30
1	B	443	ALA	O-C-N	5.57	130.00	122.59
1	B	104	ASP	O-C-N	-5.57	115.19	122.59
1	A	773	VAL	N-CA-C	5.56	116.20	110.36
1	A	185	TYR	CA-C-O	-5.56	114.60	120.55
1	B	117	ASN	N-CA-CB	-5.56	101.24	110.47
1	B	160	THR	N-CA-CB	-5.56	101.18	111.13
1	B	672	GLU	CB-CG-CD	5.56	122.05	112.60
1	A	228	ILE	N-CA-C	-5.55	104.96	110.62
1	A	658	ILE	CB-CG1-CD1	-5.55	102.14	113.80
1	B	612	ILE	N-CA-C	-5.55	105.70	111.58
1	B	719	GLU	CA-C-N	5.55	132.15	121.54
1	B	719	GLU	C-N-CA	5.55	132.15	121.54
1	A	515	ASP	CA-C-N	5.55	129.35	121.42
1	A	515	ASP	C-N-CA	5.55	129.35	121.42
1	B	427	ASP	CA-C-N	5.55	132.14	121.54
1	B	427	ASP	C-N-CA	5.55	132.14	121.54
1	B	808	THR	CA-C-N	-5.55	110.94	121.54
1	B	808	THR	C-N-CA	-5.55	110.94	121.54
1	B	313	GLU	O-C-N	5.55	129.81	122.43
1	A	192	TYR	CB-CA-C	-5.54	99.07	110.38
1	A	758	ASP	N-CA-C	-5.54	99.00	110.80
1	B	373	GLY	CA-C-O	-5.54	116.78	122.26
1	A	122	HIS	CB-CA-C	-5.54	98.87	110.17
1	A	214	TRP	N-CA-C	5.54	117.81	109.23
1	B	167	PHE	N-CA-C	-5.54	99.01	110.80
1	B	464	GLU	CA-C-N	-5.54	110.97	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	464	GLU	C-N-CA	-5.54	110.97	121.54
1	A	132	GLN	N-CA-C	5.53	116.92	108.12
1	A	587	ASP	N-CA-C	5.53	116.94	108.42
1	B	127	TYR	CA-C-O	-5.53	115.63	121.88
1	A	356	TRP	O-C-N	-5.53	115.24	122.59
1	B	807	GLU	CA-C-O	-5.53	112.61	120.51
1	A	710	MET	O-C-N	5.52	131.84	123.00
1	A	493	ASN	N-CA-CB	-5.52	103.53	111.70
1	A	746	MET	CB-CA-C	-5.52	100.54	110.37
1	B	793	TRP	CA-CB-CG	5.52	124.09	113.60
1	B	518	GLN	CB-CA-C	-5.52	99.44	110.42
1	A	12	ARG	CD-NE-CZ	-5.52	116.67	124.40
1	A	165	LEU	CA-C-N	-5.51	115.42	122.26
1	A	165	LEU	C-N-CA	-5.51	115.42	122.26
1	A	460	ARG	NH1-CZ-NH2	5.51	126.47	119.30
1	B	628	GLU	N-CA-CB	-5.51	103.57	110.90
1	B	727	ARG	O-C-N	5.51	129.40	122.23
1	A	191	SER	N-CA-C	-5.51	101.09	108.86
1	A	28	LEU	N-CA-CB	-5.51	103.87	112.41
1	B	654	ASP	N-CA-C	5.51	122.53	110.80
1	A	594	LEU	N-CA-C	-5.50	102.66	111.02
1	B	690	GLN	CB-CG-CD	5.50	121.95	112.60
1	B	25	ILE	CA-C-N	-5.50	115.00	123.14
1	B	25	ILE	C-N-CA	-5.50	115.00	123.14
1	A	794	ASN	CA-C-N	-5.49	112.26	122.09
1	A	794	ASN	C-N-CA	-5.49	112.26	122.09
1	A	363	GLY	CA-C-O	5.49	128.15	121.61
1	A	402	SER	CA-C-N	5.49	132.03	121.54
1	A	402	SER	C-N-CA	5.49	132.03	121.54
1	A	85	PRO	CA-N-CD	-5.49	104.31	112.00
1	B	393	GLU	N-CA-C	5.49	122.49	110.80
1	A	114	LEU	CA-C-N	5.49	132.02	121.54
1	A	114	LEU	C-N-CA	5.49	132.02	121.54
1	A	490	PHE	CB-CA-C	-5.49	102.44	110.95
1	B	177	TRP	N-CA-CB	5.49	118.29	110.06
1	B	314	GLN	N-CA-CB	-5.49	104.04	110.35
1	A	822	ALA	CA-C-N	5.48	129.12	120.89
1	A	822	ALA	C-N-CA	5.48	129.12	120.89
1	B	493	ASN	CB-CA-C	5.48	121.33	110.42
1	B	852	ASP	O-C-N	5.48	129.61	121.72
1	A	35	LEU	CD1-CG-CD2	-5.48	98.75	110.80
1	A	311	GLU	N-CA-CB	5.48	118.15	109.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	650	ALA	CA-C-O	-5.48	113.33	119.79
1	B	215	TYR	N-CA-C	-5.47	99.75	109.06
1	A	578	SER	CA-C-O	5.47	126.57	120.82
1	A	379	ALA	CA-C-O	-5.47	113.92	120.10
1	A	863	ALA	CA-C-N	-5.47	111.56	121.14
1	A	863	ALA	C-N-CA	-5.47	111.56	121.14
1	A	382	TRP	CA-CB-CG	-5.47	103.22	113.60
1	B	472	VAL	CA-CB-CG1	-5.47	101.11	110.40
1	B	846	THR	CA-C-O	5.47	124.70	118.47
1	A	300	ASN	N-CA-CB	-5.46	101.21	110.50
1	A	484	ILE	CA-C-O	-5.46	114.49	120.72
1	B	512	GLU	CA-CB-CG	5.46	125.02	114.10
1	A	437	GLN	CA-CB-CG	-5.46	103.18	114.10
1	B	161	LYS	CG-CD-CE	5.46	123.86	111.30
1	A	84	ASN	CA-C-O	-5.46	112.68	120.16
1	B	343	LEU	N-CA-C	-5.46	102.40	110.48
1	A	690	GLN	N-CA-CB	-5.45	102.01	110.57
1	A	243	ASN	CA-C-N	5.45	131.51	121.70
1	A	243	ASN	C-N-CA	5.45	131.51	121.70
1	A	766	ILE	CA-C-O	-5.45	115.60	121.27
1	A	810	ARG	N-CA-CB	-5.45	101.28	110.49
1	A	653	ALA	CA-C-O	-5.45	115.55	121.87
1	A	743	THR	CA-C-N	-5.45	112.43	120.38
1	A	743	THR	C-N-CA	-5.45	112.43	120.38
1	B	586	MET	N-CA-C	5.45	122.40	110.80
1	B	62	GLU	CB-CG-CD	-5.44	103.35	112.60
1	B	472	VAL	CA-C-N	-5.44	112.76	121.58
1	B	472	VAL	C-N-CA	-5.44	112.76	121.58
1	A	746	MET	CB-CG-SD	-5.44	96.38	112.70
1	A	29	ASN	N-CA-C	5.44	119.21	112.47
1	A	319	MET	CG-SD-CE	5.44	112.86	100.90
1	A	626	ALA	N-CA-C	5.44	122.38	110.80
1	A	789	PHE	CA-C-O	-5.44	112.06	120.16
1	A	218	GLN	CB-CA-C	5.43	120.38	111.41
1	B	344	THR	N-CA-C	5.43	121.82	109.81
1	B	402	SER	CA-C-O	-5.43	115.53	121.89
1	A	749	LEU	O-C-N	5.43	129.81	122.59
1	A	258	LEU	CD1-CG-CD2	-5.43	98.85	110.80
1	B	784	LEU	N-CA-C	5.43	118.03	107.71
1	B	455	LEU	CA-C-O	5.43	126.70	121.00
1	A	621	SER	CB-CA-C	5.43	118.19	109.07
1	A	92	ALA	O-C-N	5.42	129.03	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	THR	CB-CA-C	-5.42	102.63	111.68
1	B	415	GLN	CB-CG-CD	5.42	121.82	112.60
1	B	72	GLY	N-CA-C	5.42	122.69	114.61
1	B	861	LEU	CA-C-O	5.42	126.29	120.55
1	A	85	PRO	CB-CA-C	-5.41	104.48	111.46
1	B	197	GLY	N-CA-C	5.41	122.73	115.59
1	B	238	LEU	N-CA-CB	-5.41	101.60	110.42
1	A	218	GLN	CA-C-O	-5.41	115.34	121.66
1	A	120	ILE	N-CA-CB	-5.40	102.48	110.58
1	B	52	PRO	CA-C-O	-5.40	112.73	120.56
1	B	810	ARG	N-CA-C	-5.40	99.30	110.80
1	A	339	GLU	OE1-CD-OE2	5.40	135.85	122.90
1	A	343	LEU	O-C-N	-5.39	116.31	122.89
1	B	63	LEU	CD1-CG-CD2	-5.39	98.94	110.80
1	A	127	TYR	N-CA-C	-5.39	103.78	110.41
1	B	430	THR	N-CA-C	5.39	117.51	109.59
1	B	746	MET	CA-C-O	5.39	129.96	120.80
1	B	879	ILE	N-CA-C	5.39	116.13	108.42
1	A	794	ASN	N-CA-C	-5.39	106.78	113.19
1	A	116	LEU	CB-CA-C	-5.39	101.52	110.68
1	A	350	SER	CA-C-N	5.39	131.83	121.54
1	A	350	SER	C-N-CA	5.39	131.83	121.54
1	A	643	GLN	N-CA-C	5.39	116.83	111.07
1	B	502	PHE	O-C-N	5.38	129.57	123.27
1	B	503	PHE	CA-C-O	-5.38	114.40	120.32
1	B	227	ILE	CB-CA-C	-5.38	104.99	111.88
1	A	170	SER	CA-C-N	-5.38	114.08	122.42
1	A	170	SER	C-N-CA	-5.38	114.08	122.42
1	B	519	ALA	N-CA-C	-5.38	98.61	108.02
1	B	679	LYS	N-CA-C	-5.38	105.32	111.07
1	A	340	ILE	CA-CB-CG2	5.37	119.63	110.50
1	B	694	ILE	CA-C-O	5.37	126.86	121.17
1	B	385	PRO	N-CD-CG	-5.37	95.14	103.20
1	A	820	PRO	CB-CA-C	5.37	120.30	110.10
1	B	864	MET	CA-CB-CG	-5.37	103.36	114.10
1	B	30	GLN	OE1-CD-NE2	5.37	127.97	122.60
1	A	670	ARG	NE-CZ-NH1	-5.36	116.14	121.50
1	A	478	LEU	CD1-CG-CD2	5.36	122.59	110.80
1	B	161	LYS	CD-CE-NZ	5.36	129.05	111.90
1	A	305	ASN	CB-CA-C	5.36	119.04	109.29
1	A	463	SER	O-C-N	-5.36	116.43	122.97
1	A	463	SER	N-CA-C	5.36	117.79	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	667	CYS	CA-C-N	-5.36	112.03	120.60
1	A	667	CYS	C-N-CA	-5.36	112.03	120.60
1	B	354	ARG	CA-C-N	5.36	131.41	122.73
1	B	354	ARG	C-N-CA	5.36	131.41	122.73
1	A	296	PRO	CB-CA-C	5.36	116.48	109.89
1	A	384	ASN	CA-C-N	-5.36	115.22	120.52
1	A	384	ASN	C-N-CA	-5.36	115.22	120.52
1	A	612	ILE	CB-CG1-CD1	5.36	125.05	113.80
1	B	149	TRP	N-CA-C	5.36	116.86	109.15
1	B	670	ARG	NE-CZ-NH1	5.36	126.86	121.50
1	A	768	THR	CA-CB-OG1	-5.35	101.57	109.60
1	A	55	SER	O-C-N	-5.35	115.19	122.36
1	A	883	ILE	CA-C-N	-5.35	113.35	120.63
1	A	883	ILE	C-N-CA	-5.35	113.35	120.63
1	B	208	THR	OG1-CB-CG2	-5.35	98.59	109.30
1	A	577	GLU	N-CA-C	-5.35	105.11	111.69
1	B	398	ASP	CA-C-N	-5.35	113.41	121.86
1	B	398	ASP	C-N-CA	-5.35	113.41	121.86
1	A	492	PRO	N-CA-C	5.35	120.55	111.03
1	B	693	LEU	N-CA-C	-5.35	104.69	111.11
1	A	631	MET	CG-SD-CE	-5.35	89.13	100.90
1	A	240	CYS	CA-CB-SG	-5.34	102.11	114.40
1	B	426	ARG	CA-CB-CG	5.34	124.79	114.10
1	B	449	LEU	CB-CG-CD2	5.34	126.73	110.70
1	B	69	LYS	CD-CE-NZ	5.34	129.00	111.90
1	B	134	GLY	N-CA-C	-5.34	103.48	114.16
1	B	318	LYS	CA-C-O	5.34	127.75	121.08
1	A	455	LEU	CB-CG-CD1	-5.34	94.69	110.70
1	A	649	VAL	N-CA-C	5.34	119.92	112.50
1	B	323	GLU	CG-CD-OE2	-5.34	106.13	118.40
1	B	634	GLU	N-CA-C	-5.34	105.46	111.28
1	B	310	TYR	CA-C-N	5.33	130.61	122.29
1	B	310	TYR	C-N-CA	5.33	130.61	122.29
1	B	540	PHE	N-CA-CB	5.33	119.57	110.50
1	A	471	GLU	N-CA-C	5.33	122.16	110.80
1	A	123	ARG	CA-CB-CG	5.33	124.76	114.10
1	A	236	SER	CA-C-O	-5.33	115.75	121.56
1	A	891	MET	O-C-N	-5.33	116.58	122.07
1	B	480	PRO	CA-CB-CG	-5.32	94.39	104.50
1	B	130	SER	O-C-N	-5.32	117.18	123.25
1	A	737	ASP	CA-C-N	-5.32	111.38	121.54
1	A	737	ASP	C-N-CA	-5.32	111.38	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	315	LEU	CB-CG-CD2	5.32	126.66	110.70
1	A	501	ARG	CA-C-N	-5.32	115.50	123.00
1	A	501	ARG	C-N-CA	-5.32	115.50	123.00
1	A	240	CYS	CA-C-O	5.31	127.22	121.06
1	B	73	ILE	CB-CA-C	-5.31	103.27	111.08
1	A	647	VAL	N-CA-C	5.31	118.55	111.44
1	B	881	VAL	CA-C-N	-5.31	113.07	122.20
1	B	881	VAL	C-N-CA	-5.31	113.07	122.20
1	A	45	LEU	O-C-N	5.31	129.27	123.01
1	B	333	ARG	CG-CD-NE	5.31	123.67	112.00
1	B	609	TYR	N-CA-C	-5.31	105.61	111.71
1	A	376	ASN	N-CA-CB	-5.30	101.83	110.42
1	B	98	CYS	N-CA-C	5.30	117.88	109.50
1	A	31	ASP	CA-C-O	5.30	126.08	120.36
1	A	224	LEU	O-C-N	5.30	127.74	122.12
1	A	881	VAL	O-C-N	5.30	127.58	122.97
1	B	506	LYS	CA-C-N	-5.30	113.43	120.90
1	B	506	LYS	C-N-CA	-5.30	113.43	120.90
1	A	82	LEU	N-CA-C	-5.30	99.51	110.80
1	A	711	HIS	CA-C-N	5.30	131.66	121.54
1	A	711	HIS	C-N-CA	5.30	131.66	121.54
1	A	747	ASN	CA-C-N	-5.30	112.43	121.97
1	A	747	ASN	C-N-CA	-5.30	112.43	121.97
1	B	98	CYS	CA-CB-SG	5.30	126.59	114.40
1	A	258	LEU	CB-CG-CD1	5.30	126.59	110.70
1	B	879	ILE	CA-C-N	-5.29	114.59	122.74
1	B	879	ILE	C-N-CA	-5.29	114.59	122.74
1	A	392	GLU	CB-CG-CD	-5.29	103.61	112.60
1	A	354	ARG	NE-CZ-NH1	-5.29	116.22	121.50
1	A	429	GLU	CA-CB-CG	-5.29	103.53	114.10
1	A	553	LYS	N-CA-C	-5.29	99.54	110.80
1	B	172	GLN	CA-C-N	5.29	131.77	121.41
1	B	172	GLN	C-N-CA	5.29	131.77	121.41
1	B	671	LEU	N-CA-C	5.28	117.47	111.02
1	B	230	LYS	CB-CG-CD	5.28	123.44	111.30
1	A	123	ARG	NE-CZ-NH2	-5.28	114.45	119.20
1	A	319	MET	CB-CA-C	-5.28	101.57	110.43
1	B	349	LYS	CB-CA-C	-5.28	98.86	109.68
1	B	496	GLY	CA-C-O	-5.28	116.45	121.62
1	B	779	ASP	CA-C-O	5.27	124.62	119.08
1	A	772	MET	CG-SD-CE	5.27	112.50	100.90
1	B	809	ASP	O-C-N	5.27	129.60	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	414	MET	CG-SD-CE	-5.27	89.30	100.90
1	A	114	LEU	N-CA-C	-5.27	105.92	112.93
1	B	449	LEU	CD1-CG-CD2	-5.26	99.22	110.80
1	B	771	SER	CA-CB-OG	-5.26	100.58	111.10
1	A	462	GLN	CA-C-N	-5.26	113.49	120.90
1	A	462	GLN	C-N-CA	-5.26	113.49	120.90
1	B	394	VAL	CA-C-O	-5.26	116.43	121.63
1	B	881	VAL	N-CA-CB	5.25	119.90	111.23
1	B	425	GLY	O-C-N	-5.25	116.93	122.97
1	B	497	ASP	CA-C-N	-5.25	113.78	122.39
1	B	497	ASP	C-N-CA	-5.25	113.78	122.39
1	A	15	ALA	CB-CA-C	-5.25	99.97	110.42
1	B	426	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	A	133	GLU	O-C-N	-5.25	115.61	122.59
1	B	339	GLU	CB-CG-CD	-5.25	103.68	112.60
1	B	426	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	A	138	ILE	CA-C-N	-5.24	114.58	122.81
1	A	138	ILE	C-N-CA	-5.24	114.58	122.81
1	A	669	VAL	CA-C-O	5.24	126.28	120.46
1	A	686	THR	CB-CA-C	-5.24	101.04	110.37
1	B	36	ARG	NE-CZ-NH1	5.24	126.74	121.50
1	B	211	VAL	CA-C-N	-5.24	113.64	122.29
1	B	211	VAL	C-N-CA	-5.24	113.64	122.29
1	B	701	VAL	O-C-N	5.24	129.12	122.57
1	B	580	ARG	CA-CB-CG	5.24	124.58	114.10
1	B	799	TRP	CA-C-N	5.24	127.57	120.65
1	B	799	TRP	C-N-CA	5.24	127.57	120.65
1	B	24	ALA	CA-C-O	5.24	126.26	120.71
1	A	325	TRP	CA-C-O	-5.24	114.35	120.53
1	B	339	GLU	CA-C-N	-5.23	116.20	122.90
1	B	339	GLU	C-N-CA	-5.23	116.20	122.90
1	A	132	GLN	CA-C-N	-5.23	111.55	121.54
1	A	132	GLN	C-N-CA	-5.23	111.55	121.54
1	B	596	LEU	O-C-N	5.23	130.06	122.43
1	B	649	VAL	CA-C-O	5.23	127.31	120.78
1	B	700	SER	CA-C-N	5.23	131.38	121.97
1	B	700	SER	C-N-CA	5.23	131.38	121.97
1	A	53	PRO	CA-C-O	5.22	130.11	120.60
1	A	208	THR	N-CA-C	5.22	121.33	114.75
1	B	123	ARG	NE-CZ-NH2	-5.22	114.50	119.20
1	A	614	ARG	NE-CZ-NH1	5.22	126.72	121.50
1	B	676	LYS	O-C-N	-5.22	116.20	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	508	ALA	N-CA-C	5.21	118.66	108.18
1	B	48	ASP	O-C-N	-5.21	116.78	121.31
1	B	808	THR	N-CA-C	5.21	121.90	110.80
1	B	108	LEU	CA-CB-CG	-5.21	98.07	116.30
1	A	614	ARG	N-CA-CB	5.21	117.70	109.94
1	A	851	PHE	CA-C-O	-5.21	115.01	120.63
1	B	485	VAL	CB-CA-C	-5.21	103.37	110.77
1	A	351	ARG	O-C-N	5.21	129.51	122.59
1	A	674	LEU	CA-C-O	5.21	126.35	120.00
1	A	890	THR	OG1-CB-CG2	-5.21	98.89	109.30
1	A	62	GLU	N-CA-CB	5.20	119.28	110.49
1	A	165	LEU	O-C-N	-5.20	116.62	123.02
1	A	336	THR	CA-CB-OG1	5.20	117.40	109.60
1	A	550	ILE	N-CA-C	5.20	120.16	109.34
1	B	426	ARG	CB-CA-C	-5.20	100.07	110.42
1	B	227	ILE	O-C-N	-5.20	116.74	121.94
1	B	554	GLU	CA-C-O	-5.20	114.47	120.24
1	B	607	ARG	O-C-N	5.20	127.64	122.03
1	A	296	PRO	N-CD-CG	5.20	111.00	103.20
1	A	306	LYS	CG-CD-CE	5.20	123.25	111.30
1	B	494	LYS	CB-CG-CD	5.20	123.25	111.30
1	A	603	TRP	O-C-N	5.20	128.49	122.20
1	B	388	LYS	CA-C-O	-5.19	115.03	121.11
1	B	218	GLN	CB-CA-C	5.19	119.36	110.01
1	A	373	GLY	CA-C-O	-5.19	116.55	122.78
1	B	8	LEU	CD1-CG-CD2	5.19	122.22	110.80
1	B	296	PRO	CA-C-O	5.19	130.05	120.60
1	A	333	ARG	CA-C-O	-5.19	114.95	120.40
1	B	480	PRO	N-CD-CG	5.19	110.98	103.20
1	B	42	ALA	CA-C-N	-5.18	114.17	122.10
1	B	42	ALA	C-N-CA	-5.18	114.17	122.10
1	B	404	GLU	N-CA-C	5.18	117.73	109.02
1	B	798	LYS	CG-CD-CE	5.18	123.22	111.30
1	A	105	SER	N-CA-CB	-5.18	102.29	110.06
1	B	619	ASP	N-CA-CB	5.18	118.83	110.65
1	A	601	ILE	CB-CA-C	-5.18	104.49	112.05
1	A	647	VAL	CA-CB-CG2	5.18	119.20	110.40
1	A	778	SER	O-C-N	5.18	128.72	122.20
1	A	740	VAL	N-CA-C	-5.18	100.86	108.11
1	A	294	LYS	CG-CD-CE	5.17	123.20	111.30
1	A	366	ARG	CD-NE-CZ	-5.17	117.16	124.40
1	A	801	GLY	CA-C-O	-5.17	111.57	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	THR	CA-C-N	-5.17	113.34	120.28
1	B	115	THR	C-N-CA	-5.17	113.34	120.28
1	A	63	LEU	CB-CG-CD1	-5.17	95.18	110.70
1	A	104	ASP	CA-C-O	-5.17	114.83	120.36
1	A	146	PHE	O-C-N	5.17	128.96	122.55
1	B	79	THR	CA-C-N	-5.17	112.70	122.27
1	B	79	THR	C-N-CA	-5.17	112.70	122.27
1	A	662	ASP	CB-CG-OD1	-5.17	106.52	118.40
1	B	329	ARG	CA-CB-CG	5.17	124.43	114.10
1	B	481	GLY	N-CA-C	-5.17	104.81	110.96
1	A	176	PHE	CA-CB-CG	5.16	118.96	113.80
1	A	611	THR	CB-CA-C	-5.16	99.67	109.95
1	B	158	LEU	N-CA-CB	5.16	117.85	109.90
1	B	240	CYS	N-CA-CB	-5.16	102.84	111.20
1	A	684	GLU	N-CA-C	-5.16	102.70	110.70
1	A	809	ASP	N-CA-CB	-5.16	101.77	110.49
1	B	294	LYS	N-CA-C	-5.16	102.05	110.20
1	B	607	ARG	N-CA-CB	5.16	117.46	109.98
1	A	12	ARG	CB-CG-CD	5.16	123.17	111.30
1	B	780	THR	CA-C-N	5.16	131.39	121.54
1	B	780	THR	C-N-CA	5.16	131.39	121.54
1	A	803	TYR	CE1-CZ-OH	-5.16	104.44	119.90
1	B	824	GLU	CA-C-N	5.16	130.84	121.41
1	B	824	GLU	C-N-CA	5.16	130.84	121.41
1	A	390	ARG	NH1-CZ-NH2	5.15	126.00	119.30
1	A	764	PHE	N-CA-CB	5.15	117.88	109.69
1	A	845	GLU	CB-CA-C	5.15	119.89	110.10
1	B	155	ASP	O-C-N	5.15	128.71	122.94
1	A	267	THR	N-CA-C	-5.15	106.92	114.39
1	B	124	VAL	CA-CB-CG2	5.15	119.16	110.40
1	B	464	GLU	CA-C-O	-5.15	116.04	120.88
1	A	551	SER	N-CA-C	-5.15	99.83	110.80
1	A	601	ILE	N-CA-C	-5.14	104.07	111.17
1	B	523	ASP	O-C-N	-5.14	116.79	122.86
1	A	676	LYS	CA-C-N	-5.14	112.71	121.97
1	A	676	LYS	C-N-CA	-5.14	112.71	121.97
1	B	118	GLU	CA-C-N	-5.14	112.49	120.31
1	B	118	GLU	C-N-CA	-5.14	112.49	120.31
1	A	119	THR	CA-C-O	5.14	125.87	120.42
1	B	4	ILE	CA-CB-CG1	5.14	119.14	110.40
1	B	314	GLN	N-CA-C	-5.14	104.17	110.65
1	B	659	ILE	O-C-N	-5.14	117.48	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	739	GLU	N-CA-C	-5.14	101.73	109.85
1	B	206	ASP	CA-C-O	-5.14	114.30	120.10
1	A	885	GLU	N-CA-C	-5.13	105.86	111.82
1	B	71	TYR	N-CA-C	5.13	117.91	110.42
1	B	278	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	B	612	ILE	CA-C-O	-5.13	114.77	120.46
1	A	860	ARG	NE-CZ-NH2	5.13	123.81	119.20
1	B	12	ARG	NE-CZ-NH2	-5.12	114.59	119.20
1	A	236	SER	CA-CB-OG	-5.12	100.85	111.10
1	B	643	GLN	N-CA-CB	5.12	118.42	109.72
1	A	124	VAL	N-CA-C	-5.12	98.70	109.34
1	B	583	VAL	CA-C-O	5.12	126.46	121.19
1	A	452	ASP	CB-CA-C	5.12	119.55	110.85
1	B	36	ARG	CB-CA-C	-5.12	102.25	110.74
1	B	87	PHE	N-CA-C	5.12	117.26	111.02
1	A	351	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A	487	PRO	O-C-N	-5.11	116.20	123.05
1	B	282	ILE	N-CA-C	5.11	115.64	108.17
1	B	405	SER	CA-CB-OG	-5.11	100.87	111.10
1	A	479	PRO	CA-C-O	5.11	127.97	120.56
1	A	601	ILE	CA-C-O	-5.11	115.07	120.64
1	B	882	ASN	CA-C-O	-5.11	115.88	121.14
1	B	470	ARG	CA-CB-CG	-5.11	103.89	114.10
1	A	469	LEU	CB-CA-C	-5.10	101.77	109.99
1	A	601	ILE	N-CA-CB	5.10	118.55	110.54
1	A	415	GLN	CB-CA-C	-5.10	101.83	110.19
1	A	770	ARG	O-C-N	-5.10	116.03	122.20
1	A	820	PRO	N-CA-C	5.10	124.85	112.10
1	B	200	THR	N-CA-C	-5.10	106.91	113.23
1	B	256	LYS	N-CA-C	5.10	125.28	111.00
1	B	797	LYS	N-CA-C	5.10	121.66	110.80
1	A	475	ARG	CB-CG-CD	5.10	123.03	111.30
1	B	109	ALA	N-CA-C	5.10	116.84	111.28
1	B	462	GLN	OE1-CD-NE2	5.10	127.70	122.60
1	B	447	VAL	CA-C-O	5.10	127.15	120.78
1	A	222	SER	N-CA-C	-5.09	107.35	113.21
1	B	64	GLY	N-CA-C	5.09	122.73	112.34
1	A	327	SER	N-CA-C	5.09	117.25	110.53
1	B	164	LYS	CD-CE-NZ	-5.09	95.61	111.90
1	B	25	ILE	CB-CA-C	-5.09	104.67	111.13
1	A	745	LEU	CB-CG-CD2	5.08	125.95	110.70
1	B	587	ASP	N-CA-C	5.08	125.23	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	LYS	N-CA-C	-5.08	99.34	108.48
1	A	442	LEU	CA-CB-CG	5.08	134.06	116.30
1	A	101	ALA	N-CA-C	5.07	121.60	110.80
1	A	333	ARG	CD-NE-CZ	5.07	131.50	124.40
1	A	677	ILE	O-C-N	-5.07	116.23	122.57
1	B	685	ASN	CA-CB-CG	5.07	117.67	112.60
1	A	305	ASN	CA-C-O	5.07	124.72	119.14
1	A	13	GLU	CA-C-O	5.07	127.75	120.51
1	A	793	TRP	CB-CA-C	-5.07	99.49	109.67
1	A	467	ILE	O-C-N	5.06	128.74	123.02
1	A	676	LYS	CA-C-O	-5.06	115.50	120.82
1	B	877	GLY	CA-C-N	-5.06	114.38	122.53
1	B	877	GLY	C-N-CA	-5.06	114.38	122.53
1	B	242	ILE	CB-CG1-CD1	5.06	124.42	113.80
1	B	296	PRO	N-CA-CB	-5.06	97.94	103.25
1	A	808	THR	CB-CA-C	-5.06	97.97	109.10
1	B	376	ASN	CB-CG-OD1	-5.06	110.68	120.80
1	B	625	SER	N-CA-CB	5.06	119.04	110.49
1	A	458	ALA	CA-C-N	5.05	128.73	121.50
1	A	458	ALA	C-N-CA	5.05	128.73	121.50
1	B	453	PHE	CA-CB-CG	-5.05	108.75	113.80
1	B	139	PHE	O-C-N	-5.05	117.49	123.25
1	A	448	HIS	CA-C-O	-5.05	115.77	122.44
1	B	104	ASP	CB-CA-C	5.05	120.47	110.42
1	B	112	ALA	CA-C-O	5.05	125.90	120.55
1	A	618	LEU	O-C-N	5.05	129.30	122.59
1	B	372	GLY	CA-C-N	-5.05	114.47	122.65
1	B	372	GLY	C-N-CA	-5.05	114.47	122.65
1	A	18	LEU	CB-CG-CD1	5.04	125.83	110.70
1	A	158	LEU	CA-CB-CG	-5.04	98.66	116.30
1	B	393	GLU	CA-CB-CG	5.04	124.18	114.10
1	A	142	GLN	CB-CA-C	5.04	118.82	109.70
1	A	575	SER	CA-C-N	5.03	128.65	120.60
1	A	575	SER	C-N-CA	5.03	128.65	120.60
1	B	200	THR	N-CA-CB	-5.03	102.59	110.44
1	B	694	ILE	N-CA-CB	5.03	116.44	110.55
1	B	355	ASN	CA-C-O	-5.03	114.88	120.66
1	B	697	LEU	O-C-N	-5.03	115.59	122.33
1	B	135	TYR	O-C-N	-5.03	115.90	122.59
1	A	7	LYS	CB-CA-C	-5.03	100.42	110.42
1	A	330	ASP	N-CA-C	-5.03	107.12	113.20
1	A	766	ILE	O-C-N	5.03	126.97	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	852	ASP	CA-C-O	-5.03	112.53	120.37
1	A	327	SER	N-CA-CB	-5.02	103.18	110.36
1	A	242	ILE	N-CA-CB	5.02	118.23	112.15
1	A	877	GLY	N-CA-C	5.02	120.70	114.37
1	A	884	GLN	CB-CA-C	5.02	118.73	110.95
1	B	268	ASP	N-CA-C	5.02	121.50	110.80
1	B	293	TRP	CA-C-N	-5.02	114.25	121.42
1	B	293	TRP	C-N-CA	-5.02	114.25	121.42
1	B	91	GLY	CA-C-N	5.02	131.12	121.54
1	B	91	GLY	C-N-CA	5.02	131.12	121.54
1	B	282	ILE	CA-C-N	-5.01	114.94	122.81
1	B	282	ILE	C-N-CA	-5.01	114.94	122.81
1	A	296	PRO	CB-CG-CD	-5.01	90.07	106.10
1	A	306	LYS	O-C-N	-5.01	117.14	122.85
1	A	649	VAL	CA-C-N	-5.01	112.17	120.68
1	A	649	VAL	C-N-CA	-5.01	112.17	120.68
1	A	217	LEU	CA-C-O	-5.00	113.36	120.51
1	A	692	ASP	N-CA-CB	-5.00	102.82	110.42
1	A	811	SER	N-CA-CB	-5.00	102.04	110.49
1	B	555	LEU	N-CA-CB	5.00	117.21	109.91

There are no chirality outliers.

All (84) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	ILE	Mainchain
1	A	152	VAL	Mainchain
1	A	170	SER	Peptide
1	A	176	PHE	Sidechain
1	A	212	THR	Mainchain
1	A	218	GLN	Mainchain,Peptide
1	A	236	SER	Mainchain
1	A	24	ALA	Mainchain
1	A	262	HIS	Sidechain
1	A	275	GLN	Mainchain
1	A	29	ASN	Mainchain
1	A	303	GLU	Sidechain
1	A	304	TRP	Peptide
1	A	319	MET	Mainchain
1	A	324	PHE	Mainchain
1	A	328	PHE	Mainchain,Peptide
1	A	356	TRP	Mainchain

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Mol	Chain	Res	Type	Group
1	A	371	ALA	Mainchain
1	A	386	GLN	Mainchain
1	A	402	SER	Peptide
1	A	415	GLN	Sidechain
1	A	434	ALA	Mainchain
1	A	466	PHE	Sidechain
1	A	473	SER	Mainchain
1	A	494	LYS	Mainchain
1	A	546	ASP	Peptide
1	A	549	GLU	Peptide
1	A	551	SER	Peptide
1	A	559	LEU	Peptide
1	A	570	ARG	Peptide
1	A	593	LYS	Peptide
1	A	598	GLU	Peptide
1	A	623	SER	Peptide
1	A	627	TYR	Sidechain
1	A	645	HIS	Sidechain
1	A	663	ASN	Mainchain
1	A	731	VAL	Peptide
1	A	802	ILE	Peptide
1	A	833	HIS	Peptide
1	A	834	ILE	Peptide
1	A	848	ASN	Peptide
1	A	99	GLN	Mainchain,Peptide
1	B	127	TYR	Sidechain
1	B	169	HIS	Sidechain
1	B	2	ALA	Peptide
1	B	215	TYR	Sidechain
1	B	225	TYR	Sidechain
1	B	294	LYS	Peptide
1	B	31	ASP	Sidechain
1	B	314	GLN	Mainchain
1	B	331	PHE	Sidechain
1	B	348	LEU	Peptide
1	B	38	GLU	Mainchain
1	B	398	ASP	Mainchain
1	B	399	ASP	Mainchain,Peptide
1	B	405	SER	Peptide
1	B	409	PHE	Sidechain
1	B	417	HIS	Peptide
1	B	43	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	B	450	LYS	Peptide
1	B	469	LEU	Mainchain
1	B	538	THR	Mainchain
1	B	539	LEU	Mainchain
1	B	604	ASN	Peptide
1	B	621	SER	Peptide
1	B	638	PHE	Sidechain
1	B	64	GLY	Peptide
1	B	657	LEU	Peptide
1	B	700	SER	Peptide
1	B	738	MET	Peptide
1	B	785	GLY	Peptide
1	B	801	GLY	Peptide
1	B	806	PHE	Peptide
1	B	807	GLU	Peptide
1	B	821	GLY	Peptide
1	B	832	GLN	Peptide
1	B	860	ARG	Peptide
1	B	87	PHE	Sidechain
1	B	90	ASP	Peptide
1	B	92	ALA	Peptide

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	6053	0	5616	996	3
1	B	6003	0	5477	1006	1
2	A	172	0	0	53	1
2	B	140	0	0	45	1
All	All	12368	0	11093	2002	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 86.

All (2002) 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:583:VAL:CB	1:A:583:VAL:CA	1.74	1.65
1:B:0:GLU:CA	1:B:0:GLU:CB	1.75	1.64
1:A:550:ILE:CB	1:A:550:ILE:CA	1.75	1.64
1:B:786:PHE:CA	1:B:786:PHE:CB	1.74	1.64
1:B:8:LEU:CD2	1:B:8:LEU:CG	1.76	1.63
1:A:610:LEU:CD2	1:A:610:LEU:CG	1.77	1.62
1:B:89:VAL:CA	1:B:89:VAL:CB	1.77	1.62
1:A:826:ALA:CB	1:A:826:ALA:CA	1.76	1.62
1:B:284:MET:CB	1:B:284:MET:CG	1.75	1.62
1:A:688:THR:CB	1:A:688:THR:CG2	1.78	1.62
1:B:477:ARG:CG	1:B:477:ARG:CB	1.77	1.62
1:A:218:GLN:CA	1:A:218:GLN:CB	1.75	1.61
1:B:228:ILE:CB	1:B:228:ILE:CG2	1.75	1.61
1:B:256:LYS:CB	1:B:256:LYS:CG	1.74	1.61
1:A:75:TRP:CB	1:A:75:TRP:CG	1.77	1.61
1:B:343:LEU:CD2	1:B:343:LEU:CG	1.77	1.61
1:B:777:ASP:CB	1:B:777:ASP:CA	1.77	1.61
1:B:340:ILE:CG1	1:B:340:ILE:CD1	1.75	1.60
1:A:320:GLU:CA	1:A:320:GLU:CB	1.74	1.60
1:A:332:ILE:CG1	1:A:332:ILE:CB	1.75	1.60
1:A:773:VAL:CG1	1:A:773:VAL:CB	1.77	1.60
1:B:89:VAL:CB	1:B:89:VAL:CG1	1.78	1.60
1:A:89:VAL:CB	1:A:89:VAL:CG1	1.80	1.60
1:A:333:ARG:CD	1:A:333:ARG:CG	1.78	1.60
1:B:230:LYS:CE	1:B:230:LYS:CD	1.76	1.60
1:B:553:LYS:CA	1:B:553:LYS:CB	1.76	1.60
1:A:99:GLN:CA	1:A:99:GLN:CB	1.78	1.59
1:A:242:ILE:CG1	1:A:242:ILE:CD1	1.76	1.59
1:A:831:ASN:CG	1:A:831:ASN:CB	1.75	1.59
1:B:313:GLU:CB	1:B:313:GLU:CG	1.75	1.59
1:A:200:THR:CB	1:A:200:THR:CA	1.79	1.59
1:B:88:ILE:CG1	1:B:88:ILE:CD1	1.75	1.59
1:A:200:THR:CB	1:A:200:THR:CG2	1.74	1.59
1:A:413:LEU:CG	1:A:413:LEU:CD1	1.79	1.59
1:A:864:MET:CA	1:A:864:MET:CB	1.75	1.59
1:B:470:ARG:CB	1:B:470:ARG:CG	1.74	1.59
1:A:669:VAL:CG1	1:A:669:VAL:CB	1.76	1.59
1:B:729:LEU:CD2	1:B:729:LEU:CG	1.75	1.58
1:A:366:ARG:CG	1:A:366:ARG:CD	1.77	1.58
1:B:294:LYS:CG	1:B:294:LYS:CD	1.75	1.58
1:B:335:PHE:CA	1:B:335:PHE:CB	1.74	1.58
1:B:694:ILE:CA	1:B:694:ILE:CB	1.78	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ILE:CB	1:A:340:ILE:CG2	1.76	1.57
1:B:579:CYS:CA	1:B:579:CYS:CB	1.78	1.57
1:A:478:LEU:CG	1:A:478:LEU:CD1	1.82	1.57
1:B:456:ALA:C	1:B:456:ALA:CA	1.74	1.57
1:B:120:ILE:CB	1:B:120:ILE:CG2	1.75	1.57
1:B:537:LYS:CG	1:B:537:LYS:CD	1.74	1.57
1:B:669:VAL:CA	1:B:669:VAL:CB	1.82	1.57
1:B:668:LEU:CD2	1:B:668:LEU:CG	1.74	1.57
1:B:806:PHE:CB	1:B:806:PHE:CG	1.79	1.57
1:B:333:ARG:CG	1:B:333:ARG:CD	1.78	1.56
1:B:610:LEU:CD1	1:B:610:LEU:CG	1.83	1.56
1:A:477:ARG:CG	1:A:477:ARG:CD	1.77	1.56
1:A:808:THR:CB	1:A:808:THR:CG2	1.76	1.56
1:A:73:ILE:CG1	1:A:73:ILE:CD1	1.77	1.56
1:A:772:MET:CB	1:A:772:MET:CG	1.78	1.56
1:B:348:LEU:CG	1:B:348:LEU:CD1	1.75	1.56
1:B:349:LYS:NZ	1:B:349:LYS:CE	1.68	1.56
1:A:883:ILE:CB	1:A:883:ILE:CG2	1.76	1.56
1:A:7:LYS:CD	1:A:7:LYS:CE	1.78	1.55
1:A:340:ILE:CG1	1:A:340:ILE:CD1	1.78	1.55
1:B:345:PRO:CG	1:B:345:PRO:CD	1.78	1.55
1:B:277:GLN:CB	1:B:277:GLN:CG	1.76	1.55
1:B:226:GLN:CG	1:B:226:GLN:CD	1.80	1.55
1:A:602:LEU:CG	1:A:602:LEU:CD1	1.80	1.54
1:B:90:ASP:CG	1:B:90:ASP:CB	1.77	1.54
1:B:677:ILE:CD1	1:B:677:ILE:CG1	1.75	1.54
1:B:740:VAL:CG1	1:B:740:VAL:CB	1.76	1.54
1:B:780:THR:CB	1:B:780:THR:CG2	1.79	1.54
1:B:572:ASN:C	1:B:572:ASN:CA	1.77	1.54
1:A:494:LYS:NZ	1:A:494:LYS:CE	1.68	1.54
1:B:142:GLN:CB	1:B:142:GLN:CG	1.84	1.54
1:B:164:LYS:CD	1:B:164:LYS:CG	1.80	1.54
1:B:337:LYS:HZ2	1:B:337:LYS:CB	1.05	1.54
1:B:690:GLN:CB	1:B:690:GLN:CG	1.84	1.54
1:A:883:ILE:CG1	1:A:883:ILE:CD1	1.80	1.53
1:A:227:ILE:CD1	1:A:227:ILE:CG1	1.79	1.53
1:A:428:MET:CB	1:A:428:MET:CG	1.83	1.53
1:A:317:VAL:CB	1:A:317:VAL:CA	1.84	1.53
1:A:570:ARG:CB	1:A:570:ARG:CG	1.81	1.53
1:B:494:LYS:CD	1:B:494:LYS:CE	1.77	1.53
1:B:26:LYS:CB	1:B:26:LYS:CG	1.77	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:883:ILE:CA	1:B:883:ILE:CB	1.81	1.52
1:A:388:LYS:NZ	1:A:388:LYS:CE	1.68	1.52
1:A:618:LEU:CD2	1:A:618:LEU:CG	1.82	1.52
1:A:219:LYS:CG	1:A:219:LYS:CD	1.87	1.52
1:A:174:ASN:CG	1:A:174:ASN:CB	1.78	1.51
1:A:757:PRO:CG	1:A:757:PRO:CD	1.82	1.51
1:A:452:ASP:CB	1:A:452:ASP:CG	1.82	1.51
1:A:671:LEU:CB	1:A:671:LEU:CA	1.89	1.51
1:A:26:LYS:NZ	1:A:26:LYS:CE	1.73	1.50
1:A:270:LYS:NZ	1:A:270:LYS:CE	1.73	1.50
1:B:136:ALA:N	1:B:136:ALA:CA	1.67	1.50
1:B:346:ASP:CB	1:B:346:ASP:CG	1.78	1.50
1:A:115:THR:CB	1:A:115:THR:CG2	1.87	1.50
1:A:450:LYS:NZ	1:A:450:LYS:CE	1.67	1.50
1:B:643:GLN:CD	1:B:643:GLN:CG	1.78	1.50
1:B:69:LYS:CB	1:B:69:LYS:CG	1.87	1.50
1:B:480:PRO:CG	1:B:480:PRO:CB	1.80	1.50
1:B:824:GLU:CB	1:B:824:GLU:CA	1.86	1.49
1:B:440:ARG:CG	1:B:440:ARG:CD	1.86	1.49
1:A:218:GLN:CB	1:A:218:GLN:CG	1.87	1.49
1:A:615:LYS:NZ	1:A:615:LYS:CE	1.74	1.48
1:A:639:LYS:CE	1:A:639:LYS:NZ	1.77	1.48
1:B:341:CYS:SG	1:B:341:CYS:CB	2.02	1.48
1:A:652:PHE:CE1	1:A:667:CYS:HB2	1.46	1.47
1:A:120:ILE:CG1	1:A:120:ILE:CD1	1.89	1.46
1:B:312:ARG:CG	1:B:312:ARG:CD	1.90	1.46
1:A:6:MET:CE	1:A:6:MET:SD	2.04	1.46
1:A:631:MET:SD	1:A:631:MET:CG	2.02	1.46
1:B:284:MET:CE	1:B:284:MET:SD	2.03	1.46
1:B:746:MET:CE	1:B:746:MET:SD	2.04	1.46
1:A:680:GLN:CA	1:A:680:GLN:CB	1.92	1.46
1:A:731:VAL:HG21	1:A:733:LEU:CD1	1.46	1.46
1:B:319:MET:CE	1:B:319:MET:SD	2.04	1.45
1:B:869:ARG:CB	1:B:869:ARG:CA	1.92	1.45
1:B:316:ARG:CA	1:B:316:ARG:CB	1.93	1.44
1:A:582:MET:CE	1:A:582:MET:SD	2.03	1.44
1:B:837:MET:SD	1:B:837:MET:CE	2.05	1.43
1:B:67:SER:CA	1:B:67:SER:CB	1.96	1.42
1:A:414:MET:CE	1:A:414:MET:SD	2.06	1.42
1:A:891:MET:CE	1:A:891:MET:SD	2.09	1.40
1:B:582:MET:CE	1:B:582:MET:SD	2.10	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ILE:CB	1:B:332:ILE:CG2	1.98	1.39
1:A:337:LYS:NZ	1:A:337:LYS:CE	1.85	1.38
1:A:65:PRO:CB	1:A:65:PRO:CG	1.87	1.34
1:A:731:VAL:CG2	1:A:733:LEU:HD12	1.56	1.33
1:B:631:MET:CE	1:B:631:MET:SD	2.16	1.33
1:A:6:MET:SD	1:A:6:MET:CG	2.21	1.27
1:B:6:MET:CE	1:B:6:MET:SD	2.23	1.26
1:A:428:MET:CG	1:A:428:MET:SD	2.23	1.25
1:B:469:LEU:HD12	1:B:470:ARG:N	1.49	1.24
1:B:6:MET:SD	1:B:6:MET:CG	2.26	1.23
1:B:296:PRO:HG3	2:B:946:HOH:O	1.40	1.20
1:A:258:LEU:HD22	1:A:258:LEU:C	1.67	1.19
1:B:772:MET:CE	1:B:772:MET:SD	2.32	1.18
1:A:63:LEU:HD12	1:A:70:THR:HG23	1.18	1.18
1:B:86:GLN:HG3	1:B:89:VAL:CG2	1.73	1.18
1:B:440:ARG:HG2	1:B:441:GLU:N	1.54	1.17
1:B:343:LEU:H	1:B:343:LEU:CD1	1.52	1.15
1:A:710:MET:N	2:A:1030:HOH:O	1.80	1.14
1:B:337:LYS:NZ	1:B:337:LYS:HB3	1.06	1.14
1:A:327:SER:H	1:A:329:ARG:NH1	1.46	1.12
1:B:21:HIS:HE1	1:B:123:ARG:HG2	1.10	1.11
1:A:63:LEU:HD12	1:A:70:THR:CG2	1.82	1.09
1:A:468:ASN:HB3	2:A:905:HOH:O	1.49	1.09
1:B:295:GLY:HA3	1:B:298:SER:O	1.52	1.09
1:B:330:ASP:C	1:B:330:ASP:OD1	1.90	1.09
1:A:447:VAL:HG11	2:A:926:HOH:O	1.53	1.09
1:B:651:ARG:CZ	1:B:670:ARG:NH2	2.16	1.09
1:A:631:MET:SD	1:A:631:MET:CE	2.41	1.08
1:A:698:SER:O	1:A:701:VAL:N	1.85	1.08
1:B:538:THR:HG22	1:B:539:LEU:H	1.13	1.08
1:B:69:LYS:CB	1:B:69:LYS:NZ	2.16	1.08
1:B:343:LEU:HD12	1:B:343:LEU:N	1.67	1.07
1:B:440:ARG:CG	1:B:441:GLU:H	1.67	1.07
1:B:805:ARG:N	1:B:811:SER:HG	1.49	1.07
1:B:850:ASP:O	1:B:851:PHE:CB	2.02	1.07
1:B:308:ASP:OD1	1:B:308:ASP:N	1.87	1.06
1:B:576:LEU:O	1:B:578:SER:N	1.88	1.06
1:A:75:TRP:CZ3	1:A:159:PRO:HG3	1.90	1.06
1:A:832:GLN:C	1:A:832:GLN:OE1	2.00	1.05
1:A:155:ASP:C	1:A:155:ASP:OD2	1.95	1.05
1:A:306:LYS:HG3	1:A:307:VAL:N	1.47	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:ILE:HD12	1:B:389:ILE:H	1.18	1.04
1:B:86:GLN:HG3	1:B:89:VAL:HG23	1.34	1.04
1:A:599:PHE:O	1:A:599:PHE:CD2	2.10	1.03
1:B:440:ARG:HG2	1:B:441:GLU:H	0.89	1.03
1:B:525:LYS:NZ	1:B:525:LYS:HB3	1.72	1.03
1:A:665:VAL:O	1:A:669:VAL:HG23	1.59	1.03
1:B:364:THR:OG1	1:B:646:GLN:NE2	1.92	1.02
1:A:652:PHE:CE1	1:A:667:CYS:CB	2.43	1.02
1:A:689:ILE:C	1:A:689:ILE:HD12	1.83	1.02
1:B:651:ARG:CZ	1:B:670:ARG:CZ	2.37	1.02
1:B:429:GLU:O	1:B:468:ASN:HB2	1.60	1.02
1:A:223:ASP:O	1:A:227:ILE:HD12	1.58	1.01
1:B:538:THR:O	1:B:539:LEU:HB2	1.59	1.01
1:B:69:LYS:NZ	1:B:69:LYS:HB3	1.74	1.01
1:A:596:LEU:O	2:A:995:HOH:O	1.78	1.00
1:B:740:VAL:HG12	1:B:741:SER:H	1.26	1.00
1:B:850:ASP:O	1:B:851:PHE:HB2	1.20	1.00
1:A:619:ASP:O	1:A:620:LYS:C	2.03	1.00
1:B:21:HIS:CE1	1:B:123:ARG:HG2	1.96	1.00
1:B:784:LEU:HB3	1:B:788:GLU:O	1.63	0.99
1:A:106:TRP:CH2	1:A:198:GLY:HA3	1.98	0.99
1:A:702:LEU:HD21	2:A:1036:HOH:O	1.63	0.99
1:A:731:VAL:HG11	1:A:733:LEU:HD11	1.44	0.99
1:B:651:ARG:HG3	2:B:914:HOH:O	1.61	0.99
1:B:773:VAL:HA	1:B:784:LEU:HD21	1.45	0.99
1:B:61:LYS:H	1:B:65:PRO:HD2	1.28	0.98
1:B:670:ARG:HA	1:B:673:ILE:HD12	1.42	0.98
1:A:256:LYS:CD	1:A:258:LEU:HD21	1.92	0.98
1:A:256:LYS:HD3	1:A:258:LEU:HD11	1.42	0.98
1:B:343:LEU:H	1:B:343:LEU:HD12	0.81	0.98
1:B:69:LYS:HB3	1:B:69:LYS:HZ3	1.27	0.97
1:B:525:LYS:HB3	1:B:525:LYS:HZ2	1.28	0.96
1:B:331:PHE:CD2	1:B:331:PHE:N	2.20	0.96
1:B:469:LEU:HD12	1:B:470:ARG:H	1.22	0.96
1:B:375:ARG:HH11	1:B:375:ARG:HB2	1.30	0.95
1:B:389:ILE:HD12	1:B:389:ILE:N	1.75	0.95
1:A:465:HIS:N	1:A:465:HIS:ND1	2.13	0.95
1:A:270:LYS:HB2	1:A:325:TRP:CH2	2.02	0.95
1:B:839:ILE:O	1:B:843:SER:N	2.00	0.95
1:A:270:LYS:HB2	1:A:325:TRP:HH2	1.29	0.94
1:A:77:ARG:HG2	1:A:156:ASP:OD2	1.66	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:ILE:HD11	1:B:889:LEU:HA	1.49	0.94
1:A:256:LYS:HD3	1:A:258:LEU:HD21	1.48	0.94
1:B:579:CYS:O	1:B:583:VAL:HG12	1.66	0.93
1:A:881:VAL:HG12	1:A:885:GLU:OE2	1.67	0.93
1:A:75:TRP:CH2	1:A:159:PRO:HG3	2.03	0.93
1:B:440:ARG:CG	1:B:440:ARG:HH21	1.80	0.93
1:B:585:LEU:CD2	1:B:586:MET:HE3	1.97	0.93
1:B:538:THR:O	1:B:539:LEU:CB	2.16	0.93
1:B:667:CYS:O	1:B:668:LEU:C	2.09	0.93
1:A:218:GLN:CB	1:A:218:GLN:HA	1.99	0.92
1:A:132:GLN:O	1:A:133:GLU:C	2.12	0.92
1:B:256:LYS:NZ	1:B:256:LYS:HB3	1.82	0.92
1:A:332:ILE:CG1	1:A:332:ILE:HB	1.98	0.92
1:B:740:VAL:HG21	1:B:789:PHE:HD1	1.35	0.92
1:B:89:VAL:CB	1:B:89:VAL:C	2.42	0.92
1:A:306:LYS:HG3	1:A:307:VAL:H	1.26	0.91
1:A:4:ILE:HD12	1:A:5:ALA:N	1.85	0.91
1:A:228:ILE:O	1:A:232:LEU:HD23	1.71	0.91
1:B:256:LYS:HB3	1:B:256:LYS:HZ2	1.35	0.91
1:B:795:ASN:O	1:B:799:TRP:CD1	2.23	0.91
1:A:395:ASP:H	1:A:406:GLY:HA3	1.30	0.91
1:B:337:LYS:HB3	1:B:337:LYS:HZ3	1.32	0.91
1:B:4:ILE:CD1	1:B:889:LEU:HA	2.00	0.91
1:B:790:LYS:O	1:B:791:TYR:C	2.13	0.91
1:A:30:GLN:HE22	1:A:187:LYS:NZ	1.67	0.90
1:B:390:ARG:HG2	1:B:390:ARG:HH11	1.36	0.90
1:B:88:ILE:O	1:B:88:ILE:HG23	1.69	0.90
1:B:469:LEU:HD12	1:B:469:LEU:C	1.93	0.90
1:A:13:GLU:O	1:A:16:GLU:N	2.05	0.90
1:A:336:THR:HG23	1:A:337:LYS:N	1.86	0.90
1:B:701:VAL:HG13	1:B:860:ARG:HH11	1.33	0.90
1:B:468:ASN:OD1	1:B:468:ASN:O	1.90	0.90
1:B:585:LEU:HD23	1:B:586:MET:HE3	1.51	0.90
1:B:607:ARG:HB3	1:B:607:ARG:HH21	1.37	0.90
1:A:30:GLN:HE22	1:A:187:LYS:HZ1	1.12	0.90
1:A:13:GLU:O	1:A:16:GLU:HG2	1.72	0.89
1:A:73:ILE:HD11	2:A:1032:HOH:O	1.70	0.89
1:A:267:THR:OG1	1:A:319:MET:HE1	1.73	0.89
1:A:305:ASN:HD22	1:A:306:LYS:N	1.71	0.89
1:B:343:LEU:CD2	1:B:343:LEU:CB	2.50	0.89
1:A:822:ALA:HA	1:A:825:ALA:HB3	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:GLN:CD	1:A:833:HIS:H	1.79	0.89
1:B:116:LEU:HD11	1:B:287:PRO:HG3	1.53	0.88
1:A:388:LYS:HZ1	1:A:482:GLU:CD	1.81	0.88
1:A:254:THR:N	2:A:1011:HOH:O	2.05	0.88
1:B:626:ALA:HB1	1:B:649:VAL:HG22	1.56	0.88
1:A:31:ASP:OD2	1:A:31:ASP:C	2.14	0.88
1:A:327:SER:H	1:A:329:ARG:HH11	1.21	0.87
1:A:618:LEU:CD2	1:A:618:LEU:HG	2.01	0.87
1:B:517:ILE:H	1:B:517:ILE:HD12	1.36	0.87
1:B:135:TYR:C	1:B:136:ALA:CA	2.47	0.87
1:B:438:VAL:HG22	1:B:484:ILE:CD1	2.04	0.87
1:A:389:ILE:HG22	1:A:390:ARG:N	1.88	0.87
1:B:479:PRO:O	1:B:483:TYR:OH	1.92	0.86
1:A:822:ALA:C	1:A:825:ALA:HB3	2.00	0.86
1:A:358:THR:O	1:A:359:THR:HG23	1.75	0.86
1:A:327:SER:N	1:A:329:ARG:NH1	2.22	0.86
1:B:69:LYS:CB	1:B:69:LYS:HZ2	1.86	0.86
1:A:63:LEU:CD1	1:A:70:THR:HG23	2.05	0.86
1:B:651:ARG:NH1	1:B:670:ARG:NH1	2.23	0.86
1:B:629:MET:SD	1:B:633:ILE:HD11	2.16	0.85
1:B:822:ALA:O	1:B:825:ALA:HB3	1.74	0.85
1:A:258:LEU:C	1:A:258:LEU:CD2	2.46	0.85
1:A:558:ILE:HG22	1:A:559:LEU:N	1.89	0.85
1:B:331:PHE:N	1:B:331:PHE:HD2	1.70	0.85
1:B:499:LEU:HD23	2:B:948:HOH:O	1.76	0.85
1:B:554:GLU:O	1:B:557:THR:HB	1.76	0.85
1:B:555:LEU:O	1:B:556:GLN:C	2.18	0.85
1:A:832:GLN:CD	1:A:833:HIS:N	2.34	0.85
1:B:120:ILE:CG2	1:B:120:ILE:CG1	2.54	0.85
1:A:4:ILE:HD12	1:A:4:ILE:C	1.99	0.85
1:A:853:ASN:N	1:A:853:ASN:HD22	1.73	0.85
1:A:822:ALA:CA	1:A:825:ALA:HB3	2.06	0.85
1:B:8:LEU:HD13	1:B:885:GLU:HG2	1.59	0.85
1:B:95:THR:OG1	1:B:97:ILE:HG22	1.77	0.85
1:B:658:ILE:CG2	1:B:658:ILE:O	2.25	0.84
1:A:611:THR:O	1:A:611:THR:HG22	1.75	0.84
1:B:8:LEU:O	1:B:9:ALA:C	2.17	0.84
1:B:538:THR:HG22	1:B:539:LEU:N	1.90	0.84
1:B:572:ASN:C	1:B:572:ASN:HA	2.00	0.84
1:B:670:ARG:O	1:B:674:LEU:HD22	1.77	0.84
1:B:724:ARG:HH21	1:B:724:ARG:HB2	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ALA:C	1:A:52:PRO:HD3	2.02	0.84
1:A:358:THR:HG22	1:A:359:THR:N	1.92	0.84
1:B:537:LYS:HB2	1:B:537:LYS:HZ2	1.42	0.84
1:A:99:GLN:CB	1:A:99:GLN:C	2.48	0.84
1:B:97:ILE:HD11	1:B:108:LEU:CD1	2.08	0.84
1:A:329:ARG:HD2	1:A:333:ARG:HH12	1.42	0.83
1:A:296:PRO:CG	1:A:304:TRP:HB2	2.07	0.83
1:A:296:PRO:O	1:A:297:TRP:HB2	1.79	0.83
1:A:731:VAL:CG2	1:A:733:LEU:CD1	2.34	0.83
1:A:478:LEU:CD1	1:A:478:LEU:HG	2.08	0.83
1:A:766:ILE:HD11	2:A:967:HOH:O	1.77	0.83
1:B:831:ASN:HB3	1:B:833:HIS:CB	2.08	0.83
1:A:756:HIS:CB	1:A:757:PRO:HD2	2.06	0.83
1:A:41:GLU:OE2	2:A:974:HOH:O	1.97	0.83
1:A:89:VAL:CG1	1:A:89:VAL:CG2	2.56	0.83
1:B:86:GLN:HG3	1:B:89:VAL:HG21	1.59	0.83
1:A:13:GLU:OE1	1:A:13:GLU:HA	1.77	0.82
1:A:748:ILE:HG23	1:A:749:LEU:HD22	1.61	0.82
1:B:469:LEU:CD1	1:B:470:ARG:H	1.92	0.82
1:A:301:SER:O	1:A:302:TYR:O	1.98	0.82
1:A:582:MET:HB3	1:A:602:LEU:HD11	1.62	0.82
1:B:242:ILE:HD13	1:B:243:ASN:N	1.94	0.82
1:A:519:ALA:HB2	1:A:675:PHE:CE1	2.15	0.82
1:B:296:PRO:HB3	2:B:946:HOH:O	1.79	0.82
1:B:364:THR:HG1	1:B:646:GLN:HE22	1.26	0.82
1:B:801:GLY:O	2:B:975:HOH:O	1.97	0.82
1:A:198:GLY:O	1:A:199:CYS:HB2	1.80	0.82
1:B:524:GLU:OE1	1:B:524:GLU:N	2.12	0.82
1:A:799:TRP:CH2	1:A:858:LEU:O	2.32	0.82
1:B:492:PRO:HB2	1:B:493:ASN:ND2	1.95	0.82
1:B:576:LEU:O	1:B:577:GLU:C	2.22	0.82
1:A:306:LYS:O	1:A:307:VAL:C	2.22	0.81
1:A:429:GLU:OE1	1:A:494:LYS:NZ	2.12	0.81
1:B:343:LEU:CD2	1:B:343:LEU:CD1	2.58	0.81
1:A:106:TRP:CZ2	1:A:198:GLY:HA3	2.14	0.81
1:A:366:ARG:CD	1:A:366:ARG:CB	2.58	0.81
1:A:821:GLY:HA3	2:A:1015:HOH:O	1.81	0.81
1:B:86:GLN:CG	1:B:89:VAL:CG2	2.57	0.81
1:B:223:ASP:O	1:B:227:ILE:HG13	1.80	0.81
1:B:390:ARG:HG2	1:B:390:ARG:NH1	1.91	0.81
1:B:430:THR:HA	1:B:468:ASN:HB2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:PRO:HB2	1:A:223:ASP:OD2	1.79	0.81
1:A:808:THR:CG2	1:A:808:THR:O	2.29	0.81
1:A:100:GLY:HA3	1:A:103:GLY:HA3	1.61	0.81
1:B:457:ASN:HD22	1:B:457:ASN:H	1.29	0.81
1:B:651:ARG:NH2	1:B:670:ARG:CZ	2.42	0.81
1:A:665:VAL:HG23	1:A:666:ARG:N	1.96	0.81
1:B:144:TRP:CZ2	1:B:147:GLY:HA2	2.16	0.81
1:B:440:ARG:HG2	1:B:440:ARG:HH21	1.44	0.81
1:A:350:SER:C	1:A:352:THR:H	1.88	0.81
1:A:832:GLN:OE1	1:A:832:GLN:CA	2.29	0.81
1:A:68:SER:O	1:A:69:LYS:C	2.24	0.80
1:A:825:ALA:HB2	2:A:912:HOH:O	1.80	0.80
1:A:13:GLU:C	1:A:16:GLU:HG2	2.06	0.80
1:A:256:LYS:HD2	1:A:258:LEU:HD21	1.64	0.80
1:B:80:GLU:O	1:B:81:LEU:HD23	1.82	0.80
1:B:211:VAL:HG12	1:B:341:CYS:HB2	1.64	0.80
1:B:653:ALA:O	2:B:1022:HOH:O	1.98	0.80
1:A:651:ARG:NH1	1:A:651:ARG:O	2.15	0.79
1:B:677:ILE:O	1:B:681:LEU:HG	1.83	0.79
1:B:740:VAL:HG21	1:B:789:PHE:CD1	2.17	0.79
1:A:329:ARG:NH2	1:A:329:ARG:HG2	1.96	0.79
1:A:739:GLU:N	2:A:979:HOH:O	2.05	0.79
1:B:525:LYS:NZ	1:B:525:LYS:CB	2.45	0.79
1:B:264:TYR:HE2	1:B:286:ASN:HB2	1.48	0.79
1:A:652:PHE:HE1	1:A:667:CYS:HB2	1.45	0.79
1:A:808:THR:O	1:A:808:THR:HG23	1.81	0.79
1:A:211:VAL:O	1:A:211:VAL:HG23	1.81	0.79
1:A:258:LEU:CD1	1:A:258:LEU:H	1.96	0.79
1:A:365:TRP:CZ2	1:A:488:SER:HA	2.18	0.79
1:A:217:LEU:O	1:A:220:ALA:HB2	1.83	0.79
1:A:682:ASP:OD1	1:A:685:ASN:HA	1.83	0.79
1:A:605:ARG:NH1	2:A:1034:HOH:O	2.07	0.78
1:A:13:GLU:HA	1:A:16:GLU:HG2	1.65	0.78
1:A:832:GLN:OE1	1:A:833:HIS:N	2.15	0.78
1:B:69:LYS:HZ2	1:B:69:LYS:HB2	1.46	0.78
1:B:277:GLN:CG	1:B:277:GLN:CA	2.60	0.78
1:B:576:LEU:O	1:B:579:CYS:N	2.17	0.78
1:B:89:VAL:HB	1:B:89:VAL:O	1.84	0.78
1:B:170:SER:O	1:B:172:GLN:N	2.17	0.78
1:B:136:ALA:N	1:B:136:ALA:HA	1.94	0.78
1:B:553:LYS:CB	1:B:553:LYS:HA	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:GLY:O	1:B:20:SER:OG	2.01	0.78
1:A:158:LEU:HB3	1:A:165:LEU:HD11	1.66	0.78
1:B:69:LYS:CB	1:B:69:LYS:CE	2.62	0.78
1:B:309:PRO:O	1:B:313:GLU:OE1	2.02	0.78
1:B:651:ARG:NE	1:B:670:ARG:NH2	2.32	0.78
1:A:594:LEU:O	1:A:598:GLU:OE2	2.01	0.77
1:B:313:GLU:CG	1:B:313:GLU:CA	2.62	0.77
1:A:832:GLN:N	2:A:919:HOH:O	2.16	0.77
1:B:323:GLU:HA	1:B:323:GLU:OE2	1.84	0.77
1:B:439:PRO:HB2	1:B:440:ARG:HD3	1.65	0.77
1:A:493:ASN:ND2	1:A:627:TYR:OH	2.18	0.77
1:B:601:ILE:HD12	2:B:987:HOH:O	1.82	0.77
1:A:373:GLY:HA3	1:A:492:PRO:HG3	1.65	0.77
1:A:808:THR:CG2	1:A:808:THR:C	2.57	0.77
1:B:25:ILE:CD1	1:B:148:GLU:OE1	2.32	0.77
1:B:8:LEU:CD2	1:B:8:LEU:HG	2.10	0.77
1:B:61:LYS:HG3	1:B:65:PRO:O	1.84	0.77
1:A:13:GLU:CA	1:A:16:GLU:HG2	2.15	0.77
1:A:386:GLN:HB3	1:A:513:LEU:HB3	1.67	0.77
1:B:61:LYS:HG3	1:B:66:ASN:HB2	1.65	0.77
1:B:701:VAL:CG1	1:B:860:ARG:HG2	2.15	0.77
1:A:122:HIS:HA	1:A:125:VAL:O	1.84	0.77
1:A:822:ALA:HA	1:A:825:ALA:CB	2.14	0.77
1:B:601:ILE:HD13	1:B:604:ASN:ND2	1.99	0.77
1:B:202:GLU:CB	1:B:470:ARG:HH11	1.98	0.77
1:B:328:PHE:O	1:B:331:PHE:CE2	2.38	0.77
1:B:556:GLN:O	1:B:557:THR:C	2.29	0.76
1:B:361:TYR:O	1:B:499:LEU:HA	1.85	0.76
1:B:796:ILE:O	1:B:799:TRP:HB2	1.85	0.76
1:B:161:LYS:O	1:B:163:GLY:N	2.18	0.76
1:B:795:ASN:O	1:B:799:TRP:CG	2.38	0.76
1:B:86:GLN:CG	1:B:89:VAL:HG23	2.14	0.76
1:B:430:THR:HA	1:B:468:ASN:CB	2.14	0.76
1:B:740:VAL:CG1	1:B:741:SER:H	1.98	0.76
1:A:89:VAL:H	1:A:175:GLU:CD	1.93	0.76
1:A:114:LEU:HD13	1:A:121:LEU:HD23	1.67	0.76
1:A:314:GLN:HG3	1:A:315:LEU:N	1.99	0.76
1:B:537:LYS:NZ	1:B:537:LYS:CB	2.48	0.76
1:A:293:TRP:O	1:A:295:GLY:N	2.18	0.76
1:B:106:TRP:CZ3	1:B:107:LEU:HD12	2.21	0.76
1:B:607:ARG:HH21	1:B:607:ARG:CB	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LEU:C	1:A:158:LEU:HG	2.11	0.75
1:B:35:LEU:HD13	1:B:46:PHE:CE1	2.21	0.75
1:A:599:PHE:CD2	1:A:599:PHE:C	2.64	0.75
1:B:348:LEU:CD1	1:B:348:LEU:CD2	2.64	0.75
1:B:778:SER:C	1:B:779:ASP:OD1	2.29	0.75
1:A:333:ARG:O	1:A:334:GLU:HB2	1.86	0.75
1:A:84:ASN:O	1:A:84:ASN:OD1	2.03	0.75
1:A:290:GLU:CD	1:A:290:GLU:H	1.92	0.75
1:B:470:ARG:CG	1:B:470:ARG:CA	2.64	0.75
1:B:729:LEU:CD2	1:B:729:LEU:CD1	2.63	0.75
1:A:205:GLU:HG2	1:A:210:GLY:O	1.85	0.75
1:A:731:VAL:HG21	1:A:733:LEU:CG	2.15	0.75
1:B:294:LYS:CD	1:B:294:LYS:CB	2.65	0.75
1:A:75:TRP:CZ3	1:A:159:PRO:CG	2.68	0.75
1:A:329:ARG:NH2	1:A:329:ARG:CG	2.48	0.75
1:A:284:MET:HE2	1:A:326:MET:SD	2.27	0.75
1:A:306:LYS:CG	1:A:307:VAL:N	2.40	0.75
1:B:25:ILE:HD11	1:B:148:GLU:OE1	1.87	0.75
1:B:874:ASN:O	1:B:875:GLY:C	2.30	0.74
1:A:655:ASP:HB2	1:A:656:GLU:OE1	1.87	0.74
1:B:98:CYS:SG	1:B:171:ALA:HB2	2.28	0.74
1:A:296:PRO:HG2	1:A:304:TRP:HB2	1.70	0.74
1:A:411:LEU:HD11	1:A:485:VAL:HG21	1.69	0.74
1:A:833:HIS:C	1:A:833:HIS:CD2	2.64	0.74
1:B:376:ASN:C	1:B:378:PRO:HD3	2.12	0.74
1:B:820:PRO:HB2	1:B:822:ALA:H	1.51	0.74
1:A:44:ALA:HA	2:A:966:HOH:O	1.87	0.74
1:A:317:VAL:CA	1:A:317:VAL:HB	2.15	0.74
1:A:300:ASN:N	1:A:300:ASN:ND2	2.36	0.74
1:A:326:MET:SD	1:A:330:ASP:HB2	2.28	0.74
1:B:212:THR:CB	1:B:340:ILE:HD13	2.17	0.74
1:A:329:ARG:CG	1:A:329:ARG:O	2.36	0.74
1:B:457:ASN:H	1:B:457:ASN:ND2	1.86	0.74
1:B:466:PHE:CD2	1:B:490:PHE:HD1	2.05	0.74
1:A:652:PHE:CD1	1:A:667:CYS:HB2	2.23	0.73
1:B:88:ILE:HD11	1:B:121:LEU:HD21	1.70	0.73
1:B:97:ILE:HD11	1:B:108:LEU:HD11	1.70	0.73
1:A:551:SER:C	1:A:552:VAL:O	2.32	0.73
1:A:821:GLY:CA	2:A:1015:HOH:O	2.37	0.73
1:B:802:ILE:CG2	1:B:802:ILE:O	2.35	0.73
1:B:228:ILE:CG2	1:B:228:ILE:CG1	2.65	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ARG:HD2	1:A:333:ARG:NH1	2.04	0.73
1:B:469:LEU:CD1	1:B:470:ARG:N	2.40	0.73
1:A:307:VAL:HA	2:A:909:HOH:O	1.88	0.73
1:A:395:ASP:N	1:A:406:GLY:HA3	2.03	0.73
1:A:610:LEU:CD2	1:A:610:LEU:CB	2.65	0.73
1:A:652:PHE:CZ	1:A:667:CYS:HB2	2.17	0.73
1:B:204:PHE:HB3	1:B:340:ILE:HG13	1.69	0.73
1:A:731:VAL:HG11	1:A:733:LEU:CD1	2.19	0.73
1:A:692:ASP:OD1	1:A:692:ASP:C	2.32	0.73
1:B:106:TRP:CZ3	1:B:107:LEU:CD1	2.72	0.73
1:B:88:ILE:CD1	1:B:88:ILE:CB	2.66	0.73
1:A:293:TRP:NE1	2:A:1024:HOH:O	2.21	0.72
1:A:380:THR:O	1:A:382:TRP:N	2.22	0.72
1:A:517:ILE:HD12	1:A:883:ILE:HG23	1.71	0.72
1:A:74:LYS:O	1:A:160:THR:OG1	2.07	0.72
1:A:228:ILE:HG12	1:A:337:LYS:NZ	2.04	0.72
1:A:731:VAL:HG23	1:A:733:LEU:H	1.55	0.72
1:B:61:LYS:N	1:B:65:PRO:HD2	2.04	0.72
1:A:230:LYS:NZ	1:A:233:GLU:OE1	2.22	0.72
1:B:383:VAL:O	1:B:383:VAL:CG1	2.37	0.72
1:B:585:LEU:CG	1:B:586:MET:HE3	2.18	0.72
1:B:656:GLU:C	1:B:657:LEU:HG	2.14	0.72
1:A:602:LEU:CD1	1:A:602:LEU:CD2	2.67	0.72
1:B:27:TYR:CE2	1:B:28:LEU:HD12	2.25	0.72
1:B:438:VAL:HG22	1:B:484:ILE:HD11	1.71	0.72
1:A:158:LEU:O	1:A:160:THR:HG23	1.90	0.72
1:B:777:ASP:CB	1:B:777:ASP:C	2.63	0.72
1:B:670:ARG:O	1:B:674:LEU:CD2	2.37	0.71
1:B:330:ASP:OD1	1:B:330:ASP:O	2.08	0.71
1:B:120:ILE:CG2	1:B:120:ILE:CA	2.65	0.71
1:B:332:ILE:CG2	1:B:332:ILE:C	2.63	0.71
1:B:447:VAL:CB	1:B:513:LEU:CD1	2.69	0.71
1:B:521:LEU:HD11	1:B:638:PHE:CZ	2.26	0.71
1:B:729:LEU:CD2	1:B:729:LEU:HG	2.12	0.71
1:A:228:ILE:HG12	1:A:337:LYS:HZ1	1.56	0.71
1:A:414:MET:HB2	2:A:901:HOH:O	1.89	0.71
1:B:49:PRO:HG2	2:B:935:HOH:O	1.89	0.71
1:A:610:LEU:CD2	1:A:610:LEU:HG	2.13	0.71
1:B:874:ASN:O	1:B:876:THR:N	2.24	0.71
1:A:519:ALA:HB2	1:A:675:PHE:CZ	2.24	0.71
1:A:883:ILE:CG2	1:A:883:ILE:CG1	2.66	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:GLU:N	1:B:339:GLU:OE2	2.22	0.71
1:A:826:ALA:CB	1:A:826:ALA:C	2.63	0.71
1:A:97:ILE:HD13	1:A:108:LEU:HD12	1.72	0.71
1:A:335:PHE:CD1	1:A:335:PHE:C	2.69	0.71
1:A:756:HIS:CG	1:A:757:PRO:HD2	2.26	0.71
1:B:443:ALA:HB3	2:B:894:HOH:O	1.89	0.71
1:A:158:LEU:CB	1:A:165:LEU:HD11	2.21	0.71
1:A:611:THR:O	1:A:611:THR:CG2	2.38	0.71
1:B:238:LEU:N	1:B:238:LEU:HD12	2.06	0.71
1:B:390:ARG:HD2	1:B:482:GLU:HG2	1.72	0.71
1:B:538:THR:CG2	1:B:539:LEU:H	1.98	0.71
1:B:810:ARG:O	1:B:811:SER:HB2	1.91	0.71
1:A:31:ASP:OD2	1:A:32:TYR:N	2.24	0.70
1:B:607:ARG:O	1:B:610:LEU:HG	1.91	0.70
1:A:96:ASP:HB2	1:A:171:ALA:H	1.55	0.70
1:B:537:LYS:CG	1:B:537:LYS:CE	2.69	0.70
1:A:242:ILE:O	1:A:242:ILE:HG13	1.90	0.70
1:A:199:CYS:SG	1:A:202:GLU:HG3	2.31	0.70
1:A:105:SER:O	1:A:106:TRP:C	2.28	0.70
1:A:860:ARG:HD2	2:A:1023:HOH:O	1.90	0.70
1:B:784:LEU:N	1:B:784:LEU:HD12	2.07	0.70
1:B:836:SER:OG	2:B:953:HOH:O	2.07	0.70
1:A:428:MET:CE	2:A:970:HOH:O	2.38	0.70
1:A:808:THR:CG2	1:A:808:THR:CA	2.70	0.70
1:B:146:PHE:HB3	1:B:416:LYS:HG2	1.72	0.70
1:B:429:GLU:C	1:B:468:ASN:HD22	1.99	0.70
1:B:525:LYS:HB3	1:B:525:LYS:HZ3	1.57	0.70
1:B:661:PHE:O	1:B:665:VAL:HG13	1.92	0.70
1:B:697:LEU:HA	1:B:700:SER:OG	1.92	0.70
1:A:336:THR:CG2	1:A:337:LYS:N	2.55	0.70
1:A:350:SER:O	1:A:352:THR:CG2	2.40	0.70
1:B:89:VAL:CG1	1:B:89:VAL:HB	2.14	0.70
1:B:264:TYR:CE2	1:B:286:ASN:HB2	2.26	0.70
1:B:318:LYS:O	1:B:320:GLU:N	2.25	0.70
1:B:740:VAL:HG12	1:B:741:SER:N	2.06	0.70
1:A:467:ILE:HG22	1:A:468:ASN:H	1.56	0.69
1:B:296:PRO:HD2	2:B:912:HOH:O	1.91	0.69
1:B:430:THR:O	1:B:489:THR:HA	1.92	0.69
1:A:301:SER:O	1:A:302:TYR:C	2.36	0.69
1:A:364:THR:HG22	1:A:497:ASP:OD1	1.92	0.69
1:B:537:LYS:CD	1:B:537:LYS:CB	2.69	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:ARG:HG2	1:B:605:ARG:HH21	1.56	0.69
1:B:656:GLU:HA	1:B:656:GLU:OE2	1.89	0.69
1:B:123:ARG:NH1	1:B:346:ASP:OD1	2.25	0.69
1:A:224:LEU:HD22	1:A:228:ILE:HG13	1.73	0.69
1:A:296:PRO:HB3	2:A:962:HOH:O	1.92	0.69
1:A:372:GLY:O	1:A:380:THR:OG1	2.05	0.69
1:B:389:ILE:HG23	1:B:510:THR:HG22	1.74	0.69
1:A:59:GLY:HA3	1:A:193:GLU:CD	2.18	0.69
1:A:451:ARG:HG2	1:A:451:ARG:HH11	1.57	0.69
1:B:86:GLN:CG	1:B:89:VAL:HG21	2.21	0.69
1:B:517:ILE:H	1:B:517:ILE:CD1	2.02	0.69
1:B:601:ILE:HA	1:B:604:ASN:HD22	1.55	0.69
1:A:155:ASP:OD2	1:A:157:LEU:N	2.20	0.69
1:A:309:PRO:HA	2:A:949:HOH:O	1.92	0.69
1:B:291:VAL:CG2	1:B:292:GLU:H	2.05	0.69
1:A:578:SER:O	1:A:582:MET:HG3	1.93	0.69
1:B:135:TYR:O	1:B:136:ALA:HB3	1.93	0.69
1:B:256:LYS:CG	1:B:256:LYS:CA	2.70	0.69
1:A:688:THR:CG2	1:A:688:THR:CA	2.68	0.69
1:B:337:LYS:CB	1:B:337:LYS:NZ	1.90	0.69
1:B:429:GLU:C	1:B:468:ASN:HB2	2.17	0.69
1:A:329:ARG:CG	1:A:329:ARG:HH21	2.05	0.68
1:B:605:ARG:NH2	1:B:672:GLU:OE2	2.26	0.68
1:B:651:ARG:HD2	1:B:893:SER:OXT	1.94	0.68
1:B:172:GLN:OE1	1:B:172:GLN:HA	1.93	0.68
1:A:320:GLU:CB	1:A:320:GLU:N	2.54	0.68
1:A:373:GLY:O	1:A:384:ASN:ND2	2.26	0.68
1:B:62:GLU:HB3	1:B:193:GLU:OE1	1.92	0.68
1:A:780:THR:O	1:A:780:THR:HG22	1.93	0.68
1:B:376:ASN:O	1:B:378:PRO:HD3	1.93	0.68
1:A:731:VAL:CG1	1:A:733:LEU:HD11	2.21	0.68
1:B:424:PHE:CZ	1:B:711:HIS:HA	2.29	0.68
1:B:224:LEU:O	1:B:224:LEU:HD22	1.94	0.68
1:A:614:ARG:HH12	1:A:620:LYS:HB3	1.59	0.68
1:B:202:GLU:CB	1:B:470:ARG:NH1	2.57	0.68
1:B:369:SER:O	1:B:383:VAL:CG1	2.42	0.68
1:B:745:LEU:HD23	1:B:769:CYS:HB3	1.74	0.68
1:A:13:GLU:OE1	1:A:13:GLU:CA	2.41	0.67
1:A:477:ARG:CD	1:A:477:ARG:CB	2.70	0.67
1:B:270:LYS:O	1:B:281:LEU:HB2	1.94	0.67
1:B:802:ILE:O	1:B:802:ILE:HG22	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:VAL:CB	1:A:583:VAL:C	2.66	0.67
1:B:296:PRO:CB	2:B:946:HOH:O	2.30	0.67
1:B:492:PRO:CB	1:B:493:ASN:ND2	2.57	0.67
1:B:881:VAL:HG23	1:B:882:ASN:N	2.06	0.67
1:A:665:VAL:O	1:A:666:ARG:C	2.34	0.67
1:B:106:TRP:HZ3	1:B:107:LEU:HD12	1.59	0.67
1:B:582:MET:SD	1:B:606:ILE:HD11	2.33	0.67
1:A:413:LEU:CD1	1:A:413:LEU:CB	2.72	0.67
1:B:341:CYS:SG	1:B:341:CYS:CA	2.82	0.67
1:A:32:TYR:HE1	1:A:138:ILE:O	1.77	0.67
1:A:47:GLN:OE1	1:A:47:GLN:HA	1.95	0.67
1:B:784:LEU:O	1:B:785:GLY:O	2.12	0.67
1:B:838:ILE:HG23	1:B:839:ILE:N	2.10	0.67
1:A:185:TYR:OH	1:A:206:ASP:OD2	2.11	0.67
1:A:631:MET:SD	1:A:631:MET:CB	2.83	0.67
1:A:756:HIS:CD2	1:A:757:PRO:HD2	2.30	0.67
1:B:23:ARG:HG2	1:B:23:ARG:NH1	2.10	0.67
1:B:343:LEU:HB2	1:B:345:PRO:HD2	1.75	0.67
1:A:832:GLN:OE1	1:A:832:GLN:HA	1.95	0.67
1:A:283:ARG:NH1	1:A:319:MET:HB2	2.09	0.67
1:A:629:MET:HG2	1:A:659:ILE:HD12	1.75	0.67
1:B:97:ILE:HD11	1:B:108:LEU:HD12	1.77	0.67
1:B:212:THR:OG1	1:B:340:ILE:HD13	1.95	0.67
1:B:223:ASP:C	1:B:223:ASP:OD2	2.29	0.67
1:A:440:ARG:HG2	1:A:441:GLU:N	2.09	0.66
1:B:25:ILE:HG22	1:B:26:LYS:N	2.10	0.66
1:B:883:ILE:CB	1:B:883:ILE:C	2.63	0.66
1:A:219:LYS:CD	1:A:219:LYS:HA	2.26	0.66
1:A:350:SER:O	1:A:352:THR:HG22	1.93	0.66
1:A:514:ASP:OD1	1:A:515:ASP:N	2.28	0.66
1:B:51:PHE:CE1	1:B:187:LYS:HA	2.30	0.66
1:B:295:GLY:CA	1:B:298:SER:O	2.37	0.66
1:B:524:GLU:N	1:B:524:GLU:CD	2.53	0.66
1:B:552:VAL:O	1:B:555:LEU:N	2.29	0.66
1:B:724:ARG:HB3	2:B:1002:HOH:O	1.94	0.66
1:A:293:TRP:CZ2	2:A:1024:HOH:O	2.46	0.66
1:B:98:CYS:SG	1:B:169:HIS:NE2	2.69	0.66
1:A:213:GLU:OE1	1:A:475:ARG:NH2	2.28	0.66
1:A:748:ILE:HG23	1:A:749:LEU:CD2	2.25	0.66
1:A:273:THR:H	1:A:312:ARG:HH21	1.42	0.66
1:A:551:SER:O	1:A:552:VAL:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:MET:O	1:A:630:ARG:C	2.38	0.66
1:B:308:ASP:OD1	2:B:907:HOH:O	2.13	0.66
1:B:446:PRO:HG2	2:B:894:HOH:O	1.96	0.66
1:B:792:LEU:HG	1:B:792:LEU:O	1.95	0.66
1:A:35:LEU:O	1:A:36:ARG:C	2.36	0.66
1:A:620:LYS:HE2	2:A:1022:HOH:O	1.94	0.66
1:A:628:GLU:OE1	1:A:631:MET:SD	2.54	0.66
1:A:855:ILE:CG2	1:A:855:ILE:O	2.42	0.66
1:B:98:CYS:SG	1:B:169:HIS:CE1	2.89	0.66
1:B:284:MET:CB	1:B:284:MET:SD	2.82	0.66
1:B:411:LEU:HD13	1:B:502:PHE:CE1	2.31	0.66
1:A:833:HIS:C	1:A:833:HIS:HD2	2.03	0.66
1:B:161:LYS:O	1:B:162:ASP:C	2.36	0.66
1:A:205:GLU:OE1	1:A:471:GLU:OE2	2.13	0.66
1:A:333:ARG:CD	1:A:333:ARG:CB	2.73	0.66
1:A:739:GLU:O	1:A:739:GLU:CD	2.38	0.66
1:B:291:VAL:HG23	1:B:292:GLU:N	2.11	0.66
1:B:283:ARG:HH21	1:B:325:TRP:HE1	1.44	0.66
1:B:284:MET:O	1:B:323:GLU:OE2	2.13	0.66
1:B:237:LEU:HD23	1:B:237:LEU:N	2.11	0.65
1:B:613:PHE:CE1	1:B:624:MET:HG2	2.30	0.65
1:A:219:LYS:HA	1:A:219:LYS:HD3	1.78	0.65
1:A:514:ASP:OD2	1:A:642:CYS:N	2.24	0.65
1:A:193:GLU:C	1:A:195:LEU:H	2.05	0.65
1:A:330:ASP:OD2	2:A:921:HOH:O	2.14	0.65
1:B:365:TRP:O	1:B:495:GLU:HA	1.97	0.65
1:B:883:ILE:HG22	2:B:929:HOH:O	1.95	0.65
1:B:27:TYR:CD2	1:B:28:LEU:HD12	2.31	0.65
1:B:585:LEU:HG	1:B:586:MET:HE3	1.79	0.65
1:B:723:GLU:C	1:B:726:PHE:HD2	2.04	0.65
1:B:215:TYR:HB2	1:B:337:LYS:NZ	2.12	0.65
1:B:658:ILE:O	1:B:658:ILE:HG22	1.96	0.65
1:A:51:PHE:CG	1:A:187:LYS:HG3	2.32	0.65
1:A:403:ARG:HG2	1:A:477:ARG:CZ	2.27	0.65
1:B:701:VAL:HG13	1:B:860:ARG:CG	2.26	0.65
1:B:712:TYR:O	1:B:713:SER:O	2.15	0.65
1:A:273:THR:H	1:A:312:ARG:HD2	1.62	0.64
1:A:291:VAL:HG23	1:A:292:GLU:N	2.11	0.64
1:B:862:ASP:OD1	1:B:866:ARG:NE	2.31	0.64
1:A:229:LEU:O	1:A:231:ALA:N	2.29	0.64
1:A:430:THR:HA	1:A:467:ILE:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:GLY:O	1:A:574:PHE:O	2.16	0.64
1:A:669:VAL:CG1	1:A:669:VAL:CA	2.73	0.64
1:A:731:VAL:HG23	1:A:733:LEU:N	2.11	0.64
1:A:358:THR:O	1:A:359:THR:CG2	2.45	0.64
1:B:430:THR:OG1	1:B:468:ASN:HB3	1.98	0.64
1:B:487:PRO:O	1:B:488:SER:HB3	1.96	0.64
1:A:135:TYR:CG	1:A:136:ALA:N	2.62	0.64
1:A:329:ARG:O	1:A:329:ARG:HG3	1.98	0.64
1:A:599:PHE:O	1:A:599:PHE:HD2	1.80	0.64
1:A:689:ILE:HD12	1:A:690:GLN:N	2.13	0.64
1:A:803:TYR:HA	1:A:822:ALA:HB2	1.79	0.64
1:B:291:VAL:CG2	1:B:292:GLU:N	2.58	0.64
1:B:424:PHE:HA	1:B:426:ARG:HH21	1.63	0.64
1:B:0:GLU:CB	1:B:0:GLU:C	2.68	0.64
1:A:86:GLN:HB3	1:A:89:VAL:CG2	2.28	0.64
1:A:290:GLU:CD	1:A:290:GLU:N	2.55	0.64
1:A:337:LYS:NZ	1:A:337:LYS:CD	2.59	0.64
1:B:839:ILE:HD12	1:B:840:ARG:CB	2.28	0.64
1:A:13:GLU:O	1:A:16:GLU:CG	2.44	0.64
1:A:83:SER:O	1:A:84:ASN:HB3	1.96	0.64
1:A:256:LYS:HD3	1:A:258:LEU:CD1	2.22	0.64
1:A:414:MET:CB	2:A:901:HOH:O	2.46	0.64
1:B:4:ILE:HD13	1:B:889:LEU:HA	1.80	0.64
1:B:343:LEU:HD22	2:B:990:HOH:O	1.96	0.64
1:A:27:TYR:CD2	1:A:28:LEU:HG	2.32	0.64
1:A:314:GLN:HG3	1:A:315:LEU:H	1.63	0.64
1:A:389:ILE:HD11	1:A:502:PHE:HE2	1.62	0.64
1:A:435:VAL:CG1	1:A:461:ALA:HB3	2.28	0.64
1:B:296:PRO:CD	2:B:912:HOH:O	2.46	0.64
1:B:440:ARG:CG	1:B:440:ARG:NH2	2.59	0.64
1:B:795:ASN:O	1:B:799:TRP:HB2	1.98	0.64
1:A:428:MET:HB2	2:A:910:HOH:O	1.97	0.64
1:A:772:MET:CG	1:A:772:MET:CA	2.71	0.64
1:B:464:GLU:O	1:B:464:GLU:HG2	1.98	0.64
1:A:358:THR:HG22	1:A:359:THR:H	1.63	0.63
1:A:499:LEU:HB3	2:A:901:HOH:O	1.98	0.63
1:B:195:LEU:HD22	1:B:195:LEU:O	1.97	0.63
1:B:328:PHE:CE2	1:B:331:PHE:CZ	2.86	0.63
1:A:272:VAL:HA	1:A:312:ARG:HD2	1.78	0.63
1:A:365:TRP:CE2	1:A:488:SER:HA	2.33	0.63
1:A:656:GLU:OE1	1:A:656:GLU:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:VAL:HG21	1:A:733:LEU:HD12	0.70	0.63
1:B:328:PHE:O	1:B:331:PHE:HE2	1.82	0.63
1:A:228:ILE:CG1	1:A:337:LYS:HZ1	2.11	0.63
1:A:864:MET:CB	1:A:864:MET:C	2.69	0.63
1:A:177:TRP:CD2	1:A:178:SER:N	2.67	0.63
1:A:258:LEU:H	1:A:258:LEU:HD13	1.63	0.63
1:A:520:ASN:OD1	1:A:520:ASN:N	2.28	0.63
1:B:335:PHE:CA	1:B:335:PHE:CG	2.78	0.63
1:B:610:LEU:CD1	1:B:610:LEU:HG	2.19	0.63
1:B:303:GLU:OE2	1:B:304:TRP:N	2.32	0.63
1:A:87:PHE:CD2	1:A:88:ILE:HG22	2.33	0.63
1:A:94:ARG:CD	2:A:1049:HOH:O	2.46	0.63
1:A:200:THR:CB	1:A:200:THR:C	2.68	0.63
1:A:221:PRO:C	1:A:223:ASP:H	2.05	0.63
1:A:51:PHE:N	1:A:52:PRO:HD3	2.14	0.63
1:A:196:SER:O	1:A:197:GLY:C	2.42	0.63
1:A:808:THR:HG23	1:A:808:THR:C	2.23	0.63
1:B:506:LYS:O	1:B:507:LYS:C	2.32	0.63
1:A:669:VAL:CG1	1:A:669:VAL:CG2	2.72	0.63
1:A:388:LYS:NZ	1:A:482:GLU:OE1	2.32	0.62
1:B:25:ILE:HD13	1:B:148:GLU:OE1	1.99	0.62
1:B:27:TYR:CE2	1:B:28:LEU:CD1	2.82	0.62
1:B:69:LYS:CG	1:B:69:LYS:CA	2.76	0.62
1:A:17:GLY:O	1:A:18:LEU:C	2.34	0.62
1:B:74:LYS:HA	2:B:1000:HOH:O	1.98	0.62
1:B:274:TYR:O	1:B:275:GLN:C	2.40	0.62
1:B:427:ASP:HB3	2:B:1003:HOH:O	1.97	0.62
1:B:597:VAL:O	1:B:600:ASN:HB3	1.99	0.62
1:B:701:VAL:HG11	1:B:860:ARG:HG2	1.81	0.62
1:B:335:PHE:CB	1:B:335:PHE:C	2.70	0.62
1:B:831:ASN:O	1:B:833:HIS:C	2.42	0.62
1:A:193:GLU:O	1:A:195:LEU:N	2.33	0.62
1:A:204:PHE:CD1	1:A:340:ILE:HD11	2.35	0.62
1:A:317:VAL:CB	1:A:317:VAL:C	2.69	0.62
1:A:874:ASN:O	1:A:876:THR:N	2.32	0.62
1:A:883:ILE:CB	1:A:883:ILE:CD1	2.76	0.62
1:B:726:PHE:CD2	1:B:726:PHE:N	2.62	0.62
1:A:216:ASP:HB3	1:A:219:LYS:HB3	1.80	0.62
1:A:328:PHE:CZ	1:A:331:PHE:HZ	2.18	0.62
1:A:403:ARG:HG2	1:A:477:ARG:NE	2.14	0.62
1:B:103:GLY:HA3	2:B:903:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:ARG:NH1	1:B:670:ARG:CZ	2.58	0.62
1:B:724:ARG:HH21	1:B:724:ARG:CB	2.10	0.62
1:A:172:GLN:O	1:A:174:ASN:ND2	2.33	0.62
1:A:389:ILE:CG2	1:A:390:ARG:N	2.60	0.62
1:A:582:MET:CE	1:A:582:MET:CG	2.78	0.62
1:B:197:GLY:O	1:B:198:GLY:C	2.43	0.62
1:B:316:ARG:O	1:B:317:VAL:C	2.42	0.62
1:A:87:PHE:HD2	1:A:88:ILE:HG22	1.64	0.62
1:A:305:ASN:HD22	1:A:305:ASN:C	2.06	0.62
1:A:651:ARG:HH11	1:A:651:ARG:C	2.08	0.62
1:B:330:ASP:C	1:B:332:ILE:H	2.06	0.62
1:B:453:PHE:CZ	1:B:457:ASN:OD1	2.53	0.62
1:A:327:SER:H	1:A:329:ARG:HH12	1.40	0.62
1:A:328:PHE:CZ	1:A:331:PHE:CZ	2.87	0.62
1:A:448:HIS:CD2	1:A:630:ARG:NH2	2.67	0.62
1:B:523:ASP:O	1:B:524:GLU:C	2.41	0.62
1:B:616:PHE:CE1	1:B:628:GLU:HB3	2.35	0.62
1:A:63:LEU:CD1	1:A:70:THR:CG2	2.67	0.62
1:A:82:LEU:O	1:A:84:ASN:N	2.32	0.62
1:A:242:ILE:CG1	1:A:242:ILE:O	2.48	0.62
1:A:773:VAL:CG1	1:A:773:VAL:CG2	2.74	0.62
1:B:337:LYS:HZ2	1:B:337:LYS:HB3	0.46	0.62
1:B:377:TYR:N	1:B:378:PRO:HD3	2.12	0.62
1:B:379:ALA:HB2	2:B:1012:HOH:O	2.00	0.62
1:B:440:ARG:CD	1:B:440:ARG:CB	2.77	0.62
1:B:786:PHE:CB	1:B:786:PHE:N	2.56	0.62
1:A:7:LYS:CE	1:A:7:LYS:CG	2.76	0.62
1:A:75:TRP:CG	1:A:75:TRP:CA	2.80	0.62
1:A:553:LYS:O	1:A:554:GLU:HB2	1.99	0.62
1:A:380:THR:O	1:A:381:PHE:C	2.41	0.61
1:B:778:SER:O	1:B:779:ASP:OD1	2.17	0.61
1:A:759:LEU:CD1	1:A:812:GLY:O	2.48	0.61
1:B:740:VAL:CG1	1:B:740:VAL:CA	2.76	0.61
1:A:199:CYS:HB3	1:A:202:GLU:HG3	1.83	0.61
1:A:307:VAL:O	1:A:308:ASP:HB2	1.98	0.61
1:B:88:ILE:CD1	1:B:121:LEU:HD21	2.30	0.61
1:B:677:ILE:CD1	1:B:677:ILE:CB	2.73	0.61
1:A:237:LEU:C	1:A:238:LEU:HD12	2.25	0.61
1:A:701:VAL:HG13	1:A:701:VAL:O	2.00	0.61
1:B:49:PRO:CG	2:B:935:HOH:O	2.46	0.61
1:A:428:MET:HE2	2:A:970:HOH:O	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:MET:CB	1:A:772:MET:SD	2.87	0.61
1:B:789:PHE:C	1:B:789:PHE:CD2	2.79	0.61
1:A:306:LYS:CG	1:A:307:VAL:H	2.05	0.61
1:A:653:ALA:HA	1:A:659:ILE:HG12	1.82	0.61
1:B:601:ILE:HD13	1:B:604:ASN:CG	2.24	0.61
1:A:327:SER:CB	1:A:329:ARG:HH11	2.14	0.61
1:A:640:LEU:O	1:A:645:HIS:NE2	2.33	0.61
1:B:861:LEU:O	1:B:862:ASP:O	2.19	0.61
1:A:230:LYS:HE3	1:A:505:GLU:CD	2.25	0.61
1:A:451:ARG:HG2	1:A:451:ARG:NH1	2.16	0.61
1:A:680:GLN:O	1:A:682:ASP:N	2.33	0.61
1:B:519:ALA:HB2	1:B:675:PHE:CE2	2.36	0.61
1:A:140:HIS:HB3	1:A:153:VAL:HG23	1.83	0.61
1:A:228:ILE:O	1:A:229:LEU:O	2.19	0.61
1:A:366:ARG:O	1:A:367:ARG:C	2.39	0.61
1:A:602:LEU:O	1:A:603:TRP:C	2.43	0.61
1:B:60:PHE:CE2	1:B:193:GLU:HG2	2.36	0.61
1:B:883:ILE:CB	1:B:883:ILE:N	2.62	0.61
1:A:746:MET:O	1:A:746:MET:HG2	2.01	0.61
1:B:142:GLN:CB	1:B:142:GLN:CD	2.72	0.61
1:B:434:ALA:HA	1:B:462:GLN:HB3	1.83	0.61
1:B:579:CYS:CB	1:B:579:CYS:HA	2.17	0.61
1:B:798:LYS:O	1:B:802:ILE:HG13	2.00	0.61
1:A:327:SER:HB3	1:A:329:ARG:HH11	1.66	0.60
1:A:672:GLU:HA	1:A:672:GLU:OE2	1.99	0.60
1:B:89:VAL:CB	1:B:89:VAL:O	2.44	0.60
1:B:668:LEU:CD2	1:B:668:LEU:CB	2.72	0.60
1:B:853:ASN:O	1:B:857:CYS:N	2.31	0.60
1:B:8:LEU:CD2	1:B:8:LEU:CB	2.76	0.60
1:B:892:TYR:O	1:B:893:SER:CB	2.50	0.60
1:A:60:PHE:CD2	1:A:193:GLU:OE1	2.53	0.60
1:A:293:TRP:CE2	2:A:1024:HOH:O	2.54	0.60
1:B:867:ALA:C	1:B:869:ARG:N	2.55	0.60
1:A:26:LYS:O	1:A:27:TYR:C	2.40	0.60
1:A:155:ASP:OD2	1:A:156:ASP:N	2.32	0.60
1:A:549:GLU:O	1:A:595:GLY:HA2	2.01	0.60
1:A:731:VAL:CB	1:A:733:LEU:CD1	2.79	0.60
1:A:758:ASP:O	1:A:759:LEU:C	2.43	0.60
1:A:860:ARG:CB	1:A:860:ARG:NH1	2.63	0.60
1:B:120:ILE:CG2	1:B:120:ILE:C	2.74	0.60
1:B:358:THR:O	1:B:359:THR:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:LEU:O	1:A:605:ARG:HB2	2.02	0.60
1:A:655:ASP:C	1:A:656:GLU:OE1	2.45	0.60
1:B:225:TYR:CE1	1:B:280:ASN:ND2	2.69	0.60
1:B:574:PHE:CE1	1:B:661:PHE:HE1	2.20	0.60
1:A:297:TRP:CD1	1:A:297:TRP:O	2.55	0.60
1:B:277:GLN:HE21	1:B:277:GLN:HA	1.66	0.60
1:A:94:ARG:HD2	2:A:1049:HOH:O	2.01	0.60
1:B:493:ASN:HD22	1:B:493:ASN:N	2.00	0.60
1:B:582:MET:SD	1:B:602:LEU:HD21	2.42	0.60
1:B:787:GLU:C	1:B:789:PHE:H	2.10	0.60
1:A:494:LYS:NZ	1:A:494:LYS:CD	2.60	0.60
1:B:669:VAL:CB	1:B:669:VAL:C	2.71	0.60
1:B:866:ARG:HH11	1:B:866:ARG:HG3	1.67	0.60
1:A:267:THR:HG1	1:A:319:MET:HE1	1.67	0.60
1:A:413:LEU:CD1	1:A:413:LEU:CD2	2.73	0.60
1:A:614:ARG:HH12	1:A:620:LYS:HE3	1.67	0.60
1:A:860:ARG:NH1	1:A:860:ARG:HB3	2.15	0.60
1:B:457:ASN:HD22	1:B:457:ASN:N	1.93	0.60
1:A:388:LYS:NZ	1:A:482:GLU:CD	2.57	0.59
1:A:680:GLN:C	1:A:682:ASP:H	2.10	0.59
1:A:759:LEU:HD12	1:A:812:GLY:HA2	1.84	0.59
1:A:122:HIS:CD2	1:A:127:TYR:CE2	2.90	0.59
1:A:365:TRP:O	1:A:495:GLU:HA	2.02	0.59
1:A:872:ASP:CG	1:A:872:ASP:O	2.44	0.59
1:B:701:VAL:CG1	1:B:860:ARG:CG	2.80	0.59
1:A:100:GLY:HA2	1:A:167:PHE:HA	1.85	0.59
1:A:270:LYS:NZ	1:A:270:LYS:CD	2.63	0.59
1:A:273:THR:N	1:A:312:ARG:HH21	1.99	0.59
1:A:520:ASN:C	1:A:521:LEU:HG	2.27	0.59
1:B:670:ARG:HA	1:B:673:ILE:CD1	2.27	0.59
1:B:672:GLU:O	1:B:673:ILE:C	2.44	0.59
1:A:224:LEU:O	1:A:228:ILE:HG13	2.02	0.59
1:A:880:GLN:C	1:A:881:VAL:HG22	2.28	0.59
1:B:585:LEU:HD11	1:B:672:GLU:HG2	1.83	0.59
1:A:240:CYS:O	1:A:263:ALA:O	2.20	0.59
1:A:692:ASP:OD1	1:A:694:ILE:N	2.35	0.59
1:B:212:THR:OG1	1:B:340:ILE:CD1	2.51	0.59
1:B:456:ALA:C	1:B:456:ALA:HA	2.12	0.59
1:B:4:ILE:O	1:B:6:MET:N	2.36	0.59
1:B:369:SER:O	1:B:383:VAL:HG13	2.01	0.59
1:B:867:ALA:O	1:B:868:PHE:C	2.44	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:872:ASP:O	1:B:873:LYS:C	2.45	0.59
1:A:122:HIS:CA	1:A:125:VAL:O	2.50	0.59
1:B:324:PHE:HE1	1:B:326:MET:HE3	1.68	0.59
1:B:395:ASP:O	1:B:396:ASP:C	2.44	0.59
1:B:415:GLN:HE22	1:B:428:MET:HB3	1.68	0.59
1:B:656:GLU:O	1:B:657:LEU:HG	2.03	0.59
1:A:87:PHE:HA	1:A:131:PHE:HE1	1.66	0.59
1:B:773:VAL:CA	1:B:784:LEU:HD21	2.27	0.59
1:A:23:ARG:HG2	1:A:23:ARG:HH11	1.68	0.59
1:A:360:PHE:HB2	1:A:499:LEU:HD11	1.83	0.59
1:A:228:ILE:O	1:A:232:LEU:CD2	2.47	0.58
1:A:824:GLU:N	1:A:828:PHE:O	2.36	0.58
1:B:140:HIS:HD2	1:B:151:ASP:OD1	1.85	0.58
1:A:849:MET:HE2	1:A:854:PHE:HA	1.85	0.58
1:B:226:GLN:HG3	2:B:955:HOH:O	2.02	0.58
1:B:670:ARG:CA	1:B:673:ILE:HD12	2.25	0.58
1:A:619:ASP:O	1:A:620:LYS:O	2.21	0.58
1:B:291:VAL:HG23	1:B:292:GLU:H	1.68	0.58
1:B:524:GLU:CD	1:B:524:GLU:H	2.12	0.58
1:A:4:ILE:C	1:A:4:ILE:CD1	2.74	0.58
1:A:340:ILE:CG2	1:A:340:ILE:CG1	2.79	0.58
1:A:487:PRO:O	1:A:488:SER:HB3	2.02	0.58
1:A:499:LEU:HG	1:A:501:ARG:HD2	1.85	0.58
1:A:610:LEU:CD2	1:A:610:LEU:HA	2.34	0.58
1:B:410:LEU:HB2	1:B:503:PHE:HB2	1.86	0.58
1:B:740:VAL:CG1	1:B:740:VAL:HB	2.16	0.58
1:B:766:ILE:O	1:B:769:CYS:N	2.34	0.58
1:A:263:ALA:CB	1:A:288:TRP:HZ3	2.17	0.58
1:A:604:ASN:O	1:A:605:ARG:C	2.46	0.58
1:B:296:PRO:HG2	1:B:304:TRP:CG	2.38	0.58
1:B:649:VAL:O	1:B:650:ALA:C	2.37	0.58
1:B:97:ILE:HG12	1:B:98:CYS:N	2.17	0.58
1:B:272:VAL:HB	1:B:311:GLU:HG3	1.85	0.58
1:B:595:GLY:O	1:B:599:PHE:HB2	2.04	0.58
1:B:789:PHE:C	1:B:789:PHE:HD2	2.11	0.58
1:A:306:LYS:O	1:A:307:VAL:O	2.22	0.58
1:B:525:LYS:CB	1:B:525:LYS:HZ3	2.14	0.58
1:B:574:PHE:HE1	1:B:661:PHE:CE1	2.22	0.58
1:B:658:ILE:O	1:B:658:ILE:HG23	2.04	0.58
1:B:867:ALA:O	1:B:869:ARG:N	2.37	0.58
1:B:48:ASP:HB2	1:B:155:ASP:OD1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:855:ILE:CB	2:B:974:HOH:O	2.51	0.58
1:A:233:GLU:O	1:A:353:LEU:CB	2.52	0.58
1:A:309:PRO:O	1:A:311:GLU:N	2.36	0.58
1:B:28:LEU:C	1:B:30:GLN:H	2.09	0.58
1:B:46:PHE:CD2	1:B:138:ILE:HD12	2.39	0.58
1:B:242:ILE:HG23	1:B:242:ILE:O	2.02	0.58
1:B:694:ILE:CA	1:B:694:ILE:HB	2.18	0.58
1:A:316:ARG:CB	2:A:1007:HOH:O	2.52	0.57
1:B:484:ILE:HD12	1:B:513:LEU:HD22	1.85	0.57
1:B:694:ILE:CA	1:B:694:ILE:CG1	2.78	0.57
1:A:428:MET:CB	2:A:910:HOH:O	2.52	0.57
1:A:464:GLU:O	1:A:465:HIS:O	2.22	0.57
1:B:66:ASN:HD22	1:B:66:ASN:N	2.00	0.57
1:B:113:SER:C	1:B:115:THR:H	2.11	0.57
1:B:460:ARG:O	1:B:461:ALA:HB2	2.03	0.57
1:B:668:LEU:CD2	1:B:668:LEU:CD1	2.79	0.57
1:A:183:LYS:O	1:A:187:LYS:HB2	2.05	0.57
1:B:328:PHE:O	1:B:328:PHE:CG	2.56	0.57
1:B:806:PHE:O	1:B:807:GLU:HB3	2.04	0.57
1:A:193:GLU:C	1:A:195:LEU:N	2.58	0.57
1:B:376:ASN:OD1	1:B:376:ASN:N	2.22	0.57
1:B:537:LYS:HB2	1:B:537:LYS:NZ	2.09	0.57
1:B:779:ASP:O	1:B:780:THR:C	2.46	0.57
1:A:218:GLN:CB	1:A:218:GLN:CD	2.75	0.57
1:A:573:GLY:O	1:A:574:PHE:C	2.45	0.57
1:B:69:LYS:CB	1:B:69:LYS:HZ3	1.95	0.57
1:A:219:LYS:CD	1:A:219:LYS:CB	2.78	0.57
1:B:537:LYS:HZ2	1:B:537:LYS:CB	2.07	0.57
1:B:624:MET:O	1:B:658:ILE:HG13	2.05	0.57
1:A:414:MET:HE3	1:A:471:GLU:OE1	2.05	0.57
1:B:200:THR:HG23	1:B:201:SER:N	2.19	0.57
1:B:388:LYS:NZ	1:B:482:GLU:HB3	2.19	0.57
1:B:508:ALA:O	1:B:509:GLY:C	2.42	0.57
1:B:797:LYS:O	1:B:800:GLN:HB3	2.04	0.57
1:B:21:HIS:CD2	1:B:142:GLN:HE22	2.23	0.57
1:B:323:GLU:OE2	1:B:323:GLU:CA	2.47	0.57
1:B:332:ILE:CG2	1:B:332:ILE:CA	2.79	0.57
1:A:291:VAL:CG2	1:A:292:GLU:N	2.67	0.57
1:A:327:SER:OG	1:A:329:ARG:CZ	2.53	0.57
1:A:675:PHE:O	1:A:676:LYS:C	2.47	0.57
1:A:860:ARG:HB3	1:A:860:ARG:CZ	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:LEU:HD13	1:B:136:ALA:HB2	1.87	0.57
1:B:69:LYS:NZ	1:B:69:LYS:HB2	2.06	0.57
1:B:106:TRP:CZ3	1:B:107:LEU:HD13	2.40	0.57
1:B:585:LEU:HG	1:B:586:MET:CE	2.35	0.57
1:A:238:LEU:N	1:A:238:LEU:CD1	2.68	0.56
1:A:552:VAL:HA	1:A:592:GLY:O	2.05	0.56
1:B:221:PRO:O	1:B:224:LEU:HB2	2.05	0.56
1:B:519:ALA:HB2	1:B:675:PHE:CD2	2.40	0.56
1:B:678:PHE:HD2	1:B:886:TRP:CD1	2.23	0.56
1:A:305:ASN:ND2	1:A:305:ASN:H	2.03	0.56
1:A:307:VAL:HG12	2:A:909:HOH:O	2.05	0.56
1:A:695:SER:O	1:A:696:TRP:C	2.47	0.56
1:A:740:VAL:O	1:A:783:LYS:HA	2.06	0.56
1:B:8:LEU:HD13	1:B:885:GLU:CG	2.34	0.56
1:B:8:LEU:CD1	1:B:885:GLU:HB3	2.35	0.56
1:B:377:TYR:C	1:B:379:ALA:H	2.13	0.56
1:B:383:VAL:O	1:B:383:VAL:HG12	2.05	0.56
1:B:430:THR:CA	1:B:468:ASN:HB2	2.33	0.56
1:B:440:ARG:CG	1:B:441:GLU:N	2.30	0.56
1:B:810:ARG:O	1:B:811:SER:CB	2.52	0.56
1:B:835:TYR:O	1:B:837:MET:N	2.38	0.56
1:A:256:LYS:HA	1:A:258:LEU:CD1	2.35	0.56
1:A:435:VAL:HG11	1:A:461:ALA:HB3	1.87	0.56
1:B:226:GLN:CD	1:B:226:GLN:CB	2.72	0.56
1:B:238:LEU:N	1:B:238:LEU:CD1	2.69	0.56
1:B:807:GLU:HG3	1:B:808:THR:N	2.19	0.56
1:A:236:SER:C	1:A:238:LEU:CD1	2.79	0.56
1:A:278:ARG:CG	1:A:279:VAL:H	2.18	0.56
1:B:313:GLU:HA	1:B:315:LEU:HD12	1.87	0.56
1:B:582:MET:CE	1:B:582:MET:CG	2.83	0.56
1:A:296:PRO:O	1:A:297:TRP:CB	2.48	0.56
1:A:414:MET:CE	1:A:414:MET:CG	2.81	0.56
1:B:96:ASP:OD2	1:B:170:SER:OG	2.11	0.56
1:B:521:LEU:CD2	1:B:636:ALA:O	2.54	0.56
1:A:484:ILE:CD1	1:A:486:VAL:HG23	2.36	0.56
1:A:490:PHE:C	1:A:490:PHE:CD2	2.84	0.56
1:B:88:ILE:O	1:B:88:ILE:CG2	2.41	0.56
1:B:624:MET:O	1:B:658:ILE:CG1	2.53	0.56
1:A:37:ASN:C	1:A:39:CYS:H	2.14	0.56
1:A:350:SER:C	1:A:352:THR:N	2.63	0.56
1:A:698:SER:O	1:A:700:SER:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:VAL:HG13	1:A:460:ARG:O	2.05	0.56
1:B:97:ILE:CD1	1:B:108:LEU:HD11	2.35	0.56
1:B:690:GLN:CG	1:B:690:GLN:CA	2.80	0.56
1:B:780:THR:HA	1:B:892:TYR:CZ	2.41	0.56
1:A:343:LEU:O	1:A:344:THR:C	2.45	0.56
1:A:450:LYS:HE3	1:A:631:MET:HG2	1.87	0.56
1:B:161:LYS:C	1:B:163:GLY:N	2.62	0.56
1:B:389:ILE:HD13	1:B:483:TYR:HB2	1.87	0.56
1:B:609:TYR:CD2	1:B:665:VAL:HB	2.41	0.56
1:B:651:ARG:NH1	1:B:670:ARG:HH12	2.02	0.56
1:A:177:TRP:CG	1:A:178:SER:N	2.74	0.55
1:B:3:GLY:O	1:B:778:SER:OG	2.21	0.55
1:B:135:TYR:O	1:B:136:ALA:CA	2.54	0.55
1:B:555:LEU:O	1:B:556:GLN:O	2.23	0.55
1:B:605:ARG:CZ	1:B:672:GLU:OE2	2.55	0.55
1:B:868:PHE:CE2	1:B:879:ILE:HG12	2.41	0.55
1:B:696:TRP:O	1:B:700:SER:OG	2.23	0.55
1:A:278:ARG:NH2	2:A:929:HOH:O	2.38	0.55
1:A:610:LEU:HA	1:A:610:LEU:HD22	1.88	0.55
1:A:624:MET:HB3	1:A:659:ILE:O	2.06	0.55
1:A:800:GLN:HG3	1:A:851:PHE:HE1	1.70	0.55
1:B:87:PHE:CE1	1:B:180:LEU:HD12	2.40	0.55
1:B:186:ALA:O	1:B:187:LYS:C	2.43	0.55
1:B:236:SER:C	1:B:237:LEU:HD23	2.31	0.55
1:A:204:PHE:HE2	1:A:237:LEU:HD12	1.71	0.55
1:B:161:LYS:C	1:B:163:GLY:H	2.13	0.55
1:B:361:TYR:O	1:B:500:LEU:N	2.39	0.55
1:B:426:ARG:HG2	2:B:1029:HOH:O	2.05	0.55
1:A:349:LYS:HA	2:A:1006:HOH:O	2.06	0.55
1:B:370:THR:HA	1:B:383:VAL:HG12	1.87	0.55
1:B:388:LYS:HZ3	1:B:482:GLU:HB3	1.71	0.55
1:B:457:ASN:ND2	1:B:457:ASN:N	2.48	0.55
1:B:724:ARG:O	1:B:724:ARG:NH2	2.40	0.55
1:A:757:PRO:O	1:A:758:ASP:CB	2.55	0.55
1:B:507:LYS:H	1:B:507:LYS:HD2	1.72	0.55
1:B:667:CYS:O	1:B:668:LEU:O	2.24	0.55
1:B:701:VAL:CG1	1:B:860:ARG:HD3	2.37	0.55
1:B:723:GLU:O	1:B:726:PHE:HD2	1.89	0.55
1:A:591:ASN:ND2	1:A:592:GLY:H	2.05	0.55
1:A:655:ASP:CB	1:A:656:GLU:OE1	2.55	0.55
1:A:773:VAL:CG1	1:A:773:VAL:CA	2.76	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:TYR:CE2	1:B:275:GLN:HG3	2.41	0.55
1:B:493:ASN:ND2	1:B:493:ASN:N	2.55	0.55
1:B:694:ILE:CB	1:B:694:ILE:C	2.75	0.55
1:B:795:ASN:O	1:B:799:TRP:CB	2.55	0.55
1:A:204:PHE:CE2	1:A:237:LEU:HD12	2.41	0.55
1:A:332:ILE:CG1	1:A:332:ILE:CA	2.80	0.55
1:A:340:ILE:CG2	1:A:340:ILE:HB	2.18	0.55
1:A:698:SER:C	1:A:700:SER:N	2.65	0.55
1:A:855:ILE:O	1:A:855:ILE:HG22	1.99	0.55
1:B:95:THR:HG22	1:B:287:PRO:C	2.31	0.55
1:B:168:VAL:HB	1:B:182:GLU:OE2	2.07	0.55
1:B:447:VAL:CB	1:B:513:LEU:HD12	2.36	0.55
1:A:689:ILE:C	1:A:689:ILE:CD1	2.62	0.55
1:B:225:TYR:CE1	1:B:280:ASN:CG	2.84	0.55
1:A:785:GLY:HA3	1:A:788:GLU:OE1	2.07	0.54
1:A:254:THR:HG23	1:A:255:PHE:H	1.72	0.54
1:A:320:GLU:CB	1:A:320:GLU:C	2.73	0.54
1:A:370:THR:HA	1:A:383:VAL:O	2.06	0.54
1:A:613:PHE:CZ	1:A:622:GLY:O	2.61	0.54
1:B:258:LEU:O	1:B:259:VAL:HG22	2.08	0.54
1:B:273:THR:H	1:B:311:GLU:HG2	1.72	0.54
1:A:741:SER:C	1:A:743:THR:N	2.55	0.54
1:B:102:LEU:HD22	1:B:161:LYS:HE2	1.90	0.54
1:B:212:THR:CB	1:B:340:ILE:CD1	2.85	0.54
1:B:439:PRO:C	1:B:440:ARG:HD3	2.32	0.54
1:B:775:VAL:HG12	1:B:893:SER:HB2	1.89	0.54
1:A:13:GLU:O	1:A:14:ALA:C	2.49	0.54
1:A:227:ILE:CD1	1:A:227:ILE:CB	2.79	0.54
1:A:290:GLU:N	1:A:290:GLU:OE2	2.33	0.54
1:A:358:THR:C	1:A:359:THR:HG23	2.31	0.54
1:A:366:ARG:CG	1:A:366:ARG:NE	2.64	0.54
1:A:394:VAL:HG12	1:A:407:CYS:SG	2.47	0.54
1:A:831:ASN:O	1:A:832:GLN:O	2.25	0.54
1:B:583:VAL:O	1:B:584:ASN:CB	2.53	0.54
1:A:309:PRO:O	1:A:310:TYR:C	2.49	0.54
1:A:358:THR:CG2	1:A:359:THR:N	2.67	0.54
1:A:683:PRO:O	1:A:685:ASN:N	2.40	0.54
1:A:731:VAL:CG1	1:A:733:LEU:CD1	2.82	0.54
1:B:286:ASN:HD22	1:B:290:GLU:H	1.55	0.54
1:B:427:ASP:CB	2:B:1003:HOH:O	2.54	0.54
1:B:89:VAL:CA	1:B:89:VAL:CG2	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:LEU:HD22	1:B:636:ALA:O	2.08	0.54
1:B:712:TYR:CA	2:B:956:HOH:O	2.56	0.54
1:A:3:GLY:HA2	1:A:777:ASP:O	2.08	0.54
1:A:75:TRP:CH2	1:A:159:PRO:CG	2.86	0.54
1:A:575:SER:O	1:A:578:SER:N	2.41	0.54
1:B:113:SER:C	1:B:115:THR:N	2.63	0.54
1:B:135:TYR:O	1:B:136:ALA:CB	2.56	0.54
1:B:227:ILE:O	1:B:228:ILE:C	2.47	0.54
1:B:439:PRO:HB2	1:B:440:ARG:CD	2.36	0.54
1:B:447:VAL:CB	1:B:513:LEU:HD11	2.38	0.54
1:B:461:ALA:C	1:B:462:GLN:HG3	2.31	0.54
1:A:5:ALA:C	1:A:7:LYS:H	2.15	0.54
1:A:223:ASP:C	1:A:227:ILE:HD12	2.32	0.54
1:A:745:LEU:HD12	1:A:749:LEU:CD2	2.37	0.54
1:B:502:PHE:CG	1:B:510:THR:HG21	2.43	0.54
1:A:13:GLU:HA	1:A:16:GLU:CG	2.37	0.54
1:A:273:THR:N	1:A:312:ARG:HD2	2.22	0.54
1:A:386:GLN:CB	1:A:513:LEU:HB3	2.36	0.54
1:A:758:ASP:O	1:A:759:LEU:HB3	2.08	0.54
1:A:115:THR:CG2	1:A:115:THR:CA	2.80	0.54
1:B:206:ASP:OD1	1:B:206:ASP:N	2.38	0.54
1:B:651:ARG:NH2	1:B:670:ARG:NE	2.55	0.54
1:B:862:ASP:O	1:B:864:MET:N	2.40	0.54
1:A:61:LYS:O	1:A:62:GLU:CB	2.56	0.53
1:A:628:GLU:O	1:A:629:MET:C	2.51	0.53
1:A:642:CYS:O	1:A:646:GLN:HG3	2.08	0.53
1:B:99:GLN:NE2	1:B:105:SER:HB3	2.23	0.53
1:B:370:THR:HA	1:B:383:VAL:CG1	2.38	0.53
1:B:390:ARG:HD2	1:B:482:GLU:CG	2.38	0.53
1:B:831:ASN:O	1:B:834:ILE:N	2.40	0.53
1:A:824:GLU:CA	1:A:828:PHE:O	2.56	0.53
1:B:256:LYS:O	1:B:258:LEU:N	2.41	0.53
1:A:135:TYR:CD2	1:A:136:ALA:N	2.77	0.53
1:A:188:VAL:HG23	1:A:189:ASN:N	2.23	0.53
1:A:430:THR:HG22	1:A:490:PHE:HB2	1.90	0.53
1:A:484:ILE:HD13	1:A:486:VAL:HG23	1.89	0.53
1:A:576:LEU:HA	1:A:579:CYS:HB2	1.90	0.53
1:B:820:PRO:HD2	1:B:822:ALA:HB3	1.90	0.53
1:B:390:ARG:NH1	1:B:390:ARG:CG	2.58	0.53
1:B:430:THR:H	1:B:494:LYS:NZ	2.06	0.53
1:B:438:VAL:HG23	1:B:482:GLU:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:701:VAL:HG12	1:B:860:ARG:HD3	1.89	0.53
1:A:81:LEU:HD23	1:A:81:LEU:O	2.09	0.53
1:A:436:TYR:HB2	1:A:484:ILE:CG2	2.39	0.53
1:A:665:VAL:HG23	1:A:666:ARG:H	1.70	0.53
1:B:701:VAL:HG13	1:B:860:ARG:NH1	2.15	0.53
1:A:677:ILE:CG2	1:A:681:LEU:HD12	2.39	0.53
1:A:826:ALA:CB	1:A:826:ALA:N	2.66	0.53
1:A:864:MET:CB	1:A:864:MET:N	2.67	0.53
1:B:114:LEU:O	1:B:121:LEU:HD12	2.08	0.53
1:B:213:GLU:O	1:B:339:GLU:OE2	2.26	0.53
1:A:478:LEU:CD1	1:A:478:LEU:CB	2.79	0.53
1:A:690:GLN:CG	1:A:690:GLN:O	2.57	0.53
1:B:4:ILE:O	1:B:5:ALA:C	2.49	0.53
1:B:429:GLU:HB3	1:B:494:LYS:CE	2.38	0.53
1:B:438:VAL:HG22	1:B:484:ILE:HD13	1.85	0.53
1:B:574:PHE:CE1	1:B:661:PHE:CE1	2.96	0.53
1:A:571:THR:HG22	1:A:572:ASN:N	2.24	0.53
1:A:610:LEU:CD2	1:A:610:LEU:CA	2.87	0.53
1:A:633:ILE:HD11	1:A:648:ILE:HD13	1.90	0.53
1:B:124:VAL:O	1:B:126:PRO:HD3	2.08	0.53
1:B:160:THR:OG1	1:B:165:LEU:HD23	2.08	0.53
1:B:215:TYR:HB2	1:B:337:LYS:HZ1	1.73	0.53
1:B:453:PHE:CD2	1:B:453:PHE:C	2.86	0.53
1:B:453:PHE:CE2	1:B:457:ASN:OD1	2.62	0.53
1:B:701:VAL:HG13	1:B:860:ARG:HG2	1.86	0.53
1:A:307:VAL:O	1:A:308:ASP:CB	2.56	0.53
1:A:327:SER:CB	1:A:329:ARG:NH1	2.72	0.53
1:A:468:ASN:CB	2:A:905:HOH:O	2.29	0.53
1:A:824:GLU:C	1:A:826:ALA:H	2.17	0.53
1:B:440:ARG:HD3	1:B:440:ARG:N	2.24	0.53
1:B:501:ARG:HD2	2:B:948:HOH:O	2.08	0.53
1:B:601:ILE:HG21	2:B:987:HOH:O	2.09	0.53
1:A:857:CYS:C	1:A:859:VAL:H	2.16	0.53
1:B:366:ARG:N	1:B:370:THR:OG1	2.42	0.53
1:B:374:CYS:SG	1:B:376:ASN:OD1	2.67	0.53
1:A:759:LEU:HD12	1:A:812:GLY:O	2.10	0.52
1:B:145:GLN:O	1:B:146:PHE:C	2.51	0.52
1:B:677:ILE:HG22	1:B:681:LEU:HD12	1.91	0.52
1:A:343:LEU:H	1:A:343:LEU:HD12	1.74	0.52
1:A:356:TRP:CE3	1:A:356:TRP:HA	2.43	0.52
1:A:748:ILE:HG23	1:A:749:LEU:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:ASP:O	1:A:872:ASP:OD2	2.26	0.52
1:B:335:PHE:CD1	1:B:336:THR:HB	2.44	0.52
1:B:670:ARG:HG3	1:B:674:LEU:HD21	1.90	0.52
1:B:684:GLU:O	1:B:685:ASN:C	2.52	0.52
1:A:613:PHE:HZ	1:A:622:GLY:O	1.93	0.52
1:A:630:ARG:HG3	1:A:645:HIS:CE1	2.44	0.52
1:A:660:ASP:O	1:A:664:PHE:HB2	2.09	0.52
1:A:821:GLY:C	1:A:823:PHE:H	2.18	0.52
1:A:853:ASN:N	1:A:853:ASN:ND2	2.52	0.52
1:B:153:VAL:HG12	1:B:153:VAL:O	2.09	0.52
1:B:384:ASN:HB3	1:B:385:PRO:CD	2.39	0.52
1:B:540:PHE:O	1:B:540:PHE:CD1	2.62	0.52
1:B:740:VAL:CG1	1:B:741:SER:N	2.69	0.52
1:B:800:GLN:HA	1:B:851:PHE:HZ	1.74	0.52
1:B:296:PRO:HD2	1:B:304:TRP:HB3	1.91	0.52
1:B:674:LEU:O	1:B:678:PHE:HB2	2.10	0.52
1:A:124:VAL:HG13	1:A:142:GLN:O	2.10	0.52
1:A:78:PRO:HB3	1:A:176:PHE:CZ	2.45	0.52
1:A:255:PHE:CB	1:A:333:ARG:CG	2.88	0.52
1:A:862:ASP:OD2	1:A:862:ASP:C	2.50	0.52
1:B:8:LEU:O	1:B:10:LYS:N	2.43	0.52
1:B:12:ARG:HH21	1:B:885:GLU:CD	2.18	0.52
1:B:197:GLY:O	1:B:198:GLY:O	2.28	0.52
1:B:258:LEU:O	1:B:259:VAL:CG2	2.58	0.52
1:B:387:PHE:HB2	1:B:485:VAL:HG13	1.91	0.52
1:A:297:TRP:O	1:A:298:SER:OG	2.19	0.52
1:A:517:ILE:HG23	1:A:640:LEU:CD2	2.40	0.52
1:A:739:GLU:O	1:A:739:GLU:OE1	2.26	0.52
1:B:82:LEU:O	1:B:83:SER:C	2.52	0.52
1:B:274:TYR:CD2	1:B:275:GLN:HG3	2.44	0.52
1:B:435:VAL:HA	1:B:484:ILE:O	2.10	0.52
1:B:790:LYS:O	1:B:793:TRP:N	2.43	0.52
1:A:306:LYS:HE3	1:A:307:VAL:H	1.74	0.52
1:A:453:PHE:C	1:A:453:PHE:CD2	2.88	0.52
1:A:467:ILE:HG22	1:A:468:ASN:N	2.24	0.52
1:A:617:ASP:O	1:A:618:LEU:C	2.53	0.52
1:B:330:ASP:C	1:B:332:ILE:N	2.64	0.52
1:A:553:LYS:C	1:A:555:LEU:N	2.67	0.52
1:A:773:VAL:O	1:A:774:ALA:C	2.47	0.52
1:B:328:PHE:CE2	1:B:331:PHE:CE2	2.98	0.52
1:A:302:TYR:O	1:A:303:GLU:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:SER:O	1:A:352:THR:HG23	2.09	0.51
1:B:519:ALA:HB2	1:B:675:PHE:CZ	2.45	0.51
1:A:63:LEU:O	1:A:70:THR:HG21	2.09	0.51
1:A:96:ASP:C	1:A:97:ILE:O	2.50	0.51
1:A:695:SER:O	1:A:697:LEU:N	2.43	0.51
1:B:806:PHE:CB	1:B:806:PHE:CD1	2.80	0.51
1:A:81:LEU:O	1:A:81:LEU:CD2	2.57	0.51
1:B:208:THR:O	1:B:346:ASP:OD1	2.28	0.51
1:B:524:GLU:O	1:B:526:VAL:N	2.43	0.51
1:B:524:GLU:O	1:B:525:LYS:C	2.52	0.51
1:B:605:ARG:HG2	1:B:605:ARG:NH2	2.25	0.51
1:A:112:ALA:C	1:A:114:LEU:H	2.19	0.51
1:A:314:GLN:CG	1:A:315:LEU:N	2.72	0.51
1:A:698:SER:C	1:A:700:SER:H	2.17	0.51
1:A:772:MET:HE2	1:A:792:LEU:HD21	1.92	0.51
1:A:773:VAL:HG11	1:A:782:GLY:O	2.11	0.51
1:B:65:PRO:O	1:B:66:ASN:HB2	2.10	0.51
1:B:643:GLN:CG	1:B:643:GLN:NE2	2.66	0.51
1:A:4:ILE:HD11	1:A:889:LEU:HD23	1.92	0.51
1:A:37:ASN:C	1:A:39:CYS:N	2.65	0.51
1:A:121:LEU:O	1:A:121:LEU:HD22	2.10	0.51
1:A:435:VAL:O	1:A:460:ARG:O	2.27	0.51
1:A:746:MET:SD	1:A:766:ILE:N	2.83	0.51
1:A:769:CYS:O	1:A:770:ARG:C	2.49	0.51
1:B:404:GLU:OE1	1:B:404:GLU:HA	2.09	0.51
1:B:660:ASP:OD1	1:B:663:ASN:OD1	2.29	0.51
1:B:694:ILE:CB	1:B:694:ILE:HA	2.21	0.51
1:A:219:LYS:CD	1:A:219:LYS:CA	2.88	0.51
1:A:268:ASP:CG	1:A:269:ALA:H	2.19	0.51
1:A:335:PHE:CD1	1:A:335:PHE:O	2.63	0.51
1:B:526:VAL:HB	2:B:950:HOH:O	2.11	0.51
1:B:579:CYS:CB	1:B:579:CYS:N	2.69	0.51
1:B:784:LEU:N	1:B:784:LEU:CD1	2.73	0.51
1:A:238:LEU:HD12	1:A:238:LEU:N	2.24	0.51
1:B:242:ILE:HD13	1:B:242:ILE:C	2.35	0.51
1:B:493:ASN:ND2	1:B:627:TYR:OH	2.44	0.51
1:B:610:LEU:HB3	1:B:661:PHE:CE2	2.46	0.51
1:B:692:ASP:O	1:B:693:LEU:C	2.53	0.51
1:B:800:GLN:HA	1:B:851:PHE:CZ	2.46	0.51
1:A:395:ASP:OD1	1:A:408:SER:HB3	2.11	0.51
1:A:832:GLN:C	1:A:832:GLN:CD	2.70	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:THR:CA	1:B:468:ASN:CB	2.89	0.51
1:B:450:LYS:O	1:B:454:PHE:CD1	2.64	0.51
1:A:139:PHE:HE1	1:A:156:ASP:HB3	1.75	0.51
1:A:154:VAL:HG22	1:A:155:ASP:H	1.76	0.51
1:A:320:GLU:O	1:A:321:ASP:C	2.54	0.51
1:A:329:ARG:HG3	1:A:333:ARG:HH11	1.76	0.51
1:A:414:MET:CE	1:A:471:GLU:OE1	2.59	0.51
1:A:467:ILE:CD1	1:A:472:VAL:HG22	2.40	0.51
1:A:600:ASN:C	1:A:602:LEU:N	2.68	0.51
1:B:429:GLU:CA	1:B:468:ASN:HD22	2.24	0.51
1:B:470:ARG:CB	1:B:470:ARG:CD	2.81	0.51
1:B:601:ILE:CG2	2:B:987:HOH:O	2.58	0.51
1:B:723:GLU:C	1:B:726:PHE:CD2	2.87	0.51
1:A:66:ASN:O	1:A:67:SER:C	2.52	0.51
1:B:412:ALA:HB2	1:B:473:SER:HB2	1.92	0.51
1:B:660:ASP:HB2	2:B:1011:HOH:O	2.11	0.51
1:A:135:TYR:O	1:A:136:ALA:HB3	2.10	0.50
1:A:656:GLU:N	1:A:656:GLU:CD	2.70	0.50
1:A:199:CYS:CB	1:A:202:GLU:HG3	2.41	0.50
1:A:216:ASP:OD1	1:A:335:PHE:CZ	2.65	0.50
1:B:272:VAL:O	1:B:278:ARG:HA	2.12	0.50
1:A:122:HIS:CG	1:A:127:TYR:CE2	3.00	0.50
1:A:291:VAL:CG2	1:A:292:GLU:H	2.24	0.50
1:A:757:PRO:O	1:A:758:ASP:HB2	2.12	0.50
1:B:89:VAL:N	1:B:175:GLU:OE2	2.44	0.50
1:B:142:GLN:CB	1:B:142:GLN:NE2	2.75	0.50
1:B:507:LYS:HD2	2:B:934:HOH:O	2.10	0.50
1:A:6:MET:CE	1:A:6:MET:CG	2.88	0.50
1:A:117:ASN:OD1	1:A:119:THR:HB	2.12	0.50
1:A:407:CYS:HB2	1:A:478:LEU:O	2.11	0.50
1:A:800:GLN:HG3	1:A:851:PHE:CE1	2.46	0.50
1:B:400:TYR:CG	1:B:401:ASP:N	2.80	0.50
1:B:640:LEU:HD21	1:B:671:LEU:HD11	1.93	0.50
1:A:853:ASN:O	1:A:857:CYS:HB2	2.11	0.50
1:B:208:THR:HA	2:B:908:HOH:O	2.11	0.50
1:B:398:ASP:HB2	2:B:964:HOH:O	2.10	0.50
1:B:477:ARG:CB	1:B:477:ARG:CD	2.81	0.50
1:A:77:ARG:O	1:A:81:LEU:HD13	2.12	0.50
1:A:97:ILE:HG12	1:A:98:CYS:H	1.75	0.50
1:A:361:TYR:OH	1:A:510:THR:C	2.54	0.50
1:A:365:TRP:CZ2	1:A:488:SER:CA	2.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:VAL:O	1:A:670:ARG:C	2.52	0.50
1:A:746:MET:O	1:A:746:MET:CG	2.55	0.50
1:B:552:VAL:C	1:B:554:GLU:N	2.69	0.50
1:A:340:ILE:CG2	1:A:340:ILE:CA	2.78	0.50
1:A:644:LEU:O	1:A:648:ILE:HG13	2.12	0.50
1:A:881:VAL:HG12	1:A:885:GLU:HB2	1.92	0.50
1:B:20:SER:O	1:B:21:HIS:C	2.53	0.50
1:B:400:TYR:CD1	1:B:401:ASP:N	2.78	0.50
1:B:521:LEU:HB3	1:B:522:PRO:HD2	1.93	0.50
1:B:677:ILE:O	1:B:681:LEU:N	2.39	0.50
1:A:63:LEU:C	1:A:193:GLU:OE2	2.54	0.50
1:B:256:LYS:HE3	1:B:293:TRP:HA	1.94	0.50
1:B:366:ARG:HA	1:B:495:GLU:HG2	1.94	0.50
1:B:443:ALA:CB	2:B:894:HOH:O	2.54	0.50
1:B:576:LEU:C	1:B:578:SER:N	2.67	0.50
1:B:603:TRP:CD1	1:B:603:TRP:O	2.65	0.50
1:B:616:PHE:O	1:B:624:MET:HB3	2.11	0.50
1:A:168:VAL:O	1:A:169:HIS:HB3	2.11	0.50
1:A:272:VAL:CA	1:A:312:ARG:HD2	2.41	0.50
1:A:411:LEU:HD23	1:A:411:LEU:C	2.37	0.50
1:B:293:TRP:CZ2	1:B:326:MET:HE2	2.47	0.50
1:B:316:ARG:CB	1:B:316:ARG:C	2.81	0.50
1:A:489:THR:OG1	1:A:491:GLU:O	2.30	0.49
1:A:771:SER:OG	1:A:893:SER:O	2.29	0.49
1:B:60:PHE:CD2	1:B:60:PHE:N	2.79	0.49
1:B:651:ARG:NH1	1:B:891:MET:HA	2.27	0.49
1:B:856:SER:C	1:B:858:LEU:N	2.69	0.49
1:A:27:TYR:HB2	1:A:150:VAL:CG1	2.42	0.49
1:A:665:VAL:C	1:A:669:VAL:HG23	2.32	0.49
1:A:743:THR:O	1:A:744:GLU:C	2.55	0.49
1:A:579:CYS:HA	1:A:582:MET:HE2	1.94	0.49
1:B:676:LYS:O	1:B:677:ILE:C	2.55	0.49
1:A:231:ALA:O	1:A:234:ARG:HB2	2.13	0.49
1:A:314:GLN:CG	1:A:315:LEU:H	2.25	0.49
1:B:6:MET:SD	1:B:870:SER:OG	2.59	0.49
1:B:404:GLU:C	1:B:405:SER:OG	2.56	0.49
1:B:598:GLU:CD	1:B:598:GLU:H	2.20	0.49
1:A:51:PHE:HB2	1:A:187:LYS:HG3	1.93	0.49
1:A:105:SER:O	1:A:108:LEU:HB2	2.11	0.49
1:A:120:ILE:HD13	1:A:237:LEU:HD21	1.94	0.49
1:A:193:GLU:O	1:A:194:ALA:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:THR:CA	1:A:200:THR:CG2	2.87	0.49
1:A:606:ILE:O	1:A:609:TYR:N	2.45	0.49
1:A:621:SER:OG	1:A:623:SER:HB2	2.13	0.49
1:A:633:ILE:CD1	1:A:648:ILE:HD13	2.42	0.49
1:B:230:LYS:HB3	1:B:234:ARG:NH2	2.28	0.49
1:B:669:VAL:O	1:B:673:ILE:HG13	2.12	0.49
1:A:168:VAL:HB	1:A:182:GLU:OE2	2.12	0.49
1:A:619:ASP:O	1:A:621:SER:N	2.44	0.49
1:B:424:PHE:HZ	1:B:711:HIS:HA	1.74	0.49
1:B:461:ALA:C	1:B:462:GLN:CG	2.83	0.49
1:A:23:ARG:O	1:A:24:ALA:C	2.53	0.49
1:A:35:LEU:HD22	1:A:46:PHE:CE1	2.48	0.49
1:A:83:SER:O	1:A:84:ASN:CB	2.59	0.49
1:A:85:PRO:HB2	1:A:131:PHE:CG	2.48	0.49
1:A:221:PRO:C	1:A:223:ASP:N	2.71	0.49
1:A:664:PHE:CZ	1:A:668:LEU:HD11	2.48	0.49
1:A:680:GLN:C	1:A:682:ASP:N	2.71	0.49
1:B:161:LYS:HG3	1:B:166:VAL:HG11	1.94	0.49
1:B:581:SER:C	1:B:583:VAL:H	2.21	0.49
1:B:724:ARG:HB2	1:B:724:ARG:NH2	2.19	0.49
1:B:867:ALA:C	1:B:869:ARG:H	2.19	0.49
1:A:803:TYR:C	1:A:803:TYR:CD2	2.88	0.49
1:B:14:ALA:O	1:B:17:GLY:N	2.46	0.49
1:B:146:PHE:HA	1:B:414:MET:CE	2.42	0.49
1:A:734:ALA:O	1:A:736:ASP:N	2.45	0.49
1:A:831:ASN:C	2:A:919:HOH:O	2.54	0.49
1:B:6:MET:SD	1:B:6:MET:HA	2.52	0.49
1:B:25:ILE:CG2	1:B:26:LYS:N	2.75	0.49
1:B:613:PHE:C	1:B:613:PHE:CD2	2.91	0.49
1:B:861:LEU:O	1:B:862:ASP:C	2.50	0.49
1:A:67:SER:O	1:A:68:SER:C	2.52	0.49
1:A:207:PHE:C	1:A:208:THR:HG23	2.37	0.49
1:A:304:TRP:CE2	1:A:313:GLU:OE2	2.65	0.49
1:A:452:ASP:CG	1:A:452:ASP:CA	2.80	0.49
1:A:677:ILE:O	1:A:678:PHE:C	2.52	0.49
1:B:158:LEU:HB2	1:B:165:LEU:HD21	1.94	0.49
1:B:160:THR:HG1	1:B:165:LEU:HD23	1.78	0.49
1:B:652:PHE:HE1	1:B:891:MET:HE1	1.77	0.49
1:B:831:ASN:C	1:B:833:HIS:N	2.69	0.49
1:A:114:LEU:CD1	1:A:121:LEU:HD23	2.41	0.48
1:A:225:TYR:HB2	1:A:328:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:SER:HB3	1:A:352:THR:HG22	1.95	0.48
1:A:608:ASN:O	1:A:609:TYR:C	2.44	0.48
1:A:695:SER:O	1:A:698:SER:N	2.46	0.48
1:B:57:SER:O	1:B:191:SER:HB2	2.12	0.48
1:B:212:THR:HB	1:B:340:ILE:CD1	2.43	0.48
1:B:0:GLU:CB	1:B:0:GLU:HA	2.19	0.48
1:B:824:GLU:CB	1:B:824:GLU:HA	2.24	0.48
1:A:25:ILE:O	1:A:151:ASP:N	2.46	0.48
1:A:47:GLN:OE1	1:A:47:GLN:CA	2.53	0.48
1:A:106:TRP:HZ2	1:A:195:LEU:O	1.97	0.48
1:A:256:LYS:CA	1:A:258:LEU:HD13	2.44	0.48
1:B:36:ARG:O	1:B:37:ASN:C	2.54	0.48
1:B:106:TRP:HZ2	1:B:195:LEU:O	1.97	0.48
1:B:595:GLY:O	1:B:599:PHE:CB	2.61	0.48
1:A:335:PHE:HD1	1:A:336:THR:HB	1.78	0.48
1:A:462:GLN:O	1:A:463:SER:C	2.43	0.48
1:A:795:ASN:O	1:A:796:ILE:C	2.52	0.48
1:B:321:ASP:O	1:B:322:GLY:C	2.57	0.48
1:B:340:ILE:CD1	1:B:340:ILE:HG13	2.20	0.48
1:B:342:ASN:CG	1:B:346:ASP:OD2	2.56	0.48
1:B:537:LYS:CG	1:B:537:LYS:NZ	2.75	0.48
1:B:730:PHE:O	1:B:732:GLN:N	2.46	0.48
1:B:731:VAL:HG11	1:B:739:GLU:O	2.13	0.48
1:A:308:ASP:OD2	1:A:313:GLU:HG3	2.14	0.48
1:A:519:ALA:CB	1:A:675:PHE:CE1	2.91	0.48
1:A:665:VAL:O	1:A:666:ARG:O	2.30	0.48
1:B:789:PHE:O	1:B:792:LEU:HB3	2.13	0.48
1:B:838:ILE:CG2	1:B:839:ILE:N	2.75	0.48
1:A:228:ILE:O	1:A:229:LEU:C	2.51	0.48
1:A:281:LEU:HA	1:A:327:SER:HA	1.95	0.48
1:A:470:ARG:O	1:A:471:GLU:O	2.32	0.48
1:A:792:LEU:HD12	1:A:792:LEU:O	2.14	0.48
1:B:142:GLN:CB	1:B:142:GLN:HE21	2.26	0.48
1:B:330:ASP:OD1	1:B:331:PHE:N	2.44	0.48
1:A:94:ARG:C	1:A:95:THR:OG1	2.56	0.48
1:A:258:LEU:HD13	1:A:258:LEU:N	2.28	0.48
1:A:305:ASN:HD22	1:A:306:LYS:H	1.54	0.48
1:A:319:MET:CG	1:A:320:GLU:N	2.76	0.48
1:A:553:LYS:C	1:A:555:LEU:H	2.21	0.48
1:A:760:LYS:HE3	1:A:760:LYS:CA	2.42	0.48
1:A:831:ASN:CB	1:A:831:ASN:ND2	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:TRP:HB3	1:B:451:ARG:HA	1.95	0.48
1:B:415:GLN:NE2	1:B:428:MET:HB3	2.28	0.48
1:B:634:GLU:HA	1:B:638:PHE:O	2.13	0.48
1:B:642:CYS:O	1:B:643:GLN:C	2.51	0.48
1:B:729:LEU:HD22	2:B:1027:HOH:O	2.14	0.48
1:B:828:PHE:CG	1:B:861:LEU:HD23	2.48	0.48
1:A:154:VAL:HG22	1:A:155:ASP:N	2.29	0.48
1:A:258:LEU:CD1	1:A:258:LEU:N	2.73	0.48
1:B:99:GLN:HE22	1:B:105:SER:HB3	1.79	0.48
1:A:66:ASN:O	1:A:67:SER:O	2.32	0.48
1:A:105:SER:O	1:A:106:TRP:O	2.32	0.48
1:A:176:PHE:O	1:A:179:ALA:HB3	2.13	0.48
1:A:391:LEU:HB3	1:A:407:CYS:HB3	1.96	0.48
1:A:849:MET:HE2	1:A:853:ASN:O	2.14	0.48
1:A:887:LEU:HD23	1:A:887:LEU:HA	1.65	0.48
1:B:100:GLY:HA3	1:B:166:VAL:O	2.13	0.48
1:A:97:ILE:HD13	1:A:108:LEU:CD1	2.42	0.48
1:A:105:SER:O	1:A:108:LEU:CB	2.62	0.48
1:A:467:ILE:CD1	1:A:472:VAL:CG2	2.92	0.48
1:A:686:THR:HG21	2:A:977:HOH:O	2.14	0.48
1:A:850:ASP:OD2	2:A:935:HOH:O	2.20	0.48
1:B:21:HIS:HD2	1:B:142:GLN:HE22	1.59	0.48
1:B:430:THR:HG23	1:B:468:ASN:HB3	1.96	0.48
1:A:309:PRO:C	1:A:311:GLU:N	2.72	0.48
1:B:284:MET:CG	1:B:284:MET:CA	2.80	0.48
1:B:646:GLN:O	1:B:647:VAL:C	2.56	0.48
1:A:30:GLN:NE2	1:A:187:LYS:NZ	2.49	0.47
1:A:146:PHE:HB3	1:A:416:LYS:HG2	1.96	0.47
1:A:267:THR:CB	1:A:319:MET:HE1	2.43	0.47
1:A:358:THR:CG2	1:A:359:THR:H	2.25	0.47
1:A:403:ARG:HB3	1:A:477:ARG:HD2	1.96	0.47
1:B:383:VAL:O	1:B:383:VAL:HG13	2.13	0.47
1:B:525:LYS:O	1:B:526:VAL:O	2.31	0.47
1:B:616:PHE:CZ	1:B:631:MET:O	2.67	0.47
1:B:83:SER:O	1:B:85:PRO:HD3	2.14	0.47
1:B:116:LEU:CD1	1:B:287:PRO:HG3	2.34	0.47
1:B:369:SER:O	1:B:383:VAL:HG11	2.13	0.47
1:B:537:LYS:CB	1:B:537:LYS:HZ3	2.25	0.47
1:B:697:LEU:HA	1:B:700:SER:HG	1.78	0.47
1:A:60:PHE:O	1:A:61:LYS:CB	2.62	0.47
1:A:242:ILE:CD1	1:A:242:ILE:CB	2.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:LYS:CE	1:A:307:VAL:H	2.26	0.47
1:B:109:ALA:O	1:B:113:SER:HB3	2.14	0.47
1:B:115:THR:O	1:B:116:LEU:C	2.56	0.47
1:B:282:ILE:HG22	1:B:326:MET:HG3	1.96	0.47
1:B:303:GLU:O	1:B:303:GLU:HG2	2.03	0.47
1:B:412:ALA:CB	1:B:473:SER:HB2	2.43	0.47
1:B:764:PHE:CE1	1:B:851:PHE:O	2.66	0.47
1:A:117:ASN:OD1	1:A:117:ASN:C	2.57	0.47
1:A:743:THR:O	1:A:747:ASN:OD1	2.32	0.47
1:B:304:TRP:CE2	1:B:312:ARG:HD3	2.50	0.47
1:B:862:ASP:CG	1:B:866:ARG:HE	2.21	0.47
1:B:868:PHE:HZ	1:B:878:GLN:HA	1.80	0.47
1:A:258:LEU:HD22	1:A:258:LEU:O	2.09	0.47
1:A:304:TRP:CZ2	1:A:317:VAL:HG13	2.50	0.47
1:A:327:SER:N	1:A:329:ARG:HH12	2.06	0.47
1:A:576:LEU:O	1:A:580:ARG:CB	2.63	0.47
1:A:874:ASN:C	1:A:876:THR:N	2.72	0.47
1:B:8:LEU:C	1:B:10:LYS:N	2.73	0.47
1:B:228:ILE:CG2	1:B:228:ILE:CA	2.84	0.47
1:B:342:ASN:ND2	1:B:346:ASP:OD2	2.47	0.47
1:B:451:ARG:HD2	2:B:902:HOH:O	2.14	0.47
1:B:585:LEU:CD1	1:B:672:GLU:HG2	2.43	0.47
1:A:32:TYR:HB2	1:A:153:VAL:CG2	2.44	0.47
1:A:98:CYS:O	1:A:99:GLN:C	2.58	0.47
1:A:756:HIS:HB2	1:A:757:PRO:HD2	1.94	0.47
1:A:803:TYR:N	1:A:822:ALA:HB1	2.29	0.47
1:A:874:ASN:O	1:A:875:GLY:C	2.51	0.47
1:B:364:THR:HG1	1:B:646:GLN:NE2	1.95	0.47
1:B:377:TYR:O	1:B:379:ALA:N	2.47	0.47
1:B:389:ILE:N	1:B:389:ILE:CD1	2.54	0.47
1:B:764:PHE:HE1	1:B:851:PHE:O	1.97	0.47
1:A:93:THR:HB	1:A:321:ASP:OD2	2.15	0.47
1:A:100:GLY:C	1:A:103:GLY:H	2.23	0.47
1:A:174:ASN:CG	1:A:174:ASN:H	2.23	0.47
1:A:229:LEU:O	1:A:232:LEU:N	2.47	0.47
1:A:263:ALA:HB2	1:A:288:TRP:HZ3	1.78	0.47
1:A:296:PRO:HG3	1:A:304:TRP:HB2	1.93	0.47
1:A:368:GLY:HA2	1:A:627:TYR:CE1	2.49	0.47
1:A:578:SER:C	1:A:582:MET:HG3	2.40	0.47
1:A:820:PRO:HD2	2:A:928:HOH:O	2.14	0.47
1:A:822:ALA:HA	2:A:912:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:SER:OG	1:B:336:THR:HG22	2.14	0.47
1:B:328:PHE:CZ	1:B:331:PHE:CE2	3.02	0.47
1:B:517:ILE:CG2	1:B:883:ILE:HG13	2.43	0.47
1:B:553:LYS:CB	1:B:553:LYS:C	2.77	0.47
1:B:558:ILE:O	1:B:559:LEU:C	2.58	0.47
1:B:626:ALA:C	1:B:628:GLU:H	2.23	0.47
1:A:84:ASN:OD1	1:A:84:ASN:C	2.58	0.47
1:A:146:PHE:CD1	1:A:416:LYS:HA	2.50	0.47
1:A:224:LEU:HD22	1:A:224:LEU:O	2.15	0.47
1:A:429:GLU:CD	1:A:494:LYS:HE3	2.40	0.47
1:B:112:ALA:O	1:B:115:THR:HB	2.14	0.47
1:B:375:ARG:HH11	1:B:375:ARG:CB	2.15	0.47
1:A:120:ILE:CD1	1:A:237:LEU:HD21	2.45	0.47
1:B:332:ILE:HG22	1:B:333:ARG:N	2.29	0.47
1:B:538:THR:CG2	1:B:539:LEU:N	2.58	0.47
1:B:626:ALA:CB	1:B:649:VAL:HG22	2.37	0.47
1:B:663:ASN:O	1:B:664:PHE:C	2.58	0.47
1:B:670:ARG:HG3	1:B:674:LEU:CD2	2.45	0.47
1:B:789:PHE:HD2	1:B:789:PHE:O	1.98	0.47
1:B:858:LEU:C	1:B:860:ARG:N	2.70	0.47
1:B:617:ASP:CG	1:B:617:ASP:O	2.47	0.47
1:A:386:GLN:HB3	1:A:513:LEU:CB	2.41	0.46
1:A:599:PHE:C	1:A:599:PHE:HD2	2.17	0.46
1:B:108:LEU:HD12	1:B:108:LEU:HA	1.58	0.46
1:B:136:ALA:N	1:B:136:ALA:CB	2.67	0.46
1:B:411:LEU:CD1	1:B:502:PHE:CE1	2.98	0.46
1:B:675:PHE:O	1:B:678:PHE:HB3	2.15	0.46
1:B:681:LEU:C	1:B:683:PRO:CD	2.88	0.46
1:A:98:CYS:SG	1:A:169:HIS:CE1	3.08	0.46
1:A:100:GLY:HA3	1:A:103:GLY:CA	2.39	0.46
1:A:256:LYS:C	1:A:258:LEU:HD13	2.41	0.46
1:A:386:GLN:O	1:A:387:PHE:CG	2.69	0.46
1:A:411:LEU:HD22	1:A:433:PHE:CE1	2.50	0.46
1:A:478:LEU:HD23	1:A:478:LEU:HA	1.36	0.46
1:A:809:ASP:O	1:A:810:ARG:C	2.58	0.46
1:B:28:LEU:C	1:B:30:GLN:N	2.71	0.46
1:B:197:GLY:C	1:B:198:GLY:O	2.58	0.46
1:B:327:SER:OG	1:B:329:ARG:HB2	2.15	0.46
1:B:453:PHE:CD2	1:B:453:PHE:O	2.67	0.46
1:B:585:LEU:O	1:B:586:MET:O	2.33	0.46
1:A:48:ASP:OD2	1:A:187:LYS:HE3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:GLU:C	1:A:313:GLU:H	2.22	0.46
1:A:571:THR:CG2	1:A:572:ASN:H	2.29	0.46
1:A:758:ASP:O	1:A:759:LEU:CB	2.58	0.46
1:B:511:GLN:CB	2:B:899:HOH:O	2.63	0.46
1:A:46:PHE:CD2	1:A:138:ILE:HD12	2.51	0.46
1:A:50:ALA:O	1:A:52:PRO:HD3	2.13	0.46
1:A:236:SER:C	1:A:238:LEU:HD12	2.40	0.46
1:A:374:CYS:C	1:A:381:PHE:CD1	2.94	0.46
1:A:579:CYS:HA	1:A:582:MET:CE	2.46	0.46
1:A:670:ARG:O	1:A:673:ILE:N	2.48	0.46
1:B:230:LYS:CD	1:B:230:LYS:NZ	2.68	0.46
1:B:284:MET:HB2	1:B:324:PHE:CZ	2.51	0.46
1:B:476:ILE:HG22	1:B:478:LEU:HG	1.98	0.46
1:A:229:LEU:O	1:A:230:LYS:C	2.57	0.46
1:A:487:PRO:O	1:A:488:SER:CB	2.57	0.46
1:A:693:LEU:HA	1:A:868:PHE:CE2	2.50	0.46
1:B:90:ASP:OD1	1:B:92:ALA:O	2.34	0.46
1:B:146:PHE:HA	1:B:414:MET:HE2	1.98	0.46
1:B:193:GLU:O	1:B:196:SER:OG	2.24	0.46
1:B:206:ASP:CG	1:B:470:ARG:HH22	2.24	0.46
1:B:521:LEU:HB3	1:B:522:PRO:CD	2.46	0.46
1:A:51:PHE:CB	1:A:187:LYS:HG3	2.46	0.46
1:A:585:LEU:HD11	1:A:605:ARG:NH2	2.30	0.46
1:A:686:THR:CG2	2:A:977:HOH:O	2.63	0.46
1:B:279:VAL:HG23	1:B:281:LEU:HD23	1.98	0.46
1:B:492:PRO:C	1:B:494:LYS:H	2.21	0.46
1:A:429:GLU:CG	1:A:494:LYS:HE3	2.46	0.46
1:A:629:MET:HE3	1:A:633:ILE:HD11	1.98	0.46
1:A:829:HIS:CE1	2:A:917:HOH:O	2.69	0.46
1:B:430:THR:H	1:B:494:LYS:HZ1	1.63	0.46
1:B:652:PHE:HE1	1:B:891:MET:CE	2.28	0.46
1:A:96:ASP:O	1:A:97:ILE:O	2.33	0.46
1:A:652:PHE:CD1	1:A:667:CYS:CB	2.94	0.46
1:A:748:ILE:HG23	1:A:749:LEU:H	1.81	0.46
1:B:430:THR:HA	1:B:468:ASN:HB3	1.97	0.46
1:B:636:ALA:CB	1:B:668:LEU:HD13	2.46	0.46
1:A:88:ILE:HA	1:A:175:GLU:CG	2.45	0.46
1:A:693:LEU:HA	1:A:868:PHE:CZ	2.51	0.46
1:B:228:ILE:O	1:B:232:LEU:HD23	2.16	0.46
1:B:340:ILE:CD1	1:B:340:ILE:HG12	2.20	0.46
1:B:390:ARG:HH11	1:B:390:ARG:CG	2.07	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:875:GLY:C	1:B:877:GLY:H	2.22	0.46
1:A:223:ASP:CG	1:A:227:ILE:HD11	2.41	0.46
1:A:327:SER:OG	1:A:329:ARG:NE	2.49	0.46
1:A:467:ILE:HD12	1:A:472:VAL:CG2	2.45	0.46
1:A:677:ILE:HG22	1:A:678:PHE:N	2.29	0.46
1:A:677:ILE:C	1:A:679:LYS:N	2.74	0.46
1:B:110:ALA:HA	1:B:204:PHE:CE2	2.51	0.46
1:B:576:LEU:O	1:B:578:SER:CA	2.62	0.46
1:B:673:ILE:HG22	1:B:677:ILE:CD1	2.46	0.46
1:B:780:THR:CG2	1:B:780:THR:OG1	2.55	0.46
1:A:232:LEU:HA	1:A:232:LEU:HD13	1.76	0.45
1:A:328:PHE:C	1:A:330:ASP:H	2.24	0.45
1:A:450:LYS:HB3	1:A:451:ARG:H	1.62	0.45
1:A:600:ASN:C	1:A:602:LEU:H	2.22	0.45
1:A:741:SER:O	1:A:742:ALA:C	2.56	0.45
1:A:852:ASP:OD2	1:A:852:ASP:C	2.59	0.45
1:B:328:PHE:CD2	1:B:331:PHE:CE2	3.05	0.45
1:B:335:PHE:CG	1:B:335:PHE:C	2.94	0.45
1:B:456:ALA:O	1:B:457:ASN:C	2.58	0.45
1:B:552:VAL:O	1:B:554:GLU:N	2.49	0.45
1:A:745:LEU:HD12	1:A:749:LEU:HD21	1.99	0.45
1:B:66:ASN:O	1:B:67:SER:O	2.34	0.45
1:B:89:VAL:CG1	1:B:89:VAL:CG2	2.88	0.45
1:B:696:TRP:O	1:B:700:SER:CB	2.63	0.45
1:B:805:ARG:N	1:B:811:SER:OG	2.30	0.45
1:A:60:PHE:N	1:A:64:GLY:HA3	2.31	0.45
1:A:576:LEU:CA	1:A:579:CYS:HB2	2.46	0.45
1:A:628:GLU:C	1:A:630:ARG:N	2.73	0.45
1:A:731:VAL:HG23	1:A:732:GLN:N	2.31	0.45
1:B:625:SER:O	1:B:626:ALA:C	2.55	0.45
1:A:26:LYS:HD3	1:A:26:LYS:HA	1.67	0.45
1:A:27:TYR:O	1:A:30:GLN:HG3	2.17	0.45
1:A:268:ASP:HB3	1:A:283:ARG:HB3	1.97	0.45
1:A:273:THR:OG1	1:A:312:ARG:NH2	2.49	0.45
1:A:305:ASN:ND2	1:A:305:ASN:N	2.64	0.45
1:A:625:SER:O	1:A:626:ALA:C	2.54	0.45
1:A:757:PRO:HG3	2:A:1029:HOH:O	2.16	0.45
1:A:872:ASP:HB2	1:A:879:ILE:HG22	1.97	0.45
1:B:492:PRO:HB2	1:B:493:ASN:CG	2.42	0.45
1:B:583:VAL:O	1:B:584:ASN:HB2	2.16	0.45
1:B:692:ASP:C	1:B:692:ASP:OD1	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:HIS:ND1	2:A:1060:HOH:O	2.05	0.45
1:A:223:ASP:CG	1:A:227:ILE:CD1	2.90	0.45
1:B:12:ARG:O	1:B:16:GLU:HG3	2.17	0.45
1:B:61:LYS:O	1:B:62:GLU:HB2	2.15	0.45
1:B:681:LEU:O	1:B:683:PRO:HD2	2.15	0.45
1:B:719:GLU:CD	1:B:719:GLU:N	2.75	0.45
1:A:388:LYS:NZ	1:A:482:GLU:HG2	2.32	0.45
1:A:479:PRO:O	1:A:480:PRO:C	2.51	0.45
1:B:656:GLU:O	1:B:657:LEU:CB	2.64	0.45
1:B:796:ILE:O	1:B:799:TRP:CB	2.62	0.45
1:A:21:HIS:NE2	1:A:123:ARG:O	2.50	0.45
1:A:159:PRO:C	1:A:160:THR:CG2	2.89	0.45
1:A:283:ARG:HB2	1:A:325:TRP:CE2	2.51	0.45
1:A:335:PHE:C	1:A:335:PHE:HD1	2.25	0.45
1:A:433:PHE:HE2	1:A:472:VAL:HG12	1.82	0.45
1:A:674:LEU:O	1:A:675:PHE:C	2.57	0.45
1:A:739:GLU:HA	2:A:979:HOH:O	2.17	0.45
1:B:135:TYR:CG	1:B:136:ALA:N	2.83	0.45
1:B:256:LYS:HB3	1:B:256:LYS:CE	2.46	0.45
1:B:476:ILE:HG22	1:B:477:ARG:N	2.32	0.45
1:B:799:TRP:HZ2	1:B:828:PHE:HE1	1.64	0.45
1:B:822:ALA:O	1:B:825:ALA:CB	2.56	0.45
1:A:56:HIS:C	1:A:58:LEU:N	2.73	0.45
1:A:68:SER:OG	1:A:69:LYS:N	2.50	0.45
1:A:571:THR:HG22	1:A:572:ASN:H	1.81	0.45
1:A:604:ASN:HD22	1:A:604:ASN:N	2.14	0.45
1:A:760:LYS:HE3	1:A:760:LYS:HA	1.99	0.45
1:A:883:ILE:CG2	1:A:883:ILE:CA	2.84	0.45
1:B:468:ASN:O	1:B:468:ASN:CG	2.58	0.45
1:B:557:THR:HG22	1:B:558:ILE:N	2.32	0.45
1:B:828:PHE:HZ	1:B:862:ASP:OD1	2.00	0.45
1:B:871:LEU:N	1:B:871:LEU:HD12	2.31	0.45
1:A:58:LEU:O	1:A:63:LEU:HG	2.16	0.45
1:A:212:THR:HG21	1:A:340:ILE:HD12	1.99	0.45
1:A:352:THR:O	1:A:352:THR:OG1	2.34	0.45
1:A:656:GLU:O	1:A:657:LEU:CB	2.65	0.45
1:A:828:PHE:N	1:A:828:PHE:CD1	2.85	0.45
1:A:878:GLN:HE21	1:A:878:GLN:HB3	1.52	0.45
1:B:69:LYS:HG2	1:B:102:LEU:CD1	2.47	0.45
1:B:502:PHE:CB	1:B:510:THR:HG21	2.47	0.45
1:B:643:GLN:CD	1:B:643:GLN:CB	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:TRP:CE3	1:B:700:SER:HB3	2.52	0.45
1:A:32:TYR:HB2	1:A:153:VAL:HG23	1.98	0.45
1:B:242:ILE:C	1:B:242:ILE:CD1	2.90	0.45
1:B:328:PHE:CD2	1:B:331:PHE:CZ	3.04	0.45
1:B:466:PHE:O	1:B:467:ILE:C	2.60	0.45
1:B:651:ARG:CZ	1:B:670:ARG:HH22	2.23	0.45
1:A:10:LYS:N	1:A:10:LYS:HD2	2.32	0.44
1:A:14:ALA:C	1:A:16:GLU:N	2.75	0.44
1:A:78:PRO:HB3	1:A:176:PHE:CE2	2.52	0.44
1:A:355:ASN:O	1:A:356:TRP:CB	2.63	0.44
1:A:521:LEU:N	1:A:522:PRO:CD	2.79	0.44
1:B:21:HIS:CE1	1:B:123:ARG:NE	2.85	0.44
1:B:48:ASP:CB	1:B:155:ASP:OD1	2.65	0.44
1:B:87:PHE:HE1	1:B:180:LEU:HD12	1.82	0.44
1:B:856:SER:C	1:B:858:LEU:H	2.24	0.44
1:A:94:ARG:N	1:A:321:ASP:OD2	2.50	0.44
1:A:106:TRP:CZ3	1:A:198:GLY:HA3	2.49	0.44
1:A:491:GLU:H	1:A:491:GLU:HG3	1.55	0.44
1:A:618:LEU:HD23	1:A:618:LEU:H	1.82	0.44
1:A:682:ASP:HB2	1:A:689:ILE:HG22	1.99	0.44
1:B:156:ASP:OD2	1:B:156:ASP:N	2.49	0.44
1:B:348:LEU:C	1:B:349:LYS:O	2.54	0.44
1:B:628:GLU:O	1:B:631:MET:N	2.45	0.44
1:B:783:LYS:C	1:B:784:LEU:HD12	2.41	0.44
1:A:89:VAL:N	1:A:175:GLU:CD	2.68	0.44
1:A:284:MET:O	1:A:323:GLU:O	2.35	0.44
1:A:353:LEU:C	1:A:354:ARG:HG2	2.42	0.44
1:A:389:ILE:HD11	1:A:485:VAL:HG11	1.99	0.44
1:B:212:THR:O	1:B:212:THR:CG2	2.62	0.44
1:B:328:PHE:CG	1:B:331:PHE:HE2	2.35	0.44
1:B:388:LYS:NZ	1:B:388:LYS:HB2	2.32	0.44
1:B:585:LEU:HB3	1:B:586:MET:H	1.54	0.44
1:B:614:ARG:HA	1:B:614:ARG:HD2	1.56	0.44
1:B:648:ILE:O	1:B:649:VAL:C	2.60	0.44
1:A:88:ILE:HA	1:A:175:GLU:HG2	1.99	0.44
1:A:89:VAL:N	1:A:175:GLU:OE1	2.49	0.44
1:A:135:TYR:OH	1:A:156:ASP:OD1	2.27	0.44
1:A:270:LYS:CB	1:A:325:TRP:CH2	2.89	0.44
1:A:355:ASN:O	1:A:356:TRP:HB2	2.18	0.44
1:A:433:PHE:CE2	1:A:463:SER:HB3	2.53	0.44
1:A:759:LEU:CD1	1:A:812:GLY:HA2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:SER:HA	1:B:116:LEU:HD13	1.99	0.44
1:B:453:PHE:O	1:B:457:ASN:OD1	2.35	0.44
1:B:459:SER:HB2	1:B:461:ALA:H	1.82	0.44
1:B:579:CYS:O	1:B:580:ARG:C	2.60	0.44
1:B:651:ARG:CZ	1:B:891:MET:HA	2.48	0.44
1:A:23:ARG:HH11	1:A:23:ARG:CG	2.31	0.44
1:A:386:GLN:HB2	1:A:513:LEU:O	2.18	0.44
1:A:505:GLU:CG	1:A:505:GLU:O	2.66	0.44
1:A:731:VAL:CG2	1:A:733:LEU:CG	2.88	0.44
1:A:776:MET:HB3	1:A:776:MET:HE3	1.51	0.44
1:B:80:GLU:O	1:B:81:LEU:CD2	2.61	0.44
1:B:438:VAL:HG12	1:B:439:PRO:HD2	2.00	0.44
1:B:628:GLU:OE1	1:B:631:MET:HE1	2.17	0.44
1:A:114:LEU:HD13	1:A:121:LEU:CD2	2.44	0.44
1:A:502:PHE:N	1:A:502:PHE:CD1	2.85	0.44
1:A:208:THR:O	1:A:343:LEU:HD11	2.18	0.44
1:A:313:GLU:O	1:A:313:GLU:CG	2.63	0.44
1:A:380:THR:C	1:A:382:TRP:N	2.73	0.44
1:A:626:ALA:O	1:A:628:GLU:N	2.51	0.44
1:A:824:GLU:C	1:A:826:ALA:N	2.74	0.44
1:B:584:ASN:HD22	1:B:584:ASN:HA	1.62	0.44
1:B:883:ILE:CA	1:B:883:ILE:CG1	2.82	0.44
1:A:27:TYR:CE2	1:A:28:LEU:HG	2.53	0.44
1:A:200:THR:CB	1:A:200:THR:N	2.69	0.44
1:B:332:ILE:C	1:B:332:ILE:HG22	2.40	0.44
1:B:382:TRP:O	1:B:448:HIS:HE1	2.00	0.44
1:B:523:ASP:C	1:B:524:GLU:OE1	2.59	0.44
1:B:582:MET:HG2	1:B:602:LEU:HD21	1.99	0.44
1:A:94:ARG:HD3	2:A:1049:HOH:O	2.13	0.44
1:A:177:TRP:CG	1:A:178:SER:H	2.36	0.44
1:A:281:LEU:HD21	1:A:297:TRP:CZ2	2.53	0.44
1:A:319:MET:SD	1:A:322:GLY:O	2.76	0.44
1:A:677:ILE:O	1:A:679:LYS:N	2.50	0.44
1:A:869:ARG:O	1:A:870:SER:C	2.61	0.44
1:B:100:GLY:N	2:B:903:HOH:O	2.48	0.44
1:B:277:GLN:HA	1:B:277:GLN:NE2	2.32	0.44
1:B:318:LYS:O	1:B:320:GLU:HG2	2.18	0.44
1:B:651:ARG:CD	1:B:893:SER:OXT	2.64	0.44
1:A:13:GLU:O	1:A:16:GLU:CA	2.66	0.43
1:A:227:ILE:O	1:A:228:ILE:C	2.60	0.43
1:B:242:ILE:O	1:B:242:ILE:CG2	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:TRP:CD1	1:B:324:PHE:CD1	3.06	0.43
1:B:365:TRP:CZ2	1:B:488:SER:HA	2.53	0.43
1:B:644:LEU:HA	1:B:647:VAL:HG22	1.98	0.43
1:A:283:ARG:NH1	1:A:319:MET:HE3	2.33	0.43
1:A:435:VAL:HG13	1:A:461:ALA:HB3	2.00	0.43
1:A:509:GLY:C	1:A:510:THR:HG23	2.42	0.43
1:A:631:MET:SD	1:A:631:MET:HB2	2.57	0.43
1:A:632:ALA:O	1:A:633:ILE:C	2.58	0.43
1:A:803:TYR:CA	1:A:822:ALA:HB2	2.46	0.43
1:B:28:LEU:O	1:B:30:GLN:N	2.51	0.43
1:B:572:ASN:C	1:B:572:ASN:CB	2.79	0.43
1:B:697:LEU:CA	1:B:700:SER:OG	2.66	0.43
1:B:837:MET:CE	1:B:837:MET:CG	2.93	0.43
1:A:225:TYR:CZ	1:A:280:ASN:HB3	2.54	0.43
1:A:284:MET:HE2	1:A:326:MET:CG	2.48	0.43
1:A:824:GLU:HA	1:A:828:PHE:C	2.43	0.43
1:A:830:LEU:C	1:A:831:ASN:O	2.57	0.43
1:B:230:LYS:CE	1:B:230:LYS:CG	2.86	0.43
1:B:349:LYS:HG2	1:B:350:SER:N	2.34	0.43
1:B:610:LEU:CD1	1:B:610:LEU:CD2	2.86	0.43
1:B:792:LEU:HD12	1:B:792:LEU:HA	1.94	0.43
1:B:858:LEU:C	1:B:860:ARG:H	2.26	0.43
1:A:255:PHE:CB	1:A:333:ARG:HG2	2.48	0.43
1:A:679:LYS:O	1:A:682:ASP:O	2.36	0.43
1:B:60:PHE:CE2	1:B:193:GLU:CG	3.01	0.43
1:B:327:SER:C	1:B:329:ARG:N	2.74	0.43
1:B:576:LEU:O	1:B:578:SER:C	2.61	0.43
1:A:293:TRP:CH2	1:A:326:MET:CB	3.01	0.43
1:A:403:ARG:CG	1:A:477:ARG:NE	2.81	0.43
1:A:603:TRP:CD1	1:A:604:ASN:HD22	2.36	0.43
1:B:381:PHE:O	1:B:382:TRP:C	2.59	0.43
1:A:63:LEU:HD12	1:A:70:THR:HG21	1.88	0.43
1:A:291:VAL:HG23	1:A:292:GLU:H	1.83	0.43
1:A:372:GLY:C	1:A:492:PRO:HB3	2.44	0.43
1:A:411:LEU:CD1	1:A:485:VAL:HG21	2.45	0.43
1:A:464:GLU:C	1:A:465:HIS:ND1	2.76	0.43
1:A:484:ILE:CD1	1:A:486:VAL:CG2	2.97	0.43
1:A:701:VAL:O	1:A:701:VAL:CG1	2.64	0.43
1:A:881:VAL:CG1	1:A:885:GLU:HB2	2.48	0.43
1:B:312:ARG:CG	1:B:312:ARG:NE	2.74	0.43
1:B:312:ARG:HG2	1:B:313:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:LYS:CG	1:B:350:SER:N	2.77	0.43
1:B:626:ALA:C	1:B:628:GLU:N	2.77	0.43
1:B:674:LEU:HD22	1:B:674:LEU:H	1.82	0.43
1:B:701:VAL:CG1	1:B:860:ARG:CD	2.97	0.43
1:B:729:LEU:CD2	1:B:729:LEU:CB	2.84	0.43
1:B:746:MET:HE3	2:B:965:HOH:O	2.18	0.43
1:A:51:PHE:N	1:A:52:PRO:CD	2.82	0.43
1:A:69:LYS:HB2	1:A:69:LYS:HE3	1.76	0.43
1:A:75:TRP:CE3	1:A:159:PRO:HG3	2.48	0.43
1:A:157:LEU:O	1:A:158:LEU:HG	2.17	0.43
1:A:370:THR:O	1:A:384:ASN:HA	2.19	0.43
1:A:824:GLU:CB	1:A:829:HIS:HA	2.48	0.43
1:B:387:PHE:CD2	1:B:387:PHE:N	2.86	0.43
1:B:595:GLY:HA3	1:B:598:GLU:OE1	2.18	0.43
1:A:88:ILE:C	1:A:89:VAL:CG2	2.91	0.43
1:A:293:TRP:CE3	1:A:295:GLY:O	2.71	0.43
1:B:100:GLY:HA3	1:B:167:PHE:HA	2.01	0.43
1:B:200:THR:H	1:B:200:THR:HG22	1.28	0.43
1:A:54:VAL:HB	1:A:55:SER:H	1.48	0.43
1:A:144:TRP:CZ2	1:A:147:GLY:HA2	2.54	0.43
1:A:633:ILE:O	1:A:636:ALA:HB3	2.18	0.43
1:B:215:TYR:HB2	1:B:337:LYS:HZ3	1.83	0.43
1:B:282:ILE:HG21	1:B:282:ILE:HD13	1.72	0.43
1:B:285:ARG:HA	1:B:322:GLY:O	2.18	0.43
1:A:140:HIS:HB3	1:A:153:VAL:CG2	2.49	0.43
1:A:393:GLU:HB2	1:A:506:LYS:HG2	2.01	0.43
1:A:668:LEU:HA	1:A:668:LEU:HD23	1.72	0.43
1:B:13:GLU:O	1:B:14:ALA:C	2.61	0.43
1:A:273:THR:H	1:A:312:ARG:NH2	2.14	0.42
1:A:517:ILE:HG23	1:A:640:LEU:HD23	2.00	0.42
1:A:543:LEU:CB	1:A:596:LEU:CB	2.97	0.42
1:A:693:LEU:O	1:A:697:LEU:HG	2.18	0.42
1:A:800:GLN:CG	1:A:851:PHE:HE1	2.32	0.42
1:B:21:HIS:CE1	2:B:945:HOH:O	2.71	0.42
1:B:110:ALA:O	1:B:111:ILE:C	2.56	0.42
1:B:204:PHE:CB	1:B:340:ILE:HG13	2.44	0.42
1:B:860:ARG:NH1	1:B:860:ARG:HG3	2.34	0.42
1:A:174:ASN:CG	1:A:174:ASN:N	2.76	0.42
1:A:207:PHE:C	1:A:208:THR:CG2	2.92	0.42
1:A:555:LEU:HD23	1:A:582:MET:HE3	2.02	0.42
1:B:18:LEU:HA	1:B:18:LEU:HD12	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:GLU:O	1:B:578:SER:O	2.37	0.42
1:B:624:MET:O	1:B:658:ILE:HD11	2.19	0.42
1:B:641:PRO:O	1:B:642:CYS:C	2.60	0.42
1:A:129:GLN:OE1	1:A:139:PHE:HB3	2.20	0.42
1:A:240:CYS:SG	1:A:266:VAL:HG23	2.60	0.42
1:A:268:ASP:CG	1:A:269:ALA:N	2.77	0.42
1:A:386:GLN:HG2	1:A:484:ILE:HD11	2.02	0.42
1:A:758:ASP:O	1:A:759:LEU:O	2.37	0.42
1:A:775:VAL:HG12	1:A:776:MET:N	2.29	0.42
1:B:242:ILE:HD13	1:B:243:ASN:CB	2.49	0.42
1:B:484:ILE:HD12	1:B:513:LEU:CD2	2.48	0.42
1:B:644:LEU:HD23	1:B:647:VAL:HG21	2.02	0.42
1:B:652:PHE:CE1	1:B:891:MET:HE1	2.55	0.42
1:B:681:LEU:C	1:B:683:PRO:HD3	2.44	0.42
1:A:97:ILE:O	1:A:98:CYS:CB	2.64	0.42
1:A:109:ALA:HB2	1:A:262:HIS:O	2.19	0.42
1:A:237:LEU:HB2	1:A:340:ILE:HG12	2.01	0.42
1:A:329:ARG:HH21	1:A:333:ARG:NH1	2.17	0.42
1:A:660:ASP:C	1:A:660:ASP:OD1	2.61	0.42
1:A:850:ASP:O	1:A:851:PHE:C	2.63	0.42
1:B:485:VAL:HG11	1:B:502:PHE:HZ	1.84	0.42
1:B:613:PHE:HZ	1:B:623:SER:CA	2.33	0.42
1:A:503:PHE:N	1:A:503:PHE:CD1	2.87	0.42
1:A:614:ARG:NH1	1:A:620:LYS:HB3	2.31	0.42
1:A:833:HIS:CD2	1:A:834:ILE:N	2.87	0.42
1:B:118:GLU:O	1:B:119:THR:C	2.58	0.42
1:B:284:MET:O	1:B:323:GLU:HA	2.19	0.42
1:B:313:GLU:OE1	1:B:313:GLU:N	2.52	0.42
1:B:670:ARG:O	1:B:673:ILE:HB	2.20	0.42
1:A:59:GLY:HA3	1:A:193:GLU:OE2	2.19	0.42
1:A:327:SER:N	1:A:329:ARG:HH11	1.99	0.42
1:A:678:PHE:CE2	1:A:689:ILE:HG12	2.54	0.42
1:B:340:ILE:CD1	1:B:340:ILE:HG23	2.50	0.42
1:B:525:LYS:H	1:B:525:LYS:HG2	1.51	0.42
1:B:772:MET:HE3	1:B:856:SER:HA	2.01	0.42
1:B:827:GLY:O	1:B:828:PHE:CD2	2.72	0.42
1:A:204:PHE:HE2	1:A:237:LEU:CD1	2.33	0.42
1:B:2:ALA:CB	2:B:999:HOH:O	2.67	0.42
1:B:671:LEU:O	1:B:674:LEU:HB2	2.19	0.42
1:B:772:MET:CE	1:B:772:MET:CG	2.96	0.42
1:B:856:SER:O	1:B:858:LEU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:LYS:CA	1:A:258:LEU:CD1	2.97	0.42
1:A:349:LYS:CG	1:A:349:LYS:O	2.68	0.42
1:A:403:ARG:HB3	1:A:477:ARG:CD	2.50	0.42
1:A:741:SER:O	1:A:745:LEU:N	2.44	0.42
1:B:172:GLN:OE1	1:B:172:GLN:CA	2.66	0.42
1:B:579:CYS:HA	1:B:582:MET:HB2	2.00	0.42
1:B:696:TRP:O	1:B:700:SER:N	2.53	0.42
1:A:77:ARG:HG3	1:A:157:LEU:HD12	2.02	0.42
1:B:313:GLU:CG	1:B:313:GLU:HA	2.47	0.42
1:B:487:PRO:O	1:B:488:SER:CB	2.58	0.42
1:B:503:PHE:N	1:B:503:PHE:CD1	2.88	0.42
1:B:677:ILE:HG22	1:B:681:LEU:CD1	2.50	0.42
1:B:766:ILE:HG23	1:B:767:ASP:N	2.34	0.42
1:B:796:ILE:C	1:B:799:TRP:HB2	2.44	0.42
1:A:32:TYR:O	1:A:36:ARG:N	2.53	0.42
1:A:77:ARG:CG	1:A:156:ASP:OD2	2.53	0.42
1:A:715:ILE:HA	1:A:715:ILE:HD12	1.60	0.42
1:B:33:GLU:OE1	1:B:37:ASN:OD1	2.38	0.42
1:B:61:LYS:CG	1:B:66:ASN:HB2	2.42	0.42
1:B:366:ARG:HH11	1:B:366:ARG:HD3	1.39	0.42
1:B:380:THR:O	1:B:381:PHE:C	2.59	0.42
1:B:682:ASP:N	1:B:683:PRO:CD	2.83	0.42
1:B:892:TYR:O	1:B:893:SER:HB2	2.20	0.42
1:A:93:THR:CB	1:A:321:ASP:OD2	2.67	0.41
1:A:857:CYS:C	1:A:859:VAL:N	2.76	0.41
1:B:100:GLY:HA3	1:B:167:PHE:CA	2.50	0.41
1:B:539:LEU:HD23	1:B:539:LEU:C	2.45	0.41
1:B:582:MET:HE1	1:B:606:ILE:HG12	2.01	0.41
1:B:774:ALA:C	1:B:776:MET:N	2.78	0.41
1:A:256:LYS:HD3	1:A:258:LEU:CD2	2.34	0.41
1:A:631:MET:O	1:A:632:ALA:C	2.62	0.41
1:A:688:THR:CG2	1:A:688:THR:N	2.82	0.41
1:A:745:LEU:HD12	1:A:749:LEU:HD23	2.01	0.41
1:B:12:ARG:O	1:B:15:ALA:HB3	2.20	0.41
1:A:285:ARG:O	1:A:287:PRO:HD3	2.19	0.41
1:A:364:THR:CG2	1:A:497:ASP:OD1	2.65	0.41
1:A:406:GLY:O	1:A:407:CYS:C	2.63	0.41
1:A:517:ILE:HG12	1:A:641:PRO:CD	2.50	0.41
1:A:579:CYS:O	1:A:580:ARG:C	2.62	0.41
1:A:663:ASN:O	1:A:664:PHE:O	2.38	0.41
1:A:738:MET:O	1:A:739:GLU:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:PHE:O	1:A:857:CYS:HB3	2.20	0.41
1:B:35:LEU:HD13	1:B:46:PHE:CZ	2.51	0.41
1:B:113:SER:OG	1:B:204:PHE:HE2	2.04	0.41
1:B:174:ASN:HD22	1:B:174:ASN:HA	1.41	0.41
1:B:179:ALA:O	1:B:182:GLU:HB3	2.19	0.41
1:B:610:LEU:HA	1:B:661:PHE:HE2	1.84	0.41
1:A:67:SER:O	1:A:70:THR:N	2.51	0.41
1:A:88:ILE:O	1:A:89:VAL:HG22	2.19	0.41
1:A:189:ASN:OD1	1:A:195:LEU:CD2	2.68	0.41
1:A:228:ILE:CG1	1:A:337:LYS:NZ	2.77	0.41
1:A:671:LEU:CB	1:A:671:LEU:C	2.80	0.41
1:A:856:SER:O	1:A:860:ARG:HG3	2.20	0.41
1:B:321:ASP:O	1:B:323:GLU:N	2.54	0.41
1:B:453:PHE:CE1	1:B:457:ASN:OD1	2.73	0.41
1:B:644:LEU:HA	1:B:647:VAL:CG2	2.49	0.41
1:A:88:ILE:C	1:A:89:VAL:HG22	2.45	0.41
1:A:349:LYS:O	1:A:349:LYS:HG3	2.20	0.41
1:A:823:PHE:O	1:A:826:ALA:N	2.52	0.41
1:B:35:LEU:HD13	1:B:46:PHE:HE1	1.80	0.41
1:B:78:PRO:CD	1:B:156:ASP:HB2	2.51	0.41
1:B:449:LEU:HD13	1:B:453:PHE:CD1	2.55	0.41
1:B:673:ILE:O	1:B:676:LYS:N	2.53	0.41
1:A:172:GLN:O	1:A:174:ASN:N	2.53	0.41
1:A:224:LEU:O	1:A:228:ILE:N	2.49	0.41
1:A:616:PHE:HD2	1:A:628:GLU:HG2	1.86	0.41
1:B:211:VAL:HG11	1:B:410:LEU:HD23	2.02	0.41
1:B:294:LYS:CG	1:B:294:LYS:CE	2.87	0.41
1:B:430:THR:N	1:B:468:ASN:HB2	2.35	0.41
1:B:469:LEU:O	1:B:470:ARG:C	2.63	0.41
1:A:177:TRP:CE3	1:A:178:SER:N	2.89	0.41
1:A:393:GLU:OE1	1:A:506:LYS:HG3	2.20	0.41
1:A:415:GLN:HE22	1:A:428:MET:HB3	1.86	0.41
1:B:581:SER:O	1:B:583:VAL:N	2.54	0.41
1:B:632:ALA:O	1:B:635:ALA:HB3	2.20	0.41
1:A:61:LYS:O	1:A:62:GLU:HB2	2.21	0.41
1:A:196:SER:O	1:A:197:GLY:O	2.38	0.41
1:A:435:VAL:CG1	1:A:461:ALA:O	2.69	0.41
1:A:571:THR:CG2	1:A:572:ASN:N	2.84	0.41
1:A:573:GLY:C	1:A:574:PHE:O	2.63	0.41
1:B:13:GLU:CD	1:B:18:LEU:HD23	2.45	0.41
1:B:95:THR:HG23	1:B:288:TRP:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:PHE:CD2	1:B:181:LEU:HD12	2.56	0.41
1:B:256:LYS:CB	1:B:256:LYS:CD	2.80	0.41
1:B:429:GLU:OE2	1:B:494:LYS:HB3	2.21	0.41
1:B:577:GLU:O	1:B:578:SER:C	2.64	0.41
1:A:10:LYS:HE3	2:A:1021:HOH:O	2.21	0.41
1:A:88:ILE:HG21	1:A:88:ILE:HD13	1.40	0.41
1:A:297:TRP:CD1	1:A:297:TRP:C	2.99	0.41
1:A:449:LEU:H	1:A:449:LEU:HG	1.55	0.41
1:A:575:SER:C	1:A:577:GLU:N	2.79	0.41
1:A:640:LEU:O	1:A:645:HIS:CD2	2.74	0.41
1:A:657:LEU:C	1:A:658:ILE:HD12	2.46	0.41
1:A:697:LEU:HD23	1:A:697:LEU:HA	1.66	0.41
1:A:756:HIS:O	1:A:757:PRO:O	2.39	0.41
1:A:765:GLY:O	1:A:766:ILE:C	2.63	0.41
1:B:37:ASN:HD22	1:B:37:ASN:HA	1.56	0.41
1:B:40:LEU:CD1	1:B:136:ALA:HB2	2.50	0.41
1:B:113:SER:HA	1:B:116:LEU:CD1	2.51	0.41
1:B:131:PHE:HA	1:B:135:TYR:CD1	2.56	0.41
1:B:284:MET:HB2	1:B:324:PHE:CE2	2.56	0.41
1:B:499:LEU:O	2:B:948:HOH:O	2.22	0.41
1:B:574:PHE:CZ	1:B:606:ILE:HD13	2.55	0.41
1:B:647:VAL:HG23	1:B:648:ILE:N	2.36	0.41
1:B:739:GLU:OE2	1:B:785:GLY:HA2	2.21	0.41
1:B:773:VAL:CB	1:B:784:LEU:HD11	2.51	0.41
1:A:56:HIS:C	1:A:58:LEU:H	2.27	0.41
1:A:388:LYS:HZ2	1:A:482:GLU:HG2	1.86	0.41
1:A:620:LYS:HB3	1:A:620:LYS:HE3	1.67	0.41
1:B:413:LEU:O	1:B:471:GLU:HA	2.21	0.41
1:B:651:ARG:HH12	1:B:670:ARG:NH1	2.09	0.41
1:B:853:ASN:HB3	1:B:854:PHE:H	1.71	0.41
1:B:865:PHE:O	1:B:866:ARG:C	2.60	0.41
1:A:64:GLY:HA3	1:A:65:PRO:HD3	1.89	0.40
1:A:440:ARG:HH21	1:A:440:ARG:HD2	1.71	0.40
1:A:479:PRO:HA	1:A:480:PRO:HD3	1.90	0.40
1:B:34:THR:O	1:B:35:LEU:C	2.62	0.40
1:B:35:LEU:O	1:B:36:ARG:C	2.62	0.40
1:B:120:ILE:HD11	1:B:342:ASN:HD21	1.86	0.40
1:B:237:LEU:C	1:B:238:LEU:HD12	2.46	0.40
1:B:409:PHE:N	1:B:409:PHE:CD2	2.88	0.40
1:B:438:VAL:CG2	1:B:484:ILE:HD11	2.47	0.40
1:B:456:ALA:O	1:B:457:ASN:O	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:VAL:HG23	1:B:594:LEU:HD13	2.02	0.40
1:B:696:TRP:CD2	1:B:700:SER:HB3	2.56	0.40
1:B:768:THR:O	1:B:772:MET:HG3	2.21	0.40
1:B:797:LYS:O	1:B:800:GLN:CB	2.68	0.40
1:A:317:VAL:HB	1:A:317:VAL:C	2.44	0.40
1:A:829:HIS:HE1	2:A:917:HOH:O	2.04	0.40
1:B:76:LYS:HD2	1:B:81:LEU:HD21	2.02	0.40
1:B:97:ILE:HG23	1:B:97:ILE:HD13	1.72	0.40
1:B:120:ILE:C	1:B:120:ILE:HG22	2.46	0.40
1:B:176:PHE:O	1:B:177:TRP:C	2.63	0.40
1:B:487:PRO:O	1:B:487:PRO:HG2	2.20	0.40
1:B:790:LYS:O	1:B:792:LEU:N	2.51	0.40
1:A:450:LYS:CE	1:A:631:MET:HG2	2.49	0.40
1:A:831:ASN:CA	2:A:919:HOH:O	2.68	0.40
1:B:242:ILE:CD1	1:B:243:ASN:N	2.74	0.40
1:B:327:SER:O	1:B:328:PHE:C	2.63	0.40
1:B:605:ARG:C	1:B:607:ARG:N	2.77	0.40
1:A:63:LEU:HB3	1:A:193:GLU:HG3	2.03	0.40
1:A:415:GLN:NE2	1:A:428:MET:HB3	2.37	0.40
1:A:756:HIS:CD2	1:A:757:PRO:CD	3.00	0.40
1:B:27:TYR:CE2	1:B:28:LEU:HD11	2.56	0.40
1:B:291:VAL:H	1:B:291:VAL:HG22	1.30	0.40
1:B:369:SER:OG	1:B:646:GLN:HG2	2.21	0.40
1:B:390:ARG:NH1	1:B:392:GLU:OE1	2.53	0.40
1:B:440:ARG:CD	1:B:440:ARG:N	2.85	0.40
1:B:525:LYS:O	1:B:526:VAL:C	2.63	0.40
1:A:87:PHE:HB2	1:A:131:PHE:CE1	2.57	0.40
1:A:189:ASN:OD1	1:A:195:LEU:HD21	2.22	0.40
1:A:263:ALA:HB2	1:A:288:TRP:CZ3	2.56	0.40
1:A:766:ILE:HG21	1:A:766:ILE:HD13	1.52	0.40
1:B:413:LEU:HD22	1:B:487:PRO:HB2	2.02	0.40
1:B:492:PRO:O	1:B:494:LYS:N	2.55	0.40
1:B:648:ILE:HG22	1:B:649:VAL:N	2.37	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:A:457:ASN:OD1	2:B:1033:HOH:O[1_454]	1.56	0.64
1:A:442:LEU:CD2	2:A:922:HOH:O[1_455]	1.95	0.25
1:A:300:ASN:OD1	1:B:303:GLU:N[2_656]	2.08	0.12

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	747/900 (83%)	500 (67%)	143 (19%)	104 (14%)	0	0
1	B	748/900 (83%)	497 (66%)	146 (20%)	105 (14%)	0	0
All	All	1495/1800 (83%)	997 (67%)	289 (19%)	209 (14%)	0	0

All (209) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	A	60	PHE
1	A	63	LEU
1	A	67	SER
1	A	83	SER
1	A	84	ASN
1	A	101	ALA
1	A	135	TYR
1	A	199	CYS
1	A	219	LYS
1	A	255	PHE
1	A	279	VAL
1	A	297	TRP
1	A	302	TYR
1	A	307	VAL
1	A	324	PHE
1	A	353	LEU
1	A	356	TRP
1	A	381	PHE
1	A	403	ARG
1	A	406	GLY
1	A	465	HIS
1	A	471	GLU
1	A	548	MET
1	A	550	ILE

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Mol	Chain	Res	Type
1	A	552	VAL
1	A	574	PHE
1	A	586	MET
1	A	620	LYS
1	A	624	MET
1	A	627	TYR
1	A	678	PHE
1	A	681	LEU
1	A	685	ASN
1	A	714	ASN
1	A	735	GLY
1	A	750	ASN
1	A	757	PRO
1	A	758	ASP
1	A	832	GLN
1	A	833	HIS
1	A	834	ILE
1	A	835	TYR
1	A	849	MET
1	A	875	GLY
1	B	15	ALA
1	B	62	GLU
1	B	67	SER
1	B	92	ALA
1	B	135	TYR
1	B	162	ASP
1	B	171	ALA
1	B	175	GLU
1	B	198	GLY
1	B	263	ALA
1	B	295	GLY
1	B	304	TRP
1	B	317	VAL
1	B	320	GLU
1	B	322	GLY
1	B	346	ASP
1	B	398	ASP
1	B	400	TYR
1	B	403	ARG
1	B	428	MET
1	B	440	ARG
1	B	441	GLU

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Mol	Chain	Res	Type
1	B	456	ALA
1	B	457	ASN
1	B	465	HIS
1	B	467	ILE
1	B	539	LEU
1	B	558	ILE
1	B	574	PHE
1	B	577	GLU
1	B	586	MET
1	B	617	ASP
1	B	618	LEU
1	B	620	LYS
1	B	647	VAL
1	B	654	ASP
1	B	657	LEU
1	B	713	SER
1	B	725	GLN
1	B	731	VAL
1	B	808	THR
1	B	810	ARG
1	B	833	HIS
1	B	839	ILE
1	B	850	ASP
1	B	851	PHE
1	B	863	ALA
1	B	875	GLY
1	A	4	ILE
1	A	14	ALA
1	A	15	ALA
1	A	99	GLN
1	A	173	GLY
1	A	174	ASN
1	A	263	ALA
1	A	264	TYR
1	A	313	GLU
1	A	317	VAL
1	A	326	MET
1	A	334	GLU
1	A	349	LYS
1	A	404	GLU
1	A	461	ALA
1	A	559	LEU

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Mol	Chain	Res	Type
1	A	606	ILE
1	A	618	LEU
1	A	664	PHE
1	A	809	ASP
1	A	810	ARG
1	B	5	ALA
1	B	61	LYS
1	B	81	LEU
1	B	97	ILE
1	B	172	GLN
1	B	262	HIS
1	B	268	ASP
1	B	334	GLU
1	B	396	ASP
1	B	461	ALA
1	B	515	ASP
1	B	525	LYS
1	B	552	VAL
1	B	576	LEU
1	B	585	LEU
1	B	627	TYR
1	B	632	ALA
1	B	648	ILE
1	B	673	ILE
1	B	684	GLU
1	B	785	GLY
1	B	807	GLU
1	B	811	SER
1	B	836	SER
1	B	837	MET
1	B	857	CYS
1	B	873	LYS
1	A	42	ALA
1	A	61	LYS
1	A	69	LYS
1	A	79	THR
1	A	98	CYS
1	A	108	LEU
1	A	194	ALA
1	A	229	LEU
1	A	318	LYS
1	A	351	ARG

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Mol	Chain	Res	Type
1	A	440	ARG
1	A	441	GLU
1	B	56	HIS
1	B	316	ARG
1	B	448	HIS
1	B	490	PHE
1	B	551	SER
1	B	582	MET
1	B	822	ALA
1	B	849	MET
1	B	853	ASN
1	A	13	GLU
1	A	24	ALA
1	A	278	ARG
1	A	316	ARG
1	A	329	ARG
1	A	517	ILE
1	A	543	LEU
1	A	626	ALA
1	A	699	PHE
1	A	731	VAL
1	A	749	LEU
1	A	825	ALA
1	B	69	LYS
1	B	319	MET
1	B	393	GLU
1	B	453	PHE
1	B	557	THR
1	B	605	ARG
1	B	630	ARG
1	B	646	GLN
1	B	770	ARG
1	B	798	LYS
1	B	806	PHE
1	B	829	HIS
1	B	868	PHE
1	A	90	ASP
1	A	97	ILE
1	A	100	GLY
1	A	557	THR
1	A	575	SER
1	A	683	PRO

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Mol	Chain	Res	Type
1	A	870	SER
1	B	14	ALA
1	B	732	GLN
1	B	794	ASN
1	B	823	PHE
1	A	677	ILE
1	B	88	ILE
1	B	447	VAL
1	A	521	LEU
1	A	701	VAL
1	A	592	GLY
1	A	802	ILE
1	B	740	VAL
1	A	291	VAL
1	B	54	VAL
1	A	89	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	606/782 (78%)	450 (74%)	156 (26%)	0	2
1	B	584/782 (75%)	419 (72%)	165 (28%)	0	1
All	All	1190/1564 (76%)	869 (73%)	321 (27%)	0	1

All (321) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	MET
1	A	7	LYS
1	A	12	ARG
1	A	13	GLU
1	A	22	GLU
1	A	25	ILE
1	A	30	GLN

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Mol	Chain	Res	Type
1	A	36	ARG
1	A	38	GLU
1	A	41	GLU
1	A	52	PRO
1	A	53	PRO
1	A	55	SER
1	A	57	SER
1	A	66	ASN
1	A	67	SER
1	A	69	LYS
1	A	70	THR
1	A	81	LEU
1	A	85	PRO
1	A	88	ILE
1	A	89	VAL
1	A	90	ASP
1	A	96	ASP
1	A	97	ILE
1	A	98	CYS
1	A	108	LEU
1	A	115	THR
1	A	116	LEU
1	A	121	LEU
1	A	132	GLN
1	A	151	ASP
1	A	153	VAL
1	A	155	ASP
1	A	161	LYS
1	A	165	LEU
1	A	174	ASN
1	A	181	LEU
1	A	191	SER
1	A	201	SER
1	A	204	PHE
1	A	211	VAL
1	A	218	GLN
1	A	224	LEU
1	A	228	ILE
1	A	229	LEU
1	A	230	LYS
1	A	242	ILE
1	A	258	LEU

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Mol	Chain	Res	Type
1	A	264	TYR
1	A	270	LYS
1	A	275	GLN
1	A	278	ARG
1	A	284	MET
1	A	296	PRO
1	A	300	ASN
1	A	305	ASN
1	A	306	LYS
1	A	310	TYR
1	A	313	GLU
1	A	317	VAL
1	A	324	PHE
1	A	325	TRP
1	A	329	ARG
1	A	330	ASP
1	A	332	ILE
1	A	334	GLU
1	A	335	PHE
1	A	336	THR
1	A	343	LEU
1	A	344	THR
1	A	352	THR
1	A	354	ARG
1	A	355	ASN
1	A	356	TRP
1	A	369	SER
1	A	370	THR
1	A	388	LYS
1	A	393	GLU
1	A	394	VAL
1	A	408	SER
1	A	428	MET
1	A	429	GLU
1	A	435	VAL
1	A	442	LEU
1	A	447	VAL
1	A	465	HIS
1	A	467	ILE
1	A	468	ASN
1	A	469	LEU
1	A	472	VAL

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Mol	Chain	Res	Type
1	A	484	ILE
1	A	487	PRO
1	A	497	ASP
1	A	499	LEU
1	A	504	SER
1	A	506	LYS
1	A	507	LYS
1	A	511	GLN
1	A	512	GLU
1	A	513	LEU
1	A	521	LEU
1	A	558	ILE
1	A	584	ASN
1	A	598	GLU
1	A	599	PHE
1	A	602	LEU
1	A	610	LEU
1	A	612	ILE
1	A	618	LEU
1	A	620	LYS
1	A	625	SER
1	A	628	GLU
1	A	643	GLN
1	A	647	VAL
1	A	656	GLU
1	A	658	ILE
1	A	663	ASN
1	A	666	ARG
1	A	667	CYS
1	A	672	GLU
1	A	674	LEU
1	A	690	GLN
1	A	701	VAL
1	A	714	ASN
1	A	715	ILE
1	A	744	GLU
1	A	748	ILE
1	A	751	LYS
1	A	759	LEU
1	A	760	LYS
1	A	766	ILE
1	A	767	ASP

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Mol	Chain	Res	Type
1	A	775	VAL
1	A	777	ASP
1	A	784	LEU
1	A	788	GLU
1	A	797	LYS
1	A	810	ARG
1	A	832	GLN
1	A	833	HIS
1	A	848	ASN
1	A	849	MET
1	A	852	ASP
1	A	853	ASN
1	A	859	VAL
1	A	860	ARG
1	A	865	PHE
1	A	871	LEU
1	A	874	ASN
1	A	876	THR
1	A	878	GLN
1	A	880	GLN
1	A	881	VAL
1	A	882	ASN
1	A	884	GLN
1	B	7	LYS
1	B	20	SER
1	B	28	LEU
1	B	33	GLU
1	B	36	ARG
1	B	38	GLU
1	B	40	LEU
1	B	41	GLU
1	B	49	PRO
1	B	54	VAL
1	B	60	PHE
1	B	61	LYS
1	B	62	GLU
1	B	66	ASN
1	B	68	SER
1	B	69	LYS
1	B	70	THR
1	B	78	PRO
1	B	79	THR

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Mol	Chain	Res	Type
1	B	84	ASN
1	B	86	GLN
1	B	90	ASP
1	B	93	THR
1	B	97	ILE
1	B	111	ILE
1	B	113	SER
1	B	118	GLU
1	B	120	ILE
1	B	153	VAL
1	B	154	VAL
1	B	159	PRO
1	B	164	LYS
1	B	172	GLN
1	B	174	ASN
1	B	181	LEU
1	B	185	TYR
1	B	188	VAL
1	B	195	LEU
1	B	196	SER
1	B	200	THR
1	B	211	VAL
1	B	223	ASP
1	B	224	LEU
1	B	229	LEU
1	B	234	ARG
1	B	237	LEU
1	B	242	ILE
1	B	256	LYS
1	B	259	VAL
1	B	265	SER
1	B	272	VAL
1	B	277	GLN
1	B	278	ARG
1	B	279	VAL
1	B	282	ILE
1	B	291	VAL
1	B	294	LYS
1	B	296	PRO
1	B	298	SER
1	B	303	GLU
1	B	304	TRP

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Mol	Chain	Res	Type
1	B	305	ASN
1	B	308	ASP
1	B	313	GLU
1	B	315	LEU
1	B	321	ASP
1	B	323	GLU
1	B	329	ARG
1	B	331	PHE
1	B	337	LYS
1	B	343	LEU
1	B	346	ASP
1	B	348	LEU
1	B	349	LYS
1	B	350	SER
1	B	359	THR
1	B	364	THR
1	B	375	ARG
1	B	376	ASN
1	B	388	LYS
1	B	389	ILE
1	B	390	ARG
1	B	394	VAL
1	B	396	ASP
1	B	398	ASP
1	B	401	ASP
1	B	405	SER
1	B	410	LEU
1	B	414	MET
1	B	418	ARG
1	B	427	ASP
1	B	429	GLU
1	B	438	VAL
1	B	440	ARG
1	B	455	LEU
1	B	457	ASN
1	B	462	GLN
1	B	464	GLU
1	B	467	ILE
1	B	468	ASN
1	B	469	LEU
1	B	472	VAL
1	B	485	VAL

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Mol	Chain	Res	Type
1	B	493	ASN
1	B	494	LYS
1	B	499	LEU
1	B	507	LYS
1	B	512	GLU
1	B	517	ILE
1	B	521	LEU
1	B	524	GLU
1	B	525	LYS
1	B	526	VAL
1	B	537	LYS
1	B	572	ASN
1	B	576	LEU
1	B	580	ARG
1	B	582	MET
1	B	584	ASN
1	B	586	MET
1	B	598	GLU
1	B	605	ARG
1	B	607	ARG
1	B	614	ARG
1	B	615	LYS
1	B	616	PHE
1	B	628	GLU
1	B	629	MET
1	B	630	ARG
1	B	631	MET
1	B	640	LEU
1	B	642	CYS
1	B	643	GLN
1	B	648	ILE
1	B	655	ASP
1	B	656	GLU
1	B	657	LEU
1	B	658	ILE
1	B	665	VAL
1	B	670	ARG
1	B	674	LEU
1	B	684	GLU
1	B	688	THR
1	B	690	GLN
1	B	691	LEU

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Mol	Chain	Res	Type
1	B	699	PHE
1	B	701	VAL
1	B	702	LEU
1	B	724	ARG
1	B	739	GLU
1	B	766	ILE
1	B	775	VAL
1	B	781	THR
1	B	784	LEU
1	B	790	LYS
1	B	797	LYS
1	B	831	ASN
1	B	837	MET
1	B	851	PHE
1	B	853	ASN
1	B	857	CYS
1	B	860	ARG
1	B	866	ARG
1	B	883	ILE
1	B	893	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	30	GLN
1	A	37	ASN
1	A	66	ASN
1	A	84	ASN
1	A	132	GLN
1	A	142	GLN
1	A	174	ASN
1	A	275	GLN
1	A	300	ASN
1	A	305	ASN
1	A	355	ASN
1	A	448	HIS
1	A	462	GLN
1	A	493	ASN
1	A	591	ASN
1	A	604	ASN
1	A	646	GLN

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Mol	Chain	Res	Type
1	A	663	ASN
1	A	690	GLN
1	A	711	HIS
1	A	714	ASN
1	A	756	HIS
1	A	795	ASN
1	A	800	GLN
1	A	829	HIS
1	A	833	HIS
1	A	853	ASN
1	A	874	ASN
1	A	878	GLN
1	A	884	GLN
1	A	888	GLN
1	B	21	HIS
1	B	37	ASN
1	B	47	GLN
1	B	84	ASN
1	B	86	GLN
1	B	140	HIS
1	B	142	GLN
1	B	174	ASN
1	B	243	ASN
1	B	257	ASN
1	B	262	HIS
1	B	277	GLN
1	B	280	ASN
1	B	286	ASN
1	B	342	ASN
1	B	417	HIS
1	B	457	ASN
1	B	468	ASN
1	B	493	ASN
1	B	556	GLN
1	B	584	ASN
1	B	604	ASN
1	B	646	GLN
1	B	663	ASN
1	B	831	ASN
1	B	853	ASN
1	B	884	GLN
1	B	888	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	783/900 (87%)	0.22	31 (3%) 42 33	16, 49, 81, 98	0
1	B	788/900 (87%)	0.43	50 (6%) 26 19	17, 51, 84, 102	0
All	All	1571/1800 (87%)	0.32	81 (5%) 33 25	16, 50, 83, 102	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	843	SER	5.4
1	B	835	TYR	5.0
1	B	601	ILE	4.1
1	B	702	LEU	4.0
1	B	259	VAL	4.0
1	B	398	ASP	4.0
1	B	659	ILE	3.9
1	B	777	ASP	3.9
1	A	550	ILE	3.9
1	A	702	LEU	3.8
1	B	731	VAL	3.8
1	B	417	HIS	3.8
1	A	812	GLY	3.4
1	A	820	PRO	3.4
1	B	560	ASN	3.4
1	B	855	ILE	3.3
1	A	522	PRO	3.2
1	B	603	TRP	3.2
1	B	788	GLU	3.2
1	A	332	ILE	3.1
1	B	832	GLN	3.1
1	A	734	ALA	3.1
1	B	742	ALA	3.0
1	A	551	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	712	TYR	2.9
1	B	701	VAL	2.9
1	B	824	GLU	2.9
1	A	712	TYR	2.8
1	A	821	GLY	2.8
1	B	92	ALA	2.8
1	B	594	LEU	2.7
1	B	786	PHE	2.7
1	A	733	LEU	2.7
1	B	714	ASN	2.6
1	B	718	ASN	2.6
1	B	844	ASP	2.6
1	B	397	ALA	2.6
1	B	64	GLY	2.6
1	B	443	ALA	2.6
1	A	89	VAL	2.5
1	A	170	SER	2.5
1	A	345	PRO	2.5
1	B	743	THR	2.5
1	A	255	PHE	2.5
1	B	95	THR	2.5
1	A	553	LYS	2.4
1	A	301	SER	2.4
1	B	697	LEU	2.4
1	B	587	ASP	2.4
1	A	836	SER	2.4
1	A	302	TYR	2.4
1	B	522	PRO	2.3
1	A	576	LEU	2.3
1	B	833	HIS	2.3
1	B	794	ASN	2.3
1	A	586	MET	2.3
1	B	654	ASP	2.3
1	B	839	ILE	2.3
1	B	699	PHE	2.2
1	B	456	ALA	2.2
1	B	612	ILE	2.2
1	A	173	GLY	2.2
1	A	545	GLY	2.2
1	A	699	PHE	2.2
1	B	347	ALA	2.2
1	B	394	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	244	ILE	2.2
1	A	64	GLY	2.2
1	B	540	PHE	2.2
1	A	521	LEU	2.2
1	A	731	VAL	2.2
1	A	546	ASP	2.1
1	B	67	SER	2.1
1	B	314	GLN	2.1
1	B	634	GLU	2.1
1	B	820	PRO	2.1
1	B	729	LEU	2.1
1	B	713	SER	2.0
1	A	793	TRP	2.0
1	A	701	VAL	2.0
1	B	425	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.