



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:51 PM GMT

PDB ID : 1QXP
Title : Crystal Structure of a mu-like calpain
Authors : Pal, G.P.; Veyra, T.D.; Elce, J.S.; Jia, Z.
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

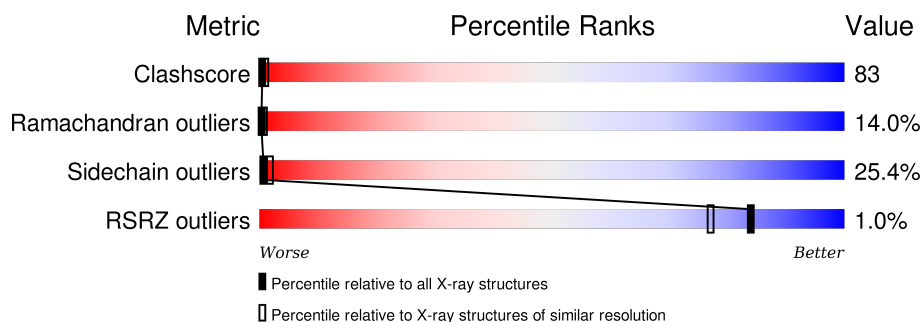
1 Overall quality at a glance

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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	UNP P97571
B	105	SER	CYS	ENGINEERED	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

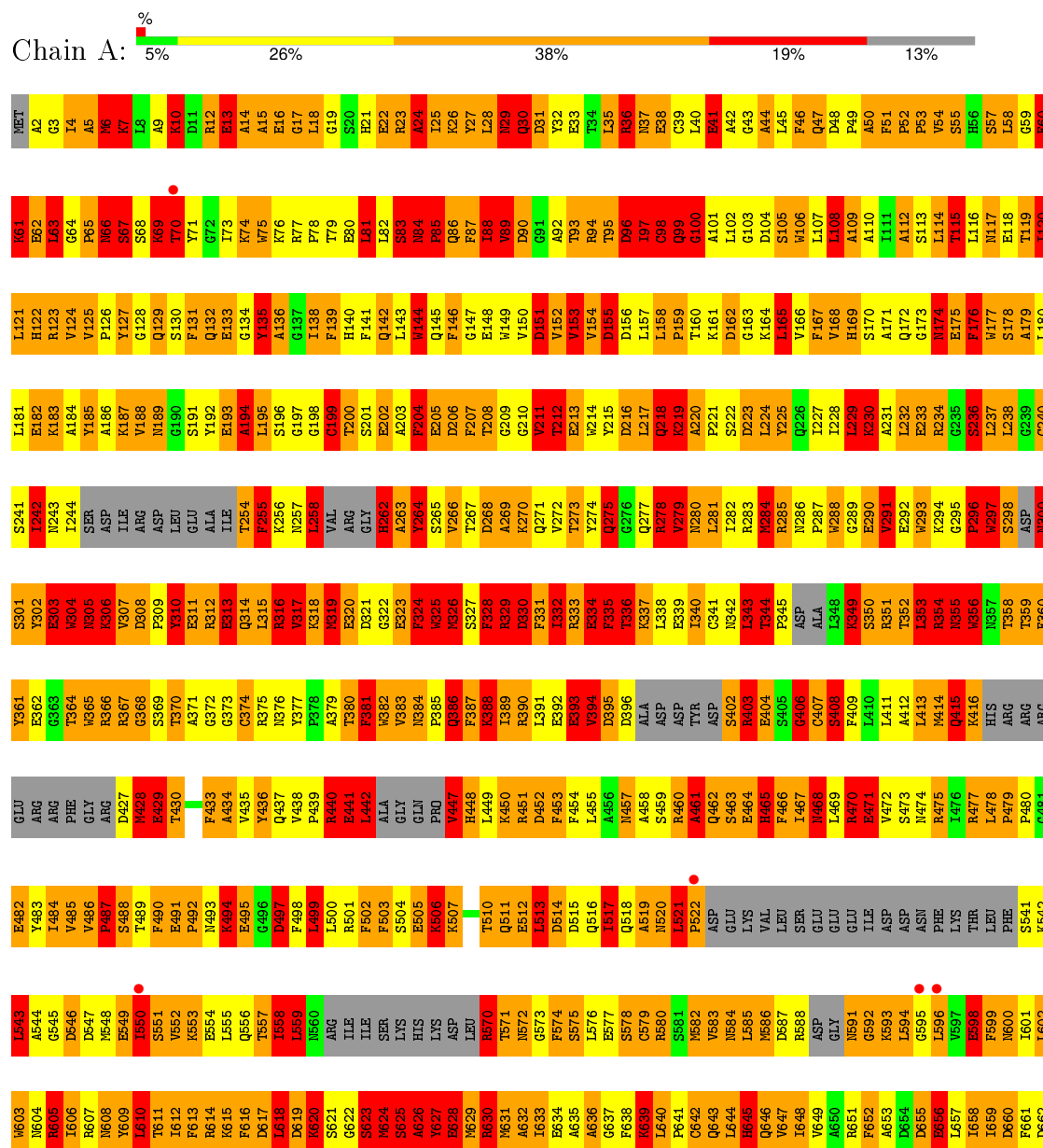
- Molecule 2 is water.

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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

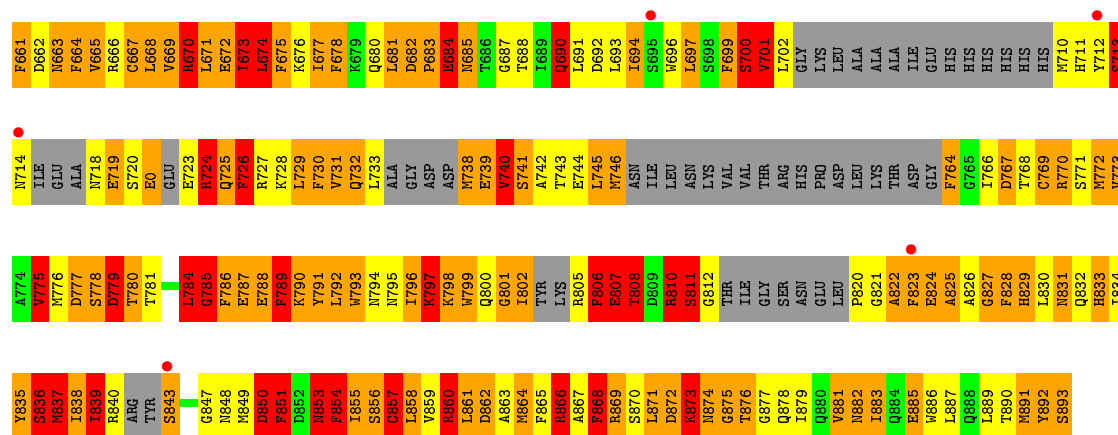
- Molecule 1: mu-like calpain



L601	SER	G481	GLU	Y361	SER	S241	L181	L121	K81	ME1	S836	H776	GLU	S663
L602	LYS	E482	ARG	E362	TYR	I242	E182	H122	E82	ALA	ME1	D777	ALA	F664
M603	LEU	Y483	ARG	G363	ASP	I243	A183	G123	G43	ASN	ILE	S778	ASN	F665
M604	ALA	I484	F424	T364	ASP	ILE	A184	V124	G64	GLU	ILE	D779	GLU	F666
R605	GLY	V485	G425	R365	LYS	ASP	Y185	V125	P85	ARG	ARG	T780	SER	C667
I606	ASP	V486	R426	R366	VAL	ASP	A186	P126	M66	GLY	ARG	T781	GLY	L668
R607	ASP	P487	D427	R367	VAL	ASP	K187	V127	S87	TYR	TYR	G782	GLU	V669
M608	MET	S488	M428	G368	D308	ARG	V188	G128	S88	SER	SER	K783	GLU	A670
Y609	GLU	T489	E429	S369	P309	ASP	M189	Q129	K69	ASP	ASP	L784	ARG	L671
T610	L610	F490	T430	T370	Y310	LEU	G190	F130	T70	GLN	T345	F785	GLN	E672
I612	S551	E491	I431	A371	GLU	S191	S191	F131	Y71	PHE	T346	F786	PHE	L673
F613	V552	P492	G432	G372	ALA	ALA	Y192	G132	G72	ARG	G347	E787	ARG	L674
K614	K553	M493	F433	G373	E193	ILE	E193	E133	I73	LYS	M848	F788	LYS	F675
R614	E554	K494	A434	C374	THR	THR	A194	G134	K74	LEU	M849	F789	LEU	L676
K615	L555	E495	V435	R375	PHE	PHE	L195	Y135	W75	LEU	M850	K790	LEU	L677
F616	L556	G496	F436	R376	LYS	K256	S196	L135	W75	LEU	F851	K791	LEU	F678
D617	T557	D497	Q437	Y377	LYS	K257	G197	G137	R77	ARG	F852	L792	ARG	K679
L618	L558	F498	V438	P378	K318	L258	G198	T138	P78	LYS	M853	L793	LYS	C680
D619	L559	A499	P439	A379	M319	V259	C199	F139	T79	ARG	F854	N794	ARG	L681
K620	M560	L500	R440	T380	E320	ARG	T200	H140	E80	GLY	I855	N795	GLY	D682
S621	ARG	R501	R441	F381	D321	G261	S201	H141	L81	GLY	S856	L796	GLY	F683
G622	ILE	F502	L442	V382	G322	H262	E202	Q142	L82	ARG	S857	K797	ARG	E684
S623	ILE	F503	A443	V383	E323	A263	A203	L143	S83	LYS	L858	K798	LYS	K685
M624	SER	S504	G444	N384	F324	Y264	F204	Y144	M84	ARG	L859	H799	ARG	T686
S625	SER	E505	GLN	P385	H325	S265	E205	Q145	P85	ARG	R860	Q800	ARG	L687
A626	HIS	K506	P446	Q386	M326	Y266	D206	F146	Q86	GLY	L861	G801	GLY	T688
Y627	LYS	K507	V447	R387	S327	T267	F207	G147	F87	THR	D862	L802	THR	L689
E628	ASP	A508	H448	K388	F328	D268	L188	E148	L88	ARG	L863	Y803	ARG	Q690
M629	LEU	G509	L449	I389	R329	A269	G209	Y149	V89	LYS	M864	L745	LYS	L691
R630	LEU	T510	K450	R390	D330	K270	G210	V150	D90	ARG	F865	L746	ARG	D692
M631	LYS	Q511	R451	L391	F331	Q271	V211	D151	G91	ARG	R866	M746	ARG	L693
A632	LYS	E512	D452	E392	I332	V272	T212	V152	A82	GLY	A867	GLU	GLY	T694
I633	GLY	E513	F453	E393	R333	T273	E213	V153	T93	THR	F868	T808	THR	L695
E634	LYS	D514	F454	V394	E334	Y274	W214	V154	R94	THR	R869	D809	THR	L696
A635	LYS	D515	L455	D395	F335	Q275	Y215	D155	T95	ARG	S870	L810	ARG	L697
A636	LYS	Q516	A456	D396	T336	G276	D216	D156	D96	LYS	L871	S811	LYS	S698
G637	LYS	I517	V457	A397	K337	Q277	L217	L157	I97	VAL	D872	G812	VAL	F699
R638	LYS	Q518	A458	D398	L338	R278	Q218	L158	C98	VAL	K873	THR	VAL	S700
K639	LYS	A519	S459	D399	E339	V279	K219	P159	C99	THR	M874	ILE	THR	L701
L640	LYS	M520	R460	Y400	I340	N280	A220	T160	Q99	ARG	G875	GLY	ARG	L702
P641	LYS	L521	A461	D401	C341	L281	A221	K161	A101	LYS	T876	GLY	LYS	GLY
C642	LYS	P522	Q462	S402	N342	L282	S222	D162	A42	LYS	G877	ASN	LYS	LYS
Q643	LYS	D523	S463	R403	R343	R283	D223	G163	G43	LYS	Q878	GLY	LYS	LEU
L644	LYS	E524	E464	E404	T344	N284	L224	K164	D104	LYS	I879	LEU	LYS	ALA
H645	LYS	K525	H465	S405	P345	N285	Y225	L165	S105	LYS	Q880	P820	LYS	ALA
Q646	LYS	V526	F466	G406	D346	N286	Q226	V166	W106	LYS	V881	G821	LYS	ALA
V647	LYS	LEU	I467	C407	A347	P287	I227	F167	F46	LYS	M882	A822	LYS	ALA
I648	LYS	SER	M468	F408	L348	N288	I228	V168	L107	LYS	I883	A823	LYS	ASP
V649	LYS	GLY	L469	S409	K349	G289	L229	H169	L108	LYS	F883	F823	GLY	GLY
A650	LYS	GLY	R470	L410	S350	E290	K230	S170	A109	LYS	Q884	E824	GLY	GLY
M651	ASN	GLY	E471	L411	R351	Y291	A231	A171	A110	LYS	E885	A825	LYS	HIS
F652	GLY	ILE	V472	A412	THR	E292	L232	Q172	I111	LYS	W886	A826	LYS	HIS
A653	LYS	ASP	S473	L413	LEU	E293	E233	G173	A112	LYS	L887	G827	LYS	HIS
D654	LYS	ASP	M474	M414	R354	K294	R234	N174	S113	LYS	Q888	F828	LYS	HIS
D655	LYS	ASN	R475	Q415	N355	G295	G235	E175	V54	LYS	L889	H829	LYS	HIS
E656	LYS	PHE	I476	K416	N356	P296	S236	F176	T115	LYS	T890	L830	LYS	W710
L657	LYS	LYS	R477	H417	N357	K297	L237	H177	H56	LYS	M891	L831	LYS	H711
M658	LYS	T538	L478	R418	T358	K298	L238	S178	N117	LYS	Y892	Q832	LYS	W712
L659	LYS	F539	P479	A419	ASP	S298	G239	S179	E118	LYS	S893	H833	LYS	S713
D660	LYS	F540	P480	ARG	ASN	ASN	C240	L180	I120	LYS	F60	L834	LYS	W714
														L715

• Molecule 1: mu-like calpain





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 49.81 – 2.69	Depositor EDS
% Data completeness (in resolution range)	91.6 (91.29-2.80) 87.3 (49.81-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (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.	DCC
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 98.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 55542 reflections	Xtriage
F_o, F_c correlation	0.90	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 6.85% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	3.70	964/6177 (15.6%)	2.67	470/8354 (5.6%)
1	B	3.71	932/6128 (15.2%)	2.67	489/8288 (5.9%)
All	All	3.70	1896/12305 (15.4%)	2.67	959/16642 (5.8%)

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

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

All (1896) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	SER	CA-CB	28.73	1.96	1.52
1	A	339	GLU	CD-OE1	23.66	1.51	1.25
1	A	320	GLU	CD-OE2	20.06	1.47	1.25
1	B	429	GLU	CD-OE1	19.54	1.47	1.25
1	A	811	SER	CA-CB	-18.37	1.25	1.52
1	B	185	TYR	CD1-CE1	-18.14	1.12	1.39
1	B	316	ARG	CA-CB	17.98	1.93	1.53
1	B	6	MET	CG-SD	17.54	2.26	1.81
1	A	680	GLN	CA-CB	17.33	1.92	1.53
1	B	869	ARG	CA-CB	17.27	1.92	1.53
1	B	806	PHE	CB-CG	16.50	1.79	1.51
1	A	428	MET	CG-SD	16.32	2.23	1.81
1	A	310	TYR	CG-CD2	16.27	1.60	1.39
1	A	310	TYR	CE2-CZ	15.93	1.59	1.38
1	A	6	MET	CG-SD	15.67	2.21	1.81
1	A	671	LEU	CA-CB	15.34	1.89	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	436	TYR	CD1-CE1	15.24	1.62	1.39
1	B	312	ARG	CG-CD	15.22	1.90	1.51
1	B	609	TYR	CD1-CE1	15.16	1.62	1.39
1	B	291	VAL	CA-CB	-15.02	1.23	1.54
1	A	75	TRP	CB-CG	15.01	1.77	1.50
1	B	332	ILE	CB-CG2	14.84	1.98	1.52
1	A	452	ASP	CB-CG	14.82	1.82	1.51
1	A	193	GLU	CD-OE2	14.79	1.42	1.25
1	A	460	ARG	CZ-NH2	14.75	1.52	1.33
1	A	803	TYR	CD1-CE1	14.67	1.61	1.39
1	B	824	GLU	CA-CB	14.57	1.86	1.53
1	A	337	LYS	CE-NZ	14.46	1.85	1.49
1	B	320	GLU	CD-OE2	14.46	1.41	1.25
1	A	110	ALA	CA-CB	-14.36	1.22	1.52
1	B	154	VAL	CB-CG2	-14.26	1.23	1.52
1	B	324	PHE	CD1-CE1	14.19	1.67	1.39
1	A	331	PHE	CE1-CZ	14.07	1.64	1.37
1	B	233	GLU	CD-OE1	13.99	1.41	1.25
1	A	317	VAL	CA-CB	13.98	1.84	1.54
1	B	440	ARG	CG-CD	13.94	1.86	1.51
1	B	726	PHE	CE1-CZ	13.87	1.63	1.37
1	B	328	PHE	CD1-CE1	-13.85	1.11	1.39
1	B	323	GLU	CD-OE1	13.82	1.40	1.25
1	A	463	SER	C-O	-13.50	0.97	1.23
1	B	176	PHE	CE1-CZ	-13.37	1.11	1.37
1	B	669	VAL	CA-CB	13.31	1.82	1.54
1	A	429	GLU	CD-OE1	13.31	1.40	1.25
1	A	360	PHE	CE1-CZ	13.30	1.62	1.37
1	A	225	TYR	CD2-CE2	13.28	1.59	1.39
1	B	744	GLU	CD-OE1	13.23	1.40	1.25
1	A	149	TRP	CE3-CZ3	-13.14	1.16	1.38
1	A	656	GLU	CD-OE1	13.13	1.40	1.25
1	A	218	GLN	CB-CG	13.06	1.87	1.52
1	B	672	GLU	CD-OE1	13.00	1.40	1.25
1	A	89	VAL	CB-CG1	12.99	1.80	1.52
1	A	485	VAL	CB-CG1	-12.97	1.25	1.52
1	A	193	GLU	CD-OE1	12.94	1.39	1.25
1	B	495	GLU	CD-OE1	12.90	1.39	1.25
1	A	133	GLU	CD-OE1	12.89	1.39	1.25
1	A	204	PHE	CE2-CZ	12.89	1.61	1.37
1	B	69	LYS	CB-CG	12.86	1.87	1.52
1	A	860	ARG	CZ-NH2	12.81	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	616	PHE	CE1-CZ	-12.78	1.13	1.37
1	B	361	TYR	CD1-CE1	12.76	1.58	1.39
1	B	135	TYR	CD1-CE1	-12.75	1.20	1.39
1	B	297	TRP	CZ3-CH2	-12.64	1.19	1.40
1	B	226	GLN	CG-CD	12.60	1.80	1.51
1	B	441	GLU	CA-CB	-12.58	1.26	1.53
1	A	329	ARG	CZ-NH1	12.55	1.49	1.33
1	A	627	TYR	CE2-CZ	-12.51	1.22	1.38
1	A	177	TRP	CG-CD1	-12.50	1.19	1.36
1	B	346	ASP	CB-CG	12.48	1.77	1.51
1	A	584	ASN	CB-CG	-12.45	1.22	1.51
1	B	360	PHE	CB-CG	-12.43	1.30	1.51
1	B	366	ARG	NE-CZ	-12.41	1.17	1.33
1	A	41	GLU	CG-CD	12.39	1.70	1.51
1	B	328	PHE	CE1-CZ	-12.34	1.13	1.37
1	B	90	ASP	CB-CG	12.34	1.77	1.51
1	B	678	PHE	CD2-CE2	-12.34	1.14	1.39
1	B	665	VAL	CB-CG2	-12.30	1.27	1.52
1	B	828	PHE	CE2-CZ	12.30	1.60	1.37
1	B	672	GLU	CD-OE2	12.26	1.39	1.25
1	B	335	PHE	CE2-CZ	12.25	1.60	1.37
1	B	9	ALA	CA-CB	-12.19	1.26	1.52
1	B	188	VAL	CB-CG2	-12.19	1.27	1.52
1	B	89	VAL	CB-CG1	12.18	1.78	1.52
1	B	146	PHE	CD2-CE2	-12.18	1.14	1.39
1	B	362	GLU	CG-CD	12.11	1.70	1.51
1	B	643	GLN	CG-CD	12.10	1.78	1.51
1	A	392	GLU	C-O	12.10	1.46	1.23
1	B	313	GLU	CB-CG	12.09	1.75	1.52
1	A	174	ASN	CB-CG	12.06	1.78	1.51
1	A	434	ALA	C-O	-12.04	1.00	1.23
1	B	369	SER	CB-OG	-11.97	1.26	1.42
1	A	27	TYR	CD1-CE1	11.86	1.57	1.39
1	B	690	GLN	CB-CG	11.81	1.84	1.52
1	B	142	GLN	CB-CG	11.77	1.84	1.52
1	B	341	CYS	CB-SG	11.73	2.02	1.82
1	B	87	PHE	CE2-CZ	11.72	1.59	1.37
1	B	464	GLU	CG-CD	11.71	1.69	1.51
1	B	176	PHE	CE2-CZ	-11.71	1.15	1.37
1	A	303	GLU	CD-OE2	-11.70	1.12	1.25
1	A	826	ALA	CA-CB	11.66	1.76	1.52
1	A	773	VAL	CB-CG1	11.64	1.77	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	394	VAL	CB-CG2	-11.63	1.28	1.52
1	A	124	VAL	CB-CG2	-11.57	1.28	1.52
1	B	883	ILE	CA-CB	11.57	1.81	1.54
1	A	665	VAL	CB-CG2	-11.54	1.28	1.52
1	A	616	PHE	CG-CD2	-11.52	1.21	1.38
1	B	225	TYR	CE1-CZ	-11.50	1.23	1.38
1	A	379	ALA	CA-CB	-11.49	1.28	1.52
1	A	652	PHE	CD1-CE1	11.46	1.62	1.39
1	B	811	SER	CA-CB	11.42	1.70	1.52
1	A	387	PHE	CE2-CZ	11.42	1.59	1.37
1	A	669	VAL	CB-CG1	11.40	1.76	1.52
1	A	631	MET	SD-CE	11.37	2.41	1.77
1	B	13	GLU	CD-OE2	11.36	1.38	1.25
1	B	13	GLU	CD-OE1	11.35	1.38	1.25
1	A	504	SER	CB-OG	11.32	1.56	1.42
1	B	68	SER	C-O	-11.28	1.01	1.23
1	B	320	GLU	CD-OE1	11.27	1.38	1.25
1	A	639	LYS	CE-NZ	11.26	1.77	1.49
1	A	280	ASN	CG-OD1	-11.23	0.99	1.24
1	B	199	CYS	CB-SG	11.18	2.01	1.82
1	B	198	GLY	C-O	11.17	1.41	1.23
1	A	613	PHE	CB-CG	-11.09	1.32	1.51
1	B	881	VAL	CB-CG2	-11.08	1.29	1.52
1	B	740	VAL	CB-CG1	11.02	1.76	1.52
1	A	41	GLU	CD-OE1	11.00	1.37	1.25
1	A	831	ASN	CG-OD1	10.99	1.48	1.24
1	B	579	CYS	CA-CB	10.99	1.78	1.53
1	A	503	PHE	CE2-CZ	-10.97	1.16	1.37
1	A	99	GLN	CA-CB	10.96	1.78	1.53
1	A	274	TYR	CE1-CZ	-10.96	1.24	1.38
1	A	215	TYR	CE1-CZ	10.96	1.52	1.38
1	A	505	GLU	CG-CD	10.96	1.68	1.51
1	B	335	PHE	CD1-CE1	10.95	1.61	1.39
1	A	739	GLU	CD-OE2	10.94	1.37	1.25
1	B	661	PHE	CE2-CZ	10.88	1.58	1.37
1	B	857	CYS	CB-SG	10.86	2.00	1.82
1	A	175	GLU	CG-CD	10.84	1.68	1.51
1	A	627	TYR	CB-CG	10.80	1.67	1.51
1	A	570	ARG	CB-CG	10.80	1.81	1.52
1	A	831	ASN	CB-CG	10.79	1.75	1.51
1	A	630	ARG	CZ-NH2	10.78	1.47	1.33
1	A	166	VAL	CB-CG2	-10.75	1.30	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	LYS	CD-CE	10.73	1.78	1.51
1	B	638	PHE	CG-CD1	-10.73	1.22	1.38
1	B	328	PHE	CG-CD2	-10.73	1.22	1.38
1	B	135	TYR	CD2-CE2	-10.73	1.23	1.39
1	A	471	GLU	C-O	-10.73	1.02	1.23
1	B	62	GLU	CD-OE2	10.72	1.37	1.25
1	B	377	TYR	CD1-CE1	10.72	1.55	1.39
1	A	115	THR	CB-CG2	10.72	1.87	1.52
1	B	89	VAL	CA-CB	10.64	1.77	1.54
1	B	333	ARG	CG-CD	10.61	1.78	1.51
1	B	146	PHE	CB-CG	10.59	1.69	1.51
1	B	136	ALA	N-CA	10.56	1.67	1.46
1	A	112	ALA	CA-CB	-10.56	1.30	1.52
1	B	577	GLU	CD-OE1	10.54	1.37	1.25
1	B	778	SER	CB-OG	10.54	1.55	1.42
1	A	350	SER	CB-OG	10.53	1.55	1.42
1	B	699	PHE	CE1-CZ	10.53	1.57	1.37
1	A	362	GLU	CG-CD	-10.53	1.36	1.51
1	B	123	ARG	CZ-NH1	10.52	1.46	1.33
1	B	131	PHE	CE1-CZ	10.48	1.57	1.37
1	A	333	ARG	CG-CD	10.47	1.78	1.51
1	B	777	ASP	CA-CB	10.47	1.76	1.53
1	A	133	GLU	CD-OE2	10.47	1.37	1.25
1	B	494	LYS	CD-CE	10.46	1.77	1.51
1	B	415	GLN	CB-CG	-10.45	1.24	1.52
1	B	429	GLU	CG-CD	10.45	1.67	1.51
1	B	88	ILE	CB-CG2	-10.44	1.20	1.52
1	B	131	PHE	CD1-CE1	-10.42	1.18	1.39
1	A	453	PHE	CE2-CZ	10.41	1.57	1.37
1	A	483	TYR	CD1-CE1	-10.39	1.23	1.39
1	A	366	ARG	CG-CD	10.38	1.77	1.51
1	B	570	ARG	N-CA	10.37	1.67	1.46
1	A	868	PHE	CG-CD1	-10.35	1.23	1.38
1	B	193	GLU	CG-CD	-10.35	1.36	1.51
1	A	615	LYS	CE-NZ	10.33	1.74	1.49
1	A	483	TYR	CD2-CE2	-10.32	1.23	1.39
1	A	512	GLU	CG-CD	10.32	1.67	1.51
1	B	141	PHE	CE1-CZ	-10.32	1.17	1.37
1	B	338	LEU	CA-CB	-10.31	1.30	1.53
1	B	208	THR	C-O	10.30	1.43	1.23
1	B	204	PHE	CE2-CZ	10.29	1.56	1.37
1	A	477	ARG	CG-CD	10.27	1.77	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	310	TYR	CD2-CE2	-10.26	1.24	1.39
1	A	219	LYS	CG-CD	10.25	1.87	1.52
1	A	350	SER	CA-CB	10.24	1.68	1.52
1	A	436	TYR	CE2-CZ	-10.23	1.25	1.38
1	B	553	LYS	CA-CB	10.22	1.76	1.53
1	B	775	VAL	CB-CG2	-10.21	1.31	1.52
1	A	207	PHE	CD2-CE2	10.21	1.59	1.39
1	B	290	GLU	CD-OE2	10.20	1.36	1.25
1	B	694	ILE	CA-CB	10.20	1.78	1.54
1	B	285	ARG	CZ-NH1	10.19	1.46	1.33
1	B	740	VAL	CB-CG2	10.18	1.74	1.52
1	A	608	ASN	C-O	-10.18	1.04	1.23
1	A	462	GLN	CA-CB	-10.18	1.31	1.53
1	A	167	PHE	CG-CD2	-10.16	1.23	1.38
1	B	48	ASP	CB-CG	10.16	1.73	1.51
1	A	339	GLU	CD-OE2	10.13	1.36	1.25
1	B	230	LYS	CD-CE	10.10	1.76	1.51
1	B	34	THR	N-CA	10.09	1.66	1.46
1	B	799	TRP	CB-CG	10.09	1.68	1.50
1	B	690	GLN	CG-CD	10.08	1.74	1.51
1	B	243	ASN	N-CA	10.07	1.66	1.46
1	A	200	THR	CA-CB	10.06	1.79	1.53
1	A	609	TYR	CZ-OH	10.06	1.54	1.37
1	B	182	GLU	CD-OE2	10.02	1.36	1.25
1	A	428	MET	CB-CG	10.02	1.83	1.51
1	A	390	ARG	CZ-NH1	10.01	1.46	1.33
1	A	313	GLU	CD-OE2	10.01	1.36	1.25
1	A	770	ARG	C-O	-10.00	1.04	1.23
1	A	203	ALA	CA-CB	-9.99	1.31	1.52
1	B	885	GLU	C-O	-9.97	1.04	1.23
1	B	288	TRP	CD2-CE2	-9.96	1.29	1.41
1	A	301	SER	CA-CB	9.94	1.67	1.52
1	B	628	GLU	CD-OE2	9.93	1.36	1.25
1	B	295	GLY	N-CA	9.93	1.60	1.46
1	B	828	PHE	CE1-CZ	-9.92	1.18	1.37
1	B	435	VAL	CB-CG2	9.92	1.73	1.52
1	B	621	SER	CA-CB	9.92	1.67	1.52
1	B	443	ALA	CA-CB	9.90	1.73	1.52
1	A	664	PHE	CE1-CZ	9.89	1.56	1.37
1	B	210	GLY	C-O	-9.88	1.07	1.23
1	B	243	ASN	C-O	9.87	1.42	1.23
1	A	218	GLN	CA-CB	9.87	1.75	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	30	GLN	C-O	-9.83	1.04	1.23
1	B	491	GLU	CD-OE1	9.83	1.36	1.25
1	B	130	SER	CB-OG	9.81	1.55	1.42
1	B	149	TRP	CG-CD1	-9.81	1.23	1.36
1	A	215	TYR	CE2-CZ	-9.81	1.25	1.38
1	A	166	VAL	N-CA	9.79	1.66	1.46
1	A	616	PHE	CB-CG	9.78	1.68	1.51
1	B	464	GLU	CD-OE1	9.78	1.36	1.25
1	B	84	ASN	CG-OD1	9.75	1.45	1.24
1	A	360	PHE	CB-CG	-9.73	1.34	1.51
1	B	856	SER	CA-CB	9.72	1.67	1.52
1	A	265	SER	CB-OG	9.72	1.54	1.42
1	A	836	SER	CA-CB	-9.70	1.38	1.52
1	A	370	THR	C-O	-9.70	1.04	1.23
1	A	433	PHE	CD1-CE1	9.70	1.58	1.39
1	A	870	SER	CB-OG	9.69	1.54	1.42
1	B	885	GLU	CD-OE2	9.68	1.36	1.25
1	A	864	MET	CA-CB	9.68	1.75	1.53
1	B	598	GLU	CD-OE2	9.68	1.36	1.25
1	B	772	MET	SD-CE	9.68	2.32	1.77
1	B	150	VAL	CB-CG1	-9.65	1.32	1.52
1	B	324	PHE	N-CA	-9.64	1.27	1.46
1	A	488	SER	CB-OG	9.63	1.54	1.42
1	A	270	LYS	CE-NZ	9.63	1.73	1.49
1	A	757	PRO	CG-CD	9.62	1.82	1.50
1	A	176	PHE	CE1-CZ	9.62	1.55	1.37
1	A	318	LYS	N-CA	9.61	1.65	1.46
1	B	0	GLU	CA-CB	9.61	1.75	1.53
1	A	177	TRP	CD2-CE2	-9.61	1.29	1.41
1	B	291	VAL	CB-CG2	9.61	1.73	1.52
1	A	26	LYS	CE-NZ	9.61	1.73	1.49
1	A	323	GLU	CG-CD	9.60	1.66	1.51
1	A	583	VAL	CA-CB	9.60	1.75	1.54
1	B	360	PHE	CE2-CZ	9.59	1.55	1.37
1	B	313	GLU	CG-CD	9.56	1.66	1.51
1	B	362	GLU	C-O	9.55	1.41	1.23
1	B	170	SER	CB-OG	9.54	1.54	1.42
1	A	202	GLU	CD-OE2	9.54	1.36	1.25
1	A	744	GLU	CD-OE1	9.47	1.36	1.25
1	A	591	ASN	CB-CG	9.45	1.72	1.51
1	B	203	ALA	CA-CB	9.45	1.72	1.52
1	B	387	PHE	CB-CG	-9.44	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	572	ASN	CA-C	9.44	1.77	1.52
1	A	803	TYR	CE2-CZ	9.44	1.50	1.38
1	A	847	GLY	C-O	9.44	1.38	1.23
1	B	389	ILE	C-O	9.43	1.41	1.23
1	A	303	GLU	CD-OE1	9.42	1.36	1.25
1	A	734	ALA	CA-CB	9.42	1.72	1.52
1	A	177	TRP	CE3-CZ3	-9.41	1.22	1.38
1	A	182	GLU	CD-OE1	9.40	1.35	1.25
1	A	892	TYR	CG-CD2	-9.40	1.26	1.39
1	A	361	TYR	CD1-CE1	9.40	1.53	1.39
1	B	26	LYS	CB-CG	9.39	1.77	1.52
1	A	135	TYR	N-CA	-9.38	1.27	1.46
1	A	516	GLN	CA-CB	-9.37	1.33	1.53
1	A	154	VAL	CB-CG1	9.37	1.72	1.52
1	B	609	TYR	CD2-CE2	9.36	1.53	1.39
1	B	477	ARG	CB-CG	9.36	1.77	1.52
1	A	471	GLU	N-CA	9.35	1.65	1.46
1	B	95	THR	C-O	9.35	1.41	1.23
1	B	786	PHE	CA-CB	9.35	1.74	1.53
1	A	382	TRP	C-O	9.35	1.41	1.23
1	B	175	GLU	C-O	-9.34	1.05	1.23
1	A	320	GLU	CA-CB	9.32	1.74	1.53
1	A	453	PHE	CD2-CE2	-9.32	1.20	1.39
1	B	335	PHE	CA-CB	9.32	1.74	1.53
1	A	891	MET	CA-CB	-9.31	1.33	1.53
1	B	811	SER	CB-OG	9.31	1.54	1.42
1	B	503	PHE	CD2-CE2	9.31	1.57	1.39
1	A	630	ARG	NE-CZ	9.28	1.45	1.33
1	A	482	GLU	CD-OE2	9.27	1.35	1.25
1	B	256	LYS	CD-CE	9.26	1.74	1.51
1	A	448	HIS	N-CA	9.26	1.64	1.46
1	B	83	SER	C-O	9.26	1.41	1.23
1	B	627	TYR	CD1-CE1	-9.26	1.25	1.39
1	B	13	GLU	CG-CD	9.25	1.65	1.51
1	A	377	TYR	CD1-CE1	-9.23	1.25	1.39
1	A	313	GLU	CD-OE1	9.21	1.35	1.25
1	A	204	PHE	CG-CD1	9.21	1.52	1.38
1	B	409	PHE	CB-CG	-9.20	1.35	1.51
1	A	483	TYR	CA-CB	-9.19	1.33	1.53
1	B	424	PHE	C-O	9.19	1.40	1.23
1	B	144	TRP	CG-CD1	-9.18	1.24	1.36
1	B	742	ALA	N-CA	9.18	1.64	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	ARG	CG-CD	-9.16	1.29	1.51
1	A	877	GLY	CA-C	9.15	1.66	1.51
1	A	502	PHE	CE2-CZ	-9.14	1.20	1.37
1	A	609	TYR	CG-CD1	-9.14	1.27	1.39
1	A	867	ALA	CA-CB	9.14	1.71	1.52
1	A	139	PHE	CD2-CE2	9.13	1.57	1.39
1	A	188	VAL	CB-CG2	-9.13	1.33	1.52
1	A	122	HIS	C-O	9.12	1.40	1.23
1	B	487	PRO	N-CD	-9.08	1.35	1.47
1	B	791	TYR	CB-CG	9.07	1.65	1.51
1	B	214	TRP	CG-CD1	-9.07	1.24	1.36
1	B	325	TRP	CE3-CZ3	9.06	1.53	1.38
1	A	278	ARG	C-O	-9.05	1.06	1.23
1	A	474	ASN	CB-CG	9.02	1.71	1.51
1	B	305	ASN	CB-CG	9.02	1.71	1.51
1	B	699	PHE	CG-CD2	9.02	1.52	1.38
1	A	71	TYR	CE2-CZ	-9.01	1.26	1.38
1	A	323	GLU	CB-CG	8.99	1.69	1.52
1	A	381	PHE	CG-CD1	8.98	1.52	1.38
1	A	652	PHE	CE2-CZ	8.98	1.54	1.37
1	B	55	SER	CA-CB	8.96	1.66	1.52
1	B	627	TYR	CG-CD1	8.96	1.50	1.39
1	A	678	PHE	CD2-CE2	-8.96	1.21	1.39
1	A	123	ARG	CZ-NH1	8.95	1.44	1.33
1	B	133	GLU	CG-CD	8.95	1.65	1.51
1	A	113	SER	CB-OG	8.93	1.53	1.42
1	B	436	TYR	CG-CD1	8.93	1.50	1.39
1	B	277	GLN	CB-CG	8.93	1.76	1.52
1	A	297	TRP	CG-CD1	8.91	1.49	1.36
1	B	892	TYR	CE2-CZ	8.91	1.50	1.38
1	A	334	GLU	CD-OE2	8.90	1.35	1.25
1	B	504	SER	N-CA	8.90	1.64	1.46
1	A	233	GLU	CG-CD	8.89	1.65	1.51
1	B	131	PHE	CG-CD1	-8.89	1.25	1.38
1	A	799	TRP	C-O	-8.89	1.06	1.23
1	A	820	PRO	CA-C	8.88	1.70	1.52
1	B	113	SER	C-O	8.88	1.40	1.23
1	B	628	GLU	CD-OE1	8.87	1.35	1.25
1	A	810	ARG	NE-CZ	8.87	1.44	1.33
1	A	858	LEU	CA-CB	8.85	1.74	1.53
1	B	348	LEU	CA-CB	8.84	1.74	1.53
1	A	502	PHE	C-O	-8.83	1.06	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	75	TRP	CG-CD1	-8.83	1.24	1.36
1	A	168	VAL	CB-CG1	-8.81	1.34	1.52
1	A	406	GLY	C-O	-8.80	1.09	1.23
1	B	71	TYR	CE1-CZ	8.80	1.50	1.38
1	B	482	GLU	CD-OE1	8.80	1.35	1.25
1	A	233	GLU	CD-OE2	-8.79	1.16	1.25
1	B	382	TRP	CE3-CZ3	8.79	1.53	1.38
1	B	647	VAL	C-O	-8.78	1.06	1.23
1	A	570	ARG	CG-CD	8.78	1.73	1.51
1	B	166	VAL	CB-CG2	8.78	1.71	1.52
1	A	550	ILE	CA-CB	8.76	1.75	1.54
1	B	624	MET	SD-CE	-8.76	1.28	1.77
1	B	214	TRP	CB-CG	-8.75	1.34	1.50
1	A	503	PHE	CG-CD1	-8.75	1.25	1.38
1	A	696	TRP	C-O	-8.74	1.06	1.23
1	B	409	PHE	CD2-CE2	8.73	1.56	1.39
1	A	498	PHE	CB-CG	-8.73	1.36	1.51
1	A	393	GLU	CD-OE2	-8.73	1.16	1.25
1	A	453	PHE	CB-CG	-8.72	1.36	1.51
1	B	463	SER	CB-OG	8.71	1.53	1.42
1	A	477	ARG	NE-CZ	8.71	1.44	1.33
1	B	502	PHE	CD1-CE1	8.70	1.56	1.39
1	A	490	PHE	CE2-CZ	-8.69	1.20	1.37
1	A	320	GLU	CD-OE1	8.69	1.35	1.25
1	A	738	MET	CA-CB	-8.68	1.34	1.53
1	A	498	PHE	CE2-CZ	-8.67	1.20	1.37
1	B	394	VAL	C-O	8.67	1.39	1.23
1	B	52	PRO	CA-C	-8.67	1.35	1.52
1	A	389	ILE	CA-CB	-8.66	1.34	1.54
1	B	33	GLU	CD-OE1	8.65	1.35	1.25
1	A	479	PRO	CA-C	-8.65	1.35	1.52
1	A	468	ASN	CB-CG	8.64	1.71	1.51
1	B	677	ILE	C-O	8.64	1.39	1.23
1	B	791	TYR	CD1-CE1	8.63	1.52	1.39
1	A	319	MET	CG-SD	-8.62	1.58	1.81
1	B	19	GLY	N-CA	-8.62	1.33	1.46
1	B	204	PHE	CG-CD1	8.61	1.51	1.38
1	A	877	GLY	N-CA	8.61	1.58	1.46
1	A	155	ASP	CB-CG	-8.61	1.33	1.51
1	A	463	SER	CA-CB	-8.60	1.40	1.52
1	A	505	GLU	CD-OE1	8.60	1.35	1.25
1	B	684	GLU	CD-OE1	8.60	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	502	PHE	CE2-CZ	-8.59	1.21	1.37
1	B	167	PHE	CG-CD1	-8.59	1.25	1.38
1	B	610	LEU	CG-CD1	8.58	1.83	1.51
1	A	764	PHE	CE1-CZ	-8.57	1.21	1.37
1	B	259	VAL	CA-CB	8.57	1.72	1.54
1	A	459	SER	C-O	-8.56	1.07	1.23
1	B	94	ARG	CA-CB	8.56	1.72	1.53
1	B	656	GLU	CD-OE1	8.55	1.35	1.25
1	B	772	MET	C-O	8.54	1.39	1.23
1	A	315	LEU	C-O	-8.52	1.07	1.23
1	A	570	ARG	NE-CZ	8.52	1.44	1.33
1	B	385	PRO	C-O	8.51	1.40	1.23
1	B	143	LEU	C-O	-8.50	1.07	1.23
1	B	508	ALA	C-O	-8.50	1.07	1.23
1	A	799	TRP	CE3-CZ3	8.49	1.52	1.38
1	A	656	GLU	CD-OE2	8.49	1.34	1.25
1	B	465	HIS	C-O	-8.49	1.07	1.23
1	A	436	TYR	CD2-CE2	8.48	1.52	1.39
1	B	265	SER	C-O	-8.48	1.07	1.23
1	B	54	VAL	CB-CG2	-8.47	1.35	1.52
1	B	39	CYS	C-O	-8.46	1.07	1.23
1	A	186	ALA	CA-CB	-8.46	1.34	1.52
1	B	360	PHE	CD2-CE2	8.45	1.56	1.39
1	B	505	GLU	CD-OE1	8.45	1.34	1.25
1	A	361	TYR	CB-CG	8.44	1.64	1.51
1	A	796	ILE	CA-CB	8.44	1.74	1.54
1	A	41	GLU	CA-CB	8.43	1.72	1.53
1	B	185	TYR	CB-CG	8.43	1.64	1.51
1	A	57	SER	CB-OG	-8.43	1.31	1.42
1	A	353	LEU	C-O	8.41	1.39	1.23
1	A	310	TYR	CE1-CZ	8.40	1.49	1.38
1	B	418	ARG	CZ-NH2	8.40	1.44	1.33
1	A	290	GLU	C-O	8.40	1.39	1.23
1	A	461	ALA	N-CA	8.39	1.63	1.46
1	A	868	PHE	CD2-CE2	-8.39	1.22	1.39
1	B	874	ASN	N-CA	8.39	1.63	1.46
1	B	166	VAL	CB-CG1	-8.38	1.35	1.52
1	A	618	LEU	CG-CD2	8.38	1.82	1.51
1	A	454	PHE	CE1-CZ	8.38	1.53	1.37
1	B	780	THR	CB-CG2	8.36	1.79	1.52
1	A	376	ASN	N-CA	-8.36	1.29	1.46
1	A	502	PHE	CB-CG	8.35	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	546	ASP	CA-CB	8.35	1.72	1.53
1	B	211	VAL	CB-CG1	-8.35	1.35	1.52
1	A	631	MET	CG-SD	8.35	2.02	1.81
1	A	757	PRO	CA-C	8.35	1.69	1.52
1	A	772	MET	CB-CG	8.35	1.78	1.51
1	A	630	ARG	CZ-NH1	8.31	1.43	1.33
1	A	800	GLN	N-CA	-8.31	1.29	1.46
1	A	860	ARG	CG-CD	8.31	1.72	1.51
1	B	328	PHE	CE2-CZ	-8.30	1.21	1.37
1	B	835	TYR	CA-CB	8.31	1.72	1.53
1	B	345	PRO	CG-CD	8.30	1.78	1.50
1	B	334	GLU	N-CA	8.30	1.62	1.46
1	B	865	PHE	CB-CG	-8.30	1.37	1.51
1	A	670	ARG	C-O	8.29	1.39	1.23
1	B	366	ARG	CZ-NH1	8.29	1.43	1.33
1	A	355	ASN	CG-ND2	8.29	1.53	1.32
1	B	139	PHE	N-CA	-8.29	1.29	1.46
1	A	776	MET	CG-SD	-8.29	1.59	1.81
1	B	456	ALA	CA-C	8.28	1.74	1.52
1	B	839	ILE	C-O	8.28	1.39	1.23
1	A	447	VAL	N-CA	8.28	1.62	1.46
1	B	335	PHE	CG-CD2	8.27	1.51	1.38
1	A	185	TYR	CZ-OH	-8.27	1.23	1.37
1	B	642	CYS	C-O	-8.27	1.07	1.23
1	B	118	GLU	CD-OE1	8.27	1.34	1.25
1	A	175	GLU	CD-OE2	8.26	1.34	1.25
1	B	680	GLN	CA-CB	8.26	1.72	1.53
1	B	854	PHE	CE1-CZ	8.26	1.53	1.37
1	B	32	TYR	CE2-CZ	-8.26	1.27	1.38
1	B	256	LYS	CB-CG	8.26	1.74	1.52
1	A	739	GLU	CD-OE1	8.25	1.34	1.25
1	A	862	ASP	CB-CG	-8.25	1.34	1.51
1	B	851	PHE	C-O	8.24	1.39	1.23
1	B	192	TYR	CG-CD1	-8.24	1.28	1.39
1	B	34	THR	CB-CG2	-8.24	1.25	1.52
1	B	387	PHE	CD1-CE1	8.24	1.55	1.39
1	B	324	PHE	CB-CG	-8.23	1.37	1.51
1	A	739	GLU	CB-CG	8.22	1.67	1.52
1	A	775	VAL	CA-CB	-8.21	1.37	1.54
1	A	279	VAL	C-O	-8.21	1.07	1.23
1	A	502	PHE	CD1-CE1	-8.21	1.22	1.39
1	B	164	LYS	CG-CD	8.21	1.80	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	ARG	NE-CZ	8.20	1.43	1.33
1	B	182	GLU	CA-CB	-8.20	1.35	1.53
1	A	580	ARG	N-CA	-8.19	1.29	1.46
1	A	891	MET	C-O	-8.19	1.07	1.23
1	A	106	TRP	C-O	-8.19	1.07	1.23
1	B	470	ARG	CB-CG	8.19	1.74	1.52
1	A	392	GLU	CD-OE2	8.19	1.34	1.25
1	A	10	LYS	N-CA	8.19	1.62	1.46
1	A	492	PRO	C-O	-8.19	1.06	1.23
1	B	201	SER	C-O	-8.18	1.07	1.23
1	A	331	PHE	CB-CG	-8.18	1.37	1.51
1	B	396	ASP	C-O	8.18	1.38	1.23
1	A	382	TRP	CE3-CZ3	8.17	1.52	1.38
1	B	403	ARG	N-CA	8.17	1.62	1.46
1	B	118	GLU	CD-OE2	-8.17	1.16	1.25
1	A	833	HIS	CA-C	8.16	1.74	1.52
1	A	329	ARG	N-CA	8.15	1.62	1.46
1	B	74	LYS	C-O	8.15	1.38	1.23
1	A	478	LEU	CG-CD1	8.14	1.81	1.51
1	B	69	LYS	C-O	8.14	1.38	1.23
1	A	144	TRP	CB-CG	-8.13	1.35	1.50
1	A	361	TYR	CE1-CZ	-8.12	1.27	1.38
1	B	345	PRO	CA-CB	8.12	1.69	1.53
1	A	415	GLN	N-CA	8.11	1.62	1.46
1	B	417	HIS	CA-CB	8.11	1.71	1.53
1	A	367	ARG	C-O	-8.10	1.07	1.23
1	B	363	GLY	N-CA	8.10	1.58	1.46
1	B	399	ASP	C-O	8.10	1.38	1.23
1	A	436	TYR	C-O	8.10	1.38	1.23
1	B	264	TYR	CD2-CE2	-8.09	1.27	1.39
1	B	583	VAL	CA-CB	8.09	1.71	1.54
1	B	409	PHE	CG-CD2	-8.09	1.26	1.38
1	B	237	LEU	C-O	-8.09	1.07	1.23
1	B	88	ILE	CA-C	-8.08	1.31	1.52
1	A	328	PHE	C-O	-8.08	1.07	1.23
1	A	133	GLU	CA-C	8.08	1.74	1.52
1	B	61	LYS	CA-CB	8.07	1.71	1.53
1	B	6	MET	SD-CE	8.07	2.23	1.77
1	B	349	LYS	CA-C	-8.06	1.31	1.52
1	B	380	THR	C-O	8.06	1.38	1.23
1	A	436	TYR	CG-CD1	8.06	1.49	1.39
1	A	760	LYS	CA-C	8.05	1.73	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	54	VAL	CA-CB	-8.05	1.37	1.54
1	A	354	ARG	NE-CZ	8.04	1.43	1.33
1	A	19	GLY	N-CA	8.04	1.58	1.46
1	A	387	PHE	CD1-CE1	8.04	1.55	1.39
1	B	38	GLU	CD-OE2	8.03	1.34	1.25
1	A	803	TYR	CE1-CZ	-8.03	1.28	1.38
1	A	301	SER	CB-OG	8.03	1.52	1.42
1	B	400	TYR	CD2-CE2	8.01	1.51	1.39
1	A	688	THR	CB-CG2	8.00	1.78	1.52
1	B	418	ARG	N-CA	8.00	1.62	1.46
1	A	264	TYR	CD1-CE1	8.00	1.51	1.39
1	B	120	ILE	C-O	-7.99	1.08	1.23
1	A	740	VAL	CB-CG1	-7.99	1.36	1.52
1	A	213	GLU	CB-CG	-7.99	1.36	1.52
1	B	277	GLN	CG-CD	7.98	1.69	1.51
1	A	433	PHE	CG-CD1	-7.97	1.26	1.38
1	A	623	SER	C-O	-7.97	1.08	1.23
1	B	200	THR	N-CA	7.96	1.62	1.46
1	A	130	SER	CB-OG	7.96	1.52	1.42
1	A	144	TRP	N-CA	7.94	1.62	1.46
1	B	788	GLU	CA-CB	7.94	1.71	1.53
1	A	483	TYR	CB-CG	7.94	1.63	1.51
1	B	416	LYS	CD-CE	7.94	1.71	1.51
1	A	324	PHE	CD2-CE2	-7.94	1.23	1.39
1	B	656	GLU	C-O	7.94	1.38	1.23
1	B	183	LYS	CD-CE	7.93	1.71	1.51
1	A	386	GLN	C-O	-7.93	1.08	1.23
1	A	740	VAL	CB-CG2	-7.93	1.36	1.52
1	A	873	LYS	C-O	7.92	1.38	1.23
1	A	350	SER	CA-C	-7.91	1.32	1.52
1	B	398	ASP	C-N	7.90	1.52	1.34
1	A	655	ASP	CB-CG	7.88	1.68	1.51
1	A	790	LYS	CA-CB	7.86	1.71	1.53
1	B	290	GLU	CD-OE1	7.86	1.34	1.25
1	B	729	LEU	C-O	7.86	1.38	1.23
1	B	613	PHE	CE2-CZ	7.85	1.52	1.37
1	A	214	TRP	CG-CD1	-7.84	1.25	1.36
1	A	731	VAL	CB-CG1	7.84	1.69	1.52
1	A	882	ASN	C-O	7.84	1.38	1.23
1	B	843	SER	CA-CB	7.84	1.64	1.52
1	A	225	TYR	CD1-CE1	7.83	1.51	1.39
1	A	821	GLY	C-O	7.82	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	89	VAL	CB-CG2	7.82	1.69	1.52
1	B	331	PHE	CD1-CE1	-7.82	1.23	1.39
1	A	385	PRO	CA-C	-7.82	1.37	1.52
1	B	613	PHE	CB-CG	-7.82	1.38	1.51
1	A	377	TYR	C-O	-7.81	1.08	1.23
1	A	789	PHE	CA-C	-7.80	1.32	1.52
1	A	241	SER	CA-CB	7.80	1.64	1.52
1	A	649	VAL	CA-CB	7.79	1.71	1.54
1	B	331	PHE	CD2-CE2	-7.79	1.23	1.39
1	A	167	PHE	C-O	7.79	1.38	1.23
1	A	468	ASN	CG-ND2	7.79	1.52	1.32
1	B	125	VAL	C-O	7.78	1.38	1.23
1	B	647	VAL	CB-CG2	-7.78	1.36	1.52
1	A	662	ASP	CB-CG	-7.78	1.35	1.51
1	B	17	GLY	CA-C	7.78	1.64	1.51
1	A	833	HIS	C-O	7.77	1.38	1.23
1	A	332	ILE	CB-CG1	7.77	1.75	1.54
1	A	413	LEU	C-O	-7.77	1.08	1.23
1	A	616	PHE	CE2-CZ	-7.77	1.22	1.37
1	A	19	GLY	CA-C	7.76	1.64	1.51
1	A	119	THR	N-CA	-7.76	1.30	1.46
1	B	495	GLU	CD-OE2	7.76	1.34	1.25
1	A	440	ARG	C-O	7.76	1.38	1.23
1	A	450	LYS	CD-CE	7.76	1.70	1.51
1	A	213	GLU	CD-OE2	-7.75	1.17	1.25
1	A	89	VAL	CA-CB	7.75	1.71	1.54
1	A	148	GLU	CD-OE1	7.75	1.34	1.25
1	A	314	GLN	CG-CD	7.75	1.68	1.51
1	A	27	TYR	CZ-OH	-7.74	1.24	1.37
1	A	278	ARG	CA-C	-7.73	1.32	1.52
1	B	259	VAL	CA-C	7.73	1.73	1.52
1	A	311	GLU	CD-OE1	-7.72	1.17	1.25
1	A	382	TRP	CD2-CE2	-7.72	1.32	1.41
1	B	73	ILE	C-O	-7.72	1.08	1.23
1	A	242	ILE	C-O	-7.72	1.08	1.23
1	A	613	PHE	CG-CD2	-7.72	1.27	1.38
1	B	38	GLU	C-O	-7.71	1.08	1.23
1	A	177	TRP	CB-CG	-7.71	1.36	1.50
1	A	404	GLU	CD-OE1	7.71	1.34	1.25
1	A	429	GLU	N-CA	-7.70	1.30	1.46
1	B	159	PRO	C-O	-7.70	1.07	1.23
1	A	26	LYS	CD-CE	7.70	1.70	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	366	ARG	N-CA	7.70	1.61	1.46
1	B	454	PHE	CB-CG	7.70	1.64	1.51
1	A	635	ALA	N-CA	7.69	1.61	1.46
1	B	349	LYS	CE-NZ	7.69	1.68	1.49
1	A	217	LEU	CA-C	-7.68	1.32	1.52
1	A	764	PHE	N-CA	7.68	1.61	1.46
1	B	416	LYS	CB-CG	7.68	1.73	1.52
1	A	30	GLN	CD-NE2	7.68	1.52	1.32
1	A	507	LYS	CD-CE	7.68	1.70	1.51
1	A	553	LYS	CA-CB	7.66	1.70	1.53
1	B	284	MET	CB-CG	7.66	1.75	1.51
1	A	666	ARG	CZ-NH1	7.66	1.43	1.33
1	A	778	SER	C-O	7.66	1.38	1.23
1	B	470	ARG	CZ-NH1	-7.66	1.23	1.33
1	B	508	ALA	CA-CB	7.66	1.68	1.52
1	A	637	GLY	C-O	7.66	1.35	1.23
1	A	494	LYS	CE-NZ	7.65	1.68	1.49
1	A	69	LYS	CE-NZ	-7.65	1.29	1.49
1	A	141	PHE	CG-CD2	7.65	1.50	1.38
1	A	647	VAL	CB-CG1	7.65	1.69	1.52
1	A	355	ASN	CG-OD1	7.64	1.40	1.24
1	A	787	GLU	CD-OE2	7.64	1.34	1.25
1	A	803	TYR	CG-CD1	-7.64	1.29	1.39
1	A	800	GLN	CB-CG	-7.63	1.31	1.52
1	B	297	TRP	CD2-CE2	-7.63	1.32	1.41
1	B	346	ASP	CG-OD1	7.63	1.43	1.25
1	A	881	VAL	CB-CG1	-7.63	1.36	1.52
1	A	45	LEU	C-O	7.63	1.37	1.23
1	A	763	GLY	C-O	7.63	1.35	1.23
1	B	412	ALA	C-O	7.62	1.37	1.23
1	B	655	ASP	CB-CG	7.62	1.67	1.51
1	A	61	LYS	CA-CB	7.62	1.70	1.53
1	A	602	LEU	CG-CD1	7.62	1.80	1.51
1	B	451	ARG	CG-CD	7.61	1.71	1.51
1	B	472	VAL	C-O	7.61	1.37	1.23
1	A	388	LYS	CE-NZ	7.61	1.68	1.49
1	B	181	LEU	CG-CD1	-7.61	1.23	1.51
1	A	313	GLU	CG-CD	7.60	1.63	1.51
1	B	377	TYR	CD2-CE2	7.60	1.50	1.39
1	A	340	ILE	CB-CG2	7.59	1.76	1.52
1	A	356	TRP	CB-CG	-7.59	1.36	1.50
1	B	152	VAL	C-O	-7.59	1.08	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	215	TYR	CG-CD2	-7.59	1.29	1.39
1	B	278	ARG	CG-CD	7.59	1.71	1.51
1	A	543	LEU	C-O	7.58	1.37	1.23
1	B	41	GLU	CD-OE1	7.58	1.33	1.25
1	B	550	ILE	CA-CB	-7.58	1.37	1.54
1	B	331	PHE	CB-CG	-7.57	1.38	1.51
1	A	878	GLN	CD-OE1	7.57	1.40	1.24
1	A	127	TYR	CE2-CZ	7.57	1.48	1.38
1	A	797	LYS	CB-CG	7.56	1.73	1.52
1	A	800	GLN	C-O	7.56	1.37	1.23
1	A	106	TRP	CB-CG	-7.55	1.36	1.50
1	B	182	GLU	N-CA	7.55	1.61	1.46
1	A	129	GLN	CD-NE2	7.55	1.51	1.32
1	A	275	GLN	N-CA	-7.55	1.31	1.46
1	A	882	ASN	CB-CG	7.55	1.68	1.51
1	A	490	PHE	CG-CD2	-7.54	1.27	1.38
1	A	656	GLU	CG-CD	7.54	1.63	1.51
1	A	109	ALA	CA-CB	7.54	1.68	1.52
1	B	837	MET	CA-C	7.54	1.72	1.52
1	A	845	GLU	CA-C	7.54	1.72	1.52
1	B	471	GLU	CG-CD	7.54	1.63	1.51
1	B	648	ILE	CB-CG2	-7.53	1.29	1.52
1	A	579	CYS	CB-SG	7.52	1.95	1.82
1	A	628	GLU	CD-OE1	7.51	1.33	1.25
1	B	503	PHE	C-O	-7.51	1.09	1.23
1	A	225	TYR	CG-CD1	7.51	1.49	1.39
1	A	306	LYS	C-O	-7.50	1.09	1.23
1	A	385	PRO	C-O	-7.50	1.08	1.23
1	B	303	GLU	CD-OE2	7.50	1.33	1.25
1	B	192	TYR	CZ-OH	7.50	1.50	1.37
1	B	471	GLU	CD-OE1	7.50	1.33	1.25
1	A	450	LYS	CE-NZ	7.49	1.67	1.49
1	B	649	VAL	CB-CG2	-7.49	1.37	1.52
1	A	466	PHE	CD2-CE2	7.49	1.54	1.39
1	B	303	GLU	CD-OE1	7.49	1.33	1.25
1	A	883	ILE	CB-CG2	7.48	1.76	1.52
1	A	316	ARG	CA-CB	7.48	1.70	1.53
1	A	383	VAL	C-O	-7.47	1.09	1.23
1	A	65	PRO	CB-CG	7.47	1.87	1.50
1	B	50	ALA	C-O	7.46	1.37	1.23
1	B	403	ARG	CA-C	7.46	1.72	1.52
1	A	769	CYS	CB-SG	7.46	1.95	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	444	GLY	C-O	7.46	1.35	1.23
1	B	344	THR	N-CA	7.46	1.61	1.46
1	A	436	TYR	CG-CD2	-7.46	1.29	1.39
1	B	436	TYR	CZ-OH	7.46	1.50	1.37
1	A	324	PHE	CB-CG	-7.45	1.38	1.51
1	A	382	TRP	CB-CG	7.45	1.63	1.50
1	B	79	THR	CB-CG2	-7.45	1.27	1.52
1	B	560	ASN	CA-CB	7.45	1.72	1.53
1	A	808	THR	CB-CG2	7.44	1.76	1.52
1	B	101	ALA	CA-CB	7.44	1.68	1.52
1	A	636	ALA	CA-CB	-7.43	1.36	1.52
1	B	42	ALA	CA-CB	-7.43	1.36	1.52
1	A	854	PHE	CE1-CZ	7.42	1.51	1.37
1	A	777	ASP	C-O	-7.41	1.09	1.23
1	A	117	ASN	CG-ND2	7.41	1.51	1.32
1	B	634	GLU	CD-OE2	7.41	1.33	1.25
1	B	464	GLU	CD-OE2	7.40	1.33	1.25
1	A	600	ASN	CA-CB	7.39	1.72	1.53
1	B	767	ASP	CA-CB	7.39	1.70	1.53
1	A	44	ALA	N-CA	7.39	1.61	1.46
1	B	140	HIS	CA-CB	-7.39	1.37	1.53
1	B	335	PHE	CD2-CE2	7.38	1.54	1.39
1	A	131	PHE	CB-CG	-7.38	1.38	1.51
1	A	413	LEU	CG-CD1	7.38	1.79	1.51
1	B	74	LYS	CA-C	7.38	1.72	1.52
1	B	572	ASN	C-O	7.38	1.37	1.23
1	A	25	ILE	CB-CG2	-7.37	1.29	1.52
1	A	285	ARG	CB-CG	7.37	1.72	1.52
1	B	312	ARG	C-O	-7.37	1.09	1.23
1	B	312	ARG	CB-CG	7.37	1.72	1.52
1	A	297	TRP	CD2-CE2	7.36	1.50	1.41
1	B	643	GLN	CD-OE1	7.36	1.40	1.24
1	B	369	SER	C-O	-7.35	1.09	1.23
1	A	71	TYR	CB-CG	7.35	1.62	1.51
1	A	874	ASN	CB-CG	7.35	1.68	1.51
1	B	185	TYR	CD2-CE2	-7.34	1.28	1.39
1	B	351	ARG	CA-CB	7.33	1.70	1.53
1	B	429	GLU	CD-OE2	7.33	1.33	1.25
1	A	255	PHE	N-CA	7.32	1.60	1.46
1	B	288	TRP	CZ3-CH2	-7.32	1.28	1.40
1	A	174	ASN	CA-C	7.31	1.72	1.52
1	A	427	ASP	N-CA	7.30	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	399	ASP	CG-OD2	7.30	1.42	1.25
1	A	659	ILE	CA-CB	-7.30	1.38	1.54
1	A	329	ARG	CB-CG	7.30	1.72	1.52
1	B	512	GLU	CD-OE2	-7.29	1.17	1.25
1	A	504	SER	CA-CB	7.29	1.63	1.52
1	A	778	SER	CB-OG	7.29	1.51	1.42
1	B	793	TRP	CB-CG	7.28	1.63	1.50
1	A	437	GLN	C-O	7.28	1.37	1.23
1	A	375	ARG	C-O	-7.27	1.09	1.23
1	A	381	PHE	CD2-CE2	7.27	1.53	1.39
1	A	176	PHE	CG-CD2	7.27	1.49	1.38
1	A	10	LYS	CE-NZ	7.27	1.67	1.49
1	A	320	GLU	CB-CG	7.27	1.66	1.52
1	A	380	THR	N-CA	-7.26	1.31	1.46
1	A	658	ILE	CB-CG2	-7.26	1.30	1.52
1	A	120	ILE	C-O	-7.26	1.09	1.23
1	A	712	TYR	CA-CB	7.26	1.70	1.53
1	A	199	CYS	CB-SG	-7.25	1.70	1.82
1	A	593	LYS	CA-CB	7.25	1.69	1.53
1	B	96	ASP	C-O	-7.25	1.09	1.23
1	A	674	LEU	CA-CB	-7.25	1.37	1.53
1	B	479	PRO	CA-CB	-7.25	1.39	1.53
1	B	354	ARG	N-CA	7.25	1.60	1.46
1	A	119	THR	CA-CB	-7.24	1.34	1.53
1	B	791	TYR	CD2-CE2	7.24	1.50	1.39
1	A	185	TYR	CE1-CZ	-7.24	1.29	1.38
1	B	599	PHE	CE1-CZ	7.24	1.51	1.37
1	A	734	ALA	C-O	7.23	1.37	1.23
1	A	802	ILE	CA-CB	-7.22	1.38	1.54
1	B	129	GLN	C-O	-7.22	1.09	1.23
1	B	647	VAL	CB-CG1	-7.22	1.37	1.52
1	B	237	LEU	N-CA	7.21	1.60	1.46
1	B	399	ASP	CB-CG	7.21	1.66	1.51
1	B	322	GLY	CA-C	7.21	1.63	1.51
1	B	59	GLY	N-CA	7.21	1.56	1.46
1	A	812	GLY	N-CA	7.20	1.56	1.46
1	B	480	PRO	N-CD	-7.20	1.37	1.47
1	B	160	THR	N-CA	-7.20	1.31	1.46
1	A	611	THR	CA-CB	-7.20	1.34	1.53
1	A	666	ARG	CZ-NH2	7.19	1.42	1.33
1	A	369	SER	CB-OG	7.18	1.51	1.42
1	B	24	ALA	CA-CB	-7.18	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	342	ASN	C-O	-7.18	1.09	1.23
1	B	378	PRO	CA-C	-7.18	1.38	1.52
1	B	228	ILE	CB-CG2	7.18	1.75	1.52
1	B	826	ALA	CA-CB	7.18	1.67	1.52
1	B	378	PRO	CG-CD	7.17	1.74	1.50
1	A	16	GLU	CD-OE2	7.17	1.33	1.25
1	A	341	CYS	CA-C	7.17	1.71	1.52
1	A	860	ARG	CZ-NH1	7.17	1.42	1.33
1	A	516	GLN	N-CA	7.17	1.60	1.46
1	B	329	ARG	NE-CZ	7.17	1.42	1.33
1	B	90	ASP	CA-CB	7.16	1.69	1.53
1	B	764	PHE	CD2-CE2	7.16	1.53	1.39
1	B	349	LYS	CD-CE	7.15	1.69	1.51
1	A	194	ALA	CA-CB	-7.15	1.37	1.52
1	A	437	GLN	CD-NE2	7.15	1.50	1.32
1	B	278	ARG	CB-CG	7.15	1.71	1.52
1	B	167	PHE	C-O	7.14	1.36	1.23
1	A	99	GLN	N-CA	7.14	1.60	1.46
1	B	120	ILE	CB-CG2	7.14	1.75	1.52
1	B	256	LYS	N-CA	7.13	1.60	1.46
1	B	473	SER	C-O	-7.13	1.09	1.23
1	B	854	PHE	CG-CD2	7.13	1.49	1.38
1	B	281	LEU	C-O	7.12	1.36	1.23
1	B	719	GLU	CD-OE2	7.12	1.33	1.25
1	B	726	PHE	CD1-CE1	7.12	1.53	1.39
1	B	389	ILE	CB-CG1	-7.12	1.34	1.54
1	B	687	GLY	CA-C	7.12	1.63	1.51
1	A	385	PRO	N-CA	-7.11	1.35	1.47
1	B	296	PRO	CB-CG	-7.11	1.14	1.50
1	A	51	PHE	CG-CD1	7.11	1.49	1.38
1	A	448	HIS	C-O	-7.11	1.09	1.23
1	A	7	LYS	CE-NZ	7.11	1.66	1.49
1	A	434	ALA	CA-CB	-7.11	1.37	1.52
1	A	439	PRO	C-O	7.10	1.37	1.23
1	A	822	ALA	N-CA	7.10	1.60	1.46
1	B	892	TYR	CE1-CZ	7.10	1.47	1.38
1	A	92	ALA	C-O	7.09	1.36	1.23
1	A	288	TRP	CB-CG	-7.09	1.37	1.50
1	B	215	TYR	CE2-CZ	-7.09	1.29	1.38
1	B	296	PRO	CA-C	7.09	1.67	1.52
1	B	192	TYR	CG-CD2	-7.08	1.29	1.39
1	A	262	HIS	N-CA	7.08	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	586	MET	CG-SD	7.08	1.99	1.81
1	B	872	ASP	CB-CG	-7.08	1.36	1.51
1	B	539	LEU	CA-C	7.08	1.71	1.52
1	A	41	GLU	CB-CG	7.07	1.65	1.52
1	A	892	TYR	CZ-OH	-7.07	1.25	1.37
1	A	696	TRP	CB-CG	-7.07	1.37	1.50
1	B	20	SER	CB-OG	7.07	1.51	1.42
1	A	884	GLN	CD-NE2	7.06	1.50	1.32
1	B	503	PHE	CB-CG	-7.06	1.39	1.51
1	A	673	ILE	CA-CB	7.05	1.71	1.54
1	A	833	HIS	N-CA	7.05	1.60	1.46
1	B	382	TRP	C-O	7.05	1.36	1.23
1	A	41	GLU	CD-OE2	7.05	1.33	1.25
1	A	387	PHE	CG-CD2	7.05	1.49	1.38
1	B	438	VAL	CB-CG2	7.05	1.67	1.52
1	A	51	PHE	CD2-CE2	-7.04	1.25	1.39
1	A	192	TYR	CE1-CZ	-7.04	1.29	1.38
1	A	598	GLU	C-O	-7.04	1.09	1.23
1	B	409	PHE	CD1-CE1	7.04	1.53	1.39
1	B	498	PHE	C-O	7.04	1.36	1.23
1	A	204	PHE	CD2-CE2	-7.04	1.25	1.39
1	A	241	SER	CB-OG	7.03	1.51	1.42
1	A	152	VAL	CB-CG2	-7.03	1.38	1.52
1	A	110	ALA	N-CA	7.03	1.60	1.46
1	A	789	PHE	CD2-CE2	-7.03	1.25	1.39
1	A	76	LYS	CB-CG	7.03	1.71	1.52
1	B	131	PHE	C-O	-7.02	1.10	1.23
1	B	271	GLN	CG-CD	7.02	1.67	1.51
1	B	664	PHE	CD2-CE2	7.02	1.53	1.39
1	B	499	LEU	C-O	7.01	1.36	1.23
1	A	236	SER	CA-CB	-7.01	1.42	1.52
1	B	450	LYS	CB-CG	7.00	1.71	1.52
1	B	236	SER	CB-OG	7.00	1.51	1.42
1	B	22	GLU	CD-OE1	7.00	1.33	1.25
1	A	485	VAL	C-O	-6.99	1.10	1.23
1	A	183	LYS	N-CA	6.99	1.60	1.46
1	A	96	ASP	CA-C	-6.99	1.34	1.52
1	B	854	PHE	CE2-CZ	6.99	1.50	1.37
1	B	811	SER	CA-C	6.98	1.71	1.52
1	A	12	ARG	CA-C	6.98	1.71	1.52
1	B	230	LYS	CB-CG	-6.98	1.33	1.52
1	B	670	ARG	CZ-NH2	-6.98	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	VAL	CA-C	-6.96	1.34	1.52
1	B	23	ARG	CB-CG	6.96	1.71	1.52
1	B	382	TRP	CB-CG	-6.96	1.37	1.50
1	A	381	PHE	CB-CG	-6.95	1.39	1.51
1	A	384	ASN	CG-ND2	6.95	1.50	1.32
1	A	452	ASP	C-O	6.95	1.36	1.23
1	A	638	PHE	CE2-CZ	6.95	1.50	1.37
1	A	334	GLU	CB-CG	-6.95	1.39	1.52
1	B	135	TYR	CG-CD2	-6.94	1.30	1.39
1	A	412	ALA	CA-C	-6.94	1.34	1.52
1	A	736	ASP	CB-CG	6.94	1.66	1.51
1	B	504	SER	CA-CB	6.94	1.63	1.52
1	B	96	ASP	CA-C	-6.93	1.34	1.52
1	B	366	ARG	CG-CD	6.93	1.69	1.51
1	A	164	LYS	C-O	6.92	1.36	1.23
1	A	217	LEU	CG-CD2	-6.92	1.26	1.51
1	B	636	ALA	C-O	6.92	1.36	1.23
1	A	550	ILE	CA-C	6.92	1.71	1.52
1	B	192	TYR	CD2-CE2	-6.91	1.28	1.39
1	B	631	MET	SD-CE	6.90	2.16	1.77
1	B	764	PHE	CE1-CZ	6.90	1.50	1.37
1	B	636	ALA	CA-CB	-6.90	1.38	1.52
1	B	341	CYS	C-O	-6.89	1.10	1.23
1	B	777	ASP	N-CA	6.89	1.60	1.46
1	A	244	ILE	CA-CB	6.89	1.70	1.54
1	A	306	LYS	CE-NZ	6.89	1.66	1.49
1	A	623	SER	CB-OG	6.89	1.51	1.42
1	B	491	GLU	CG-CD	6.88	1.62	1.51
1	A	214	TRP	CD2-CE2	-6.88	1.33	1.41
1	A	257	ASN	C-O	6.88	1.36	1.23
1	A	610	LEU	CG-CD2	6.88	1.77	1.51
1	A	266	VAL	C-O	6.87	1.36	1.23
1	A	151	ASP	CG-OD1	6.87	1.41	1.25
1	A	139	PHE	CE1-CZ	6.87	1.50	1.37
1	B	360	PHE	CD1-CE1	6.87	1.52	1.39
1	A	281	LEU	CA-C	-6.86	1.35	1.52
1	B	398	ASP	CG-OD1	6.86	1.41	1.25
1	B	699	PHE	CD2-CE2	6.86	1.52	1.39
1	B	343	LEU	CG-CD2	6.86	1.77	1.51
1	A	178	SER	C-O	6.86	1.36	1.23
1	A	756	HIS	N-CA	6.86	1.60	1.46
1	A	67	SER	CA-CB	6.85	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	871	LEU	C-O	-6.85	1.10	1.23
1	B	2	ALA	N-CA	6.85	1.60	1.46
1	A	820	PRO	N-CA	6.85	1.58	1.47
1	A	466	PHE	CE2-CZ	6.85	1.50	1.37
1	B	164	LYS	CB-CG	6.85	1.71	1.52
1	B	11	ASP	CA-C	6.84	1.70	1.52
1	A	380	THR	CA-CB	-6.84	1.35	1.53
1	A	656	GLU	CB-CG	6.84	1.65	1.52
1	B	851	PHE	CD1-CE1	6.83	1.52	1.39
1	B	329	ARG	CZ-NH2	6.83	1.42	1.33
1	B	451	ARG	NE-CZ	6.83	1.42	1.33
1	A	222	SER	C-O	6.83	1.36	1.23
1	A	200	THR	CB-CG2	6.82	1.74	1.52
1	B	699	PHE	CD1-CE1	6.82	1.52	1.39
1	B	738	MET	CG-SD	6.82	1.98	1.81
1	B	780	THR	C-O	-6.82	1.10	1.23
1	A	312	ARG	CZ-NH2	6.82	1.42	1.33
1	B	616	PHE	CB-CG	-6.81	1.39	1.51
1	B	627	TYR	CE2-CZ	6.81	1.47	1.38
1	A	155	ASP	CG-OD1	6.80	1.41	1.25
1	A	436	TYR	CZ-OH	-6.80	1.26	1.37
1	A	374	CYS	C-O	-6.80	1.10	1.23
1	B	267	THR	N-CA	-6.80	1.32	1.46
1	B	319	MET	CG-SD	6.79	1.98	1.81
1	B	329	ARG	CA-C	6.79	1.70	1.52
1	B	452	ASP	CB-CG	6.79	1.66	1.51
1	B	843	SER	N-CA	6.79	1.59	1.46
1	B	22	GLU	CG-CD	6.79	1.62	1.51
1	B	481	GLY	C-O	6.78	1.34	1.23
1	A	678	PHE	CE2-CZ	6.78	1.50	1.37
1	B	681	LEU	C-O	6.78	1.36	1.23
1	A	803	TYR	CB-CG	-6.77	1.41	1.51
1	B	294	LYS	CG-CD	6.77	1.75	1.52
1	B	678	PHE	CD1-CE1	-6.77	1.25	1.39
1	B	885	GLU	CB-CG	6.76	1.65	1.52
1	A	871	LEU	CA-C	-6.76	1.35	1.52
1	B	505	GLU	CB-CG	6.76	1.65	1.52
1	B	231	ALA	N-CA	6.75	1.59	1.46
1	A	663	ASN	CB-CG	6.75	1.66	1.51
1	B	666	ARG	C-O	-6.75	1.10	1.23
1	A	783	LYS	C-O	6.74	1.36	1.23
1	A	863	ALA	CA-CB	-6.74	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	87	PHE	CD1-CE1	6.74	1.52	1.39
1	B	335	PHE	CB-CG	6.74	1.62	1.51
1	B	361	TYR	CG-CD1	6.74	1.48	1.39
1	B	587	ASP	CB-CG	6.74	1.66	1.51
1	B	433	PHE	CE2-CZ	-6.74	1.24	1.37
1	B	607	ARG	CB-CG	6.73	1.70	1.52
1	A	652	PHE	CE1-CZ	-6.73	1.24	1.37
1	B	491	GLU	CD-OE2	6.73	1.33	1.25
1	B	175	GLU	CB-CG	6.71	1.65	1.52
1	B	727	ARG	C-O	6.71	1.36	1.23
1	B	340	ILE	CB-CG2	-6.71	1.32	1.52
1	B	616	PHE	CD2-CE2	-6.70	1.25	1.39
1	A	167	PHE	CA-CB	-6.70	1.39	1.53
1	A	149	TRP	CE2-CZ2	-6.69	1.28	1.39
1	A	616	PHE	C-O	6.69	1.36	1.23
1	A	767	ASP	CG-OD1	6.69	1.40	1.25
1	B	177	TRP	CB-CG	-6.69	1.38	1.50
1	A	349	LYS	C-O	6.68	1.36	1.23
1	A	514	ASP	CG-OD2	6.68	1.40	1.25
1	B	424	PHE	C-N	6.68	1.45	1.33
1	A	58	LEU	C-O	6.68	1.36	1.23
1	A	780	THR	CA-CB	-6.67	1.35	1.53
1	A	273	THR	CB-CG2	6.67	1.74	1.52
1	A	214	TRP	CZ3-CH2	-6.67	1.29	1.40
1	B	483	TYR	CG-CD2	-6.67	1.30	1.39
1	A	243	ASN	N-CA	6.66	1.59	1.46
1	B	518	GLN	N-CA	6.66	1.59	1.46
1	A	278	ARG	CZ-NH2	6.65	1.41	1.33
1	A	393	GLU	C-O	6.65	1.35	1.23
1	B	113	SER	CB-OG	6.65	1.50	1.42
1	A	133	GLU	CG-CD	6.65	1.61	1.51
1	A	859	VAL	CA-CB	-6.64	1.40	1.54
1	A	702	LEU	N-CA	6.64	1.59	1.46
1	A	105	SER	CB-OG	6.64	1.50	1.42
1	A	764	PHE	CE2-CZ	-6.64	1.24	1.37
1	B	512	GLU	CG-CD	6.64	1.61	1.51
1	B	176	PHE	CG-CD1	-6.63	1.28	1.38
1	B	519	ALA	C-O	-6.63	1.10	1.23
1	A	331	PHE	CA-CB	-6.63	1.39	1.53
1	A	686	THR	N-CA	6.63	1.59	1.46
1	B	324	PHE	CA-C	-6.63	1.35	1.52
1	B	308	ASP	C-O	6.62	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	474	ASN	N-CA	-6.62	1.33	1.46
1	B	843	SER	CA-C	6.62	1.70	1.52
1	A	335	PHE	CG-CD1	6.61	1.48	1.38
1	B	639	LYS	CA-CB	6.61	1.68	1.53
1	A	408	SER	CB-OG	-6.61	1.33	1.42
1	A	148	GLU	CG-CD	6.61	1.61	1.51
1	B	344	THR	C-O	-6.61	1.10	1.23
1	A	332	ILE	CA-CB	6.61	1.70	1.54
1	B	153	VAL	CA-CB	-6.60	1.40	1.54
1	B	48	ASP	N-CA	-6.60	1.33	1.46
1	B	483	TYR	CE2-CZ	6.59	1.47	1.38
1	A	795	ASN	C-O	-6.59	1.10	1.23
1	A	760	LYS	C-O	6.59	1.35	1.23
1	A	694	ILE	CA-CB	6.59	1.70	1.54
1	B	400	TYR	CG-CD1	6.58	1.47	1.39
1	A	288	TRP	CE2-CZ2	-6.58	1.28	1.39
1	A	730	PHE	CD2-CE2	6.58	1.52	1.39
1	A	633	ILE	CB-CG2	-6.58	1.32	1.52
1	A	22	GLU	CG-CD	6.58	1.61	1.51
1	B	284	MET	CG-SD	-6.58	1.64	1.81
1	B	640	LEU	N-CA	6.58	1.59	1.46
1	B	502	PHE	CA-C	-6.57	1.35	1.52
1	B	806	PHE	CD1-CE1	6.57	1.52	1.39
1	B	135	TYR	CB-CG	6.57	1.61	1.51
1	A	355	ASN	CB-CG	6.56	1.66	1.51
1	B	726	PHE	CD2-CE2	6.56	1.52	1.39
1	B	373	GLY	C-O	-6.55	1.13	1.23
1	B	477	ARG	CD-NE	-6.55	1.35	1.46
1	A	40	LEU	C-O	-6.55	1.10	1.23
1	B	227	ILE	CA-CB	-6.55	1.39	1.54
1	B	505	GLU	C-O	-6.55	1.10	1.23
1	B	61	LYS	N-CA	6.55	1.59	1.46
1	A	661	PHE	CG-CD2	-6.55	1.28	1.38
1	A	663	ASN	CA-CB	-6.55	1.36	1.53
1	B	675	PHE	CD1-CE1	-6.54	1.26	1.39
1	B	8	LEU	CG-CD2	6.54	1.76	1.51
1	B	213	GLU	CD-OE2	6.53	1.32	1.25
1	B	483	TYR	CZ-OH	6.53	1.49	1.37
1	B	162	ASP	CA-C	6.53	1.70	1.52
1	B	277	GLN	CD-OE1	6.53	1.38	1.24
1	A	354	ARG	CG-CD	-6.53	1.35	1.51
1	A	500	LEU	C-O	6.53	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	746	MET	CG-SD	-6.53	1.64	1.81
1	B	390	ARG	CD-NE	-6.53	1.35	1.46
1	A	667	CYS	CB-SG	6.52	1.93	1.82
1	B	384	ASN	CA-CB	-6.52	1.36	1.53
1	B	92	ALA	CA-CB	6.52	1.66	1.52
1	A	100	GLY	CA-C	6.51	1.62	1.51
1	B	123	ARG	CB-CG	6.50	1.70	1.52
1	B	137	GLY	C-O	-6.50	1.13	1.23
1	B	185	TYR	CE2-CZ	6.50	1.47	1.38
1	B	524	GLU	CD-OE1	6.50	1.32	1.25
1	B	354	ARG	C-O	-6.50	1.10	1.23
1	A	629	MET	CA-CB	6.50	1.68	1.53
1	B	892	TYR	CZ-OH	6.50	1.48	1.37
1	B	613	PHE	CG-CD2	-6.50	1.29	1.38
1	B	274	TYR	CE2-CZ	-6.49	1.30	1.38
1	B	537	LYS	CG-CD	6.49	1.74	1.52
1	B	499	LEU	N-CA	-6.49	1.33	1.46
1	B	41	GLU	N-CA	-6.49	1.33	1.46
1	B	304	TRP	C-O	-6.49	1.11	1.23
1	A	615	LYS	CB-CG	6.48	1.70	1.52
1	A	33	GLU	CD-OE1	6.47	1.32	1.25
1	B	46	PHE	CE1-CZ	-6.47	1.25	1.37
1	B	331	PHE	CG-CD1	-6.46	1.29	1.38
1	B	787	GLU	CD-OE1	-6.46	1.18	1.25
1	A	291	VAL	C-O	6.46	1.35	1.23
1	B	377	TYR	CG-CD2	-6.46	1.30	1.39
1	A	465	HIS	N-CA	6.45	1.59	1.46
1	B	645	HIS	CA-C	-6.45	1.36	1.52
1	B	599	PHE	CB-CG	-6.45	1.40	1.51
1	B	294	LYS	CE-NZ	6.44	1.65	1.49
1	A	513	LEU	C-O	6.44	1.35	1.23
1	B	123	ARG	NE-CZ	6.44	1.41	1.33
1	B	177	TRP	CE3-CZ3	6.44	1.49	1.38
1	B	808	THR	CA-C	6.43	1.69	1.52
1	A	845	GLU	CA-CB	6.43	1.68	1.53
1	B	225	TYR	CG-CD1	-6.43	1.30	1.39
1	B	436	TYR	CA-CB	-6.43	1.39	1.53
1	A	133	GLU	C-O	6.43	1.35	1.23
1	B	335	PHE	CG-CD1	6.43	1.48	1.38
1	A	859	VAL	CB-CG2	6.42	1.66	1.52
1	B	398	ASP	CG-OD2	6.42	1.40	1.25
1	B	847	GLY	C-O	6.41	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	492	PRO	CA-CB	-6.41	1.40	1.53
1	B	60	PHE	CA-CB	-6.40	1.39	1.53
1	B	8	LEU	N-CA	-6.40	1.33	1.46
1	B	242	ILE	CB-CG2	-6.40	1.33	1.52
1	A	30	GLN	CG-CD	-6.40	1.36	1.51
1	A	388	LYS	CG-CD	6.40	1.74	1.52
1	A	797	LYS	CG-CD	6.40	1.74	1.52
1	A	38	GLU	CD-OE1	6.39	1.32	1.25
1	A	62	GLU	CA-C	-6.39	1.36	1.52
1	A	385	PRO	CG-CD	-6.39	1.29	1.50
1	B	264	TYR	CZ-OH	-6.39	1.26	1.37
1	A	506	LYS	CD-CE	6.39	1.67	1.51
1	B	718	ASN	CA-CB	6.38	1.69	1.53
1	B	789	PHE	C-O	6.38	1.35	1.23
1	A	368	GLY	CA-C	-6.38	1.41	1.51
1	B	603	TRP	CE3-CZ3	6.38	1.49	1.38
1	A	390	ARG	CB-CG	6.37	1.69	1.52
1	A	520	ASN	CA-CB	-6.37	1.36	1.53
1	B	348	LEU	CG-CD1	6.36	1.75	1.51
1	B	871	LEU	CA-CB	-6.36	1.39	1.53
1	A	95	THR	CA-CB	-6.36	1.36	1.53
1	A	459	SER	CA-C	-6.36	1.36	1.52
1	A	519	ALA	C-O	6.36	1.35	1.23
1	A	740	VAL	CA-CB	-6.35	1.41	1.54
1	A	831	ASN	CG-ND2	6.35	1.48	1.32
1	A	520	ASN	CB-CG	-6.35	1.36	1.51
1	A	304	TRP	CZ3-CH2	6.34	1.50	1.40
1	A	450	LYS	CA-C	-6.34	1.36	1.52
1	B	851	PHE	CB-CG	-6.34	1.40	1.51
1	B	881	VAL	CB-CG1	6.34	1.66	1.52
1	A	238	LEU	N-CA	-6.33	1.33	1.46
1	A	367	ARG	N-CA	-6.33	1.33	1.46
1	B	266	VAL	CA-CB	6.33	1.68	1.54
1	B	777	ASP	C-O	6.33	1.35	1.23
1	B	182	GLU	CG-CD	6.33	1.61	1.51
1	A	331	PHE	C-O	6.33	1.35	1.23
1	B	685	ASN	CB-CG	6.33	1.65	1.51
1	B	402	SER	C-N	6.31	1.48	1.34
1	A	628	GLU	N-CA	-6.31	1.33	1.46
1	A	793	TRP	CG-CD2	-6.31	1.32	1.43
1	B	172	GLN	CB-CG	6.30	1.69	1.52
1	A	517	ILE	CA-C	6.30	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	PHE	CB-CG	-6.29	1.40	1.51
1	B	20	SER	N-CA	6.29	1.58	1.46
1	A	511	GLN	C-O	-6.29	1.11	1.23
1	A	750	ASN	CA-CB	6.29	1.69	1.53
1	B	806	PHE	CG-CD2	6.28	1.48	1.38
1	A	282	ILE	C-O	6.28	1.35	1.23
1	A	464	GLU	CB-CG	6.28	1.64	1.52
1	B	375	ARG	CZ-NH1	6.28	1.41	1.33
1	B	729	LEU	CG-CD2	6.28	1.75	1.51
1	B	828	PHE	CG-CD1	6.28	1.48	1.38
1	B	80	GLU	CD-OE2	6.27	1.32	1.25
1	B	330	ASP	CB-CG	6.27	1.65	1.51
1	B	351	ARG	C-O	6.27	1.35	1.23
1	B	426	ARG	CG-CD	6.27	1.67	1.51
1	A	652	PHE	CA-CB	-6.27	1.40	1.53
1	B	310	TYR	CE1-CZ	6.25	1.46	1.38
1	A	628	GLU	C-O	6.25	1.35	1.23
1	B	264	TYR	CE1-CZ	-6.25	1.30	1.38
1	B	154	VAL	CA-CB	-6.24	1.41	1.54
1	A	17	GLY	C-O	-6.24	1.13	1.23
1	B	308	ASP	CG-OD2	6.24	1.39	1.25
1	A	713	SER	C-O	6.24	1.35	1.23
1	B	823	PHE	CB-CG	6.24	1.61	1.51
1	A	888	GLN	CB-CG	6.23	1.69	1.52
1	B	272	VAL	CB-CG2	6.23	1.66	1.52
1	B	374	CYS	CB-SG	-6.22	1.71	1.82
1	B	390	ARG	CG-CD	-6.22	1.36	1.51
1	A	212	THR	C-O	6.21	1.35	1.23
1	A	370	THR	CA-CB	-6.21	1.37	1.53
1	B	14	ALA	CA-CB	-6.21	1.39	1.52
1	A	557	THR	C-O	6.21	1.35	1.23
1	B	738	MET	CB-CG	6.21	1.71	1.51
1	B	510	THR	CB-CG2	6.20	1.72	1.52
1	B	402	SER	C-O	6.20	1.35	1.23
1	A	466	PHE	CE1-CZ	-6.20	1.25	1.37
1	A	609	TYR	CE1-CZ	6.20	1.46	1.38
1	B	638	PHE	CE1-CZ	-6.20	1.25	1.37
1	B	665	VAL	C-O	6.19	1.35	1.23
1	B	189	ASN	N-CA	-6.18	1.33	1.46
1	B	46	PHE	CG-CD2	-6.18	1.29	1.38
1	B	680	GLN	C-O	-6.18	1.11	1.23
1	B	61	LYS	CE-NZ	6.18	1.64	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	728	LYS	CA-CB	6.18	1.67	1.53
1	A	696	TRP	CA-C	-6.18	1.36	1.52
1	A	205	GLU	CG-CD	6.17	1.61	1.51
1	B	304	TRP	N-CA	6.17	1.58	1.46
1	A	492	PRO	CA-C	-6.17	1.40	1.52
1	A	856	SER	C-O	-6.17	1.11	1.23
1	A	511	GLN	CG-CD	6.16	1.65	1.51
1	B	46	PHE	CD1-CE1	6.16	1.51	1.39
1	B	323	GLU	CD-OE2	6.16	1.32	1.25
1	A	797	LYS	C-O	-6.16	1.11	1.23
1	A	81	LEU	C-O	-6.16	1.11	1.23
1	A	495	GLU	CD-OE1	6.16	1.32	1.25
1	B	631	MET	CG-SD	6.15	1.97	1.81
1	A	125	VAL	N-CA	6.15	1.58	1.46
1	A	361	TYR	C-O	6.15	1.35	1.23
1	A	367	ARG	NE-CZ	6.15	1.41	1.33
1	B	397	ALA	CA-C	6.14	1.69	1.52
1	B	682	ASP	CB-CG	-6.14	1.38	1.51
1	A	870	SER	CA-CB	6.14	1.62	1.52
1	B	130	SER	CA-CB	-6.14	1.43	1.52
1	B	293	TRP	CZ3-CH2	6.14	1.49	1.40
1	A	47	GLN	CA-CB	-6.14	1.40	1.53
1	A	65	PRO	CA-C	6.14	1.65	1.52
1	A	359	THR	N-CA	-6.14	1.34	1.46
1	A	264	TYR	CZ-OH	6.13	1.48	1.37
1	A	609	TYR	CD1-CE1	6.13	1.48	1.39
1	B	730	PHE	C-O	6.13	1.35	1.23
1	B	480	PRO	CB-CG	6.13	1.80	1.50
1	B	16	GLU	CD-OE2	-6.13	1.19	1.25
1	B	450	LYS	C-O	6.13	1.34	1.23
1	A	823	PHE	CB-CG	6.12	1.61	1.51
1	A	634	GLU	CG-CD	6.12	1.61	1.51
1	B	668	LEU	CG-CD2	6.12	1.74	1.51
1	B	796	ILE	CA-C	6.12	1.68	1.52
1	A	492	PRO	N-CA	-6.12	1.36	1.47
1	A	117	ASN	CB-CG	6.11	1.65	1.51
1	B	231	ALA	C-O	-6.11	1.11	1.23
1	A	511	GLN	CB-CG	6.11	1.69	1.52
1	A	518	GLN	CA-C	6.11	1.68	1.52
1	B	27	TYR	CD1-CE1	6.10	1.48	1.39
1	B	507	LYS	CB-CG	6.10	1.69	1.52
1	B	56	HIS	CA-C	6.10	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	182	GLU	CD-OE1	-6.10	1.19	1.25
1	A	780	THR	CB-CG2	-6.09	1.32	1.52
1	B	806	PHE	CE2-CZ	6.09	1.49	1.37
1	A	89	VAL	C-O	-6.09	1.11	1.23
1	B	168	VAL	CB-CG1	6.09	1.65	1.52
1	B	52	PRO	C-O	-6.09	1.11	1.23
1	B	138	ILE	CB-CG2	-6.08	1.33	1.52
1	B	192	TYR	CE2-CZ	-6.08	1.30	1.38
1	B	632	ALA	C-O	6.08	1.34	1.23
1	B	428	MET	CG-SD	-6.08	1.65	1.81
1	B	475	ARG	CB-CG	6.08	1.69	1.52
1	A	99	GLN	CA-C	-6.08	1.37	1.52
1	A	888	GLN	C-O	6.08	1.34	1.23
1	B	725	GLN	CA-CB	6.08	1.67	1.53
1	A	74	LYS	CG-CD	6.07	1.73	1.52
1	B	150	VAL	CA-C	6.07	1.68	1.52
1	B	153	VAL	C-O	6.07	1.34	1.23
1	A	298	SER	CA-CB	-6.06	1.43	1.52
1	A	304	TRP	CB-CG	6.06	1.61	1.50
1	A	772	MET	N-CA	-6.06	1.34	1.46
1	B	143	LEU	CA-CB	6.06	1.67	1.53
1	B	585	LEU	CG-CD1	6.06	1.74	1.51
1	B	859	VAL	C-O	-6.06	1.11	1.23
1	A	31	ASP	CG-OD1	6.06	1.39	1.25
1	A	394	VAL	C-O	-6.05	1.11	1.23
1	B	167	PHE	CG-CD2	-6.05	1.29	1.38
1	A	756	HIS	CG-CD2	6.05	1.46	1.35
1	B	187	LYS	CD-CE	6.05	1.66	1.51
1	A	585	LEU	CG-CD2	6.05	1.74	1.51
1	A	5	ALA	C-O	-6.04	1.11	1.23
1	A	125	VAL	CB-CG1	-6.04	1.40	1.52
1	A	558	ILE	CA-CB	-6.04	1.41	1.54
1	A	794	ASN	N-CA	-6.04	1.34	1.46
1	A	133	GLU	CB-CG	6.04	1.63	1.52
1	B	164	LYS	C-O	6.03	1.34	1.23
1	B	885	GLU	CG-CD	6.03	1.60	1.51
1	A	266	VAL	CB-CG1	-6.03	1.40	1.52
1	B	54	VAL	C-O	-6.03	1.11	1.23
1	A	178	SER	CB-OG	6.02	1.50	1.42
1	B	322	GLY	C-O	6.01	1.33	1.23
1	B	325	TRP	CG-CD1	-6.01	1.28	1.36
1	A	129	GLN	C-O	-6.01	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	483	TYR	CD2-CE2	6.01	1.48	1.39
1	A	440	ARG	C-N	6.00	1.47	1.34
1	A	885	GLU	CD-OE1	6.00	1.32	1.25
1	B	49	PRO	N-CD	-6.00	1.39	1.47
1	B	57	SER	CB-OG	6.00	1.50	1.42
1	B	502	PHE	CA-CB	6.00	1.67	1.53
1	A	613	PHE	CD2-CE2	5.99	1.51	1.39
1	B	490	PHE	C-O	-5.99	1.11	1.23
1	B	62	GLU	C-O	5.99	1.34	1.23
1	B	472	VAL	CB-CG1	-5.99	1.40	1.52
1	B	518	GLN	CG-CD	5.99	1.64	1.51
1	A	142	GLN	CB-CG	-5.98	1.36	1.52
1	B	443	ALA	N-CA	5.98	1.58	1.46
1	A	487	PRO	N-CA	-5.98	1.37	1.47
1	A	788	GLU	C-O	-5.98	1.11	1.23
1	B	387	PHE	CE2-CZ	5.98	1.48	1.37
1	A	215	TYR	CA-CB	-5.97	1.40	1.53
1	B	418	ARG	CZ-NH1	5.97	1.40	1.33
1	A	451	ARG	CZ-NH1	5.97	1.40	1.33
1	A	545	GLY	CA-C	5.97	1.61	1.51
1	A	596	LEU	N-CA	5.96	1.58	1.46
1	B	646	GLN	CG-CD	5.96	1.64	1.51
1	A	206	ASP	CB-CG	5.96	1.64	1.51
1	A	392	GLU	CA-CB	-5.96	1.40	1.53
1	B	26	LYS	CG-CD	5.96	1.72	1.52
1	B	225	TYR	CG-CD2	-5.96	1.31	1.39
1	B	176	PHE	CB-CG	-5.96	1.41	1.51
1	A	368	GLY	C-O	5.95	1.33	1.23
1	B	651	ARG	NE-CZ	5.95	1.40	1.33
1	B	342	ASN	CA-CB	-5.95	1.37	1.53
1	B	435	VAL	CB-CG1	5.95	1.65	1.52
1	A	570	ARG	CA-CB	5.95	1.67	1.53
1	B	27	TYR	CG-CD2	-5.94	1.31	1.39
1	A	713	SER	N-CA	5.94	1.58	1.46
1	B	451	ARG	CD-NE	5.94	1.56	1.46
1	B	49	PRO	N-CA	-5.94	1.37	1.47
1	B	125	VAL	CB-CG2	-5.93	1.40	1.52
1	A	114	LEU	N-CA	5.93	1.58	1.46
1	A	889	LEU	C-O	-5.93	1.12	1.23
1	B	643	GLN	CA-CB	5.93	1.67	1.53
1	B	9	ALA	C-O	5.93	1.34	1.23
1	A	124	VAL	CA-C	-5.92	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	409	PHE	CD1-CE1	5.92	1.51	1.39
1	A	542	LYS	N-CA	5.91	1.58	1.46
1	A	700	SER	CB-OG	-5.91	1.34	1.42
1	A	65	PRO	C-O	5.91	1.35	1.23
1	B	597	VAL	CA-C	5.91	1.68	1.52
1	A	167	PHE	N-CA	-5.91	1.34	1.46
1	B	673	ILE	CA-C	5.91	1.68	1.52
1	B	194	ALA	CA-CB	-5.91	1.40	1.52
1	A	503	PHE	CB-CG	-5.91	1.41	1.51
1	A	865	PHE	CE2-CZ	5.90	1.48	1.37
1	B	746	MET	CG-SD	5.90	1.96	1.81
1	B	21	HIS	C-O	-5.90	1.12	1.23
1	B	348	LEU	CB-CG	5.90	1.69	1.52
1	A	392	GLU	CD-OE1	5.90	1.32	1.25
1	A	795	ASN	CB-CG	-5.90	1.37	1.51
1	A	27	TYR	CD2-CE2	-5.89	1.30	1.39
1	A	274	TYR	CE2-CZ	-5.89	1.30	1.38
1	A	743	THR	C-O	5.89	1.34	1.23
1	A	312	ARG	CZ-NH1	5.88	1.40	1.33
1	A	789	PHE	CE2-CZ	5.88	1.48	1.37
1	B	641	PRO	CG-CD	5.88	1.70	1.50
1	A	57	SER	CA-CB	-5.88	1.44	1.52
1	B	294	LYS	CD-CE	5.88	1.66	1.51
1	B	601	ILE	CA-CB	5.88	1.68	1.54
1	B	172	GLN	CG-CD	-5.88	1.37	1.51
1	A	676	LYS	CA-CB	5.88	1.66	1.53
1	A	331	PHE	CE2-CZ	-5.88	1.26	1.37
1	A	192	TYR	CE2-CZ	5.87	1.46	1.38
1	B	372	GLY	C-O	5.87	1.33	1.23
1	A	134	GLY	CA-C	5.87	1.61	1.51
1	B	453	PHE	CE1-CZ	5.87	1.48	1.37
1	B	447	VAL	C-O	-5.86	1.12	1.23
1	A	643	GLN	CG-CD	-5.86	1.37	1.51
1	A	713	SER	CA-C	5.86	1.68	1.52
1	A	124	VAL	CA-CB	5.86	1.67	1.54
1	B	232	LEU	CG-CD1	-5.86	1.30	1.51
1	A	325	TRP	CG-CD1	-5.85	1.28	1.36
1	B	360	PHE	CG-CD2	-5.85	1.29	1.38
1	B	789	PHE	CG-CD2	5.85	1.47	1.38
1	B	876	THR	CA-C	-5.85	1.37	1.52
1	A	451	ARG	C-O	5.84	1.34	1.23
1	B	351	ARG	CA-C	5.84	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	241	SER	CB-OG	5.84	1.49	1.42
1	A	109	ALA	CA-C	5.84	1.68	1.52
1	B	487	PRO	C-O	5.84	1.34	1.23
1	B	383	VAL	CB-CG2	-5.83	1.40	1.52
1	A	586	MET	C-O	5.83	1.34	1.23
1	A	149	TRP	CB-CG	-5.83	1.39	1.50
1	B	57	SER	N-CA	-5.83	1.34	1.46
1	B	404	GLU	CD-OE1	5.83	1.32	1.25
1	B	33	GLU	CB-CG	5.83	1.63	1.52
1	A	273	THR	CA-CB	-5.82	1.38	1.53
1	B	99	GLN	C-O	-5.82	1.12	1.23
1	B	342	ASN	CG-OD1	5.82	1.36	1.24
1	B	582	MET	SD-CE	5.82	2.10	1.77
1	A	594	LEU	CA-C	-5.82	1.37	1.52
1	B	105	SER	N-CA	-5.82	1.34	1.46
1	B	835	TYR	C-O	5.82	1.34	1.23
1	A	62	GLU	CG-CD	5.81	1.60	1.51
1	B	163	GLY	C-O	-5.81	1.14	1.23
1	A	556	GLN	C-O	5.80	1.34	1.23
1	B	607	ARG	NE-CZ	5.80	1.40	1.33
1	A	365	TRP	CG-CD1	-5.80	1.28	1.36
1	A	294	LYS	C-O	5.80	1.34	1.23
1	A	642	CYS	N-CA	5.80	1.57	1.46
1	A	800	GLN	CA-CB	-5.80	1.41	1.53
1	B	882	ASN	CB-CG	5.80	1.64	1.51
1	B	148	GLU	CD-OE1	-5.79	1.19	1.25
1	A	71	TYR	CD2-CE2	-5.79	1.30	1.39
1	B	259	VAL	C-O	5.79	1.34	1.23
1	B	647	VAL	CA-CB	5.79	1.67	1.54
1	A	176	PHE	CA-CB	-5.79	1.41	1.53
1	A	767	ASP	CG-OD2	5.79	1.38	1.25
1	B	76	LYS	CD-CE	5.79	1.65	1.51
1	A	175	GLU	C-O	5.79	1.34	1.23
1	A	97	ILE	C-O	-5.79	1.12	1.23
1	A	165	LEU	CA-CB	5.79	1.67	1.53
1	B	15	ALA	CA-CB	5.79	1.64	1.52
1	B	193	GLU	CA-C	-5.79	1.38	1.52
1	A	454	PHE	CD1-CE1	-5.78	1.27	1.39
1	A	862	ASP	CG-OD2	-5.78	1.12	1.25
1	B	207	PHE	CD2-CE2	5.78	1.50	1.39
1	B	229	LEU	CG-CD1	-5.78	1.30	1.51
1	B	386	GLN	CA-CB	-5.78	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	98	CYS	C-O	-5.77	1.12	1.23
1	B	46	PHE	C-O	-5.77	1.12	1.23
1	B	887	LEU	CG-CD2	-5.77	1.30	1.51
1	A	634	GLU	CD-OE2	5.77	1.31	1.25
1	B	178	SER	N-CA	5.77	1.57	1.46
1	B	216	ASP	CB-CG	-5.76	1.39	1.51
1	A	437	GLN	N-CA	-5.76	1.34	1.46
1	A	647	VAL	CB-CG2	5.76	1.65	1.52
1	B	415	GLN	CD-NE2	5.75	1.47	1.32
1	B	311	GLU	CD-OE1	5.75	1.31	1.25
1	B	277	GLN	CA-C	-5.75	1.38	1.52
1	B	269	ALA	N-CA	5.75	1.57	1.46
1	B	663	ASN	CA-C	-5.75	1.38	1.52
1	B	329	ARG	C-N	5.74	1.47	1.34
1	A	751	LYS	N-CA	5.74	1.57	1.46
1	A	134	GLY	C-O	5.74	1.32	1.23
1	A	80	GLU	CD-OE1	5.74	1.31	1.25
1	A	511	GLN	CD-OE1	5.74	1.36	1.24
1	B	185	TYR	CE1-CZ	-5.74	1.31	1.38
1	A	175	GLU	N-CA	5.73	1.57	1.46
1	A	778	SER	CA-CB	5.73	1.61	1.52
1	A	744	GLU	CD-OE2	5.73	1.31	1.25
1	A	696	TRP	CG-CD1	-5.73	1.28	1.36
1	A	33	GLU	CD-OE2	5.73	1.31	1.25
1	A	86	GLN	CD-OE1	5.72	1.36	1.24
1	B	384	ASN	C-O	5.72	1.34	1.23
1	A	671	LEU	C-O	-5.72	1.12	1.23
1	B	72	GLY	C-O	5.72	1.32	1.23
1	B	456	ALA	N-CA	5.72	1.57	1.46
1	A	289	GLY	N-CA	-5.72	1.37	1.46
1	B	807	GLU	CD-OE2	5.72	1.31	1.25
1	A	831	ASN	CA-C	-5.71	1.38	1.52
1	A	127	TYR	CD2-CE2	-5.71	1.30	1.39
1	A	387	PHE	CG-CD1	5.71	1.47	1.38
1	B	425	GLY	N-CA	5.71	1.54	1.46
1	B	873	LYS	CA-CB	5.71	1.66	1.53
1	B	436	TYR	CG-CD2	-5.71	1.31	1.39
1	B	223	ASP	CA-C	-5.70	1.38	1.52
1	B	292	GLU	CA-CB	5.70	1.66	1.53
1	B	638	PHE	CB-CG	-5.70	1.41	1.51
1	B	714	ASN	C-O	5.70	1.34	1.23
1	A	627	TYR	CG-CD1	-5.70	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	664	PHE	CE2-CZ	-5.70	1.26	1.37
1	A	601	ILE	C-O	5.70	1.34	1.23
1	A	871	LEU	CG-CD1	5.70	1.73	1.51
1	A	179	ALA	C-O	-5.70	1.12	1.23
1	B	883	ILE	CB-CG2	5.70	1.70	1.52
1	B	225	TYR	CA-C	-5.70	1.38	1.52
1	B	321	ASP	C-O	5.69	1.34	1.23
1	B	713	SER	CA-C	5.69	1.67	1.52
1	A	768	THR	CA-CB	-5.69	1.38	1.53
1	A	791	TYR	CG-CD2	5.69	1.46	1.39
1	B	278	ARG	CD-NE	5.69	1.56	1.46
1	A	541	SER	N-CA	5.68	1.57	1.46
1	A	362	GLU	N-CA	5.68	1.57	1.46
1	B	217	LEU	N-CA	5.68	1.57	1.46
1	A	333	ARG	CB-CG	5.68	1.67	1.52
1	A	407	CYS	CA-CB	-5.68	1.41	1.53
1	A	603	TRP	CE2-CZ2	-5.68	1.30	1.39
1	A	737	ASP	C-O	5.68	1.34	1.23
1	B	288	TRP	CG-CD1	-5.68	1.28	1.36
1	A	867	ALA	C-N	-5.67	1.21	1.34
1	A	831	ASN	N-CA	-5.67	1.35	1.46
1	A	646	GLN	CB-CG	5.67	1.67	1.52
1	A	510	THR	C-O	-5.67	1.12	1.23
1	A	739	GLU	CG-CD	-5.67	1.43	1.51
1	B	51	PHE	CB-CG	-5.67	1.41	1.51
1	B	473	SER	N-CA	-5.67	1.35	1.46
1	A	390	ARG	CA-C	5.66	1.67	1.52
1	B	501	ARG	CB-CG	5.66	1.67	1.52
1	A	886	TRP	CD2-CE2	-5.66	1.34	1.41
1	B	368	GLY	CA-C	5.66	1.60	1.51
1	A	186	ALA	C-O	5.66	1.34	1.23
1	A	891	MET	SD-CE	5.66	2.09	1.77
1	A	660	ASP	CA-CB	-5.65	1.41	1.53
1	B	75	TRP	CZ3-CH2	-5.65	1.31	1.40
1	B	478	LEU	CG-CD2	-5.65	1.30	1.51
1	B	855	ILE	N-CA	5.65	1.57	1.46
1	B	53	PRO	CA-C	-5.64	1.41	1.52
1	A	402	SER	CA-CB	5.64	1.61	1.52
1	B	478	LEU	CB-CG	5.64	1.69	1.52
1	A	790	LYS	CA-C	5.64	1.67	1.52
1	A	70	THR	CA-CB	5.64	1.68	1.53
1	A	603	TRP	CG-CD1	5.64	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	619	ASP	N-CA	-5.64	1.35	1.46
1	B	8	LEU	C-O	5.64	1.34	1.23
1	A	477	ARG	CD-NE	5.64	1.56	1.46
1	A	572	ASN	CG-OD1	5.64	1.36	1.24
1	A	120	ILE	CG1-CD1	5.63	1.89	1.50
1	A	404	GLU	CD-OE2	5.63	1.31	1.25
1	A	695	SER	N-CA	5.63	1.57	1.46
1	B	624	MET	CA-C	5.63	1.67	1.52
1	A	185	TYR	CD1-CE1	5.63	1.47	1.39
1	A	479	PRO	C-O	-5.63	1.11	1.23
1	A	854	PHE	C-O	5.63	1.34	1.23
1	A	438	VAL	CB-CG2	-5.63	1.41	1.52
1	A	850	ASP	C-O	-5.63	1.12	1.23
1	A	43	GLY	C-O	-5.62	1.14	1.23
1	A	141	PHE	CA-CB	-5.62	1.41	1.53
1	A	578	SER	N-CA	5.62	1.57	1.46
1	A	854	PHE	CA-CB	-5.62	1.41	1.53
1	A	189	ASN	C-O	5.62	1.34	1.23
1	B	683	PRO	CG-CD	5.62	1.69	1.50
1	B	157	LEU	CA-CB	5.62	1.66	1.53
1	A	238	LEU	CG-CD1	5.62	1.72	1.51
1	A	145	GLN	CA-CB	-5.62	1.41	1.53
1	A	608	ASN	C-N	-5.62	1.21	1.34
1	A	685	ASN	CA-C	5.61	1.67	1.52
1	B	138	ILE	N-CA	5.61	1.57	1.46
1	A	415	GLN	CB-CG	-5.61	1.37	1.52
1	B	126	PRO	C-O	-5.60	1.12	1.23
1	A	122	HIS	CB-CG	-5.60	1.40	1.50
1	B	575	SER	CA-CB	-5.60	1.44	1.52
1	A	13	GLU	N-CA	-5.60	1.35	1.46
1	A	607	ARG	CG-CD	-5.60	1.38	1.51
1	B	280	ASN	CB-CG	5.60	1.64	1.51
1	B	11	ASP	CG-OD2	5.60	1.38	1.25
1	B	789	PHE	CE1-CZ	5.60	1.48	1.37
1	A	869	ARG	CZ-NH1	5.59	1.40	1.33
1	A	153	VAL	CB-CG2	5.59	1.64	1.52
1	A	388	LYS	C-O	5.59	1.33	1.23
1	A	233	GLU	CB-CG	-5.59	1.41	1.52
1	B	134	GLY	C-O	-5.58	1.14	1.23
1	A	674	LEU	CG-CD1	-5.58	1.31	1.51
1	A	866	ARG	C-O	5.58	1.33	1.23
1	B	274	TYR	CG-CD1	-5.58	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	LYS	C-O	-5.57	1.12	1.23
1	B	452	ASP	CG-OD1	5.57	1.38	1.25
1	A	114	LEU	CG-CD1	5.57	1.72	1.51
1	A	265	SER	C-O	-5.57	1.12	1.23
1	B	580	ARG	CG-CD	5.57	1.65	1.51
1	A	174	ASN	CG-OD1	5.57	1.36	1.24
1	A	491	GLU	CD-OE1	5.57	1.31	1.25
1	A	324	PHE	CG-CD2	-5.57	1.30	1.38
1	A	631	MET	C-O	5.57	1.33	1.23
1	B	310	TYR	CA-C	-5.57	1.38	1.52
1	B	643	GLN	C-O	-5.57	1.12	1.23
1	B	467	ILE	CB-CG2	5.56	1.70	1.52
1	A	229	LEU	N-CA	-5.56	1.35	1.46
1	B	854	PHE	CG-CD1	5.56	1.47	1.38
1	A	498	PHE	CG-CD2	-5.56	1.30	1.38
1	A	632	ALA	CA-CB	-5.56	1.40	1.52
1	A	94	ARG	C-O	-5.55	1.12	1.23
1	A	120	ILE	CA-CB	5.55	1.67	1.54
1	A	617	ASP	CG-OD1	5.55	1.38	1.25
1	B	656	GLU	CG-CD	5.55	1.60	1.51
1	B	439	PRO	CA-CB	-5.55	1.42	1.53
1	B	868	PHE	N-CA	-5.55	1.35	1.46
1	A	146	PHE	CD1-CE1	5.55	1.50	1.39
1	A	475	ARG	CG-CD	5.54	1.65	1.51
1	A	714	ASN	C-O	5.54	1.33	1.23
1	A	334	GLU	CD-OE1	5.54	1.31	1.25
1	B	206	ASP	CB-CG	-5.54	1.40	1.51
1	B	488	SER	C-O	5.54	1.33	1.23
1	B	640	LEU	C-O	-5.54	1.12	1.23
1	B	710	MET	CA-CB	5.54	1.66	1.53
1	A	320	GLU	CG-CD	-5.53	1.43	1.51
1	A	388	LYS	CD-CE	5.53	1.65	1.51
1	B	90	ASP	CG-OD2	5.53	1.38	1.25
1	B	583	VAL	CB-CG1	-5.53	1.41	1.52
1	A	454	PHE	CB-CG	-5.53	1.42	1.51
1	A	204	PHE	CB-CG	-5.53	1.42	1.51
1	B	615	LYS	CB-CG	5.53	1.67	1.52
1	B	264	TYR	CB-CG	-5.53	1.43	1.51
1	B	89	VAL	CA-C	-5.53	1.38	1.52
1	B	381	PHE	CB-CG	-5.52	1.42	1.51
1	B	460	ARG	CG-CD	5.52	1.65	1.51
1	B	524	GLU	CA-C	5.52	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	36	ARG	NE-CZ	5.52	1.40	1.33
1	A	678	PHE	CD1-CE1	5.52	1.50	1.39
1	A	12	ARG	NE-CZ	5.52	1.40	1.33
1	A	616	PHE	CG-CD1	-5.52	1.30	1.38
1	A	9	ALA	CA-CB	5.52	1.64	1.52
1	B	196	SER	CB-OG	-5.52	1.35	1.42
1	B	157	LEU	CG-CD1	-5.51	1.31	1.51
1	B	454	PHE	CE1-CZ	5.51	1.47	1.37
1	A	665	VAL	N-CA	5.51	1.57	1.46
1	A	663	ASN	N-CA	5.51	1.57	1.46
1	A	468	ASN	C-O	5.50	1.33	1.23
1	A	214	TRP	CZ2-CH2	-5.50	1.26	1.37
1	A	571	THR	CA-CB	5.50	1.67	1.53
1	B	491	GLU	CB-CG	5.50	1.62	1.52
1	A	884	GLN	N-CA	-5.50	1.35	1.46
1	A	344	THR	N-CA	-5.49	1.35	1.46
1	A	83	SER	C-O	-5.49	1.12	1.23
1	A	830	LEU	N-CA	5.49	1.57	1.46
1	B	377	TYR	C-O	5.48	1.33	1.23
1	B	684	GLU	CD-OE2	5.48	1.31	1.25
1	A	503	PHE	CD2-CE2	-5.48	1.28	1.39
1	B	183	LYS	CE-NZ	5.48	1.62	1.49
1	B	521	LEU	C-O	5.48	1.33	1.23
1	B	661	PHE	CB-CG	5.48	1.60	1.51
1	B	837	MET	C-O	5.48	1.33	1.23
1	B	475	ARG	N-CA	-5.47	1.35	1.46
1	A	138	ILE	CB-CG2	5.47	1.69	1.52
1	B	634	GLU	CB-CG	5.47	1.62	1.52
1	A	459	SER	CB-OG	-5.47	1.35	1.42
1	A	460	ARG	CA-C	-5.47	1.38	1.52
1	B	325	TRP	CZ2-CH2	5.47	1.47	1.37
1	B	31	ASP	CG-OD1	5.47	1.38	1.25
1	A	497	ASP	CB-CG	5.47	1.63	1.51
1	B	349	LYS	CB-CG	-5.47	1.37	1.52
1	B	27	TYR	CA-CB	-5.46	1.42	1.53
1	A	209	GLY	C-O	-5.46	1.15	1.23
1	B	87	PHE	CD2-CE2	5.46	1.50	1.39
1	B	697	LEU	CA-CB	5.46	1.66	1.53
1	A	661	PHE	CA-C	5.46	1.67	1.52
1	B	223	ASP	CB-CG	-5.46	1.40	1.51
1	A	860	ARG	NE-CZ	5.46	1.40	1.33
1	B	28	LEU	C-O	5.46	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	377	TYR	N-CA	-5.46	1.35	1.46
1	A	51	PHE	CE2-CZ	5.45	1.47	1.37
1	A	129	GLN	N-CA	5.45	1.57	1.46
1	A	311	GLU	C-O	5.45	1.33	1.23
1	A	271	GLN	CA-C	5.45	1.67	1.52
1	A	495	GLU	CA-CB	-5.45	1.42	1.53
1	A	118	GLU	CB-CG	5.45	1.62	1.52
1	A	243	ASN	CA-C	5.45	1.67	1.52
1	B	60	PHE	N-CA	5.45	1.57	1.46
1	B	61	LYS	CD-CE	5.45	1.64	1.51
1	A	364	THR	CA-C	5.44	1.67	1.52
1	A	23	ARG	CA-C	5.44	1.67	1.52
1	B	660	ASP	C-O	5.44	1.33	1.23
1	B	742	ALA	CA-CB	5.44	1.63	1.52
1	B	824	GLU	CA-C	5.43	1.67	1.52
1	A	84	ASN	C-N	5.43	1.44	1.34
1	B	400	TYR	N-CA	5.43	1.57	1.46
1	A	652	PHE	C-O	5.43	1.33	1.23
1	A	127	TYR	CE1-CZ	-5.43	1.31	1.38
1	B	31	ASP	CB-CG	5.43	1.63	1.51
1	B	608	ASN	CA-C	5.43	1.67	1.52
1	B	797	LYS	CB-CG	5.42	1.67	1.52
1	A	518	GLN	CA-CB	-5.42	1.42	1.53
1	B	392	GLU	CD-OE2	5.42	1.31	1.25
1	A	861	LEU	CG-CD2	5.42	1.71	1.51
1	B	267	THR	CA-CB	5.42	1.67	1.53
1	A	177	TRP	CG-CD2	5.42	1.52	1.43
1	B	77	ARG	CG-CD	-5.41	1.38	1.51
1	A	749	LEU	CG-CD2	5.41	1.71	1.51
1	A	892	TYR	CA-CB	5.41	1.65	1.53
1	A	648	ILE	CA-CB	-5.40	1.42	1.54
1	B	149	TRP	CZ3-CH2	-5.40	1.31	1.40
1	B	197	GLY	CA-C	5.40	1.60	1.51
1	B	206	ASP	C-O	-5.40	1.13	1.23
1	B	219	LYS	CA-C	5.40	1.67	1.52
1	A	277	GLN	C-O	5.40	1.33	1.23
1	B	7	LYS	CE-NZ	5.40	1.62	1.49
1	B	400	TYR	CA-C	5.40	1.67	1.52
1	B	129	GLN	CA-CB	-5.39	1.42	1.53
1	B	319	MET	C-O	5.39	1.33	1.23
1	A	240	CYS	N-CA	-5.39	1.35	1.46
1	A	409	PHE	CG-CD1	5.39	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	283	ARG	CA-C	-5.39	1.39	1.52
1	A	168	VAL	CA-CB	-5.39	1.43	1.54
1	B	555	LEU	N-CA	5.39	1.57	1.46
1	B	467	ILE	CB-CG1	5.38	1.69	1.54
1	A	202	GLU	CD-OE1	5.38	1.31	1.25
1	A	288	TRP	CE3-CZ3	-5.38	1.29	1.38
1	A	225	TYR	CB-CG	-5.38	1.43	1.51
1	B	169	HIS	N-CA	-5.38	1.35	1.46
1	B	382	TRP	CG-CD1	-5.37	1.29	1.36
1	B	557	THR	CB-CG2	5.37	1.70	1.52
1	B	304	TRP	CA-CB	5.37	1.65	1.53
1	A	884	GLN	CG-CD	5.36	1.63	1.51
1	B	15	ALA	N-CA	5.36	1.57	1.46
1	B	152	VAL	CA-CB	-5.36	1.43	1.54
1	B	700	SER	CB-OG	-5.36	1.35	1.42
1	B	615	LYS	CD-CE	5.36	1.64	1.51
1	B	214	TRP	CZ3-CH2	5.36	1.48	1.40
1	A	298	SER	N-CA	5.35	1.57	1.46
1	A	311	GLU	CD-OE2	5.35	1.31	1.25
1	A	770	ARG	C-N	-5.35	1.21	1.34
1	B	577	GLU	CD-OE2	5.35	1.31	1.25
1	B	609	TYR	CA-CB	5.35	1.65	1.53
1	A	831	ASN	CA-CB	5.35	1.67	1.53
1	B	607	ARG	CZ-NH1	5.35	1.40	1.33
1	B	584	ASN	CA-C	5.35	1.66	1.52
1	A	873	LYS	CA-C	5.35	1.66	1.52
1	A	359	THR	CB-CG2	-5.34	1.34	1.52
1	B	784	LEU	C-O	-5.34	1.13	1.23
1	A	623	SER	N-CA	-5.34	1.35	1.46
1	B	23	ARG	C-N	-5.34	1.21	1.34
1	B	225	TYR	CZ-OH	5.34	1.47	1.37
1	A	668	LEU	C-O	5.34	1.33	1.23
1	B	521	LEU	N-CA	5.34	1.57	1.46
1	A	338	LEU	CG-CD2	-5.34	1.32	1.51
1	B	596	LEU	C-O	5.33	1.33	1.23
1	A	107	LEU	CG-CD2	-5.33	1.32	1.51
1	A	166	VAL	CA-CB	-5.33	1.43	1.54
1	A	458	ALA	CA-CB	-5.33	1.41	1.52
1	B	261	GLY	CA-C	5.33	1.60	1.51
1	B	283	ARG	NE-CZ	5.33	1.40	1.33
1	A	313	GLU	CB-CG	-5.33	1.42	1.52
1	A	645	HIS	C-N	-5.33	1.21	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	660	ASP	N-CA	-5.33	1.35	1.46
1	A	777	ASP	CA-CB	5.33	1.65	1.53
1	B	664	PHE	CD1-CE1	5.33	1.50	1.39
1	A	271	GLN	CD-OE1	5.33	1.35	1.24
1	B	851	PHE	CG-CD1	-5.33	1.30	1.38
1	A	730	PHE	N-CA	5.33	1.56	1.46
1	A	87	PHE	CG-CD2	-5.32	1.30	1.38
1	A	313	GLU	CA-CB	-5.32	1.42	1.53
1	A	60	PHE	CG-CD2	5.32	1.46	1.38
1	A	809	ASP	CA-C	5.32	1.66	1.52
1	B	33	GLU	CG-CD	5.32	1.59	1.51
1	B	326	MET	N-CA	-5.32	1.35	1.46
1	B	188	VAL	N-CA	5.31	1.56	1.46
1	B	502	PHE	CG-CD1	-5.31	1.30	1.38
1	A	470	ARG	CZ-NH2	-5.31	1.26	1.33
1	A	503	PHE	CE1-CZ	-5.31	1.27	1.37
1	A	213	GLU	C-O	-5.31	1.13	1.23
1	B	356	TRP	CA-CB	-5.30	1.42	1.53
1	B	95	THR	N-CA	5.30	1.56	1.46
1	A	123	ARG	CB-CG	-5.30	1.38	1.52
1	A	544	ALA	CA-CB	5.30	1.63	1.52
1	A	670	ARG	CZ-NH1	5.30	1.40	1.33
1	B	634	GLU	CG-CD	5.30	1.59	1.51
1	B	181	LEU	CA-C	-5.29	1.39	1.52
1	A	230	LYS	CE-NZ	5.29	1.62	1.49
1	A	66	ASN	C-O	-5.29	1.13	1.23
1	B	720	SER	CA-CB	5.29	1.60	1.52
1	A	335	PHE	CB-CG	5.29	1.60	1.51
1	A	498	PHE	CG-CD1	-5.29	1.30	1.38
1	B	892	TYR	C-O	5.28	1.33	1.23
1	A	464	GLU	CG-CD	5.28	1.59	1.51
1	A	626	ALA	N-CA	-5.28	1.35	1.46
1	B	18	LEU	N-CA	-5.28	1.35	1.46
1	A	784	LEU	C-O	5.28	1.33	1.23
1	B	133	GLU	N-CA	5.28	1.56	1.46
1	B	391	LEU	CA-CB	5.28	1.65	1.53
1	B	456	ALA	CA-CB	5.28	1.63	1.52
1	A	669	VAL	C-N	-5.27	1.22	1.34
1	A	789	PHE	C-O	-5.27	1.13	1.23
1	B	388	LYS	CA-C	-5.27	1.39	1.52
1	B	540	PHE	CB-CG	5.27	1.60	1.51
1	B	655	ASP	CA-CB	5.27	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	TYR	CD2-CE2	-5.27	1.31	1.39
1	B	415	GLN	N-CA	5.27	1.56	1.46
1	B	2	ALA	C-O	5.27	1.33	1.23
1	B	315	LEU	CA-C	-5.26	1.39	1.52
1	B	318	LYS	C-O	5.26	1.33	1.23
1	A	511	GLN	CD-NE2	5.26	1.46	1.32
1	B	392	GLU	C-O	5.26	1.33	1.23
1	A	434	ALA	CA-C	-5.26	1.39	1.52
1	A	475	ARG	CZ-NH1	5.26	1.39	1.33
1	A	691	LEU	C-O	-5.26	1.13	1.23
1	B	509	GLY	CA-C	-5.25	1.43	1.51
1	B	325	TRP	CB-CG	5.25	1.59	1.50
1	B	396	ASP	C-N	5.25	1.46	1.34
1	A	675	PHE	CE2-CZ	-5.25	1.27	1.37
1	B	726	PHE	CB-CG	-5.25	1.42	1.51
1	B	769	CYS	CA-C	-5.25	1.39	1.52
1	A	308	ASP	CG-OD1	5.25	1.37	1.25
1	A	275	GLN	CD-NE2	-5.24	1.19	1.32
1	A	520	ASN	C-O	5.24	1.33	1.23
1	B	156	ASP	C-O	5.24	1.33	1.23
1	B	583	VAL	N-CA	-5.24	1.35	1.46
1	A	28	LEU	N-CA	5.24	1.56	1.46
1	A	218	GLN	C-O	-5.24	1.13	1.23
1	A	218	GLN	CD-OE1	5.23	1.35	1.24
1	A	254	THR	C-O	5.23	1.33	1.23
1	A	315	LEU	CA-CB	5.23	1.65	1.53
1	B	241	SER	CA-C	-5.23	1.39	1.52
1	B	376	ASN	CG-ND2	5.23	1.46	1.32
1	A	38	GLU	CD-OE2	5.22	1.31	1.25
1	B	456	ALA	C-O	5.22	1.33	1.23
1	A	670	ARG	NE-CZ	-5.22	1.26	1.33
1	A	672	GLU	CD-OE1	5.22	1.31	1.25
1	A	892	TYR	CD2-CE2	5.22	1.47	1.39
1	A	50	ALA	C-O	5.21	1.33	1.23
1	B	36	ARG	NE-CZ	5.21	1.39	1.33
1	B	155	ASP	CA-CB	-5.21	1.42	1.53
1	B	426	ARG	C-O	5.21	1.33	1.23
1	B	514	ASP	C-O	5.21	1.33	1.23
1	A	187	LYS	CD-CE	5.21	1.64	1.51
1	B	263	ALA	N-CA	5.21	1.56	1.46
1	B	297	TRP	CA-CB	-5.21	1.42	1.53
1	A	503	PHE	CG-CD2	-5.21	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	ALA	C-O	5.20	1.33	1.23
1	A	614	ARG	CZ-NH1	5.20	1.39	1.33
1	B	519	ALA	C-N	-5.20	1.22	1.34
1	A	23	ARG	CG-CD	5.20	1.65	1.51
1	A	558	ILE	CB-CG2	5.20	1.69	1.52
1	A	275	GLN	C-N	-5.20	1.23	1.33
1	B	305	ASN	CG-ND2	5.20	1.45	1.32
1	A	414	MET	SD-CE	5.20	2.06	1.77
1	A	774	ALA	C-O	-5.19	1.13	1.23
1	B	81	LEU	CG-CD2	5.19	1.71	1.51
1	B	226	GLN	CA-C	5.19	1.66	1.52
1	B	345	PRO	C-O	-5.19	1.12	1.23
1	A	220	ALA	C-N	-5.19	1.24	1.34
1	A	238	LEU	CA-CB	-5.19	1.41	1.53
1	B	284	MET	C-O	5.19	1.33	1.23
1	B	475	ARG	CZ-NH2	-5.19	1.26	1.33
1	B	454	PHE	CD1-CE1	-5.19	1.28	1.39
1	A	374	CYS	CB-SG	5.19	1.91	1.82
1	A	639	LYS	CD-CE	5.19	1.64	1.51
1	B	341	CYS	CA-C	-5.18	1.39	1.52
1	A	358	THR	CA-C	5.18	1.66	1.52
1	B	494	LYS	CG-CD	5.18	1.70	1.52
1	B	36	ARG	CG-CD	-5.18	1.39	1.51
1	B	174	ASN	CA-CB	5.18	1.66	1.53
1	A	490	PHE	CG-CD1	-5.17	1.30	1.38
1	B	311	GLU	N-CA	5.17	1.56	1.46
1	B	854	PHE	N-CA	-5.17	1.36	1.46
1	A	677	ILE	N-CA	-5.17	1.36	1.46
1	B	771	SER	CA-CB	-5.17	1.45	1.52
1	B	78	PRO	CA-CB	-5.17	1.43	1.53
1	B	313	GLU	CD-OE1	5.17	1.31	1.25
1	B	806	PHE	CA-CB	5.17	1.65	1.53
1	A	237	LEU	N-CA	5.17	1.56	1.46
1	A	323	GLU	C-O	5.17	1.33	1.23
1	B	288	TRP	CE3-CZ3	-5.16	1.29	1.38
1	B	313	GLU	CD-OE2	-5.16	1.20	1.25
1	B	617	ASP	CB-CG	-5.16	1.41	1.51
1	A	823	PHE	CD2-CE2	-5.16	1.28	1.39
1	B	618	LEU	CA-C	5.16	1.66	1.52
1	A	702	LEU	CA-CB	5.16	1.65	1.53
1	A	337	LYS	CG-CD	-5.15	1.34	1.52
1	A	593	LYS	N-CA	-5.15	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	144	TRP	CZ3-CH2	-5.15	1.31	1.40
1	A	874	ASN	CG-ND2	5.15	1.45	1.32
1	B	891	MET	C-O	5.15	1.33	1.23
1	A	681	LEU	C-O	-5.15	1.13	1.23
1	A	94	ARG	NE-CZ	5.14	1.39	1.33
1	A	601	ILE	N-CA	5.14	1.56	1.46
1	B	839	ILE	CA-C	5.14	1.66	1.52
1	A	582	MET	CA-CB	-5.14	1.42	1.53
1	B	829	HIS	C-O	-5.14	1.13	1.23
1	B	30	GLN	CG-CD	-5.14	1.39	1.51
1	B	47	GLN	CB-CG	5.14	1.66	1.52
1	B	207	PHE	CD1-CE1	5.14	1.49	1.39
1	B	581	SER	CA-CB	5.14	1.60	1.52
1	A	286	ASN	CA-CB	-5.13	1.39	1.53
1	A	88	ILE	C-O	5.13	1.33	1.23
1	A	124	VAL	C-O	-5.13	1.13	1.23
1	B	426	ARG	CZ-NH2	5.13	1.39	1.33
1	B	467	ILE	N-CA	5.13	1.56	1.46
1	A	491	GLU	CA-CB	-5.13	1.42	1.53
1	B	375	ARG	C-O	5.13	1.33	1.23
1	A	356	TRP	CD2-CE2	5.12	1.47	1.41
1	A	603	TRP	CZ3-CH2	-5.12	1.31	1.40
1	B	17	GLY	N-CA	5.12	1.53	1.46
1	A	470	ARG	CG-CD	-5.12	1.39	1.51
1	B	311	GLU	C-O	-5.12	1.13	1.23
1	B	48	ASP	CG-OD2	5.12	1.37	1.25
1	B	133	GLU	CD-OE1	5.12	1.31	1.25
1	A	741	SER	CA-CB	5.12	1.60	1.52
1	B	678	PHE	C-O	5.12	1.33	1.23
1	A	383	VAL	CA-CB	-5.11	1.44	1.54
1	B	57	SER	CA-C	-5.11	1.39	1.52
1	B	94	ARG	C-O	-5.11	1.13	1.23
1	B	468	ASN	CB-CG	5.11	1.62	1.51
1	A	679	LYS	CA-CB	-5.11	1.42	1.53
1	A	648	ILE	CB-CG2	-5.11	1.37	1.52
1	B	47	GLN	C-O	-5.11	1.13	1.23
1	A	131	PHE	CG-CD2	-5.11	1.31	1.38
1	A	317	VAL	CB-CG2	-5.11	1.42	1.52
1	B	192	TYR	CE1-CZ	-5.11	1.31	1.38
1	A	27	TYR	CE1-CZ	-5.10	1.31	1.38
1	B	580	ARG	CZ-NH1	5.10	1.39	1.33
1	B	427	ASP	CA-C	5.10	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	638	PHE	CD2-CE2	-5.09	1.29	1.39
1	B	690	GLN	C-O	-5.09	1.13	1.23
1	B	827	GLY	C-O	-5.09	1.15	1.23
1	A	135	TYR	CB-CG	5.09	1.59	1.51
1	A	356	TRP	CZ3-CH2	5.09	1.48	1.40
1	A	385	PRO	CA-CB	-5.09	1.43	1.53
1	A	644	LEU	CG-CD1	-5.09	1.33	1.51
1	B	572	ASN	C-N	5.09	1.42	1.33
1	A	415	GLN	C-O	-5.09	1.13	1.23
1	B	447	VAL	C-N	-5.09	1.22	1.34
1	B	349	LYS	N-CA	5.08	1.56	1.46
1	B	674	LEU	C-O	5.08	1.33	1.23
1	A	208	THR	C-O	5.08	1.32	1.23
1	B	161	LYS	CG-CD	5.08	1.69	1.52
1	B	627	TYR	CD2-CE2	5.08	1.47	1.39
1	B	356	TRP	CZ3-CH2	5.07	1.48	1.40
1	B	6	MET	CA-C	-5.07	1.39	1.52
1	A	625	SER	N-CA	5.07	1.56	1.46
1	B	112	ALA	CA-C	5.07	1.66	1.52
1	B	220	ALA	C-N	-5.07	1.24	1.34
1	B	773	VAL	N-CA	5.07	1.56	1.46
1	B	810	ARG	C-O	5.07	1.32	1.23
1	A	18	LEU	CA-C	-5.07	1.39	1.52
1	A	763	GLY	N-CA	5.07	1.53	1.46
1	B	881	VAL	C-O	5.07	1.32	1.23
1	A	876	THR	CB-OG1	5.07	1.53	1.43
1	B	213	GLU	CA-CB	5.06	1.65	1.53
1	A	199	CYS	N-CA	-5.06	1.36	1.46
1	A	293	TRP	CA-C	-5.06	1.39	1.52
1	B	482	GLU	CG-CD	5.06	1.59	1.51
1	A	886	TRP	CB-CG	5.06	1.59	1.50
1	A	482	GLU	CG-CD	5.06	1.59	1.51
1	A	336	THR	CA-C	-5.05	1.39	1.52
1	A	751	LYS	CD-CE	5.05	1.63	1.51
1	B	376	ASN	C-O	-5.05	1.13	1.23
1	B	638	PHE	CG-CD2	-5.05	1.31	1.38
1	B	384	ASN	CB-CG	-5.05	1.39	1.51
1	A	381	PHE	CE1-CZ	5.05	1.47	1.37
1	A	614	ARG	CB-CG	5.05	1.66	1.52
1	A	734	ALA	N-CA	5.05	1.56	1.46
1	B	222	SER	CA-CB	-5.05	1.45	1.52
1	B	370	THR	C-O	5.05	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	361	TYR	CA-C	-5.04	1.39	1.52
1	B	329	ARG	CB-CG	5.04	1.66	1.52
1	A	856	SER	CA-C	-5.04	1.39	1.52
1	B	701	VAL	CB-CG1	-5.04	1.42	1.52
1	B	621	SER	C-O	5.03	1.32	1.23
1	B	673	ILE	CG1-CD1	-5.03	1.15	1.50
1	A	351	ARG	CB-CG	5.03	1.66	1.52
1	B	295	GLY	CA-C	5.03	1.59	1.51
1	A	46	PHE	CE1-CZ	5.03	1.47	1.37
1	A	323	GLU	CD-OE1	5.03	1.31	1.25
1	A	416	LYS	CB-CG	5.03	1.66	1.52
1	A	146	PHE	C-O	-5.03	1.13	1.23
1	A	868	PHE	CE1-CZ	-5.03	1.27	1.37
1	B	205	GLU	CD-OE1	5.03	1.31	1.25
1	B	95	THR	CB-CG2	5.02	1.69	1.52
1	A	457	ASN	CG-OD1	5.02	1.34	1.24
1	B	117	ASN	C-O	5.02	1.32	1.23
1	B	435	VAL	C-O	-5.02	1.13	1.23
1	A	351	ARG	NE-CZ	5.02	1.39	1.33
1	B	225	TYR	CD1-CE1	-5.02	1.31	1.39
1	A	875	GLY	N-CA	-5.01	1.38	1.46
1	B	365	TRP	C-O	-5.01	1.13	1.23
1	A	200	THR	CB-OG1	5.01	1.53	1.43
1	B	343	LEU	CB-CG	-5.01	1.38	1.52
1	B	853	ASN	CB-CG	5.01	1.62	1.51
1	B	836	SER	CA-CB	5.00	1.60	1.52
1	A	547	ASP	N-CA	5.00	1.56	1.46
1	B	27	TYR	CB-CG	-5.00	1.44	1.51
1	A	105	SER	CA-C	5.00	1.66	1.52
1	A	375	ARG	C-N	-5.00	1.22	1.34
1	A	579	CYS	C-O	5.00	1.32	1.23
1	B	700	SER	C-O	5.00	1.32	1.23

All (959) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	ARG	NE-CZ-NH1	-29.77	105.41	120.30
1	A	329	ARG	NE-CZ-NH1	26.14	133.37	120.30
1	A	329	ARG	NE-CZ-NH2	-24.17	108.22	120.30
1	B	514	ASP	CB-CG-OD2	-18.56	101.59	118.30
1	A	285	ARG	NE-CZ-NH2	-15.96	112.32	120.30
1	B	285	ARG	NE-CZ-NH1	15.90	128.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	614	ARG	NE-CZ-NH2	-15.75	112.43	120.30
1	A	278	ARG	NE-CZ-NH1	-15.65	112.48	120.30
1	B	501	ARG	NE-CZ-NH2	-15.59	112.50	120.30
1	B	315	LEU	CA-CB-CG	15.47	150.88	115.30
1	B	514	ASP	CB-CG-OD1	15.47	132.22	118.30
1	B	501	ARG	NE-CZ-NH1	15.35	127.97	120.30
1	B	375	ARG	NE-CZ-NH1	15.28	127.94	120.30
1	A	477	ARG	NE-CZ-NH2	15.27	127.93	120.30
1	A	460	ARG	NE-CZ-NH2	15.14	127.87	120.30
1	B	285	ARG	NE-CZ-NH2	-15.11	112.74	120.30
1	B	779	ASP	CB-CG-OD2	14.97	131.78	118.30
1	A	31	ASP	CB-CG-OD2	-14.81	104.97	118.30
1	A	396	ASP	CB-CG-OD1	14.80	131.62	118.30
1	B	330	ASP	CB-CG-OD2	14.77	131.59	118.30
1	B	308	ASP	CB-CG-OD1	-14.67	105.09	118.30
1	B	366	ARG	NE-CZ-NH1	-14.67	112.96	120.30
1	B	470	ARG	NE-CZ-NH2	14.62	127.61	120.30
1	A	497	ASP	CB-CG-OD1	-14.24	105.48	118.30
1	B	375	ARG	NE-CZ-NH2	-14.23	113.19	120.30
1	A	756	HIS	C-N-CD	-13.92	89.97	120.60
1	A	354	ARG	NE-CZ-NH2	13.84	127.22	120.30
1	A	860	ARG	NE-CZ-NH1	-13.83	113.39	120.30
1	A	175	GLU	OE1-CD-OE2	-13.59	107.00	123.30
1	B	398	ASP	CA-C-N	13.51	146.92	117.20
1	B	670	ARG	NE-CZ-NH1	13.11	126.86	120.30
1	A	662	ASP	CB-CG-OD1	-13.09	106.52	118.30
1	B	470	ARG	NE-CZ-NH1	-12.92	113.84	120.30
1	B	36	ARG	NE-CZ-NH1	12.89	126.74	120.30
1	A	614	ARG	NE-CZ-NH1	12.84	126.72	120.30
1	B	512	GLU	OE1-CD-OE2	-12.72	108.03	123.30
1	B	497	ASP	CB-CG-OD1	12.69	129.72	118.30
1	A	390	ARG	NE-CZ-NH2	-12.41	114.10	120.30
1	A	810	ARG	NE-CZ-NH2	12.39	126.50	120.30
1	A	94	ARG	NE-CZ-NH1	12.34	126.47	120.30
1	B	216	ASP	CB-CG-OD1	-12.28	107.25	118.30
1	B	346	ASP	CB-CG-OD1	12.20	129.28	118.30
1	A	395	ASP	CB-CG-OD1	-12.12	107.39	118.30
1	B	850	ASP	CB-CG-OD1	11.94	129.05	118.30
1	B	139	PHE	CB-CG-CD2	11.88	129.11	120.80
1	A	310	TYR	CB-CG-CD1	-11.87	113.88	121.00
1	B	866	ARG	NE-CZ-NH1	11.76	126.18	120.30
1	B	850	ASP	CB-CG-OD2	11.73	128.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	ARG	NE-CZ-NH2	-11.70	114.45	120.30
1	B	123	ARG	NE-CZ-NH2	-11.60	114.50	120.30
1	A	155	ASP	CB-CG-OD2	-11.54	107.91	118.30
1	B	862	ASP	CB-CG-OD2	11.51	128.66	118.30
1	A	514	ASP	CB-CG-OD1	-11.47	107.98	118.30
1	B	12	ARG	NE-CZ-NH2	-11.43	114.59	120.30
1	B	850	ASP	OD1-CG-OD2	-11.29	101.85	123.30
1	B	104	ASP	CB-CG-OD2	11.19	128.37	118.30
1	B	657	LEU	CB-CG-CD2	11.16	129.97	111.00
1	B	193	GLU	OE1-CD-OE2	11.02	136.53	123.30
1	B	123	ARG	NE-CZ-NH1	11.00	125.80	120.30
1	A	232	LEU	CB-CG-CD1	-10.97	92.34	111.00
1	A	478	LEU	CB-CG-CD2	-10.91	92.45	111.00
1	B	865	PHE	N-CA-C	-10.84	81.72	111.00
1	B	399	ASP	CB-CG-OD2	10.83	128.04	118.30
1	B	366	ARG	NH1-CZ-NH2	10.81	131.29	119.40
1	A	497	ASP	CB-CG-OD2	10.80	128.02	118.30
1	B	31	ASP	CB-CG-OD1	10.77	127.99	118.30
1	A	31	ASP	CB-CG-OD1	10.73	127.96	118.30
1	A	151	ASP	CB-CG-OD2	-10.71	108.66	118.30
1	B	216	ASP	CB-CG-OD2	10.66	127.89	118.30
1	A	618	LEU	CB-CG-CD2	10.53	128.90	111.00
1	A	339	GLU	OE1-CD-OE2	10.46	135.85	123.30
1	B	872	ASP	CB-CG-OD2	10.46	127.71	118.30
1	B	398	ASP	CB-CG-OD2	10.40	127.67	118.30
1	B	402	SER	C-N-CA	10.36	147.60	121.70
1	A	862	ASP	CB-CG-OD1	10.35	127.62	118.30
1	A	358	THR	CA-CB-CG2	-10.35	97.92	112.40
1	A	830	LEU	CB-CG-CD2	10.30	128.51	111.00
1	A	513	LEU	CB-CG-CD1	-10.29	93.50	111.00
1	B	451	ARG	NE-CZ-NH2	10.28	125.44	120.30
1	A	237	LEU	CB-CG-CD2	10.19	128.33	111.00
1	A	332	ILE	CG1-CB-CG2	10.18	133.80	111.40
1	A	165	LEU	CB-CG-CD2	10.18	128.30	111.00
1	A	809	ASP	CB-CG-OD2	10.16	127.45	118.30
1	A	211	VAL	CB-CA-C	-10.15	92.12	111.40
1	B	428	MET	CG-SD-CE	10.12	116.40	100.20
1	A	88	ILE	CG1-CB-CG2	-10.12	89.14	111.40
1	B	362	GLU	OE1-CD-OE2	-10.12	111.16	123.30
1	B	58	LEU	CA-CB-CG	10.09	138.51	115.30
1	B	188	VAL	CA-CB-CG1	10.08	126.03	110.90
1	A	165	LEU	CA-CB-CG	-10.08	92.11	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	580	ARG	NE-CZ-NH1	10.07	125.33	120.30
1	A	640	LEU	CB-CG-CD2	10.04	128.07	111.00
1	B	396	ASP	CB-CG-OD2	10.03	127.33	118.30
1	B	436	TYR	CB-CG-CD1	9.98	126.99	121.00
1	A	522	PRO	CA-C-O	-9.95	96.31	120.20
1	A	312	ARG	NE-CZ-NH1	-9.88	115.36	120.30
1	B	23	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	A	310	TYR	CZ-CE2-CD2	-9.83	110.95	119.80
1	B	446	PRO	N-CD-CG	-9.77	88.55	103.20
1	B	36	ARG	CG-CD-NE	9.73	132.24	111.80
1	A	736	ASP	CB-CG-OD2	9.72	127.05	118.30
1	B	315	LEU	CB-CA-C	-9.66	91.84	110.20
1	B	862	ASP	CB-CG-OD1	-9.62	109.64	118.30
1	B	472	VAL	CB-CA-C	-9.60	93.16	111.40
1	A	396	ASP	OD1-CG-OD2	-9.60	105.06	123.30
1	A	455	LEU	CB-CG-CD1	-9.59	94.69	111.00
1	A	339	GLU	CG-CD-OE2	-9.58	99.14	118.30
1	A	282	ILE	CG1-CB-CG2	-9.57	90.35	111.40
1	B	366	ARG	NE-CZ-NH2	-9.57	115.52	120.30
1	A	831	ASN	CB-CA-C	9.56	129.53	110.40
1	A	328	PHE	O-C-N	-9.56	107.40	122.70
1	B	294	LYS	CA-CB-CG	9.56	134.43	113.40
1	B	587	ASP	CB-CG-OD2	9.50	126.85	118.30
1	A	326	MET	CG-SD-CE	9.43	115.28	100.20
1	A	570	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	B	402	SER	O-C-N	9.37	137.69	122.70
1	A	812	GLY	CA-C-O	-9.32	103.82	120.60
1	A	6	MET	CG-SD-CE	-9.31	85.30	100.20
1	A	63	LEU	CB-CG-CD1	-9.30	95.18	111.00
1	B	208	THR	CA-CB-CG2	-9.30	99.39	112.40
1	B	449	LEU	CB-CG-CD2	9.25	126.73	111.00
1	B	308	ASP	CB-CG-OD2	9.25	126.63	118.30
1	A	682	ASP	CB-CG-OD2	9.24	126.62	118.30
1	B	330	ASP	CB-CG-OD1	-9.24	109.98	118.30
1	A	185	TYR	CD1-CE1-CZ	-9.23	111.49	119.80
1	B	315	LEU	CB-CG-CD2	9.21	126.66	111.00
1	A	258	LEU	CB-CG-CD1	9.17	126.59	111.00
1	B	344	THR	OG1-CB-CG2	-9.17	88.92	110.00
1	A	742	ALA	N-CA-C	-9.16	86.27	111.00
1	B	647	VAL	CG1-CB-CG2	-9.15	96.26	110.90
1	B	469	LEU	CB-CA-C	9.12	127.53	110.20
1	A	216	ASP	CB-CG-OD1	9.12	126.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	ASP	CB-CG-OD2	9.11	126.50	118.30
1	A	367	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	A	803	TYR	CA-C-O	9.07	139.16	120.10
1	B	630	ARG	NE-CZ-NH1	-9.05	115.77	120.30
1	B	398	ASP	O-C-N	-9.04	108.24	122.70
1	B	631	MET	CA-CB-CG	9.01	128.61	113.30
1	B	155	ASP	CB-CG-OD1	-9.00	110.20	118.30
1	A	233	GLU	OE1-CD-OE2	-8.82	112.71	123.30
1	A	362	GLU	OE1-CD-OE2	8.81	133.88	123.30
1	B	181	LEU	CB-CG-CD2	-8.80	96.05	111.00
1	A	745	LEU	CB-CG-CD2	8.79	125.95	111.00
1	A	36	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	A	18	LEU	CB-CG-CD1	8.73	125.83	111.00
1	B	714	ASN	CA-C-O	8.72	138.41	120.10
1	B	433	PHE	N-CA-CB	-8.71	94.93	110.60
1	A	665	VAL	CA-CB-CG2	-8.70	97.85	110.90
1	B	400	TYR	N-CA-C	8.70	134.49	111.00
1	A	682	ASP	CB-CG-OD1	-8.69	110.48	118.30
1	B	792	LEU	CA-CB-CG	-8.68	95.35	115.30
1	A	591	ASN	N-CA-C	-8.64	87.66	111.00
1	A	89	VAL	CA-CB-CG1	8.61	123.81	110.90
1	B	697	LEU	CB-CA-C	8.59	126.52	110.20
1	B	291	VAL	CG1-CB-CG2	8.56	124.60	110.90
1	B	601	ILE	CG1-CB-CG2	-8.54	92.62	111.40
1	B	331	PHE	CB-CA-C	-8.52	93.36	110.40
1	B	485	VAL	CA-CB-CG2	-8.50	98.16	110.90
1	A	268	ASP	CB-CG-OD2	8.46	125.91	118.30
1	B	430	THR	OG1-CB-CG2	-8.45	90.56	110.00
1	B	436	TYR	CZ-CE2-CD2	8.44	127.39	119.80
1	A	605	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	B	682	ASP	CB-CG-OD2	8.41	125.87	118.30
1	A	303	GLU	CB-CG-CD	-8.40	91.53	114.20
1	B	331	PHE	CB-CG-CD2	-8.39	114.92	120.80
1	A	58	LEU	CB-CG-CD2	-8.38	96.76	111.00
1	B	629	MET	CG-SD-CE	8.38	113.60	100.20
1	A	447	VAL	CB-CA-C	-8.37	95.49	111.40
1	B	583	VAL	N-CA-C	-8.36	88.42	111.00
1	A	175	GLU	CG-CD-OE2	8.35	135.01	118.30
1	B	436	TYR	CB-CG-CD2	-8.34	116.00	121.00
1	B	651	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	A	670	ARG	NE-CZ-NH1	-8.33	116.14	120.30
1	A	306	LYS	CA-CB-CG	-8.32	95.08	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	CYS	CA-CB-SG	-8.32	99.02	114.00
1	A	475	ARG	NE-CZ-NH2	-8.31	116.14	120.30
1	B	858	LEU	N-CA-C	8.28	133.35	111.00
1	B	724	ARG	NE-CZ-NH2	8.27	124.43	120.30
1	A	319	MET	C-N-CA	-8.26	101.04	121.70
1	A	547	ASP	CB-CG-OD2	8.26	125.73	118.30
1	B	860	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	B	398	ASP	N-CA-C	8.22	133.19	111.00
1	B	641	PRO	N-CD-CG	-8.20	90.90	103.20
1	B	319	MET	CG-SD-CE	8.18	113.29	100.20
1	A	354	ARG	NE-CZ-NH1	-8.17	116.22	120.30
1	A	442	LEU	CA-CB-CG	8.16	134.06	115.30
1	B	830	LEU	CB-CG-CD1	-8.15	97.14	111.00
1	B	32	TYR	CB-CG-CD2	8.13	125.88	121.00
1	A	237	LEU	CB-CG-CD1	-8.10	97.23	111.00
1	A	427	ASP	CB-CG-OD2	8.10	125.59	118.30
1	B	426	ARG	NE-CZ-NH1	-8.09	116.25	120.30
1	B	11	ASP	CB-CG-OD2	8.09	125.58	118.30
1	B	644	LEU	CA-CB-CG	-8.04	96.80	115.30
1	B	521	LEU	CB-CG-CD1	-8.03	97.35	111.00
1	B	398	ASP	CA-C-O	-7.95	103.40	120.10
1	A	350	SER	N-CA-CB	7.95	122.42	110.50
1	A	585	LEU	CB-CG-CD1	-7.94	97.50	111.00
1	B	256	LYS	CD-CE-NZ	7.92	129.91	111.70
1	A	319	MET	CG-SD-CE	7.92	112.86	100.20
1	A	462	GLN	O-C-N	-7.89	110.07	122.70
1	B	90	ASP	CB-CA-C	7.88	126.17	110.40
1	A	303	GLU	N-CA-C	7.85	132.20	111.00
1	A	702	LEU	CA-C-O	-7.85	103.61	120.10
1	A	7	LYS	CB-CG-CD	7.84	131.98	111.60
1	B	619	ASP	CB-CG-OD2	7.83	125.35	118.30
1	A	733	LEU	CB-CG-CD2	-7.81	97.72	111.00
1	A	350	SER	O-C-N	7.81	135.19	122.70
1	B	96	ASP	CB-CG-OD2	7.80	125.32	118.30
1	A	159	PRO	O-C-N	7.78	135.15	122.70
1	B	440	ARG	CB-CA-C	-7.77	94.87	110.40
1	B	436	TYR	CE1-CZ-OH	7.72	140.94	120.10
1	B	298	SER	CA-CB-OG	-7.70	90.40	111.20
1	B	17	GLY	N-CA-C	7.69	132.32	113.10
1	A	772	MET	CG-SD-CE	7.69	112.50	100.20
1	A	803	TYR	OH-CZ-CE2	7.68	140.85	120.10
1	B	44	ALA	N-CA-CB	-7.65	99.39	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ASP	CB-CG-OD1	-7.64	111.42	118.30
1	A	616	PHE	CB-CG-CD1	7.61	126.13	120.80
1	B	36	ARG	NH1-CZ-NH2	-7.59	111.05	119.40
1	B	346	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	A	809	ASP	OD1-CG-OD2	-7.58	108.89	123.30
1	B	675	PHE	CB-CG-CD2	7.58	126.11	120.80
1	B	776	MET	CB-CG-SD	-7.58	89.67	112.40
1	A	585	LEU	CB-CG-CD2	7.57	123.87	111.00
1	B	93	THR	CA-CB-CG2	7.56	122.99	112.40
1	B	161	LYS	CD-CE-NZ	7.54	129.05	111.70
1	A	389	ILE	CB-CA-C	-7.54	96.52	111.60
1	A	499	LEU	CB-CA-C	-7.54	95.87	110.20
1	B	882	ASN	N-CA-C	-7.54	90.66	111.00
1	A	500	LEU	CB-CG-CD2	7.53	123.79	111.00
1	B	388	LYS	CB-CA-C	-7.52	95.35	110.40
1	B	69	LYS	CD-CE-NZ	7.52	129.00	111.70
1	B	830	LEU	CA-CB-CG	7.51	132.58	115.30
1	B	657	LEU	CA-CB-CG	7.50	132.56	115.30
1	B	16	GLU	OE1-CD-OE2	-7.50	114.31	123.30
1	B	108	LEU	CA-CB-CG	-7.49	98.07	115.30
1	A	607	ARG	NE-CZ-NH1	-7.49	116.56	120.30
1	A	514	ASP	CB-CG-OD2	7.48	125.03	118.30
1	A	340	ILE	CB-CG1-CD1	7.47	134.82	113.90
1	A	872	ASP	CB-CG-OD1	-7.46	111.58	118.30
1	B	263	ALA	CB-CA-C	-7.46	98.91	110.10
1	A	278	ARG	CB-CA-C	-7.46	95.49	110.40
1	A	338	LEU	CB-CG-CD1	7.45	123.66	111.00
1	A	350	SER	N-CA-C	-7.43	90.95	111.00
1	A	175	GLU	CA-CB-CG	7.41	129.70	113.40
1	A	216	ASP	OD1-CG-OD2	-7.41	109.23	123.30
1	A	833	HIS	N-CA-C	7.40	130.97	111.00
1	B	651	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	A	151	ASP	CB-CG-OD1	7.39	124.95	118.30
1	A	628	GLU	CB-CG-CD	-7.39	94.24	114.20
1	B	121	LEU	CB-CG-CD2	-7.38	98.46	111.00
1	A	751	LYS	CA-C-O	-7.37	104.63	120.10
1	A	620	LYS	CB-CA-C	7.37	125.13	110.40
1	B	862	ASP	N-CA-C	-7.36	91.12	111.00
1	A	670	ARG	CD-NE-CZ	-7.35	113.31	123.60
1	A	803	TYR	CB-CG-CD2	7.34	125.41	121.00
1	B	151	ASP	OD1-CG-OD2	-7.34	109.35	123.30
1	B	267	THR	O-C-N	-7.34	110.96	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	802	ILE	CA-C-O	-7.34	104.69	120.10
1	B	65	PRO	N-CD-CG	7.33	114.20	103.20
1	B	0	GLU	CA-C-O	-7.33	104.70	120.10
1	A	803	TYR	CB-CG-CD1	-7.33	116.60	121.00
1	A	165	LEU	CB-CA-C	7.29	124.05	110.20
1	B	92	ALA	N-CA-CB	7.29	120.31	110.10
1	B	233	GLU	OE1-CD-OE2	7.29	132.05	123.30
1	B	348	LEU	CB-CG-CD1	7.29	123.39	111.00
1	B	585	LEU	CB-CG-CD1	7.27	123.36	111.00
1	A	12	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	A	759	LEU	CB-CG-CD1	-7.25	98.67	111.00
1	B	426	ARG	NE-CZ-NH2	7.25	123.92	120.30
1	A	158	LEU	CA-CB-CG	-7.24	98.66	115.30
1	B	139	PHE	CB-CG-CD1	-7.24	115.73	120.80
1	A	310	TYR	CE1-CZ-OH	-7.23	100.57	120.10
1	B	391	LEU	CB-CG-CD1	7.18	123.21	111.00
1	A	455	LEU	CB-CG-CD2	7.18	123.21	111.00
1	A	440	ARG	NE-CZ-NH1	-7.15	116.72	120.30
1	A	758	ASP	CB-CG-OD1	7.13	124.72	118.30
1	B	28	LEU	CB-CG-CD1	7.13	123.13	111.00
1	B	674	LEU	CB-CG-CD1	7.13	123.12	111.00
1	A	218	GLN	C-N-CA	7.12	139.51	121.70
1	B	155	ASP	CB-CG-OD2	7.11	124.70	118.30
1	B	378	PRO	N-CD-CG	-7.11	92.53	103.20
1	B	151	ASP	CB-CG-OD1	7.11	124.70	118.30
1	A	861	LEU	CB-CG-CD2	-7.09	98.94	111.00
1	B	609	TYR	N-CA-CB	7.08	123.35	110.60
1	B	83	SER	C-N-CA	-7.08	104.00	121.70
1	B	538	THR	CB-CA-C	-7.07	92.51	111.60
1	B	746	MET	CG-SD-CE	7.05	111.48	100.20
1	A	691	LEU	CB-CG-CD1	7.04	122.97	111.00
1	A	40	LEU	CB-CG-CD2	7.04	122.96	111.00
1	B	278	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	A	860	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	B	89	VAL	CA-CB-CG1	7.02	121.43	110.90
1	B	594	LEU	CB-CG-CD2	7.01	122.91	111.00
1	A	351	ARG	NE-CZ-NH2	7.01	123.80	120.30
1	B	340	ILE	CG1-CB-CG2	-7.00	96.00	111.40
1	B	164	LYS	CD-CE-NZ	-7.00	95.61	111.70
1	B	98	CYS	CA-CB-SG	6.99	126.59	114.00
1	B	617	ASP	CB-CA-C	-6.98	96.43	110.40
1	B	281	LEU	CB-CG-CD2	6.97	122.85	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	825	ALA	N-CA-CB	-6.97	100.34	110.10
1	A	702	LEU	CA-CB-CG	6.95	131.29	115.30
1	A	413	LEU	CB-CG-CD2	-6.95	99.19	111.00
1	A	655	ASP	CB-CG-OD2	6.94	124.55	118.30
1	A	343	LEU	CB-CG-CD2	6.94	122.79	111.00
1	B	449	LEU	O-C-N	6.93	133.79	122.70
1	A	601	ILE	O-C-N	6.93	133.78	122.70
1	B	461	ALA	N-CA-CB	-6.92	100.42	110.10
1	A	631	MET	CG-SD-CE	-6.92	89.13	100.20
1	B	199	CYS	CA-CB-SG	-6.91	101.56	114.00
1	A	570	ARG	NH1-CZ-NH2	-6.91	111.80	119.40
1	B	389	ILE	N-CA-C	-6.91	92.35	111.00
1	B	418	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	A	789	PHE	N-CA-C	-6.90	92.38	111.00
1	A	237	LEU	CA-CB-CG	-6.89	99.45	115.30
1	B	162	ASP	CB-CG-OD2	6.88	124.50	118.30
1	B	159	PRO	N-CD-CG	-6.88	92.88	103.20
1	B	200	THR	OG1-CB-CG2	-6.87	94.19	110.00
1	A	756	HIS	N-CA-C	-6.87	92.45	111.00
1	B	396	ASP	C-N-CA	6.87	138.87	121.70
1	B	476	ILE	CG1-CB-CG2	-6.87	96.29	111.40
1	B	296	PRO	N-CD-CG	-6.87	92.90	103.20
1	B	806	PHE	CB-CG-CD2	6.87	125.61	120.80
1	B	808	THR	O-C-N	-6.86	111.72	122.70
1	A	429	GLU	CB-CA-C	6.86	124.12	110.40
1	A	102	LEU	CB-CG-CD2	-6.86	99.34	111.00
1	A	358	THR	OG1-CB-CG2	-6.85	94.24	110.00
1	A	786	PHE	N-CA-C	-6.85	92.50	111.00
1	B	580	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	A	768	THR	N-CA-CB	-6.85	97.28	110.30
1	A	521	LEU	CB-CG-CD1	6.85	122.64	111.00
1	B	811	SER	CB-CA-C	6.84	123.10	110.10
1	A	94	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	B	466	PHE	CB-CA-C	-6.83	96.73	110.40
1	A	27	TYR	CD1-CE1-CZ	-6.83	113.65	119.80
1	A	430	THR	CA-CB-CG2	6.82	121.95	112.40
1	B	454	PHE	CG-CD2-CE2	6.82	128.31	120.80
1	A	89	VAL	CG1-CB-CG2	-6.81	100.00	110.90
1	B	414	MET	CG-SD-CE	-6.81	89.30	100.20
1	A	810	ARG	NH1-CZ-NH2	-6.81	111.91	119.40
1	A	324	PHE	CB-CG-CD2	-6.80	116.04	120.80
1	B	274	TYR	CG-CD2-CE2	6.80	126.74	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	447	VAL	CA-CB-CG1	6.79	121.09	110.90
1	A	356	TRP	N-CA-C	-6.79	92.66	111.00
1	A	355	ASN	N-CA-CB	-6.79	98.38	110.60
1	A	550	ILE	C-N-CA	6.78	138.66	121.70
1	B	866	ARG	CA-CB-CG	6.78	128.32	113.40
1	B	471	GLU	OE1-CD-OE2	-6.78	115.16	123.30
1	A	339	GLU	N-CA-CB	-6.76	98.44	110.60
1	A	15	ALA	CB-CA-C	-6.75	99.97	110.10
1	A	756	HIS	CB-CA-C	6.75	123.90	110.40
1	A	108	LEU	CB-CG-CD2	-6.74	99.53	111.00
1	B	63	LEU	CB-CG-CD1	6.73	122.44	111.00
1	A	628	GLU	N-CA-CB	-6.72	98.50	110.60
1	A	492	PRO	N-CD-CG	-6.72	93.12	103.20
1	B	308	ASP	N-CA-CB	-6.72	98.51	110.60
1	A	448	HIS	N-CA-CB	6.71	122.67	110.60
1	B	861	LEU	CA-CB-CG	-6.70	99.88	115.30
1	A	2	ALA	N-CA-C	-6.70	92.91	111.00
1	A	234	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	A	889	LEU	CB-CG-CD2	-6.70	99.61	111.00
1	B	233	GLU	CG-CD-OE2	-6.70	104.91	118.30
1	B	93	THR	OG1-CB-CG2	-6.69	94.62	110.00
1	A	96	ASP	N-CA-C	-6.68	92.97	111.00
1	B	284	MET	CG-SD-CE	6.66	110.86	100.20
1	B	672	GLU	OE1-CD-OE2	6.66	131.29	123.30
1	A	463	SER	CB-CA-C	-6.66	97.45	110.10
1	B	139	PHE	CG-CD1-CE1	6.66	128.12	120.80
1	B	290	GLU	OE1-CD-OE2	6.65	131.28	123.30
1	A	303	GLU	CG-CD-OE2	-6.64	105.01	118.30
1	A	492	PRO	CA-C-N	-6.64	102.59	117.20
1	B	670	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	634	GLU	CG-CD-OE2	6.64	131.58	118.30
1	B	887	LEU	CA-CB-CG	-6.63	100.05	115.30
1	A	104	ASP	CB-CG-OD2	6.62	124.26	118.30
1	B	432	GLY	O-C-N	6.62	133.29	122.70
1	A	216	ASP	CB-CG-OD2	6.62	124.26	118.30
1	B	724	ARG	CD-NE-CZ	6.62	132.86	123.60
1	A	522	PRO	N-CA-C	6.62	129.30	112.10
1	A	635	ALA	CB-CA-C	-6.62	100.18	110.10
1	A	240	CYS	CA-CB-SG	-6.61	102.11	114.00
1	A	831	ASN	N-CA-CB	6.59	122.46	110.60
1	B	62	GLU	OE1-CD-OE2	6.59	131.21	123.30
1	A	630	ARG	NE-CZ-NH2	6.58	123.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	830	LEU	CB-CG-CD1	-6.58	99.81	111.00
1	A	317	VAL	CA-CB-CG2	6.58	120.76	110.90
1	A	232	LEU	CA-CB-CG	6.56	130.38	115.30
1	A	477	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	B	598	GLU	CA-CB-CG	6.55	127.82	113.40
1	B	390	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	B	436	TYR	OH-CZ-CE2	-6.54	102.44	120.10
1	A	612	ILE	CG1-CB-CG2	-6.54	97.02	111.40
1	B	291	VAL	CB-CA-C	-6.54	98.98	111.40
1	B	6	MET	N-CA-CB	6.53	122.36	110.60
1	B	472	VAL	CA-CB-CG1	-6.53	101.11	110.90
1	B	396	ASP	O-C-N	6.53	133.14	122.70
1	A	447	VAL	O-C-N	-6.52	112.27	122.70
1	A	28	LEU	CB-CG-CD1	-6.52	99.92	111.00
1	A	136	ALA	N-CA-C	6.52	128.59	111.00
1	B	477	ARG	NE-CZ-NH2	6.51	123.56	120.30
1	A	312	ARG	N-CA-C	-6.50	93.44	111.00
1	B	483	TYR	CG-CD1-CE1	6.50	126.50	121.30
1	A	505	GLU	CG-CD-OE1	6.50	131.30	118.30
1	B	133	GLU	OE1-CD-OE2	6.50	131.09	123.30
1	A	477	ARG	CD-NE-CZ	6.49	132.69	123.60
1	A	319	MET	N-CA-C	6.49	128.52	111.00
1	B	185	TYR	CB-CA-C	-6.48	97.43	110.40
1	B	121	LEU	CA-CB-CG	6.48	130.19	115.30
1	A	269	ALA	O-C-N	6.47	133.06	122.70
1	A	513	LEU	CB-CG-CD2	6.47	122.01	111.00
1	B	628	GLU	OE1-CD-OE2	6.47	131.07	123.30
1	A	205	GLU	CA-CB-CG	6.47	127.64	113.40
1	B	90	ASP	CB-CG-OD2	6.47	124.12	118.30
1	A	820	PRO	N-CD-CG	-6.46	93.50	103.20
1	B	200	THR	CA-CB-CG2	-6.46	103.35	112.40
1	B	890	THR	OG1-CB-CG2	-6.46	95.14	110.00
1	A	710	MET	C-N-CA	6.46	137.86	121.70
1	B	497	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	B	321	ASP	CB-CG-OD2	6.45	124.11	118.30
1	A	264	TYR	CB-CG-CD1	6.45	124.87	121.00
1	A	266	VAL	N-CA-C	-6.45	93.58	111.00
1	B	61	LYS	CA-CB-CG	6.45	127.59	113.40
1	A	672	GLU	OE1-CD-OE2	6.45	131.04	123.30
1	A	404	GLU	OE1-CD-OE2	6.44	131.03	123.30
1	A	278	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	B	389	ILE	CB-CA-C	-6.44	98.72	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	TYR	CG-CD1-CE1	-6.43	116.15	121.30
1	B	364	THR	CA-CB-CG2	-6.43	103.40	112.40
1	A	242	ILE	CG1-CB-CG2	-6.43	97.26	111.40
1	A	460	ARG	NH1-CZ-NH2	6.43	126.47	119.40
1	B	315	LEU	CB-CG-CD1	6.41	121.90	111.00
1	B	193	GLU	CG-CD-OE1	-6.41	105.48	118.30
1	A	486	VAL	O-C-N	6.41	133.27	121.10
1	A	889	LEU	O-C-N	-6.41	112.45	122.70
1	A	455	LEU	CA-CB-CG	-6.40	100.57	115.30
1	B	18	LEU	CB-CG-CD1	-6.40	100.11	111.00
1	A	645	HIS	N-CA-CB	6.40	122.12	110.60
1	B	452	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	76	LYS	CD-CE-NZ	6.39	126.39	111.70
1	A	193	GLU	CB-CA-C	-6.38	97.63	110.40
1	A	434	ALA	N-CA-CB	-6.38	101.17	110.10
1	B	242	ILE	CG1-CB-CG2	-6.38	97.37	111.40
1	A	128	GLY	CA-C-O	-6.38	109.12	120.60
1	A	243	ASN	N-CA-C	6.37	128.21	111.00
1	B	23	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	233	GLU	CA-CB-CG	6.37	127.41	113.40
1	B	507	LYS	CD-CE-NZ	6.36	126.33	111.70
1	B	658	ILE	O-C-N	6.36	132.88	122.70
1	B	312	ARG	CD-NE-CZ	6.36	132.50	123.60
1	A	759	LEU	C-N-CA	6.36	137.59	121.70
1	A	570	ARG	N-CA-C	-6.34	93.89	111.00
1	B	470	ARG	N-CA-CB	-6.33	99.20	110.60
1	B	825	ALA	CA-C-N	-6.33	103.28	117.20
1	B	477	ARG	NE-CZ-NH1	-6.31	117.14	120.30
1	A	297	TRP	CB-CA-C	6.31	123.02	110.40
1	A	324	PHE	N-CA-CB	6.30	121.94	110.60
1	B	131	PHE	CZ-CE2-CD2	-6.30	112.55	120.10
1	B	654	ASP	CA-C-N	-6.29	103.36	117.20
1	A	640	LEU	CB-CG-CD1	-6.29	100.31	111.00
1	B	362	GLU	CA-CB-CG	-6.28	99.59	113.40
1	A	110	ALA	CB-CA-C	-6.27	100.69	110.10
1	B	336	THR	OG1-CB-CG2	-6.27	95.58	110.00
1	B	135	TYR	CZ-CE2-CD2	6.26	125.43	119.80
1	B	451	ARG	CA-CB-CG	6.25	127.16	113.40
1	B	166	VAL	CA-CB-CG2	6.25	120.27	110.90
1	A	588	ARG	CA-C-O	6.24	133.21	120.10
1	A	330	ASP	CB-CG-OD2	6.24	123.92	118.30
1	A	486	VAL	CA-C-O	-6.24	107.00	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	THR	N-CA-CB	-6.23	98.46	110.30
1	A	591	ASN	CB-CA-C	6.23	122.86	110.40
1	A	609	TYR	CG-CD2-CE2	6.23	126.29	121.30
1	A	387	PHE	CG-CD1-CE1	-6.22	113.95	120.80
1	A	637	GLY	C-N-CA	-6.22	106.16	121.70
1	A	570	ARG	CA-CB-CG	6.21	127.07	113.40
1	A	617	ASP	CB-CG-OD1	6.21	123.89	118.30
1	B	13	GLU	N-CA-CB	6.20	121.76	110.60
1	A	499	LEU	CB-CG-CD2	-6.19	100.48	111.00
1	A	587	ASP	CB-CG-OD1	-6.19	112.73	118.30
1	A	291	VAL	CG1-CB-CG2	6.19	120.80	110.90
1	B	729	LEU	CB-CA-C	6.18	121.94	110.20
1	B	396	ASP	CB-CG-OD1	-6.17	112.74	118.30
1	B	681	LEU	N-CA-C	6.17	127.67	111.00
1	A	500	LEU	N-CA-C	-6.17	94.34	111.00
1	B	151	ASP	CB-CG-OD2	6.16	123.85	118.30
1	B	23	ARG	CG-CD-NE	-6.15	98.88	111.80
1	A	112	ALA	CB-CA-C	-6.14	100.89	110.10
1	A	114	LEU	CA-CB-CG	6.14	129.43	115.30
1	B	323	GLU	OE1-CD-OE2	6.14	130.67	123.30
1	A	808	THR	N-CA-CB	6.14	121.97	110.30
1	B	32	TYR	CG-CD2-CE2	6.13	126.21	121.30
1	A	616	PHE	CZ-CE2-CD2	6.12	127.45	120.10
1	B	89	VAL	CB-CA-C	-6.12	99.78	111.40
1	B	123	ARG	CD-NE-CZ	-6.12	115.04	123.60
1	B	147	GLY	CA-C-O	-6.12	109.59	120.60
1	B	349	LYS	N-CA-C	-6.11	94.49	111.00
1	B	662	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	697	LEU	CA-CB-CG	-6.09	101.28	115.30
1	B	671	LEU	CB-CG-CD1	6.09	121.36	111.00
1	B	124	VAL	CG1-CB-CG2	-6.09	101.15	110.90
1	B	323	GLU	CG-CD-OE2	-6.09	106.13	118.30
1	A	96	ASP	CB-CG-OD2	6.08	123.78	118.30
1	A	100	GLY	N-CA-C	6.08	128.31	113.10
1	A	547	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	B	232	LEU	CA-CB-CG	6.08	129.29	115.30
1	A	390	ARG	N-CA-CB	-6.08	99.66	110.60
1	A	627	TYR	CB-CG-CD1	6.08	124.65	121.00
1	B	277	GLN	CB-CG-CD	6.08	127.40	111.60
1	B	743	THR	O-C-N	6.07	132.41	122.70
1	B	627	TYR	CG-CD2-CE2	-6.07	116.44	121.30
1	A	284	MET	CA-CB-CG	6.07	123.61	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	LEU	CA-C-O	-6.06	107.38	120.10
1	B	41	GLU	CA-CB-CG	6.05	126.72	113.40
1	A	780	THR	OG1-CB-CG2	-6.05	96.09	110.00
1	B	700	SER	CA-C-N	-6.05	103.90	117.20
1	A	341	CYS	CA-CB-SG	6.04	124.87	114.00
1	B	475	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	A	310	TYR	CD1-CG-CD2	6.03	124.53	117.90
1	A	507	LYS	CD-CE-NZ	6.02	125.55	111.70
1	B	221	PRO	N-CD-CG	-6.02	94.18	103.20
1	B	297	TRP	CA-CB-CG	6.01	125.12	113.70
1	B	609	TYR	CZ-CE2-CD2	6.01	125.21	119.80
1	B	490	PHE	CB-CA-C	-6.00	98.39	110.40
1	B	76	LYS	CD-CE-NZ	6.00	125.50	111.70
1	B	700	SER	O-C-N	6.00	132.30	122.70
1	A	390	ARG	NH1-CZ-NH2	6.00	126.00	119.40
1	A	333	ARG	NE-CZ-NH2	5.99	123.29	120.30
1	B	838	ILE	CA-C-O	-5.99	107.53	120.10
1	B	682	ASP	N-CA-CB	-5.99	99.83	110.60
1	B	667	CYS	C-N-CA	-5.98	106.74	121.70
1	A	202	GLU	OE1-CD-OE2	5.98	130.48	123.30
1	A	329	ARG	CB-CA-C	-5.98	98.43	110.40
1	A	830	LEU	C-N-CA	-5.98	106.75	121.70
1	B	404	GLU	OE1-CD-OE2	5.98	130.47	123.30
1	A	808	THR	O-C-N	5.97	132.26	122.70
1	B	91	GLY	CA-C-O	-5.97	109.85	120.60
1	A	892	TYR	CD1-CE1-CZ	-5.96	114.43	119.80
1	B	779	ASP	CB-CG-OD1	-5.96	112.94	118.30
1	A	516	GLN	CB-CA-C	-5.96	98.49	110.40
1	B	428	MET	CA-CB-CG	5.95	123.42	113.30
1	A	809	ASP	CB-CG-OD1	5.95	123.65	118.30
1	A	275	GLN	O-C-N	-5.95	113.09	123.20
1	A	792	LEU	CB-CA-C	-5.95	98.91	110.20
1	A	312	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	B	34	THR	OG1-CB-CG2	-5.94	96.34	110.00
1	B	399	ASP	CB-CG-OD1	-5.94	112.95	118.30
1	B	167	PHE	CG-CD2-CE2	5.94	127.33	120.80
1	B	358	THR	N-CA-C	5.94	127.03	111.00
1	A	582	MET	CG-SD-CE	-5.94	90.70	100.20
1	B	825	ALA	C-N-CA	5.93	136.53	121.70
1	A	393	GLU	OE1-CD-OE2	-5.93	116.18	123.30
1	A	876	THR	N-CA-CB	5.93	121.56	110.30
1	B	223	ASP	CB-CG-OD2	-5.92	112.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	578	SER	CA-C-N	-5.92	104.18	117.20
1	B	602	LEU	CB-CG-CD2	5.91	121.05	111.00
1	B	447	VAL	O-C-N	-5.91	113.25	122.70
1	A	268	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	B	402	SER	N-CA-C	5.91	126.95	111.00
1	B	410	LEU	CB-CG-CD1	5.91	121.04	111.00
1	B	454	PHE	CZ-CE2-CD2	-5.90	113.02	120.10
1	A	328	PHE	CA-C-N	5.90	130.18	117.20
1	B	340	ILE	CB-CG1-CD1	5.90	130.42	113.90
1	B	377	TYR	CZ-CE2-CD2	5.90	125.11	119.80
1	B	18	LEU	CB-CG-CD2	5.89	121.02	111.00
1	B	32	TYR	CD1-CE1-CZ	5.89	125.10	119.80
1	B	701	VAL	CA-CB-CG1	-5.88	102.08	110.90
1	B	107	LEU	CA-CB-CG	-5.88	101.78	115.30
1	B	295	GLY	N-CA-C	5.88	127.79	113.10
1	A	53	PRO	N-CA-CB	-5.87	96.14	102.60
1	B	443	ALA	N-CA-CB	5.86	118.31	110.10
1	B	193	GLU	N-CA-C	-5.86	95.19	111.00
1	A	644	LEU	CB-CG-CD1	5.85	120.95	111.00
1	A	166	VAL	CA-CB-CG2	-5.85	102.13	110.90
1	A	193	GLU	OE1-CD-OE2	5.85	130.32	123.30
1	A	776	MET	CB-CG-SD	-5.85	94.86	112.40
1	B	864	MET	CA-CB-CG	-5.85	103.36	113.30
1	A	333	ARG	N-CA-C	-5.84	95.23	111.00
1	A	491	GLU	OE1-CD-OE2	5.84	130.31	123.30
1	B	241	SER	O-C-N	5.84	132.04	122.70
1	B	649	VAL	CG1-CB-CG2	-5.83	101.58	110.90
1	A	274	TYR	CD1-CE1-CZ	5.82	125.04	119.80
1	A	141	PHE	CG-CD1-CE1	-5.82	114.40	120.80
1	A	660	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	281	LEU	N-CA-C	-5.82	95.29	111.00
1	A	577	GLU	OE1-CD-OE2	-5.82	116.32	123.30
1	B	521	LEU	N-CA-C	5.82	126.71	111.00
1	A	510	THR	CA-CB-CG2	-5.82	104.25	112.40
1	A	107	LEU	CB-CG-CD2	-5.81	101.12	111.00
1	B	168	VAL	CG1-CB-CG2	5.81	120.20	110.90
1	A	229	LEU	N-CA-C	-5.81	95.31	111.00
1	B	806	PHE	N-CA-C	-5.81	95.31	111.00
1	A	638	PHE	CG-CD1-CE1	5.81	127.19	120.80
1	B	180	LEU	CB-CG-CD2	-5.81	101.12	111.00
1	A	115	THR	O-C-N	-5.80	113.41	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	361	TYR	CZ-CE2-CD2	5.80	125.03	119.80
1	A	803	TYR	CE1-CZ-OH	-5.80	104.44	120.10
1	B	116	LEU	CD1-CG-CD2	-5.80	93.09	110.50
1	B	866	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	B	114	LEU	CB-CG-CD1	-5.79	101.15	111.00
1	A	161	LYS	CB-CG-CD	5.78	126.63	111.60
1	B	76	LYS	N-CA-CB	-5.78	100.19	110.60
1	B	48	ASP	CB-CA-C	5.78	121.95	110.40
1	A	429	GLU	N-CA-CB	-5.77	100.21	110.60
1	B	95	THR	OG1-CB-CG2	-5.77	96.73	110.00
1	B	136	ALA	N-CA-C	5.77	126.58	111.00
1	B	508	ALA	O-C-N	-5.77	113.39	123.20
1	A	775	VAL	CB-CA-C	-5.77	100.44	111.40
1	B	349	LYS	CB-CA-C	-5.77	98.86	110.40
1	A	311	GLU	O-C-N	5.76	131.92	122.70
1	B	418	ARG	CA-CB-CG	5.76	126.08	113.40
1	A	122	HIS	CB-CA-C	-5.76	98.87	110.40
1	A	36	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	570	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	B	828	PHE	CG-CD2-CE2	-5.75	114.47	120.80
1	B	348	LEU	N-CA-CB	5.75	121.90	110.40
1	B	407	CYS	N-CA-C	-5.75	95.49	111.00
1	A	619	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	691	LEU	N-CA-C	-5.74	95.50	111.00
1	B	303	GLU	CB-CA-C	-5.73	98.93	110.40
1	B	624	MET	CB-CA-C	5.73	121.86	110.40
1	B	264	TYR	CG-CD2-CE2	-5.72	116.72	121.30
1	A	710	MET	O-C-N	5.71	131.84	122.70
1	B	289	GLY	N-CA-C	5.71	127.38	113.10
1	B	572	ASN	N-CA-C	5.71	126.40	111.00
1	A	820	PRO	CA-C-O	5.70	133.88	120.20
1	B	294	LYS	CD-CE-NZ	5.70	124.81	111.70
1	B	772	MET	CG-SD-CE	-5.70	91.08	100.20
1	A	331	PHE	CG-CD1-CE1	-5.70	114.53	120.80
1	A	506	LYS	CA-CB-CG	5.70	125.93	113.40
1	B	77	ARG	NE-CZ-NH2	5.69	123.15	120.30
1	B	162	ASP	O-C-N	-5.69	113.52	123.20
1	B	625	SER	N-CA-CB	5.69	119.04	110.50
1	B	631	MET	CB-CA-C	5.69	121.78	110.40
1	A	757	PRO	N-CD-CG	-5.69	94.67	103.20
1	B	159	PRO	CA-CB-CG	-5.68	93.22	104.00
1	B	174	ASN	O-C-N	5.67	131.78	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	631	MET	N-CA-CB	5.67	120.81	110.60
1	A	96	ASP	CB-CA-C	-5.67	99.06	110.40
1	A	192	TYR	CB-CA-C	-5.66	99.07	110.40
1	A	185	TYR	O-C-N	5.66	131.76	122.70
1	A	324	PHE	CB-CA-C	-5.66	99.08	110.40
1	A	470	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	614	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	340	ILE	CA-CB-CG1	-5.66	100.25	111.00
1	B	282	ILE	CG1-CB-CG2	-5.65	98.96	111.40
1	B	333	ARG	CG-CD-NE	5.65	123.67	111.80
1	A	638	PHE	CD1-CE1-CZ	-5.65	113.32	120.10
1	A	195	LEU	CB-CG-CD1	-5.65	101.39	111.00
1	A	333	ARG	CD-NE-CZ	5.64	131.50	123.60
1	A	811	SER	N-CA-CB	-5.64	102.04	110.50
1	B	145	GLN	N-CA-CB	-5.64	100.45	110.60
1	A	831	ASN	N-CA-C	-5.64	95.78	111.00
1	A	126	PRO	O-C-N	5.63	131.72	122.70
1	B	263	ALA	N-CA-CB	5.63	117.99	110.10
1	B	876	THR	CA-CB-CG2	-5.63	104.51	112.40
1	B	499	LEU	N-CA-CB	-5.63	99.14	110.40
1	A	168	VAL	CG1-CB-CG2	-5.63	101.90	110.90
1	A	367	ARG	NH1-CZ-NH2	-5.63	113.21	119.40
1	A	204	PHE	CB-CG-CD1	-5.62	116.86	120.80
1	A	441	GLU	OE1-CD-OE2	-5.62	116.55	123.30
1	B	372	GLY	N-CA-C	5.62	127.16	113.10
1	A	281	LEU	CA-CB-CG	5.62	128.23	115.30
1	B	513	LEU	CB-CG-CD1	5.62	120.56	111.00
1	B	34	THR	CA-CB-OG1	-5.62	97.20	109.00
1	B	42	ALA	CB-CA-C	-5.62	101.67	110.10
1	A	205	GLU	CG-CD-OE2	5.62	129.53	118.30
1	A	185	TYR	CE1-CZ-CE2	5.61	128.78	119.80
1	B	311	GLU	C-N-CA	5.61	135.74	121.70
1	A	180	LEU	CB-CG-CD2	-5.61	101.46	111.00
1	B	435	VAL	CG1-CB-CG2	-5.61	101.92	110.90
1	A	740	VAL	CA-CB-CG2	-5.60	102.50	110.90
1	B	131	PHE	N-CA-CB	-5.60	100.52	110.60
1	B	333	ARG	CA-CB-CG	-5.60	101.08	113.40
1	B	394	VAL	O-C-N	5.60	131.66	122.70
1	A	128	GLY	CA-C-N	5.60	129.51	117.20
1	B	296	PRO	CB-CA-C	5.60	125.99	112.00
1	A	766	ILE	CG1-CB-CG2	-5.59	99.09	111.40
1	B	828	PHE	CG-CD1-CE1	5.59	126.95	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	808	THR	C-N-CA	5.59	135.68	121.70
1	A	821	GLY	N-CA-C	-5.59	99.12	113.10
1	A	305	ASN	N-CA-C	-5.59	95.91	111.00
1	B	12	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	B	641	PRO	CA-C-N	5.59	129.49	117.20
1	B	93	THR	N-CA-C	-5.58	95.92	111.00
1	A	389	ILE	CA-CB-CG2	-5.58	99.74	110.90
1	A	396	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	573	GLY	N-CA-C	-5.58	99.16	113.10
1	A	63	LEU	CB-CG-CD2	5.57	120.47	111.00
1	B	733	LEU	CA-C-O	-5.57	108.39	120.10
1	B	87	PHE	CZ-CE2-CD2	-5.57	113.42	120.10
1	A	666	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	B	359	THR	OG1-CB-CG2	-5.56	97.21	110.00
1	B	729	LEU	CB-CG-CD1	-5.56	101.55	111.00
1	B	660	ASP	CB-CG-OD1	5.56	123.30	118.30
1	B	812	GLY	CA-C-O	-5.56	110.59	120.60
1	A	854	PHE	CB-CG-CD2	-5.55	116.91	120.80
1	B	61	LYS	CD-CE-NZ	5.55	124.47	111.70
1	B	332	ILE	CG1-CB-CG2	5.55	123.62	111.40
1	B	78	PRO	CB-CG-CD	-5.55	84.86	106.50
1	B	340	ILE	CA-CB-CG2	5.54	121.98	110.90
1	A	647	VAL	CA-CB-CG2	5.54	119.20	110.90
1	B	728	LYS	N-CA-C	-5.54	96.06	111.00
1	B	378	PRO	N-CA-CB	5.53	109.94	103.30
1	A	776	MET	CA-CB-CG	5.53	122.69	113.30
1	B	102	LEU	CB-CG-CD1	-5.53	101.61	111.00
1	A	204	PHE	CD1-CE1-CZ	-5.52	113.48	120.10
1	A	382	TRP	CA-CB-CG	-5.52	103.22	113.70
1	A	786	PHE	N-CA-CB	5.51	120.53	110.60
1	A	37	ASN	N-CA-C	-5.51	96.12	111.00
1	B	631	MET	CG-SD-CE	5.51	109.02	100.20
1	A	852	ASP	N-CA-C	-5.51	96.12	111.00
1	B	101	ALA	CB-CA-C	5.51	118.36	110.10
1	B	184	ALA	CB-CA-C	-5.51	101.83	110.10
1	A	124	VAL	CB-CA-C	-5.50	100.94	111.40
1	A	861	LEU	N-CA-C	-5.50	96.14	111.00
1	B	124	VAL	CA-CB-CG2	5.50	119.16	110.90
1	A	503	PHE	CB-CA-C	-5.50	99.40	110.40
1	B	413	LEU	CB-CG-CD2	5.50	120.35	111.00
1	B	473	SER	CA-C-N	5.50	129.31	117.20
1	B	195	LEU	CB-CG-CD1	5.50	120.35	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	TRP	CG-CD1-NE1	5.50	115.60	110.10
1	B	559	LEU	O-C-N	5.50	131.49	122.70
1	A	223	ASP	CA-C-N	-5.49	105.12	117.20
1	B	605	ARG	NE-CZ-NH2	5.49	123.05	120.30
1	B	377	TYR	CA-C-O	5.49	131.62	120.10
1	A	745	LEU	CB-CG-CD1	5.48	120.32	111.00
1	B	312	ARG	CB-CG-CD	5.48	125.85	111.60
1	B	389	ILE	N-CA-CB	5.48	123.41	110.80
1	B	518	GLN	CB-CA-C	-5.48	99.44	110.40
1	B	476	ILE	CA-CB-CG1	5.48	121.41	111.00
1	B	303	GLU	C-N-CA	5.48	135.39	121.70
1	A	105	SER	N-CA-CB	-5.47	102.29	110.50
1	A	163	GLY	O-C-N	5.47	131.45	122.70
1	A	23	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	744	GLU	CG-CD-OE2	-5.47	107.36	118.30
1	B	793	TRP	CA-CB-CG	5.47	124.09	113.70
1	B	493	ASN	CB-CA-C	5.47	121.33	110.40
1	B	848	ASN	C-N-CA	5.46	135.36	121.70
1	B	374	CYS	CA-CB-SG	-5.46	104.17	114.00
1	B	51	PHE	CZ-CE2-CD2	5.46	126.65	120.10
1	B	376	ASN	CB-CG-OD1	-5.46	110.68	121.60
1	A	319	MET	O-C-N	-5.46	113.97	122.70
1	A	392	GLU	N-CA-CB	-5.46	100.78	110.60
1	A	793	TRP	CB-CA-C	-5.46	99.49	110.40
1	A	184	ALA	N-CA-C	-5.45	96.29	111.00
1	A	588	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	127	TYR	CG-CD1-CE1	5.44	125.65	121.30
1	B	264	TYR	CB-CG-CD1	-5.44	117.74	121.00
1	B	645	HIS	N-CA-CB	5.44	120.39	110.60
1	A	624	MET	N-CA-CB	5.43	120.38	110.60
1	A	134	GLY	O-C-N	5.43	131.39	122.70
1	A	442	LEU	CA-C-O	-5.42	108.71	120.10
1	A	681	LEU	CB-CG-CD1	5.42	120.22	111.00
1	A	336	THR	OG1-CB-CG2	-5.42	97.55	110.00
1	B	102	LEU	CA-CB-CG	5.41	127.75	115.30
1	A	374	CYS	O-C-N	-5.41	114.04	122.70
1	B	95	THR	CA-CB-CG2	5.41	119.97	112.40
1	B	236	SER	N-CA-CB	-5.41	102.39	110.50
1	B	193	GLU	CA-C-O	-5.41	108.75	120.10
1	B	424	PHE	C-N-CA	5.41	133.65	122.30
1	B	579	CYS	CB-CA-C	5.40	121.19	110.40
1	A	433	PHE	CG-CD2-CE2	5.39	126.73	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	398	ASP	N-CA-CB	-5.39	100.90	110.60
1	A	652	PHE	N-CA-C	5.38	125.52	111.00
1	A	834	ILE	N-CA-C	-5.38	96.49	111.00
1	A	291	VAL	N-CA-CB	5.37	123.32	111.50
1	B	348	LEU	CB-CG-CD2	5.37	120.14	111.00
1	B	389	ILE	CA-C-N	-5.37	105.38	117.20
1	A	436	TYR	CG-CD1-CE1	-5.37	117.00	121.30
1	B	385	PRO	N-CD-CG	-5.37	95.14	103.20
1	B	329	ARG	C-N-CA	5.37	135.11	121.70
1	A	109	ALA	CB-CA-C	5.36	118.14	110.10
1	A	464	GLU	N-CA-C	-5.36	96.52	111.00
1	A	646	GLN	CG-CD-OE1	-5.36	110.88	121.60
1	A	615	LYS	CD-CE-NZ	5.36	124.02	111.70
1	B	314	GLN	CA-C-O	5.34	131.32	120.10
1	A	871	LEU	N-CA-CB	5.34	121.09	110.40
1	A	746	MET	CB-CG-SD	-5.34	96.38	112.40
1	A	701	VAL	C-N-CA	5.34	135.05	121.70
1	A	149	TRP	CG-CD1-NE1	-5.33	104.77	110.10
1	A	630	ARG	CB-CA-C	5.33	121.06	110.40
1	A	290	GLU	CA-CB-CG	-5.33	101.68	113.40
1	B	109	ALA	CA-C-N	-5.32	105.51	117.20
1	B	329	ARG	CB-CG-CD	5.31	125.41	111.60
1	A	453	PHE	CD1-CE1-CZ	-5.31	113.73	120.10
1	A	243	ASN	CB-CA-C	-5.30	99.79	110.40
1	B	745	LEU	CA-CB-CG	5.30	127.50	115.30
1	A	162	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	181	LEU	CB-CA-C	-5.30	100.13	110.20
1	A	634	GLU	CG-CD-OE1	-5.30	107.70	118.30
1	A	797	LYS	CD-CE-NZ	-5.30	99.51	111.70
1	B	860	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	63	LEU	C-N-CA	-5.29	111.18	122.30
1	A	375	ARG	N-CA-CB	-5.29	101.07	110.60
1	B	349	LYS	CB-CG-CD	-5.29	97.84	111.60
1	B	256	LYS	N-CA-C	5.29	125.28	111.00
1	B	118	GLU	O-C-N	-5.29	114.24	122.70
1	B	441	GLU	CA-C-N	-5.28	105.58	117.20
1	B	512	GLU	CA-CB-CG	5.28	125.02	113.40
1	B	388	LYS	O-C-N	5.28	131.15	122.70
1	B	143	LEU	O-C-N	-5.27	114.26	122.70
1	B	402	SER	CA-C-N	-5.27	105.60	117.20
1	A	242	ILE	CA-CB-CG2	5.27	121.44	110.90
1	B	587	ASP	N-CA-C	5.27	125.23	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	388	LYS	N-CA-C	5.27	125.22	111.00
1	B	440	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	B	610	LEU	CA-CB-CG	5.27	127.41	115.30
1	A	218	GLN	N-CA-CB	5.26	120.07	110.60
1	B	524	GLU	OE1-CD-OE2	5.26	129.61	123.30
1	B	377	TYR	CA-C-N	-5.26	102.38	117.10
1	B	540	PHE	CA-C-O	-5.26	109.06	120.10
1	A	188	VAL	CG1-CB-CG2	-5.25	102.50	110.90
1	A	862	ASP	OD1-CG-OD2	-5.25	113.32	123.30
1	B	188	VAL	N-CA-C	-5.25	96.82	111.00
1	A	648	ILE	CG1-CB-CG2	-5.25	99.85	111.40
1	B	331	PHE	CB-CG-CD1	-5.25	117.13	120.80
1	A	323	GLU	OE1-CD-OE2	-5.24	117.01	123.30
1	B	872	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	B	94	ARG	C-N-CA	5.24	134.79	121.70
1	A	384	ASN	N-CA-CB	5.24	120.02	110.60
1	A	237	LEU	N-CA-CB	5.23	120.87	110.40
1	A	448	HIS	N-CA-C	5.23	125.13	111.00
1	B	291	VAL	CA-CB-CG1	-5.23	103.05	110.90
1	B	416	LYS	CD-CE-NZ	5.23	123.74	111.70
1	B	770	ARG	CA-C-N	5.23	128.71	117.20
1	A	354	ARG	CB-CA-C	5.23	120.86	110.40
1	A	345	PRO	CB-CG-CD	-5.23	86.11	106.50
1	B	499	LEU	CB-CG-CD2	5.23	119.89	111.00
1	A	310	TYR	OH-CZ-CE2	5.22	134.21	120.10
1	A	58	LEU	CB-CG-CD1	5.22	119.88	111.00
1	A	823	PHE	CG-CD2-CE2	5.22	126.54	120.80
1	B	345	PRO	CA-N-CD	-5.22	104.19	111.50
1	B	337	LYS	CA-CB-CG	-5.22	101.92	113.40
1	B	308	ASP	CB-CA-C	5.22	120.84	110.40
1	A	300	ASN	N-CA-CB	-5.22	101.21	110.60
1	A	343	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	630	ARG	N-CA-C	-5.21	96.95	111.00
1	B	117	ASN	N-CA-CB	-5.20	101.24	110.60
1	A	296	PRO	N-CD-CG	5.20	111.00	103.20
1	B	58	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	B	133	GLU	C-N-CA	5.20	133.21	122.30
1	A	711	HIS	N-CA-CB	5.19	119.95	110.60
1	A	855	ILE	CB-CA-C	-5.19	101.22	111.60
1	B	480	PRO	N-CD-CG	5.19	110.98	103.20
1	A	40	LEU	CD1-CG-CD2	-5.19	94.94	110.50
1	B	671	LEU	CB-CG-CD2	-5.19	102.18	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	868	PHE	CB-CG-CD1	-5.18	117.17	120.80
1	B	858	LEU	CB-CA-C	-5.18	100.35	110.20
1	B	31	ASP	OD1-CG-OD2	-5.18	113.45	123.30
1	B	336	THR	N-CA-C	-5.18	97.00	111.00
1	A	49	PRO	C-N-CA	-5.18	108.75	121.70
1	B	185	TYR	CZ-CE2-CD2	-5.18	115.14	119.80
1	A	93	THR	CA-CB-CG2	-5.18	105.15	112.40
1	A	810	ARG	N-CA-CB	-5.18	101.28	110.60
1	B	876	THR	OG1-CB-CG2	-5.18	98.09	110.00
1	A	447	VAL	C-N-CA	-5.18	108.76	121.70
1	B	148	GLU	OE1-CD-OE2	-5.18	117.09	123.30
1	B	426	ARG	CA-CB-CG	5.18	124.79	113.40
1	A	62	GLU	O-C-N	5.17	130.98	122.70
1	B	383	VAL	O-C-N	5.17	130.98	122.70
1	A	498	PHE	CB-CG-CD2	-5.17	117.18	120.80
1	B	426	ARG	CB-CA-C	-5.17	100.07	110.40
1	A	123	ARG	CA-CB-CG	5.17	124.76	113.40
1	A	257	ASN	C-N-CA	5.16	134.61	121.70
1	A	69	LYS	CD-CE-NZ	-5.16	99.83	111.70
1	A	331	PHE	CB-CA-C	-5.16	100.08	110.40
1	B	684	GLU	N-CA-C	5.16	124.92	111.00
1	B	104	ASP	OD1-CG-OD2	-5.15	113.51	123.30
1	B	324	PHE	CZ-CE2-CD2	5.15	126.28	120.10
1	B	450	LYS	CD-CE-NZ	5.15	123.55	111.70
1	B	141	PHE	CZ-CE2-CD2	5.15	126.28	120.10
1	B	349	LYS	O-C-N	5.15	130.94	122.70
1	B	594	LEU	CB-CG-CD1	-5.14	102.26	111.00
1	A	308	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	A	520	ASN	N-CA-C	5.14	124.87	111.00
1	B	320	GLU	CA-CB-CG	-5.13	102.11	113.40
1	B	725	GLN	N-CA-C	-5.13	97.14	111.00
1	A	684	GLU	OE1-CD-OE2	5.13	129.46	123.30
1	B	333	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	A	85	PRO	CA-N-CD	-5.13	104.31	111.50
1	A	167	PHE	N-CA-C	5.13	124.86	111.00
1	A	387	PHE	CD1-CE1-CZ	5.13	126.26	120.10
1	B	478	LEU	CA-CB-CG	5.13	127.10	115.30
1	A	429	GLU	O-C-N	-5.13	114.49	122.70
1	A	212	THR	N-CA-C	5.13	124.85	111.00
1	B	743	THR	C-N-CA	5.13	134.52	121.70
1	B	611	THR	N-CA-C	5.13	124.84	111.00
1	A	143	LEU	N-CA-CB	-5.12	100.15	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	341	CYS	CA-CB-SG	-5.12	104.78	114.00
1	A	454	PHE	CB-CG-CD1	-5.12	117.22	120.80
1	A	381	PHE	CB-CG-CD2	-5.12	117.22	120.80
1	B	329	ARG	CD-NE-CZ	5.11	130.76	123.60
1	A	98	CYS	CA-CB-SG	-5.11	104.81	114.00
1	B	67	SER	N-CA-CB	5.11	118.16	110.50
1	B	84	ASN	CB-CA-C	5.11	120.61	110.40
1	A	159	PRO	CA-C-O	-5.11	107.95	120.20
1	A	330	ASP	OD1-CG-OD2	-5.10	113.60	123.30
1	A	317	VAL	CG1-CB-CG2	-5.10	102.74	110.90
1	A	860	ARG	CB-CG-CD	5.10	124.87	111.60
1	A	225	TYR	CG-CD2-CE2	-5.10	117.22	121.30
1	B	388	LYS	CB-CG-CD	-5.10	98.34	111.60
1	A	281	LEU	CB-CG-CD1	5.10	119.67	111.00
1	B	150	VAL	CG1-CB-CG2	-5.09	102.76	110.90
1	A	183	LYS	CD-CE-NZ	5.08	123.39	111.70
1	B	213	GLU	CG-CD-OE2	5.08	128.47	118.30
1	A	153	VAL	CA-CB-CG1	5.08	118.52	110.90
1	B	580	ARG	CA-CB-CG	5.08	124.58	113.40
1	A	207	PHE	CZ-CE2-CD2	-5.08	114.00	120.10
1	A	403	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	608	ASN	O-C-N	-5.08	114.58	122.70
1	A	602	LEU	CB-CG-CD1	5.08	119.63	111.00
1	B	339	GLU	N-CA-C	5.08	124.70	111.00
1	A	647	VAL	CA-CB-CG1	5.07	118.51	110.90
1	A	777	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	B	391	LEU	CB-CG-CD2	-5.07	102.38	111.00
1	B	660	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	788	GLU	N-CA-CB	5.07	119.72	110.60
1	B	868	PHE	O-C-N	-5.07	114.60	122.70
1	A	285	ARG	N-CA-C	5.06	124.67	111.00
1	B	195	LEU	CA-CB-CG	5.06	126.94	115.30
1	A	462	GLN	N-CA-CB	-5.06	101.49	110.60
1	B	345	PRO	C-N-CA	5.06	134.35	121.70
1	B	480	PRO	CA-CB-CG	-5.06	94.39	104.00
1	B	789	PHE	O-C-N	5.06	130.79	122.70
1	A	468	ASN	N-CA-CB	5.06	119.70	110.60
1	B	610	LEU	CB-CG-CD1	5.06	119.60	111.00
1	A	343	LEU	CD1-CG-CD2	-5.06	95.33	110.50
1	A	764	PHE	CB-CG-CD1	5.05	124.34	120.80
1	A	93	THR	C-N-CA	5.05	134.33	121.70
1	A	623	SER	N-CA-CB	-5.05	102.92	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	343	LEU	CA-CB-CG	-5.05	103.69	115.30
1	B	701	VAL	C-N-CA	5.05	134.32	121.70
1	B	726	PHE	CG-CD2-CE2	5.05	126.36	120.80
1	A	29	ASN	CB-CA-C	5.05	120.50	110.40
1	B	283	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	808	THR	CB-CA-C	-5.05	97.97	111.60
1	A	94	ARG	N-CA-C	-5.04	97.39	111.00
1	B	217	LEU	CB-CG-CD1	-5.04	102.43	111.00
1	A	434	ALA	CA-C-O	-5.04	109.52	120.10
1	B	237	LEU	O-C-N	-5.04	114.64	122.70
1	B	362	GLU	CB-CG-CD	5.04	127.80	114.20
1	B	104	ASP	CB-CA-C	5.04	120.47	110.40
1	A	114	LEU	O-C-N	5.03	130.75	122.70
1	A	280	ASN	CB-CG-OD1	-5.03	111.53	121.60
1	B	191	SER	N-CA-CB	5.03	118.05	110.50
1	B	259	VAL	CA-CB-CG2	5.03	118.45	110.90
1	A	285	ARG	NH1-CZ-NH2	5.03	124.93	119.40
1	A	633	ILE	O-C-N	5.03	130.75	122.70
1	B	660	ASP	OD1-CG-OD2	-5.02	113.76	123.30
1	A	50	ALA	CB-CA-C	5.02	117.63	110.10
1	A	628	GLU	OE1-CD-OE2	5.02	129.32	123.30
1	A	801	GLY	CA-C-O	-5.02	111.57	120.60
1	A	35	LEU	C-N-CA	-5.02	109.16	121.70
1	B	329	ARG	CA-CB-CG	5.02	124.43	113.40
1	A	469	LEU	N-CA-CB	5.01	120.43	110.40
1	A	105	SER	O-C-N	-5.01	114.69	122.70
1	B	436	TYR	CD1-CE1-CZ	-5.01	115.30	119.80
1	A	169	HIS	N-CA-CB	-5.00	101.59	110.60
1	B	598	GLU	CG-CD-OE2	5.00	128.31	118.30

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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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	5615	959	3
1	B	6003	0	5477	969	1
2	A	172	0	0	53	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	140	0	0	45	1
All	All	12368	0	11092	1928	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 83.

All (1928) 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:B:786:PHE:CA	1:B:786:PHE:CB	1.74	1.64
1:A:550:ILE:CB	1:A:550:ILE:CA	1.75	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:CB	1:B:89:VAL:CA	1.77	1.62
1:A:826:ALA:CB	1:A:826:ALA:CA	1.76	1.62
1:B:284:MET:CG	1:B:284:MET:CB	1.75	1.62
1:B:477:ARG:CG	1:B:477:ARG:CB	1.77	1.62
1:A:688:THR:CB	1:A:688:THR:CG2	1.78	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:CG	1:B:256:LYS:CB	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:CD1	1:B:340:ILE:CG1	1.75	1.60
1:B:89:VAL:CG1	1:B:89:VAL:CB	1.78	1.60
1:A:320:GLU:CB	1:A:320:GLU:CA	1.74	1.60
1:A:773:VAL:CG1	1:A:773:VAL:CB	1.77	1.60
1:A:332:ILE:CB	1:A:332:ILE:CG1	1.75	1.60
1:A:89:VAL:CB	1:A:89:VAL:CG1	1.80	1.60
1:B:230:LYS:CE	1:B:230:LYS:CD	1.76	1.60
1:A:333:ARG:CD	1:A:333:ARG:CG	1.78	1.60
1:B:553:LYS:CA	1:B:553:LYS:CB	1.76	1.60
1:A:99:GLN:CB	1:A:99:GLN:CA	1.78	1.59
1:A:242:ILE:CD1	1:A:242:ILE:CG1	1.76	1.59
1:B:313:GLU:CB	1:B:313:GLU:CG	1.75	1.59
1:A:200:THR:CA	1:A:200:THR:CB	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:LEU:CD1	1:A:413:LEU:CG	1.79	1.59
1:A:864:MET:CB	1:A:864:MET:CA	1.75	1.59
1:B:470:ARG:CB	1:B:470:ARG:CG	1.74	1.59
1:A:669:VAL:CB	1:A:669:VAL:CG1	1.76	1.59
1:B:729:LEU:CG	1:B:729:LEU:CD2	1.75	1.58
1:A:366:ARG:CG	1:A:366:ARG:CD	1.77	1.58
1:B:335:PHE:CA	1:B:335:PHE:CB	1.74	1.58
1:B:294:LYS:CG	1:B:294:LYS:CD	1.75	1.58
1:B:694:ILE:CB	1:B:694:ILE:CA	1.78	1.58
1:B:579:CYS:CB	1:B:579:CYS:CA	1.78	1.57
1:A:340:ILE:CB	1:A:340:ILE:CG2	1.76	1.57
1:A:478:LEU:CD1	1:A:478:LEU:CG	1.82	1.57
1:B:669:VAL:CA	1:B:669:VAL:CB	1.82	1.57
1:B:120:ILE:CG2	1:B:120:ILE:CB	1.75	1.57
1:B:537:LYS:CG	1:B:537:LYS:CD	1.74	1.57
1:B:668:LEU:CG	1:B:668:LEU:CD2	1.74	1.57
1:B:806:PHE:CB	1:B:806:PHE:CG	1.79	1.57
1:B:610:LEU:CD1	1:B:610:LEU:CG	1.83	1.56
1:B:333:ARG:CD	1:B:333:ARG:CG	1.78	1.56
1:A:808:THR:CB	1:A:808:THR:CG2	1.76	1.56
1:A:477:ARG:CD	1:A:477:ARG:CG	1.77	1.56
1:A:73:ILE:CD1	1:A:73:ILE:CG1	1.77	1.56
1:B:348:LEU:CD1	1:B:348:LEU:CG	1.75	1.56
1:B:349:LYS:CE	1:B:349:LYS:NZ	1.68	1.56
1:A:772:MET:CB	1:A:772:MET:CG	1.78	1.56
1:A:883:ILE:CB	1:A:883:ILE:CG2	1.76	1.56
1:A:340:ILE:CG1	1:A:340:ILE:CD1	1.78	1.55
1:A:7:LYS:CE	1:A:7:LYS:CD	1.78	1.55
1:B:345:PRO:CG	1:B:345:PRO:CD	1.78	1.55
1:B:277:GLN:CG	1:B:277:GLN:CB	1.76	1.55
1:A:831:ASN:CB	1:A:831:ASN:CG	1.75	1.55
1:B:677:ILE:CG1	1:B:677:ILE:CD1	1.75	1.54
1:B:780:THR:CG2	1:B:780:THR:CB	1.79	1.54
1:B:740:VAL:CB	1:B:740:VAL:CG1	1.76	1.54
1:A:602:LEU:CG	1:A:602:LEU:CD1	1.80	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:A:494:LYS:CE	1:A:494:LYS:NZ	1.68	1.54
1:B:337:LYS:HZ2	1:B:337:LYS:CB	1.05	1.54
1:B:690:GLN:CG	1:B:690:GLN:CB	1.84	1.54
1:A:883:ILE:CG1	1:A:883:ILE:CD1	1.80	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ILE:CG1	1:A:227:ILE:CD1	1.79	1.53
1:A:428:MET:CB	1:A:428:MET:CG	1.83	1.53
1:A:317:VAL:CA	1:A:317:VAL:CB	1.84	1.53
1:B:456:ALA:C	1:B:456:ALA:CA	1.74	1.53
1:A:570:ARG:CB	1:A:570:ARG:CG	1.81	1.53
1:B:494:LYS:CE	1:B:494:LYS:CD	1.77	1.53
1:B:883:ILE:CA	1:B:883:ILE:CB	1.81	1.52
1:B:26:LYS:CG	1:B:26:LYS:CB	1.77	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:B:90:ASP:CB	1:B:90:ASP:CG	1.77	1.52
1:A:757:PRO:CG	1:A:757:PRO:CD	1.82	1.51
1:A:671:LEU:CA	1:A:671:LEU:CB	1.89	1.51
1:A:270:LYS:NZ	1:A:270:LYS:CE	1.73	1.50
1:A:26:LYS:NZ	1:A:26:LYS:CE	1.73	1.50
1:B:136:ALA:CA	1:B:136:ALA:N	1.67	1.50
1:A:450:LYS:NZ	1:A:450:LYS:CE	1.67	1.50
1:A:115:THR:CB	1:A:115:THR:CG2	1.87	1.50
1:B:226:GLN:CG	1:B:226:GLN:CD	1.80	1.50
1:B:69:LYS:CG	1:B:69:LYS:CB	1.87	1.50
1:B:572:ASN:C	1:B:572:ASN:CA	1.77	1.50
1:B:480:PRO:CB	1:B:480:PRO:CG	1.80	1.50
1:B:824:GLU:CB	1:B:824:GLU:CA	1.86	1.49
1:B:440:ARG:CD	1:B:440:ARG:CG	1.86	1.49
1:A:218:GLN:CG	1:A:218:GLN:CB	1.87	1.49
1:A:174:ASN:CG	1:A:174:ASN:CB	1.78	1.48
1:A:615:LYS:CE	1:A:615:LYS:NZ	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:B:346:ASP:CG	1:B:346:ASP:CB	1.78	1.47
1:B:643:GLN:CG	1:B:643:GLN:CD	1.78	1.47
1:A:652:PHE:CE1	1:A:667:CYS:HB2	1.46	1.47
1:A:452:ASP:CG	1:A:452:ASP:CB	1.82	1.47
1:A:120:ILE:CD1	1:A:120:ILE:CG1	1.89	1.46
1:B:312:ARG:CG	1:B:312:ARG:CD	1.90	1.46
1:B:284:MET:CE	1:B:284:MET:SD	2.03	1.46
1:A:631:MET:SD	1:A:631:MET:CG	2.02	1.46
1:A:6:MET:CE	1:A:6:MET:SD	2.04	1.46
1:B:746:MET:CE	1:B:746:MET:SD	2.04	1.46
1:A:680:GLN:CB	1:A:680:GLN:CA	1.92	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CB	1:B:316:ARG:CA	1.93	1.44
1:A:582:MET:SD	1:A:582:MET:CE	2.03	1.44
1:B:837:MET:SD	1:B:837:MET:CE	2.05	1.43
1:B:67:SER:CB	1:B:67:SER:CA	1.96	1.42
1:A:414:MET:CE	1:A:414:MET:SD	2.06	1.42
1:A:891:MET:SD	1:A:891:MET:CE	2.09	1.40
1:B:582:MET:SD	1:B:582:MET:CE	2.10	1.40
1:B:332:ILE:CG2	1:B:332:ILE:CB	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:CG	1:A:6:MET:SD	2.21	1.27
1:B:6:MET:SD	1:B:6:MET:CE	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:B:772:MET:CE	1:B:772:MET:SD	2.32	1.18
1:B:86:GLN:HG3	1:B:89:VAL:CG2	1.73	1.18
1:A:63:LEU:HD12	1:A:70:THR:HG23	1.18	1.18
1:B:440:ARG:HG2	1:B:441:GLU:N	1.54	1.17
1:B:343:LEU:CD1	1:B:343:LEU:H	1.52	1.15
1:A:710:MET:N	2:A:1030:HOH:O	1.80	1.14
1:A:258:LEU:HD22	1:A:258:LEU:C	1.67	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:651:ARG:CZ	1:B:670:ARG:NH2	2.16	1.09
1:A:447:VAL:HG11	2:A:926:HOH:O	1.53	1.09
1:A:631:MET:SD	1:A:631:MET:CE	2.41	1.08
1:B:538:THR:HG22	1:B:539:LEU:H	1.13	1.08
1:A:698:SER:O	1:A:701:VAL:N	1.85	1.08
1:B:69:LYS:NZ	1:B:69:LYS:CB	2.16	1.08
1:B:343:LEU:N	1:B:343:LEU:HD12	1.67	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:576:LEU:O	1:B:578:SER:N	1.88	1.06
1:B:308:ASP:OD1	1:B:308:ASP:N	1.87	1.06
1:A:75:TRP:CZ3	1:A:159:PRO:HG3	1.90	1.06
1:A:306:LYS:HG3	1:A:307:VAL:N	1.47	1.05
1:B:330:ASP:C	1:B:330:ASP:OD1	1.90	1.04
1:B:389:ILE:H	1:B:389:ILE:HD12	1.18	1.04
1:B:86:GLN:HG3	1:B:89:VAL:HG23	1.34	1.04
1:A:599:PHE:CD2	1:A:599:PHE:O	2.10	1.03
1:B:440:ARG:HG2	1:B:441:GLU:H	0.89	1.03
1:B:525:LYS:HB3	1:B:525:LYS:NZ	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:B:651:ARG:CZ	1:B:670:ARG:CZ	2.37	1.02
1:A:652:PHE:CE1	1:A:667:CYS:CB	2.43	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:A:832:GLN:OE1	1:A:832:GLN:C	2.00	1.01
1:B:69:LYS:HB3	1:B:69:LYS:NZ	1.74	1.01
1:B:740:VAL:HG12	1:B:741:SER:H	1.26	1.00
1:A:596:LEU:O	2:A:995:HOH:O	1.78	1.00
1:A:155:ASP:C	1:A:155:ASP:OD2	1.95	1.00
1:B:850:ASP:O	1:B:851:PHE:HB2	1.20	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:B:651:ARG:HG3	2:B:914:HOH:O	1.61	0.99
1:A:731:VAL:HG11	1:A:733:LEU:HD11	1.44	0.99
1:A:702:LEU:HD21	2:A:1036:HOH:O	1.63	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:B:343:LEU:HD12	1:B:343:LEU:H	0.81	0.98
1:A:256:LYS:HD3	1:A:258:LEU:HD11	1.42	0.98
1:A:689:ILE:C	1:A:689:ILE:HD12	1.83	0.97
1:B:69:LYS:HZ3	1:B:69:LYS:HB3	1.27	0.97
1:B:525:LYS:HB3	1:B:525:LYS:HZ2	1.28	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:PHE:N	1:B:331:PHE:CD2	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:N	1:B:389:ILE:HD12	1.75	0.95
1:A:465:HIS:ND1	1:A:465:HIS:N	2.13	0.95
1:A:619:ASP:O	1:A:620:LYS:C	2.03	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
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:HG	1:B:586:MET:HE2	1.50	0.93
1:B:538:THR:O	1:B:539:LEU:CB	2.16	0.93
1:A:218:GLN:HA	1:A:218:GLN:CB	1.99	0.92
1:B:256:LYS:HB3	1:B:256:LYS:NZ	1.82	0.92
1:A:332:ILE:HB	1:A:332:ILE:CG1	1.98	0.92
1:B:740:VAL:HG21	1:B:789:PHE:HD1	1.35	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:795:ASN:O	1:B:799:TRP:CD1	2.23	0.91
1:B:337:LYS:HZ3	1:B:337:LYS:HB3	1.32	0.91
1:A:395:ASP:H	1:A:406:GLY:HA3	1.30	0.91
1:B:4:ILE:CD1	1:B:889:LEU:HA	2.00	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:HG23	1:B:88:ILE:O	1.69	0.90
1:A:336:THR:HG23	1:A:337:LYS:N	1.86	0.90
1:A:13:GLU:O	1:A:16:GLU:N	2.05	0.90
1:B:701:VAL:HG13	1:B:860:ARG:HH11	1.33	0.90
1:B:468:ASN:O	1:B:468:ASN:OD1	1.90	0.90
1:B:607:ARG:HH21	1:B:607:ARG:HB3	1.37	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:B:343:LEU:CD2	1:B:343:LEU:CB	2.50	0.89
1:A:305:ASN:HD22	1:A:306:LYS:N	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:ALA:HA	1:A:825:ALA:HB3	1.54	0.89
1:B:116:LEU:HD11	1:B:287:PRO:HG3	1.53	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:B:667:CYS:O	1:B:668:LEU:C	2.09	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:438:VAL:HG22	1:B:484:ILE:CD1	2.04	0.87
1:A:132:GLN:O	1:A:133:GLU:C	2.12	0.87
1:B:89:VAL:CB	1:B:89:VAL:C	2.42	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: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:HZ2	1:B:69:LYS:CB	1.86	0.86
1:B:790:LYS:O	1:B:791:TYR:C	2.13	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:469:LEU:C	1:B:469:LEU:HD12	1.93	0.85
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:B:331:PHE:HD2	1:B:331:PHE:N	1.70	0.85
1:A:558:ILE:HG22	1:A:559:LEU:N	1.89	0.85
1:B:554:GLU:O	1:B:557:THR:HB	1.76	0.85
1:B:499:LEU:HD23	2:B:948:HOH:O	1.76	0.85
1:B:120:ILE:CG2	1:B:120:ILE:CG1	2.54	0.85
1:A:853:ASN:N	1:A:853:ASN:HD22	1.73	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:A:822:ALA:CA	1:A:825:ALA:HB3	2.06	0.85
1:A:388:LYS:HZ1	1:A:482:GLU:CD	1.81	0.84
1:B:658:ILE:CG2	1:B:658:ILE:O	2.25	0.84
1:B:538:THR:HG22	1:B:539:LEU:N	1.90	0.84
1:A:611:THR:O	1:A:611:THR:HG22	1.75	0.84
1:B:670:ARG:O	1:B:674:LEU:HD22	1.77	0.84
1:B:724:ARG:HB2	1:B:724:ARG:HH21	1.41	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:B:97:ILE:HD11	1:B:108:LEU:CD1	2.08	0.84
1:A:832:GLN:CD	1:A:833:HIS:H	1.79	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG	1:A:478:LEU:CD1	2.08	0.83
1:A:31:ASP:C	1:A:31:ASP:OD2	2.14	0.83
1:B:831:ASN:HB3	1:B:833:HIS:CB	2.08	0.83
1:A:766:ILE:HD11	2:A:967:HOH:O	1.77	0.83
1:A:756:HIS:CB	1:A:757:PRO:HD2	2.06	0.83
1:B:86:GLN:HG3	1:B:89:VAL:HG21	1.59	0.83
1:A:89:VAL:CG2	1:A:89:VAL:CG1	2.56	0.83
1:A:41:GLU:OE2	2:A:974:HOH:O	1.97	0.83
1:B:135:TYR:C	1:B:136:ALA:CA	2.47	0.82
1:A:13:GLU:HA	1:A:13:GLU:OE1	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: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:301:SER:O	1:A:302:TYR:O	1.98	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:A:519:ALA:HB2	1:A:675:PHE:CE1	2.15	0.82
1:B:801:GLY:O	2:B:975:HOH:O	1.97	0.82
1:B:8:LEU:O	1:B:9:ALA:C	2.17	0.82
1:A:198:GLY:O	1:A:199:CYS:HB2	1.80	0.82
1:B:524:GLU:N	1:B:524:GLU:OE1	2.12	0.82
1:A:822:ALA:C	1:A:825:ALA:HB3	2.00	0.82
1:B:492:PRO:HB2	1:B:493:ASN:ND2	1.95	0.82
1:A:799:TRP:CH2	1:A:858:LEU:O	2.32	0.82
1:B:343:LEU:CD2	1:B:343:LEU:CD1	2.58	0.81
1:A:429:GLU:OE1	1:A:494:LYS:NZ	2.12	0.81
1:B:86:GLN:CG	1:B:89:VAL:CG2	2.57	0.81
1:A:821:GLY:HA3	2:A:1015:HOH:O	1.81	0.81
1:B:223:ASP:O	1:B:227:ILE:HG13	1.80	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:B:430:THR:HA	1:B:468:ASN:HB2	1.62	0.81
1:B:390:ARG:HG2	1:B:390:ARG:NH1	1.91	0.81
1:A:221:PRO:HB2	1:A:223:ASP:OD2	1.79	0.81
1:A:808:THR:O	1:A:808:THR:CG2	2.29	0.81
1:B:651:ARG:NH2	1:B:670:ARG:CZ	2.42	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:ASN:H	1:B:457:ASN:HD22	1.29	0.81
1:A:100:GLY:HA3	1:A:103:GLY:HA3	1.61	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:555:LEU:O	1:B:556:GLN:C	2.18	0.81
1:A:832:GLN:CD	1:A:833:HIS:N	2.34	0.81
1:B:440:ARG:HG2	1:B:440:ARG:HH21	1.44	0.81
1:A:832:GLN:OE1	1:A:832:GLN:CA	2.29	0.81
1:A:825:ALA:HB2	2:A:912:HOH:O	1.80	0.80
1:B:572:ASN:HA	1:B:572:ASN:C	2.00	0.80
1:A:256:LYS:HD2	1:A:258:LEU:HD21	1.64	0.80
1:A:4:ILE:HD12	1:A:4:ILE:C	1.99	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:A:50:ALA:C	1:A:52:PRO:HD3	2.02	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:HG2	1:A:329:ARG:NH2	1.96	0.79
1:A:99:GLN:CB	1:A:99:GLN:C	2.48	0.79
1:A:258:LEU:CD2	1:A:258:LEU:C	2.46	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:808:THR:O	1:A:808:THR:HG23	1.81	0.79
1:A:652:PHE:HE1	1:A:667:CYS:HB2	1.45	0.79
1:A:258:LEU:H	1:A:258:LEU:CD1	1.96	0.79
1:A:365:TRP:CZ2	1:A:488:SER:HA	2.18	0.79
1:A:211:VAL:HG23	1:A:211:VAL:O	1.81	0.79
1:A:682:ASP:OD1	1:A:685:ASN:HA	1.83	0.79
1:A:217:LEU:O	1:A:220:ALA:HB2	1.83	0.79
1:A:605:ARG:NH1	2:A:1034:HOH:O	2.07	0.78
1:A:832:GLN:OE1	1:A:833:HIS:N	2.15	0.78
1:A:13:GLU:HA	1:A:16:GLU:HG2	1.65	0.78
1:B:69:LYS:HZ2	1:B:69:LYS:HB2	1.46	0.78
1:B:576:LEU:O	1:B:579:CYS:N	2.17	0.78
1:B:277:GLN:CG	1:B:277:GLN:CA	2.60	0.78
1:B:89:VAL:O	1:B:89:VAL:HB	1.84	0.78
1:B:170:SER:O	1:B:172:GLN:N	2.17	0.78
1:B:136:ALA:HA	1:B:136:ALA:N	1.94	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:LYS:CB	1:B:553:LYS:HA	2.12	0.78
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: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:B:69:LYS:CE	1:B:69:LYS:CB	2.62	0.78
1:B:313:GLU:CA	1:B:313:GLU:CG	2.62	0.77
1:A:594:LEU:O	1:A:598:GLU:OE2	2.01	0.77
1:B:323:GLU:OE2	1:B:323:GLU:HA	1.84	0.77
1:A:832:GLN:N	2:A:919:HOH:O	2.16	0.77
1:B:439:PRO:HB2	1:B:440:ARG:HD3	1.65	0.77
1:B:601:ILE:HD12	2:B:987:HOH:O	1.82	0.77
1:A:493:ASN:ND2	1:A:627:TYR:OH	2.18	0.77
1:B:25:ILE:CD1	1:B:148:GLU:OE1	2.32	0.77
1:A:373:GLY:HA3	1:A:492:PRO:HG3	1.65	0.77
1:B:8:LEU:CD2	1:B:8:LEU:HG	2.10	0.77
1:B:576:LEU:O	1:B:577:GLU:C	2.22	0.77
1:B:61:LYS:HG3	1:B:65:PRO:O	1.84	0.77
1:A:306:LYS:O	1:A:307:VAL:C	2.22	0.77
1:B:61:LYS:HG3	1:B:66:ASN:HB2	1.65	0.77
1:A:13:GLU:CA	1:A:16:GLU:HG2	2.15	0.77
1:B:701:VAL:CG1	1:B:860:ARG:HG2	2.15	0.77
1:A:386:GLN:HB3	1:A:513:LEU:HB3	1.67	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:A:122:HIS:HA	1:A:125:VAL:O	1.84	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:796:ILE:O	1:B:799:TRP:HB2	1.85	0.76
1:B:361:TYR:O	1:B:499:LEU:HA	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:740:VAL:CG1	1:B:741:SER:H	1.98	0.76
1:B:430:THR:HA	1:B:468:ASN:CB	2.14	0.76
1:A:350:SER:C	1:A:352:THR:H	1.88	0.76
1:A:68:SER:O	1:A:69:LYS:C	2.24	0.76
1:B:537:LYS:CB	1:B:537:LYS:NZ	2.48	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:607:ARG:CB	1:B:607:ARG:HH21	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:TRP:CZ3	1:B:107:LEU:HD12	2.21	0.76
1:A:293:TRP:O	1:A:295:GLY:N	2.18	0.76
1:B:35:LEU:HD13	1:B:46:PHE:CE1	2.21	0.75
1:B:348:LEU:CD1	1:B:348:LEU:CD2	2.64	0.75
1:A:333:ARG:O	1:A:334:GLU:HB2	1.86	0.75
1:B:470:ARG:CG	1:B:470:ARG:CA	2.64	0.75
1:B:729:LEU:CD1	1:B:729:LEU:CD2	2.63	0.75
1:A:84:ASN:O	1:A:84:ASN:OD1	2.03	0.75
1:A:13:GLU:C	1:A:16:GLU:HG2	2.06	0.75
1:A:731:VAL:HG21	1:A:733:LEU:CG	2.15	0.75
1:A:205:GLU:HG2	1:A:210:GLY:O	1.85	0.75
1:B:294:LYS:CB	1:B:294:LYS:CD	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: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:98:CYS:SG	1:B:171:ALA:HB2	2.28	0.74
1:A:655:ASP:HB2	1:A:656:GLU:OE1	1.87	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: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:HB	1:A:317:VAL:CA	2.15	0.74
1:B:585:LEU:CG	1:B:586:MET:HE2	2.18	0.74
1:B:212:THR:CB	1:B:340:ILE:HD13	2.17	0.74
1:A:326:MET:SD	1:A:330:ASP:HB2	2.28	0.74
1:A:300:ASN:N	1:A:300:ASN:ND2	2.36	0.74
1:A:329:ARG:O	1:A:329:ARG:CG	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:821:GLY:CA	2:A:1015:HOH:O	2.37	0.73
1:B:802:ILE:O	1:B:802:ILE:CG2	2.35	0.73
1:B:228:ILE:CG1	1:B:228:ILE:CG2	2.65	0.73
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:610:LEU:CD2	1:A:610:LEU:CB	2.65	0.73
1:B:204:PHE:HB3	1:B:340:ILE:HG13	1.69	0.73
1:A:307:VAL:HA	2:A:909:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:PHE:CZ	1:A:667:CYS:HB2	2.17	0.73
1:A:395:ASP:N	1:A:406:GLY:HA3	2.03	0.73
1:A:731:VAL:HG11	1:A:733:LEU:CD1	2.19	0.73
1:B:106:TRP:CZ3	1:B:107:LEU:CD1	2.72	0.73
1:B:88:ILE:CB	1:B:88:ILE:CD1	2.66	0.73
1:A:517:ILE:HD12	1:A:883:ILE:HG23	1.71	0.72
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: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:808:THR:C	1:A:808:THR:CG2	2.57	0.72
1:A:230:LYS:NZ	1:A:233:GLU:OE1	2.22	0.72
1:B:383:VAL:CG1	1:B:383:VAL:O	2.37	0.72
1:A:602:LEU:CD1	1:A:602:LEU:CD2	2.67	0.72
1:B:438:VAL:HG22	1:B:484:ILE:HD11	1.71	0.72
1:B:27:TYR:CE2	1:B:28:LEU:HD12	2.25	0.72
1:A:158:LEU:O	1:A:160:THR:HG23	1.90	0.72
1:B:556:GLN:O	1:B:557:THR:C	2.29	0.72
1:B:670:ARG:O	1:B:674:LEU:CD2	2.37	0.71
1:B:330:ASP:O	1:B:330:ASP:OD1	2.08	0.71
1:B:729:LEU:HG	1:B:729:LEU:CD2	2.12	0.71
1:B:120:ILE:CG2	1:B:120:ILE:CA	2.65	0.71
1:B:521:LEU:HD11	1:B:638:PHE:CZ	2.26	0.71
1:B:447:VAL:CB	1:B:513:LEU:CD1	2.69	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:HG	1:A:610:LEU:CD2	2.13	0.71
1:A:89:VAL:H	1:A:175:GLU:CD	1.93	0.71
1:B:874:ASN:O	1:B:876:THR:N	2.24	0.71
1:A:883:ILE:CG1	1:A:883:ILE:CG2	2.66	0.71
1:A:519:ALA:HB2	1:A:675:PHE:CZ	2.24	0.71
1:B:339:GLU:OE2	1:B:339:GLU:N	2.22	0.71
1:B:836:SER:OG	2:B:953:HOH:O	2.07	0.71
1:A:97:ILE:HD13	1:A:108:LEU:HD12	1.72	0.71
1:B:778:SER:C	1:B:779:ASP:OD1	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:810:ARG:O	1:B:811:SER:HB2	1.91	0.71
1:A:599:PHE:C	1:A:599:PHE:CD2	2.64	0.71
1:A:611:THR:O	1:A:611:THR:CG2	2.38	0.71
1:B:238:LEU:HD12	1:B:238:LEU:N	2.06	0.71
1:B:607:ARG:O	1:B:610:LEU:HG	1.91	0.70
1:A:31:ASP:OD2	1:A:32:TYR:N	2.24	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:HG13	1:A:242:ILE:O	1.90	0.70
1:A:199:CYS:SG	1:A:202:GLU:HG3	2.31	0.70
1:B:784:LEU:HD12	1:B:784:LEU:N	2.07	0.70
1:A:860:ARG:HD2	2:A:1023:HOH:O	1.90	0.70
1:A:105:SER:O	1:A:106:TRP:C	2.28	0.70
1:A:30:GLN:HE22	1:A:187:LYS:HZ3	1.38	0.70
1:B:661:PHE:O	1:B:665:VAL:HG13	1.92	0.70
1:A:808:THR:CA	1:A:808:THR:CG2	2.70	0.70
1:A:428:MET:CE	2:A:970:HOH:O	2.38	0.70
1:B:525:LYS:HB3	1:B:525:LYS:HZ3	1.57	0.70
1:B:874:ASN:O	1:B:875:GLY:C	2.30	0.70
1:B:146:PHE:HB3	1:B:416:LYS:HG2	1.72	0.70
1:B:697:LEU:HA	1:B:700:SER:OG	1.92	0.70
1:A:290:GLU:CD	1:A:290:GLU:H	1.92	0.70
1:A:157:LEU:C	1:A:158:LEU:HG	2.11	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:740:VAL:HG12	1:B:741:SER:N	2.06	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:256:LYS:HB3	1:B:256:LYS:HZ2	1.57	0.69
1:B:296:PRO:HD2	2:B:912:HOH:O	1.91	0.69
1:A:833:HIS:CD2	1:A:833:HIS:C	2.64	0.69
1:B:430:THR:O	1:B:489:THR:HA	1.92	0.69
1:A:467:ILE:HG22	1:A:468:ASN:H	1.56	0.69
1:B:376:ASN:C	1:B:378:PRO:HD3	2.12	0.69
1:B:605:ARG:HG2	1:B:605:ARG:HH21	1.56	0.69
1:B:537:LYS:CB	1:B:537:LYS:CD	2.69	0.69
1:A:364:THR:HG22	1:A:497:ASP:OD1	1.92	0.69
1:B:656:GLU:OE2	1:B:656:GLU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:PRO:HB3	2:A:962:HOH:O	1.92	0.69
1:B:389:ILE:HG23	1:B:510:THR:HG22	1.74	0.69
1:A:30:GLN:HE22	1:A:187:LYS:HZ1	1.37	0.69
1:B:86:GLN:CG	1:B:89:VAL:HG21	2.21	0.69
1:A:451:ARG:HH11	1:A:451:ARG:HG2	1.57	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:B:256:LYS:CG	1:B:256:LYS:CA	2.70	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:A:688:THR:CA	1:A:688:THR:CG2	2.68	0.69
1:B:337:LYS:NZ	1:B:337:LYS:CB	1.90	0.69
1:A:551:SER:C	1:A:552:VAL:O	2.32	0.69
1:A:329:ARG:HH21	1:A:329:ARG:CG	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:HA	1:B:172:GLN:OE1	1.93	0.68
1:A:320:GLU:N	1:A:320:GLU:CB	2.54	0.68
1:B:62:GLU:HB3	1:B:193:GLU:OE1	1.92	0.68
1:A:373:GLY:O	1:A:384:ASN:ND2	2.26	0.68
1:B:376:ASN:O	1:B:378:PRO:HD3	1.93	0.68
1:A:780:THR:HG22	1:A:780:THR:O	1.93	0.68
1:A:692:ASP:OD1	1:A:692:ASP:C	2.32	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:656:GLU:C	1:B:657:LEU:HG	2.14	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:477:ARG:CD	1:A:477:ARG:CB	2.70	0.67
1:A:13:GLU:CA	1:A:13:GLU:OE1	2.41	0.67
1:B:802:ILE:O	1:B:802:ILE:HG22	1.94	0.67
1:B:270:LYS:O	1:B:281:LEU:HB2	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:MET:SD	1:B:606:ILE:HD11	2.33	0.67
1:B:106:TRP:HZ3	1:B:107:LEU:HD12	1.59	0.67
1:B:341:CYS:CA	1:B:341:CYS:SG	2.82	0.67
1:A:413:LEU:CB	1:A:413:LEU:CD1	2.72	0.67
1:B:777:ASP:CB	1:B:777:ASP:C	2.63	0.67
1:A:32:TYR:HE1	1:A:138:ILE:O	1.77	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:47:GLN:HA	1:A:47:GLN:OE1	1.95	0.67
1:B:343:LEU:HB2	1:B:345:PRO:HD2	1.75	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:A:185:TYR:OH	1:A:206:ASP:OD2	2.11	0.67
1:B:23:ARG:NH1	1:B:23:ARG:HG2	2.10	0.67
1:B:332:ILE:CG2	1:B:332:ILE:C	2.63	0.67
1:A:832:GLN:HA	1:A:832:GLN:OE1	1.95	0.67
1:B:212:THR:OG1	1:B:340:ILE:HD13	1.95	0.67
1:B:97:ILE:HD11	1:B:108:LEU:HD12	1.77	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:25:ILE:HG22	1:B:26:LYS:N	2.10	0.66
1:A:440:ARG:HG2	1:A:441:GLU:N	2.09	0.66
1:A:219:LYS:HA	1:A:219:LYS:CD	2.26	0.66
1:B:295:GLY:CA	1:B:298:SER:O	2.37	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:350:SER:O	1:A:352:THR:HG22	1.93	0.66
1:B:51:PHE:CE1	1:B:187:LYS:HA	2.30	0.66
1:A:514:ASP:OD1	1:A:515:ASP:N	2.28	0.66
1:B:98:CYS:SG	1:B:169:HIS:NE2	2.69	0.66
1:A:293:TRP:CZ2	2:A:1024:HOH:O	2.46	0.66
1:A:748:ILE:HG23	1:A:749:LEU:CD2	2.25	0.66
1:A:213:GLU:OE1	1:A:475:ARG:NH2	2.28	0.66
1:B:792:LEU:HG	1:B:792:LEU:O	1.95	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:A:551:SER:O	1:A:552:VAL:O	2.13	0.66
1:A:273:THR:H	1:A:312:ARG:HH21	1.42	0.66
1:A:335:PHE:C	1:A:335:PHE:CD1	2.69	0.66
1:A:620:LYS:HE2	2:A:1022:HOH:O	1.94	0.66
1:B:284:MET:SD	1:B:284:MET:CB	2.82	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:CYS:SG	1:B:169:HIS:CE1	2.89	0.66
1:A:628:GLU:OE1	1:A:631:MET:SD	2.54	0.66
1:B:411:LEU:HD13	1:B:502:PHE:CE1	2.31	0.66
1:A:855:ILE:CG2	1:A:855:ILE:O	2.42	0.66
1:A:333:ARG:CB	1:A:333:ARG:CD	2.73	0.66
1:A:205:GLU:OE1	1:A:471:GLU:OE2	2.13	0.66
1:B:291:VAL:HG23	1:B:292:GLU:N	2.11	0.66
1:B:284:MET:O	1:B:323:GLU:OE2	2.13	0.66
1:B:283:ARG:HH21	1:B:325:TRP:HE1	1.44	0.66
1:B:613:PHE:CE1	1:B:624:MET:HG2	2.30	0.65
1:B:237:LEU:N	1:B:237:LEU:HD23	2.11	0.65
1:A:219:LYS:HA	1:A:219:LYS:HD3	1.78	0.65
1:B:429:GLU:C	1:B:468:ASN:HD22	1.99	0.65
1:A:514:ASP:OD2	1:A:642:CYS:N	2.24	0.65
1:B:883:ILE:HG22	2:B:929:HOH:O	1.95	0.65
1:B:365:TRP:O	1:B:495:GLU:HA	1.97	0.65
1:A:330:ASP:OD2	2:A:921:HOH:O	2.14	0.65
1:B:27:TYR:CD2	1:B:28:LEU:HD12	2.31	0.65
1:A:135:TYR:CG	1:A:136:ALA:N	2.62	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:403:ARG:HG2	1:A:477:ARG:CZ	2.27	0.65
1:A:51:PHE:CG	1:A:187:LYS:HG3	2.32	0.65
1:B:701:VAL:HG13	1:B:860:ARG:CG	2.26	0.65
1:B:223:ASP:OD2	1:B:223:ASP:C	2.29	0.65
1:B:712:TYR:O	1:B:713:SER:O	2.15	0.65
1:A:301:SER:O	1:A:302:TYR:C	2.36	0.65
1:B:256:LYS:HZ3	1:B:256:LYS:HB3	1.61	0.64
1:A:59:GLY:HA3	1:A:193:GLU:CD	2.18	0.64
1:B:862:ASP:OD1	1:B:866:ARG:NE	2.31	0.64
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:A:669:VAL:CA	1:A:669:VAL:CG1	2.73	0.64
1:A:229:LEU:O	1:A:231:ALA:N	2.29	0.64
1:A:731:VAL:HG23	1:A:733:LEU:N	2.11	0.64
1:A:430:THR:HA	1:A:467:ILE:O	1.97	0.64
1:A:573:GLY:O	1:A:574:PHE:O	2.16	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:358:THR:O	1:A:359:THR:CG2	2.45	0.64
1:A:329:ARG:HG3	1:A:329:ARG:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ILE:HG12	1:A:337:LYS:HZ3	1.61	0.64
1:A:689:ILE:HD12	1:A:690:GLN:N	2.13	0.64
1:A:599:PHE:HD2	1:A:599:PHE:O	1.80	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:A:86:GLN:HB3	1:A:89:VAL:CG2	2.28	0.64
1:A:337:LYS:CD	1:A:337:LYS:NZ	2.59	0.64
1:B:839:ILE:HD12	1:B:840:ARG:CB	2.28	0.64
1:B:429:GLU:C	1:B:468:ASN:HB2	2.17	0.64
1:A:13:GLU:O	1:A:16:GLU:CG	2.44	0.64
1:B:343:LEU:HD22	2:B:990:HOH:O	1.96	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:A:256:LYS:HD3	1:A:258:LEU:CD1	2.22	0.64
1:A:83:SER:O	1:A:84:ASN:HB3	1.96	0.64
1:B:296:PRO:CD	2:B:912:HOH:O	2.46	0.64
1:A:27:TYR:CD2	1:A:28:LEU:HG	2.32	0.64
1:B:440:ARG:NH2	1:B:440:ARG:CG	2.59	0.64
1:A:389:ILE:HD11	1:A:502:PHE:HE2	1.62	0.64
1:B:795:ASN:O	1:B:799:TRP:HB2	1.98	0.64
1:A:314:GLN:HG3	1:A:315:LEU:H	1.63	0.64
1:A:520:ASN:OD1	1:A:520:ASN:N	2.28	0.64
1:A:435:VAL:CG1	1:A:461:ALA:HB3	2.28	0.64
1:A:772:MET:CG	1:A:772:MET:CA	2.71	0.64
1:A:428:MET:HB2	2:A:910:HOH:O	1.97	0.64
1:B:464:GLU:HG2	1:B:464:GLU:O	1.98	0.64
1:B:328:PHE:CE2	1:B:331:PHE:CZ	2.86	0.63
1:A:499:LEU:HB3	2:A:901:HOH:O	1.98	0.63
1:A:358:THR:HG22	1:A:359:THR:H	1.63	0.63
1:B:195:LEU:O	1:B:195:LEU:HD22	1.97	0.63
1:A:74:LYS:O	1:A:160:THR:OG1	2.07	0.63
1:A:272:VAL:HA	1:A:312:ARG:HD2	1.78	0.63
1:B:328:PHE:O	1:B:331:PHE:HE2	1.82	0.63
1:A:731:VAL:HG21	1:A:733:LEU:HD12	0.70	0.63
1:A:365:TRP:CE2	1:A:488:SER:HA	2.33	0.63
1:A:656:GLU:N	1:A:656:GLU:OE1	2.31	0.63
1:B:335:PHE:CG	1:B:335:PHE:CA	2.78	0.63
1:B:610:LEU:CD1	1:B:610:LEU:HG	2.19	0.63
1:A:258:LEU:H	1:A:258:LEU:HD13	1.63	0.63
1:A:177:TRP:CD2	1:A:178:SER:N	2.67	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:GLU:OE2	1:B:304:TRP:N	2.32	0.63
1:A:94:ARG:CD	2:A:1049:HOH:O	2.46	0.63
1:A:87:PHE:CD2	1:A:88:ILE:HG22	2.33	0.63
1:A:51:PHE:N	1:A:52:PRO:HD3	2.14	0.63
1:A:669:VAL:CG2	1:A:669:VAL:CG1	2.72	0.63
1:A:665:VAL:O	1:A:666:ARG:C	2.34	0.62
1:B:25:ILE:HD13	1:B:148:GLU:OE1	1.99	0.62
1:A:388:LYS:NZ	1:A:482:GLU:OE1	2.32	0.62
1:B:69:LYS:CA	1:B:69:LYS:CG	2.76	0.62
1:B:27:TYR:CE2	1:B:28:LEU:CD1	2.82	0.62
1:B:701:VAL:HG11	1:B:860:ARG:HG2	1.81	0.62
1:B:427:ASP:HB3	2:B:1003:HOH:O	1.97	0.62
1:B:74:LYS:HA	2:B:1000:HOH:O	1.98	0.62
1:B:597:VAL:O	1:B:600:ASN:HB3	1.99	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: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:874:ASN:O	1:A:876:THR:N	2.32	0.62
1:B:651:ARG:NH1	1:B:670:ARG:CZ	2.58	0.62
1:A:403:ARG:HG2	1:A:477:ARG:NE	2.14	0.62
1:A:216:ASP:HB3	1:A:219:LYS:HB3	1.80	0.62
1:B:103:GLY:HA3	2:B:903:HOH:O	2.00	0.62
1:B:724:ARG:HH21	1:B:724:ARG:CB	2.10	0.62
1:A:328:PHE:CZ	1:A:331:PHE:HZ	2.18	0.62
1:A:582:MET:CE	1:A:582:MET:CG	2.78	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:855:ILE:HG22	1:A:855:ILE:O	1.99	0.62
1:A:87:PHE:HD2	1:A:88:ILE:HG22	1.64	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:448:HIS:CD2	1:A:630:ARG:NH2	2.67	0.62
1:B:616:PHE:CE1	1:B:628:GLU:HB3	2.35	0.62
1:A:328:PHE:CZ	1:A:331:PHE:CZ	2.87	0.62
1:B:786:PHE:N	1:B:786:PHE:CB	2.56	0.62
1:A:826:ALA:CB	1:A:826:ALA:C	2.63	0.62
1:A:773:VAL:CG2	1:A:773:VAL:CG1	2.74	0.62
1:A:63:LEU:CD1	1:A:70:THR:CG2	2.67	0.62
1:A:242:ILE:O	1:A:242:ILE:CG1	2.48	0.62
1:B:337:LYS:HB3	1:B:337:LYS:HZ2	0.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:ARG:CD	1:B:440:ARG:CB	2.77	0.62
1:A:82:LEU:O	1:A:84:ASN:N	2.32	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:A:75:TRP:CG	1:A:75:TRP:CA	2.80	0.62
1:A:7:LYS:CG	1:A:7:LYS:CE	2.76	0.62
1:A:833:HIS:HD2	1:A:833:HIS:C	2.03	0.62
1:B:883:ILE:C	1:B:883:ILE:CB	2.63	0.62
1:A:553:LYS:O	1:A:554:GLU:HB2	1.99	0.62
1:B:778:SER:O	1:B:779:ASP:OD1	2.17	0.61
1:B:740:VAL:CA	1:B:740:VAL:CG1	2.76	0.61
1:A:759:LEU:CD1	1:A:812:GLY:O	2.48	0.61
1:A:307:VAL:O	1:A:308:ASP:HB2	1.98	0.61
1:A:199:CYS:HB3	1:A:202:GLU:HG3	1.83	0.61
1:B:88:ILE:CD1	1:B:121:LEU:HD21	2.30	0.61
1:B:677:ILE:CB	1:B:677:ILE:CD1	2.73	0.61
1:A:629:MET:O	1:A:630:ARG:C	2.38	0.61
1:B:649:VAL:O	1:B:650:ALA:C	2.37	0.61
1:A:701:VAL:O	1:A:701:VAL:HG13	2.00	0.61
1:A:35:LEU:O	1:A:36:ARG:C	2.36	0.61
1:B:49:PRO:CG	2:B:935:HOH:O	2.46	0.61
1:A:772:MET:CB	1:A:772:MET:SD	2.87	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: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:161:LYS:O	1:B:162:ASP:C	2.36	0.61
1:B:861:LEU:O	1:B:862:ASP:O	2.19	0.61
1:A:739:GLU:O	1:A:739:GLU:CD	2.38	0.61
1:B:519:ALA:HB2	1:B:675:PHE:CE2	2.36	0.61
1:A:451:ARG:NH1	1:A:451:ARG:HG2	2.16	0.61
1:A:680:GLN:O	1:A:682:ASP:N	2.33	0.61
1:B:883:ILE:N	1:B:883:ILE:CB	2.62	0.61
1:A:228:ILE:O	1:A:229:LEU:O	2.19	0.61
1:B:60:PHE:CE2	1:B:193:GLU:HG2	2.36	0.61
1:A:140:HIS:HB3	1:A:153:VAL:HG23	1.83	0.61
1:B:579:CYS:HA	1:B:579:CYS:CB	2.17	0.61
1:A:746:MET:O	1:A:746:MET:HG2	2.01	0.61
1:B:798:LYS:O	1:B:802:ILE:HG13	2.00	0.61
1:B:434:ALA:HA	1:B:462:GLN:HB3	1.83	0.61
1:B:89:VAL:O	1:B:89:VAL:CB	2.44	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:SER:HB3	1:A:329:ARG:HH11	1.66	0.60
1:B:668:LEU:CD2	1:B:668:LEU:CB	2.72	0.60
1:A:672:GLU:HA	1:A:672:GLU:OE2	1.99	0.60
1:B:853:ASN:O	1:B:857:CYS:N	2.31	0.60
1:B:8:LEU:CB	1:B:8:LEU:CD2	2.76	0.60
1:A:155:ASP:OD2	1:A:156:ASP:N	2.32	0.60
1:A:193:GLU:C	1:A:195:LEU:H	2.05	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:723:GLU:C	1:B:726:PHE:HD2	2.04	0.60
1:A:731:VAL:CB	1:A:733:LEU:CD1	2.79	0.60
1:A:860:ARG:NH1	1:A:860:ARG:CB	2.63	0.60
1:B:358:THR:O	1:B:359:THR:HG23	2.02	0.60
1:A:549:GLU:O	1:A:595:GLY:HA2	2.01	0.60
1:B:574:PHE:CE1	1:B:661:PHE:HE1	2.20	0.60
1:A:602:LEU:O	1:A:605:ARG:HB2	2.02	0.60
1:B:225:TYR:CE1	1:B:280:ASN:ND2	2.69	0.60
1:A:297:TRP:CD1	1:A:297:TRP:O	2.55	0.60
1:B:277:GLN:HA	1:B:277:GLN:HE21	1.66	0.60
1:A:94:ARG:HD2	2:A:1049:HOH:O	2.01	0.60
1:B:582:MET:SD	1:B:602:LEU:HD21	2.42	0.60
1:B:493:ASN:N	1:B:493:ASN:HD22	2.00	0.60
1:A:494:LYS:NZ	1:A:494:LYS:CD	2.60	0.60
1:B:866:ARG:HH11	1:B:866:ARG:HG3	1.67	0.60
1:A:413:LEU:CD2	1:A:413:LEU:CD1	2.73	0.60
1:B:457:ASN:HD22	1:B:457:ASN:N	1.93	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:A:759:LEU:HD12	1:A:812:GLY:HA2	1.84	0.59
1:A:365:TRP:O	1:A:495:GLU:HA	2.02	0.59
1:A:122:HIS:CD2	1:A:127:TYR:CE2	2.90	0.59
1:A:26:LYS:O	1:A:27:TYR:C	2.40	0.59
1:B:701:VAL:CG1	1:B:860:ARG:CG	2.80	0.59
1:A:290:GLU:N	1:A:290:GLU:CD	2.55	0.59
1:A:270:LYS:CD	1:A:270:LYS:NZ	2.63	0.59
1:B:670:ARG:HA	1:B:673:ILE:CD1	2.27	0.59
1:B:524:GLU:CD	1:B:524:GLU:N	2.53	0.59
1:A:100:GLY:HA2	1:A:167:PHE:HA	1.85	0.59
1:A:273:THR:N	1:A:312:ARG:HH21	1.99	0.59
1:B:585:LEU:HD11	1:B:672:GLU:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:O	1:A:228:ILE:HG13	2.02	0.59
1:B:212:THR:OG1	1:B:340:ILE:CD1	2.51	0.59
1:A:692:ASP:OD1	1:A:694:ILE:N	2.35	0.59
1:A:240:CYS:O	1:A:263:ALA:O	2.20	0.59
1:B:369:SER:O	1:B:383:VAL:HG13	2.01	0.59
1:B:4:ILE:O	1:B:6:MET:N	2.36	0.59
1:A:122:HIS:CA	1:A:125:VAL:O	2.50	0.59
1:B:656:GLU:O	1:B:657:LEU:HG	2.03	0.59
1:B:415:GLN:HE22	1:B:428:MET:HB3	1.68	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:B:242:ILE:HG23	1:B:242:ILE:O	2.02	0.59
1:A:360:PHE:HB2	1:A:499:LEU:HD11	1.83	0.59
1:A:23:ARG:HH11	1:A:23:ARG:HG2	1.68	0.59
1:B:506:LYS:O	1:B:507:LYS:C	2.32	0.59
1:A:824:GLU:N	1:A:828:PHE:O	2.36	0.58
1:A:228:ILE:O	1:A:232:LEU:CD2	2.47	0.58
1:B:140:HIS:HD2	1:B:151:ASP:OD1	1.85	0.58
1:A:864:MET:CB	1:A:864:MET:C	2.69	0.58
1:A:221:PRO:C	1:A:223:ASP:H	2.05	0.58
1:B:670:ARG:CA	1:B:673:ILE:HD12	2.25	0.58
1:B:226:GLN:HG3	2:B:955:HOH:O	2.02	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: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:A:340:ILE:CG1	1:A:340:ILE:CG2	2.79	0.58
1:B:740:VAL:CG1	1:B:740:VAL:HB	2.16	0.58
1:A:499:LEU:HG	1:A:501:ARG:HD2	1.85	0.58
1:A:487:PRO:O	1:A:488:SER:HB3	2.02	0.58
1:B:766:ILE:O	1:B:769:CYS:N	2.34	0.58
1:B:296:PRO:HG2	1:B:304:TRP:CG	2.38	0.58
1:A:263:ALA:CB	1:A:288:TRP:HZ3	2.17	0.58
1:A:196:SER:O	1:A:197:GLY:C	2.42	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:A:306:LYS:O	1:A:307:VAL:O	2.22	0.58
1:B:574:PHE:HE1	1:B:661:PHE:CE1	2.22	0.58
1:B:867:ALA:O	1:B:869:ARG:N	2.37	0.58
1:B:658:ILE:HG23	1:B:658:ILE:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:LYS:HZ3	1:B:525:LYS:CB	2.14	0.58
1:A:17:GLY:O	1:A:18:LEU:C	2.34	0.58
1:B:48:ASP:HB2	1:B:155:ASP:OD1	2.04	0.58
1:B:274:TYR:O	1:B:275:GLN:C	2.40	0.58
1:B:855:ILE:CB	2:B:974:HOH:O	2.51	0.58
1:A:309:PRO:O	1:A:311:GLU:N	2.36	0.58
1:B:335:PHE:CB	1:B:335:PHE:C	2.70	0.58
1:B:694:ILE:HB	1:B:694:ILE:CA	2.18	0.58
1:A:233:GLU:O	1:A:353:LEU:CB	2.52	0.58
1:B:831:ASN:O	1:B:833:HIS:C	2.42	0.58
1:B:46:PHE:CD2	1:B:138:ILE:HD12	2.39	0.58
1:A:317:VAL:CB	1:A:317:VAL:C	2.69	0.57
1:B:694:ILE:CG1	1:B:694:ILE:CA	2.78	0.57
1:B:484:ILE:HD12	1:B:513:LEU:HD22	1.85	0.57
1:A:316:ARG:CB	2:A:1007:HOH:O	2.52	0.57
1:B:668:LEU:CD2	1:B:668:LEU:CD1	2.79	0.57
1:B:330:ASP:C	1:B:332:ILE:H	2.06	0.57
1:A:428:MET:CB	2:A:910:HOH:O	2.52	0.57
1:B:66:ASN:HD22	1:B:66:ASN:N	2.00	0.57
1:A:464:GLU:O	1:A:465:HIS:O	2.22	0.57
1:B:460:ARG:O	1:B:461:ALA:HB2	2.03	0.57
1:A:237:LEU:C	1:A:238:LEU:HD12	2.25	0.57
1:B:806:PHE:O	1:B:807:GLU:HB3	2.04	0.57
1:B:328:PHE:O	1:B:328:PHE:CG	2.56	0.57
1:A:183:LYS:O	1:A:187:LYS:HB2	2.05	0.57
1:B:316:ARG:O	1:B:317:VAL:C	2.42	0.57
1:B:523:ASP:O	1:B:524:GLU:C	2.41	0.57
1:B:197:GLY:O	1:B:198:GLY:C	2.43	0.57
1:A:305:ASN:C	1:A:305:ASN:HD22	2.06	0.57
1:B:537:LYS:HB2	1:B:537:LYS:NZ	2.09	0.57
1:A:651:ARG:C	1:A:651:ARG:HH11	2.08	0.57
1:B:376:ASN:N	1:B:376:ASN:OD1	2.22	0.57
1:B:69:LYS:HZ3	1:B:69:LYS:CB	1.95	0.57
1:B:537:LYS:CB	1:B:537:LYS:HZ2	2.07	0.57
1:A:219:LYS:CD	1:A:219:LYS:CB	2.78	0.57
1:B:624:MET:O	1:B:658:ILE:HG13	2.05	0.57
1:B:388:LYS:NZ	1:B:482:GLU:HB3	2.19	0.57
1:B:797:LYS:O	1:B:800:GLN:HB3	2.04	0.57
1:B:200:THR:HG23	1:B:201:SER:N	2.19	0.57
1:B:323:GLU:CA	1:B:323:GLU:OE2	2.47	0.57
1:B:21:HIS:CD2	1:B:142:GLN:HE22	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ILE:CG2	1:B:332:ILE:CA	2.79	0.57
1:A:327:SER:OG	1:A:329:ARG:CZ	2.53	0.57
1:A:230:LYS:HE3	1:A:505:GLU:CD	2.25	0.57
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:A:860:ARG:CZ	1:A:860:ARG:HB3	2.35	0.57
1:A:291:VAL:CG2	1:A:292:GLU:N	2.67	0.57
1:A:238:LEU:CD1	1:A:238:LEU:N	2.68	0.56
1:B:519:ALA:HB2	1:B:675:PHE:CD2	2.40	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:678:PHE:HD2	1:B:886:TRP:CD1	2.23	0.56
1:B:789:PHE:C	1:B:789:PHE:CD2	2.79	0.56
1:B:8:LEU:CD1	1:B:885:GLU:HB3	2.35	0.56
1:B:8:LEU:HD13	1:B:885:GLU:CG	2.34	0.56
1:A:307:VAL:HG12	2:A:909:HOH:O	2.05	0.56
1:A:305:ASN:H	1:A:305:ASN:ND2	2.03	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:835:TYR:O	1:B:837:MET:N	2.38	0.56
1:B:383:VAL:HG12	1:B:383:VAL:O	2.05	0.56
1:B:810:ARG:O	1:B:811:SER:CB	2.52	0.56
1:B:601:ILE:HD13	1:B:604:ASN:CG	2.24	0.56
1:A:740:VAL:O	1:A:783:LYS:HA	2.06	0.56
1:B:807:GLU:HG3	1:B:808:THR:N	2.19	0.56
1:A:256:LYS:HA	1:A:258:LEU:CD1	2.35	0.56
1:B:238:LEU:CD1	1:B:238:LEU:N	2.69	0.56
1:A:435:VAL:HG11	1:A:461:ALA:HB3	1.87	0.56
1:B:313:GLU:HA	1:B:315:LEU:HD12	1.87	0.56
1:A:366:ARG:O	1:A:367:ARG:C	2.39	0.56
1:B:582:MET:CG	1:B:582:MET:CE	2.83	0.56
1:A:602:LEU:O	1:A:603:TRP:C	2.43	0.56
1:A:278:ARG:CG	1:A:279:VAL:H	2.18	0.56
1:A:296:PRO:O	1:A:297:TRP:CB	2.48	0.56
1:B:672:GLU:O	1:B:673:ILE:C	2.44	0.56
1:B:521:LEU:CD2	1:B:636:ALA:O	2.54	0.56
1:A:388:LYS:NZ	1:A:482:GLU:CD	2.57	0.56
1:A:414:MET:CG	1:A:414:MET:CE	2.81	0.56
1:B:96:ASP:OD2	1:B:170:SER:OG	2.11	0.56
1:B:88:ILE:O	1:B:88:ILE:CG2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:MET:O	1:B:658:ILE:CG1	2.53	0.56
1:A:484:ILE:CD1	1:A:486:VAL:HG23	2.36	0.56
1:A:462:GLN:O	1:A:463:SER:C	2.43	0.56
1:A:698:SER:O	1:A:700:SER:N	2.38	0.56
1:B:97:ILE:CD1	1:B:108:LEU:HD11	2.35	0.56
1:B:780:THR:HA	1:B:892:TYR:CZ	2.41	0.56
1:B:690:GLN:CG	1:B:690:GLN:CA	2.80	0.56
1:B:867:ALA:C	1:B:869:ARG:N	2.55	0.56
1:A:435:VAL:HG13	1:A:460:ARG:O	2.05	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:B:120:ILE:CG2	1:B:120:ILE:C	2.74	0.56
1:A:450:LYS:HE3	1:A:631:MET:HG2	1.87	0.56
1:A:758:ASP:O	1:A:759:LEU:C	2.43	0.56
1:B:389:ILE:HD13	1:B:483:TYR:HB2	1.87	0.56
1:B:605:ARG:CZ	1:B:672:GLU:OE2	2.55	0.55
1:A:808:THR:C	1:A:808:THR:HG23	2.23	0.55
1:B:135:TYR:O	1:B:136:ALA:CA	2.54	0.55
1:B:868:PHE:CE2	1:B:879:ILE:HG12	2.41	0.55
1:B:555:LEU:O	1:B:556:GLN:O	2.23	0.55
1:A:655:ASP:C	1:A:656:GLU:OE1	2.45	0.55
1:A:177:TRP:CG	1:A:178:SER:N	2.74	0.55
1:B:696:TRP:O	1:B:700:SER:OG	2.23	0.55
1:B:395:ASP:O	1:B:396:ASP:C	2.44	0.55
1:A:610:LEU:HD22	1:A:610:LEU:HA	1.88	0.55
1:A:624:MET:HB3	1:A:659:ILE:O	2.06	0.55
1:A:278:ARG:NH2	2:A:929:HOH:O	2.38	0.55
1:B:87:PHE:CE1	1:B:180:LEU:HD12	2.40	0.55
1:A:800:GLN:HG3	1:A:851:PHE:HE1	1.70	0.55
1:A:204:PHE:HE2	1:A:237:LEU:HD12	1.71	0.55
1:B:669:VAL:CB	1:B:669:VAL:C	2.71	0.55
1:B:361:TYR:O	1:B:500:LEU:N	2.39	0.55
1:A:380:THR:O	1:A:381:PHE:C	2.41	0.55
1:B:426:ARG:HG2	2:B:1029:HOH:O	2.05	0.55
1:B:370:THR:HA	1:B:383:VAL:HG12	1.87	0.55
1:A:520:ASN:C	1:A:521:LEU:HG	2.27	0.55
1:B:723:GLU:O	1:B:726:PHE:HD2	1.89	0.55
1:A:349:LYS:HA	2:A:1006:HOH:O	2.06	0.55
1:B:787:GLU:C	1:B:789:PHE:H	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:667:CYS:O	1:B:668:LEU:O	2.24	0.55
1:A:757:PRO:O	1:A:758:ASP:CB	2.55	0.55
1:B:701:VAL:CG1	1:B:860:ARG:HD3	2.37	0.55
1:B:507:LYS:HD2	1:B:507:LYS:H	1.72	0.55
1:A:773:VAL:CG1	1:A:773:VAL:CA	2.76	0.55
1:B:493:ASN:ND2	1:B:493:ASN:N	2.55	0.55
1:A:680:GLN:C	1:A:682:ASP:H	2.10	0.55
1:B:795:ASN:O	1:B:799:TRP:CB	2.55	0.55
1:A:655:ASP:CB	1:A:656:GLU:OE1	2.55	0.55
1:A:591:ASN:ND2	1:A:592:GLY:H	2.05	0.55
1:B:274:TYR:CE2	1:B:275:GLN:HG3	2.41	0.55
1:A:332:ILE:CA	1:A:332:ILE:CG1	2.80	0.55
1:A:204:PHE:CE2	1:A:237:LEU:HD12	2.41	0.55
1:A:340:ILE:HB	1:A:340:ILE:CG2	2.18	0.55
1:B:447:VAL:CB	1:B:513:LEU:HD12	2.36	0.55
1:B:168:VAL:HB	1:B:182:GLU:OE2	2.07	0.55
1:A:872:ASP:O	1:A:872:ASP:CG	2.44	0.55
1:B:0:GLU:CB	1:B:0:GLU:C	2.68	0.54
1:A:785:GLY:HA3	1:A:788:GLU:OE1	2.07	0.54
1:A:583:VAL:C	1:A:583:VAL:CB	2.66	0.54
1:B:258:LEU:O	1:B:259:VAL:HG22	2.08	0.54
1:A:254:THR:HG23	1:A:255:PHE:H	1.72	0.54
1:A:880:GLN:C	1:A:881:VAL:HG22	2.28	0.54
1:A:370:THR:HA	1:A:383:VAL:O	2.06	0.54
1:B:273:THR:H	1:B:311:GLU:HG2	1.72	0.54
1:A:613:PHE:CZ	1:A:622:GLY:O	2.61	0.54
1:A:776:MET:HE1	1:A:791:TYR:CD2	2.42	0.54
1:B:212:THR:CB	1:B:340:ILE:CD1	2.85	0.54
1:B:775:VAL:HG12	1:B:893:SER:HB2	1.89	0.54
1:A:428:MET:HE2	2:A:970:HOH:O	2.04	0.54
1:B:102:LEU:HD22	1:B:161:LYS:HE2	1.90	0.54
1:B:867:ALA:O	1:B:868:PHE:C	2.44	0.54
1:B:28:LEU:C	1:B:30:GLN:H	2.09	0.54
1:B:872:ASP:O	1:B:873:LYS:C	2.45	0.54
1:A:366:ARG:NE	1:A:366:ARG:CG	2.64	0.54
1:B:583:VAL:O	1:B:584:ASN:CB	2.53	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:A:227:ILE:CB	1:A:227:ILE:CD1	2.79	0.54
1:A:290:GLU:N	1:A:290:GLU:OE2	2.33	0.54
1:A:683:PRO:O	1:A:685:ASN:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:VAL:CG1	1:A:733:LEU:CD1	2.82	0.54
1:A:358:THR:CG2	1:A:359:THR:N	2.67	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:CG2	1:B:89:VAL:CA	2.81	0.54
1:A:193:GLU:C	1:A:195:LEU:N	2.58	0.54
1:B:521:LEU:HD22	1:B:636:ALA:O	2.08	0.54
1:A:4:ILE:CD1	1:A:4:ILE:C	2.74	0.54
1:B:712:TYR:CA	2:B:956:HOH:O	2.56	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:135:TYR:O	1:B:136:ALA:CB	2.56	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:A:3:GLY:HA2	1:A:777:ASP:O	2.08	0.54
1:B:502:PHE:CG	1:B:510:THR:HG21	2.43	0.54
1:A:745:LEU:HD12	1:A:749:LEU:CD2	2.37	0.54
1:A:758:ASP:O	1:A:759:LEU:HB3	2.08	0.54
1:A:13:GLU:HA	1:A:16:GLU:CG	2.37	0.54
1:A:386:GLN:CB	1:A:513:LEU:HB3	2.36	0.54
1:B:146:PHE:HA	1:B:414:MET:HE2	1.90	0.54
1:A:273:THR:N	1:A:312:ARG:HD2	2.22	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:A:115:THR:CG2	1:A:115:THR:CA	2.80	0.54
1:B:524:GLU:CD	1:B:524:GLU:H	2.12	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:B:390:ARG:HD2	1:B:482:GLU:CG	2.38	0.53
1:B:370:THR:HA	1:B:383:VAL:CG1	2.38	0.53
1:B:831:ASN:O	1:B:834:ILE:N	2.40	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: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:604:ASN:O	1:A:605:ARG:C	2.46	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:B:789:PHE:C	1:B:789:PHE:HD2	2.11	0.53
1:A:576:LEU:HA	1:A:579:CYS:HB2	1.90	0.53
1:A:430:THR:HG22	1:A:490:PHE:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:820:PRO:HD2	1:B:822:ALA:HB3	1.90	0.53
1:A:484:ILE:HD13	1:A:486:VAL:HG23	1.89	0.53
1:B:430:THR:H	1:B:494:LYS:NZ	2.06	0.53
1:B:390:ARG:NH1	1:B:390:ARG:CG	2.58	0.53
1:B:438:VAL:HG23	1:B:482:GLU:O	2.09	0.53
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: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:436:TYR:HB2	1:A:484:ILE:CG2	2.39	0.53
1:A:826:ALA:N	1:A:826:ALA:CB	2.66	0.53
1:B:114:LEU:O	1:B:121:LEU:HD12	2.08	0.53
1:A:864:MET:CB	1:A:864:MET:N	2.67	0.53
1:A:677:ILE:CG2	1:A:681:LEU:HD12	2.39	0.53
1:B:213:GLU:O	1:B:339:GLU:OE2	2.26	0.53
1:B:574:PHE:CE1	1:B:661:PHE:CE1	2.96	0.53
1:A:478:LEU:CB	1:A:478:LEU:CD1	2.79	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:A:690:GLN:CG	1:A:690:GLN:O	2.57	0.53
1:A:610:LEU:CD2	1:A:610:LEU:CA	2.87	0.53
1:B:113:SER:C	1:B:115:THR:H	2.11	0.53
1:B:215:TYR:HB2	1:B:337:LYS:HZ1	1.73	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:B:160:THR:OG1	1:B:165:LEU:HD23	2.08	0.53
1:A:633:ILE:HD11	1:A:648:ILE:HD13	1.90	0.53
1:A:571:THR:HG22	1:A:572:ASN:N	2.24	0.53
1:B:124:VAL:O	1:B:126:PRO:HD3	2.08	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:B:440:ARG:N	1:B:440:ARG:HD3	2.24	0.53
1:A:468:ASN:CB	2:A:905:HOH:O	2.29	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:B:186:ALA:O	1:B:187:LYS:C	2.43	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:B:677:ILE:HG22	1:B:681:LEU:HD12	1.91	0.52
1:B:779:ASP:O	1:B:780:THR:C	2.46	0.52
1:A:759:LEU:HD12	1:A:812:GLY:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:GLN:CD	1:A:218:GLN:CB	2.75	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:A:748:ILE:HG23	1:A:749:LEU:N	2.24	0.52
1:A:573:GLY:O	1:A:574:PHE:C	2.45	0.52
1:A:872:ASP:O	1:A:872:ASP:OD2	2.26	0.52
1:A:343:LEU:H	1:A:343:LEU:HD12	1.74	0.52
1:A:356:TRP:HA	1:A:356:TRP:CE3	2.43	0.52
1:A:630:ARG:HG3	1:A:645:HIS:CE1	2.44	0.52
1:A:613:PHE:HZ	1:A:622:GLY:O	1.93	0.52
1:A:660:ASP:O	1:A:664:PHE:HB2	2.09	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:A:853:ASN:ND2	1:A:853:ASN:N	2.52	0.52
1:B:508:ALA:O	1:B:509:GLY:C	2.42	0.52
1:B:384:ASN:HB3	1:B:385:PRO:CD	2.39	0.52
1:B:153:VAL:O	1:B:153:VAL:HG12	2.09	0.52
1:B:540:PHE:O	1:B:540:PHE:CD1	2.62	0.52
1:B:113:SER:C	1:B:115:THR:N	2.63	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:675:PHE:O	1:A:676:LYS:C	2.47	0.52
1:A:124:VAL:HG13	1:A:142:GLN:O	2.10	0.52
1:B:8:LEU:O	1:B:10:LYS:N	2.43	0.52
1:B:258:LEU:O	1:B:259:VAL:CG2	2.58	0.52
1:A:255:PHE:CB	1:A:333:ARG:CG	2.88	0.52
1:B:330:ASP:C	1:B:332:ILE:N	2.64	0.52
1:B:387:PHE:HB2	1:B:485:VAL:HG13	1.91	0.52
1:B:197:GLY:O	1:B:198:GLY:O	2.28	0.52
1:A:78:PRO:HB3	1:A:176:PHE:CZ	2.45	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:B:790:LYS:O	1:B:793:TRP:N	2.43	0.52
1:B:435:VAL:HA	1:B:484:ILE:O	2.10	0.52
1:A:739:GLU:O	1:A:739:GLU:OE1	2.26	0.52
1:B:274:TYR:CD2	1:B:275:GLN:HG3	2.44	0.52
1:A:306:LYS:HE3	1:A:307:VAL:H	1.74	0.52
1:A:467:ILE:HG22	1:A:468:ASN:N	2.24	0.52
1:A:372:GLY:O	1:A:380:THR:OG1	2.05	0.52
1:B:585:LEU:CD2	1:B:586:MET:CE	2.89	0.52
1:B:328:PHE:CE2	1:B:331:PHE:CE2	2.98	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:SER:O	1:A:696:TRP:C	2.47	0.52
1:B:519:ALA:HB2	1:B:675:PHE:CZ	2.45	0.51
1:A:302:TYR:O	1:A:303:GLU:HB3	2.10	0.51
1:A:350:SER:O	1:A:352:THR:HG23	2.09	0.51
1:A:63:LEU:O	1:A:70:THR:HG21	2.09	0.51
1:A:236:SER:C	1:A:238:LEU:CD1	2.79	0.51
1:B:806:PHE:CD1	1:B:806:PHE:CB	2.80	0.51
1:A:695:SER:O	1:A:697:LEU:N	2.43	0.51
1:A:343:LEU:O	1:A:344:THR:C	2.45	0.51
1:A:81:LEU:CD2	1:A:81:LEU:O	2.57	0.51
1:B:605:ARG:HG2	1:B:605:ARG:NH2	2.25	0.51
1:B:208:THR:O	1:B:346:ASP:OD1	2.28	0.51
1:B:161:LYS:C	1:B:163:GLY:H	2.13	0.51
1:B:524:GLU:O	1:B:526:VAL:N	2.43	0.51
1:B:377:TYR:C	1:B:379:ALA:H	2.13	0.51
1:A:135:TYR:O	1:A:136:ALA:HB3	2.10	0.51
1:A:773:VAL:HG11	1:A:782:GLY:O	2.11	0.51
1:B:643:GLN:NE2	1:B:643:GLN:CG	2.66	0.51
1:B:65:PRO:O	1:B:66:ASN:HB2	2.10	0.51
1:A:490:PHE:CD2	1:A:490:PHE:C	2.84	0.51
1:A:314:GLN:CG	1:A:315:LEU:N	2.72	0.51
1:A:37:ASN:C	1:A:39:CYS:H	2.14	0.51
1:A:267:THR:OG1	1:A:319:MET:CE	2.59	0.51
1:B:694:ILE:HA	1:B:694:ILE:CB	2.21	0.51
1:A:4:ILE:HD11	1:A:889:LEU:HD23	1.92	0.51
1:A:746:MET:SD	1:A:766:ILE:N	2.83	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: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:579:CYS:CB	1:B:579:CYS:N	2.69	0.51
1:B:429:GLU:CA	1:B:468:ASN:HD22	2.24	0.51
1:A:219:LYS:CD	1:A:219:LYS:CA	2.88	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:784:LEU:N	1:B:784:LEU:CD1	2.73	0.51
1:B:610:LEU:HB3	1:B:661:PHE:CE2	2.46	0.51
1:A:238:LEU:HD12	1:A:238:LEU:N	2.24	0.51
1:B:493:ASN:ND2	1:B:627:TYR:OH	2.44	0.51
1:B:161:LYS:C	1:B:163:GLY:N	2.62	0.51
1:B:800:GLN:HA	1:B:851:PHE:CZ	2.46	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:A:395:ASP:OD1	1:A:408:SER:HB3	2.11	0.51
1:B:450:LYS:O	1:B:454:PHE:CD1	2.64	0.51
1:A:154:VAL:HG22	1:A:155:ASP:H	1.76	0.51
1:A:139:PHE:HE1	1:A:156:ASP:HB3	1.75	0.51
1:A:329:ARG:HG3	1:A:333:ARG:HH11	1.76	0.51
1:B:470:ARG:CB	1:B:470:ARG:CD	2.81	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:B:601:ILE:CG2	2:B:987:HOH:O	2.58	0.51
1:B:95:THR:HG22	1:B:287:PRO:C	2.31	0.51
1:B:236:SER:C	1:B:237:LEU:HD23	2.31	0.51
1:B:660:ASP:HB2	2:B:1011:HOH:O	2.11	0.51
1:B:412:ALA:HB2	1:B:473:SER:HB2	1.92	0.51
1:A:199:CYS:CB	1:A:202:GLU:HG3	2.41	0.50
1:A:200:THR:CB	1:A:200:THR:C	2.68	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:B:89:VAL:N	1:B:175:GLU:OE2	2.44	0.50
1:B:652:PHE:HE1	1:B:891:MET:HE3	1.76	0.50
1:B:142:GLN:CB	1:B:142:GLN:NE2	2.75	0.50
1:A:757:PRO:O	1:A:758:ASP:HB2	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:B:507:LYS:HD2	2:B:934:HOH:O	2.10	0.50
1:A:407:CYS:HB2	1:A:478:LEU:O	2.11	0.50
1:B:640:LEU:HD21	1:B:671:LEU:HD11	1.93	0.50
1:A:6:MET:CE	1:A:6:MET:CG	2.88	0.50
1:A:800:GLN:HG3	1:A:851:PHE:CE1	2.46	0.50
1:A:117:ASN:OD1	1:A:119:THR:HB	2.12	0.50
1:B:400:TYR:CG	1:B:401:ASP:N	2.80	0.50
1:B:477:ARG:CB	1:B:477:ARG:CD	2.81	0.50
1:B:694:ILE:C	1:B:694:ILE:CB	2.75	0.50
1:B:208:THR:HA	2:B:908:HOH:O	2.11	0.50
1:B:226:GLN:CD	1:B:226:GLN:CB	2.72	0.50
1:B:4:ILE:O	1:B:5:ALA:C	2.49	0.50
1:A:853:ASN:O	1:A:857:CYS:HB2	2.11	0.50
1:B:398:ASP:HB2	2:B:964:HOH:O	2.10	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:746:MET:CG	1:A:746:MET:O	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:TRP:CZ2	1:A:488:SER:CA	2.91	0.50
1:A:340:ILE:CG2	1:A:340:ILE:CA	2.78	0.50
1:B:677:ILE:O	1:B:681:LEU:N	2.39	0.50
1:B:521:LEU:HB3	1:B:522:PRO:HD2	1.93	0.50
1:A:881:VAL:HG12	1:A:885:GLU:HB2	1.92	0.50
1:A:13:GLU:O	1:A:14:ALA:C	2.49	0.50
1:B:225:TYR:CE1	1:B:280:ASN:CG	2.84	0.50
1:A:644:LEU:O	1:A:648:ILE:HG13	2.12	0.50
1:A:37:ASN:C	1:A:39:CYS:N	2.65	0.50
1:B:400:TYR:CD1	1:B:401:ASP:N	2.78	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:616:PHE:O	1:B:624:MET:HB3	2.11	0.50
1:B:443:ALA:CB	2:B:894:HOH:O	2.54	0.50
1:B:603:TRP:O	1:B:603:TRP:CD1	2.65	0.50
1:A:168:VAL:O	1:A:169:HIS:HB3	2.11	0.50
1:B:456:ALA:C	1:B:456:ALA:HA	2.12	0.50
1:A:272:VAL:CA	1:A:312:ARG:HD2	2.41	0.50
1:A:320:GLU:C	1:A:320:GLU:CB	2.73	0.49
1:B:651:ARG:NH1	1:B:891:MET:HA	2.27	0.49
1:B:439:PRO:C	1:B:440:ARG:HD3	2.32	0.49
1:B:60:PHE:CD2	1:B:60:PHE:N	2.79	0.49
1:A:741:SER:C	1:A:743:THR:N	2.55	0.49
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:A:27:TYR:HB2	1:A:150:VAL:CG1	2.42	0.49
1:A:698:SER:C	1:A:700:SER:N	2.65	0.49
1:B:838:ILE:CG2	1:B:839:ILE:N	2.75	0.49
1:A:309:PRO:O	1:A:310:TYR:C	2.49	0.49
1:B:461:ALA:C	1:B:462:GLN:HG3	2.31	0.49
1:A:231:ALA:O	1:A:234:ARG:HB2	2.13	0.49
1:B:6:MET:SD	1:B:870:SER:OG	2.59	0.49
1:A:350:SER:C	1:A:352:THR:N	2.63	0.49
1:A:314:GLN:CG	1:A:315:LEU:H	2.25	0.49
1:B:230:LYS:HB3	1:B:234:ARG:NH2	2.28	0.49
1:A:105:SER:O	1:A:108:LEU:HB2	2.11	0.49
1:A:200:THR:CA	1:A:200:THR:CG2	2.87	0.49
1:A:120:ILE:HD13	1:A:237:LEU:HD21	1.94	0.49
1:B:669:VAL:O	1:B:673:ILE:HG13	2.12	0.49
1:A:5:ALA:C	1:A:7:LYS:H	2.15	0.49
1:A:51:PHE:HB2	1:A:187:LYS:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:606:ILE:O	1:A:609:TYR:N	2.45	0.49
1:A:168:VAL:HB	1:A:182:GLU:OE2	2.12	0.49
1:B:142:GLN:CB	1:B:142:GLN:CD	2.72	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:A:85:PRO:HB2	1:A:131:PHE:CG	2.48	0.49
1:B:303:GLU:HG2	1:B:303:GLU:O	2.03	0.49
1:B:161:LYS:HG3	1:B:166:VAL:HG11	1.94	0.49
1:B:724:ARG:HB2	1:B:724:ARG:NH2	2.19	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:664:PHE:CZ	1:A:668:LEU:HD11	2.48	0.49
1:B:14:ALA:O	1:B:17:GLY:N	2.46	0.49
1:A:228:ILE:O	1:A:229:LEU:C	2.51	0.49
1:B:146:PHE:HA	1:B:414:MET:CE	2.42	0.49
1:A:769:CYS:O	1:A:770:ARG:C	2.49	0.49
1:B:585:LEU:CD2	1:B:586:MET:HE2	2.43	0.49
1:A:628:GLU:O	1:A:629:MET:C	2.51	0.49
1:A:832:GLN:CD	1:A:832:GLN:C	2.70	0.49
1:B:25:ILE:CG2	1:B:26:LYS:N	2.75	0.49
1:B:6:MET:SD	1:B:6:MET:HA	2.52	0.49
1:A:734:ALA:O	1:A:736:ASP:N	2.45	0.49
1:A:304:TRP:CE2	1:A:313:GLU:OE2	2.65	0.49
1:B:585:LEU:HD23	1:B:586:MET:CE	2.43	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:0:GLU:HA	1:B:0:GLU:CB	2.19	0.48
1:B:212:THR:HB	1:B:340:ILE:CD1	2.43	0.48
1:B:824:GLU:CB	1:B:824:GLU:HA	2.24	0.48
1:A:695:SER:O	1:A:698:SER:N	2.46	0.48
1:A:350:SER:HB3	1:A:352:THR:HG22	1.95	0.48
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
1:B:57:SER:O	1:B:191:SER:HB2	2.12	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:A:358:THR:C	1:A:359:THR:HG23	2.31	0.48
1:B:106:TRP:HZ2	1:B:195:LEU:O	1.97	0.48
1:A:47:GLN:OE1	1:A:47:GLN:CA	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:GLY:O	1:B:599:PHE:CB	2.61	0.48
1:A:25:ILE:O	1:A:151:ASP:N	2.46	0.48
1:B:340:ILE:HG13	1:B:340:ILE:CD1	2.20	0.48
1:B:537:LYS:CG	1:B:537:LYS:NZ	2.75	0.48
1:A:335:PHE:HD1	1:A:336:THR:HB	1.78	0.48
1:B:731:VAL:HG11	1:B:739:GLU:O	2.13	0.48
1:B:730:PHE:O	1:B:732:GLN:N	2.46	0.48
1:A:308:ASP:OD2	1:A:313:GLU:HG3	2.14	0.48
1:A:665:VAL:O	1:A:666:ARG:O	2.30	0.48
1:B:585:LEU:HG	1:B:586:MET:CE	2.35	0.48
1:B:789:PHE:O	1:B:792:LEU:HB3	2.13	0.48
1:A:519:ALA:CB	1:A:675:PHE:CE1	2.91	0.48
1:B:227:ILE:O	1:B:228:ILE:C	2.47	0.48
1:A:281:LEU:HA	1:A:327:SER:HA	1.95	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:470:ARG:O	1:A:471:GLU:O	2.32	0.48
1:B:697:LEU:HA	1:B:700:SER:HG	1.78	0.48
1:A:792:LEU:O	1:A:792:LEU:HD12	2.14	0.48
1:B:684:GLU:O	1:B:685:ASN:C	2.52	0.48
1:A:319:MET:CG	1:A:320:GLU:N	2.76	0.48
1:A:305:ASN:HD22	1:A:306:LYS:H	1.54	0.48
1:B:729:LEU:HD22	2:B:1027:HOH:O	2.14	0.48
1:B:634:GLU:HA	1:B:638:PHE:O	2.13	0.48
1:A:831:ASN:CB	1:A:831:ASN:ND2	2.67	0.48
1:B:453:PHE:CD2	1:B:453:PHE:C	2.86	0.48
1:B:572:ASN:CA	1:B:573:GLY:N	2.70	0.48
1:A:258:LEU:HD13	1:A:258:LEU:N	2.28	0.48
1:B:828:PHE:CG	1:B:861:LEU:HD23	2.48	0.48
1:B:415:GLN:NE2	1:B:428:MET:HB3	2.28	0.48
1:B:382:TRP:HB3	1:B:451:ARG:HA	1.95	0.48
1:A:760:LYS:CA	1:A:760:LYS:HE3	2.42	0.48
1:A:154:VAL:HG22	1:A:155:ASP:N	2.29	0.48
1:A:258:LEU:N	1:A:258:LEU:CD1	2.73	0.48
1:A:857:CYS:C	1:A:859:VAL:H	2.16	0.48
1:B:99:GLN:HE22	1:B:105:SER:HB3	1.79	0.48
1:A:824:GLU:C	1:A:826:ALA:H	2.17	0.48
1:A:267:THR:OG1	1:A:319:MET:HE3	2.14	0.48
1:A:105:SER:O	1:A:106:TRP:O	2.32	0.48
1:A:66:ASN:O	1:A:67:SER:O	2.32	0.48
1:A:391:LEU:HB3	1:A:407:CYS:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:GLY:HA3	1:B:166:VAL:O	2.13	0.48
1:A:176:PHE:O	1:A:179:ALA:HB3	2.13	0.48
1:A:887:LEU:HD23	1:A:887:LEU:HA	1.65	0.48
1:A:105:SER:O	1:A:108:LEU:CB	2.62	0.48
1:A:97:ILE:HD13	1:A:108:LEU:CD1	2.42	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:467:ILE:CD1	1:A:472:VAL:CG2	2.92	0.48
1:B:145:GLN:O	1:B:146:PHE:C	2.51	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:284:MET:CA	1:B:284:MET:CG	2.80	0.48
1:A:579:CYS:HA	1:A:582:MET:HE3	1.96	0.48
1:A:403:ARG:HB3	1:A:477:ARG:HD2	1.96	0.47
1:A:30:GLN:NE2	1:A:187:LYS:NZ	2.49	0.47
1:B:383:VAL:HG13	1:B:383:VAL:O	2.13	0.47
1:B:616:PHE:CZ	1:B:631:MET:O	2.67	0.47
1:B:525:LYS:O	1:B:526:VAL:O	2.31	0.47
1:A:358:THR:CG2	1:A:359:THR:H	2.25	0.47
1:A:146:PHE:HB3	1:A:416:LYS:HG2	1.96	0.47
1:B:116:LEU:CD1	1:B:287:PRO:HG3	2.34	0.47
1:B:537:LYS:CB	1:B:537:LYS:HZ3	2.25	0.47
1:B:369:SER:O	1:B:383:VAL:HG11	2.13	0.47
1:B:83:SER:O	1:B:85:PRO:HD3	2.14	0.47
1:B:109:ALA:O	1:B:113:SER:HB3	2.14	0.47
1:A:306:LYS:CE	1:A:307:VAL:H	2.26	0.47
1:A:60:PHE:O	1:A:61:LYS:CB	2.62	0.47
1:A:242:ILE:CB	1:A:242:ILE:CD1	2.75	0.47
1:B:764:PHE:CE1	1:B:851:PHE:O	2.66	0.47
1:B:412:ALA:CB	1:B:473:SER:HB2	2.43	0.47
1:B:282:ILE:HG22	1:B:326:MET:HG3	1.96	0.47
1:A:773:VAL:O	1:A:774:ALA:C	2.47	0.47
1:B:304:TRP:CE2	1:B:312:ARG:HD3	2.50	0.47
1:B:349:LYS:CG	1:B:350:SER:N	2.77	0.47
1:B:868:PHE:HZ	1:B:878:GLN:HA	1.80	0.47
1:A:743:THR:O	1:A:747:ASN:OD1	2.32	0.47
1:B:242:ILE:CG2	1:B:242:ILE:O	2.62	0.47
1:B:12:ARG:HH21	1:B:885:GLU:CD	2.18	0.47
1:B:228:ILE:CG2	1:B:228:ILE:CA	2.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:LEU:CD1	1:B:672:GLU:HG2	2.43	0.47
1:B:342:ASN:ND2	1:B:346:ASP:OD2	2.47	0.47
1:A:576:LEU:O	1:A:580:ARG:CB	2.63	0.47
1:B:388:LYS:HZ3	1:B:482:GLU:HB3	1.78	0.47
1:A:258:LEU:O	1:A:258:LEU:HD22	2.09	0.47
1:B:451:ARG:HD2	2:B:902:HOH:O	2.14	0.47
1:A:862:ASP:OD2	1:A:862:ASP:C	2.50	0.47
1:A:821:GLY:C	1:A:823:PHE:H	2.18	0.47
1:A:756:HIS:HB2	1:A:757:PRO:HD2	1.94	0.47
1:B:364:THR:HG1	1:B:646:GLN:NE2	1.95	0.47
1:B:764:PHE:HE1	1:B:851:PHE:O	1.97	0.47
1:B:389:ILE:CD1	1:B:389:ILE:N	2.54	0.47
1:B:524:GLU:O	1:B:525:LYS:C	2.52	0.47
1:A:803:TYR:N	1:A:822:ALA:HB1	2.29	0.47
1:A:32:TYR:HB2	1:A:153:VAL:CG2	2.44	0.47
1:B:377:TYR:O	1:B:379:ALA:N	2.47	0.47
1:B:82:LEU:O	1:B:83:SER:C	2.52	0.47
1:A:93:THR:HB	1:A:321:ASP:OD2	2.15	0.47
1:A:296:PRO:HG3	1:A:304:TRP:HB2	1.93	0.47
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:A:617:ASP:O	1:A:618:LEU:C	2.53	0.47
1:A:229:LEU:O	1:A:232:LEU:N	2.47	0.47
1:A:228:ILE:HG12	1:A:337:LYS:HZ1	1.78	0.47
1:A:822:ALA:HA	2:A:912:HOH:O	2.14	0.47
1:A:368:GLY:HA2	1:A:627:TYR:CE1	2.49	0.47
1:A:553:LYS:C	1:A:555:LEU:N	2.67	0.47
1:A:263:ALA:HB2	1:A:288:TRP:HZ3	1.78	0.47
1:A:453:PHE:C	1:A:453:PHE:CD2	2.88	0.47
1:A:820:PRO:HD2	2:A:928:HOH:O	2.14	0.47
1:B:112:ALA:O	1:B:115:THR:HB	2.14	0.47
1:A:669:VAL:O	1:A:670:ARG:C	2.52	0.47
1:A:224:LEU:HD22	1:A:224:LEU:O	2.15	0.47
1:A:50:ALA:O	1:A:52:PRO:HD3	2.13	0.47
1:B:375:ARG:CB	1:B:375:ARG:HH11	2.15	0.47
1:A:146:PHE:CD1	1:A:416:LYS:HA	2.50	0.47
1:A:96:ASP:C	1:A:97:ILE:O	2.50	0.47
1:A:120:ILE:CD1	1:A:237:LEU:HD21	2.45	0.47
1:B:670:ARG:HG3	1:B:674:LEU:CD2	2.45	0.47
1:B:332:ILE:HG22	1:B:333:ARG:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:789:PHE:O	1:B:789:PHE:HD2	1.98	0.47
1:B:626:ALA:CB	1:B:649:VAL:HG22	2.37	0.47
1:B:538:THR:CG2	1:B:539:LEU:N	2.58	0.47
1:A:23:ARG:O	1:A:24:ALA:C	2.53	0.47
1:B:108:LEU:HD12	1:B:108:LEU:HA	1.58	0.46
1:B:675:PHE:O	1:B:678:PHE:HB3	2.15	0.46
1:B:136:ALA:CB	1:B:136:ALA:N	2.67	0.46
1:B:411:LEU:CD1	1:B:502:PHE:CE1	2.98	0.46
1:A:386:GLN:HB3	1:A:513:LEU:CB	2.41	0.46
1:A:112:ALA:C	1:A:114:LEU:H	2.19	0.46
1:A:608:ASN:O	1:A:609:TYR:C	2.44	0.46
1:A:98:CYS:SG	1:A:169:HIS:CE1	3.08	0.46
1:A:478:LEU:HA	1:A:478:LEU:HD23	1.36	0.46
1:B:585:LEU:O	1:B:586:MET:O	2.33	0.46
1:B:453:PHE:O	1:B:453:PHE:CD2	2.67	0.46
1:A:411:LEU:HD22	1:A:433:PHE:CE1	2.50	0.46
1:A:100:GLY:HA3	1:A:103:GLY:CA	2.39	0.46
1:A:386:GLN:O	1:A:387:PHE:CG	2.69	0.46
1:B:327:SER:OG	1:B:329:ARG:HB2	2.15	0.46
1:A:67:SER:O	1:A:68:SER:C	2.52	0.46
1:A:758:ASP:O	1:A:759:LEU:CB	2.58	0.46
1:A:48:ASP:OD2	1:A:187:LYS:HE3	2.15	0.46
1:A:571:THR:CG2	1:A:572:ASN:H	2.29	0.46
1:B:511:GLN:CB	2:B:899:HOH:O	2.63	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:320:GLU:O	1:A:321:ASP:C	2.54	0.46
1:B:230:LYS:CD	1:B:230:LYS:NZ	2.68	0.46
1:A:670:ARG:O	1:A:673:ILE:N	2.48	0.46
1:A:579:CYS:HA	1:A:582:MET:CE	2.46	0.46
1:A:46:PHE:CD2	1:A:138:ILE:HD12	2.51	0.46
1:B:242:ILE:C	1:B:242:ILE:HD13	2.35	0.46
1:B:692:ASP:O	1:B:693:LEU:C	2.53	0.46
1:B:521:LEU:HB3	1:B:522:PRO:CD	2.46	0.46
1:B:90:ASP:OD1	1:B:92:ALA:O	2.34	0.46
1:B:193:GLU:O	1:B:196:SER:OG	2.24	0.46
1:A:693:LEU:HA	1:A:868:PHE:CE2	2.50	0.46
1:A:487:PRO:O	1:A:488:SER:CB	2.57	0.46
1:B:723:GLU:C	1:B:726:PHE:CD2	2.87	0.46
1:A:585:LEU:HD11	1:A:605:ARG:NH2	2.30	0.46
1:A:600:ASN:C	1:A:602:LEU:N	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:PHE:CB	1:A:187:LYS:HG3	2.46	0.46
1:B:279:VAL:HG23	1:B:281:LEU:HD23	1.98	0.46
1:A:686:THR:CG2	2:A:977:HOH:O	2.63	0.46
1:A:829:HIS:CE1	2:A:917:HOH:O	2.69	0.46
1:A:66:ASN:O	1:A:67:SER:C	2.52	0.46
1:B:652:PHE:HE1	1:B:891:MET:CE	2.28	0.46
1:A:429:GLU:CG	1:A:494:LYS:HE3	2.46	0.46
1:A:96:ASP:O	1:A:97:ILE:O	2.33	0.46
1:B:636:ALA:CB	1:B:668:LEU:HD13	2.46	0.46
1:B:430:THR:HA	1:B:468:ASN:HB3	1.97	0.46
1:A:652:PHE:CD1	1:A:667:CYS:CB	2.94	0.46
1:A:698:SER:C	1:A:700:SER:H	2.17	0.46
1:A:748:ILE:HG23	1:A:749:LEU:H	1.81	0.46
1:A:284:MET:HE2	1:A:326:MET:SD	2.56	0.46
1:A:656:GLU:CD	1:A:656:GLU:N	2.70	0.46
1:B:228:ILE:O	1:B:232:LEU:HD23	2.16	0.46
1:B:340:ILE:HG12	1:B:340:ILE:CD1	2.20	0.46
1:A:88:ILE:HA	1:A:175:GLU:CG	2.45	0.46
1:B:390:ARG:HH11	1:B:390:ARG:CG	2.07	0.46
1:A:693:LEU:HA	1:A:868:PHE:CZ	2.51	0.46
1:B:110:ALA:HA	1:B:204:PHE:CE2	2.51	0.46
1:A:327:SER:OG	1:A:329:ARG:NE	2.49	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:677:ILE:HG22	1:A:678:PHE:N	2.29	0.46
1:A:467:ILE:HD12	1:A:472:VAL:CG2	2.45	0.46
1:B:328:PHE:CD2	1:B:331:PHE:CE2	3.05	0.45
1:A:450:LYS:HB3	1:A:451:ARG:H	1.62	0.45
1:A:232:LEU:HA	1:A:232:LEU:HD13	1.76	0.45
1:A:30:GLN:NE2	1:A:187:LYS:HZ3	2.09	0.45
1:B:552:VAL:O	1:B:554:GLU:N	2.49	0.45
1:B:89:VAL:CG1	1:B:89:VAL:CG2	2.88	0.45
1:B:66:ASN:O	1:B:67:SER:O	2.34	0.45
1:B:805:ARG:N	1:B:811:SER:OG	2.30	0.45
1:B:552:VAL:C	1:B:554:GLU:N	2.69	0.45
1:A:745:LEU:HD12	1:A:749:LEU:HD21	1.99	0.45
1:B:696:TRP:O	1:B:700:SER:CB	2.63	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:731:VAL:HG23	1:A:732:GLN:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASP:HB3	1:A:283:ARG:HB3	1.97	0.45
1:A:305:ASN:ND2	1:A:305:ASN:N	2.64	0.45
1:A:63:LEU:C	1:A:193:GLU:OE2	2.54	0.45
1:B:583:VAL:O	1:B:584:ASN:HB2	2.16	0.45
1:B:20:SER:O	1:B:21:HIS:C	2.53	0.45
1:A:757:PRO:HG3	2:A:1029:HOH:O	2.16	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:273:THR:OG1	1:A:312:ARG:NH2	2.49	0.45
1:A:872:ASP:HB2	1:A:879:ILE:HG22	1.97	0.45
1:A:361:TYR:OH	1:A:510:THR:C	2.54	0.45
1:B:12:ARG:O	1:B:16:GLU:HG3	2.17	0.45
1:B:576:LEU:C	1:B:578:SER:N	2.67	0.45
1:B:681:LEU:O	1:B:683:PRO:HD2	2.15	0.45
1:B:61:LYS:O	1:B:62:GLU:HB2	2.15	0.45
1:A:414:MET:HE3	1:A:471:GLU:OE1	2.17	0.45
1:B:656:GLU:O	1:B:657:LEU:CB	2.64	0.45
1:A:21:HIS:ND1	2:A:1060:HOH:O	2.05	0.45
1:A:388:LYS:NZ	1:A:482:GLU:HG2	2.32	0.45
1:B:796:ILE:O	1:B:799:TRP:CB	2.62	0.45
1:B:856:SER:C	1:B:858:LEU:N	2.69	0.45
1:B:831:ASN:C	1:B:833:HIS:N	2.69	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:A:283:ARG:HB2	1:A:325:TRP:CE2	2.51	0.45
1:A:223:ASP:C	1:A:227:ILE:HD12	2.32	0.45
1:B:135:TYR:CG	1:B:136:ALA:N	2.83	0.45
1:A:433:PHE:HE2	1:A:472:VAL:HG12	1.82	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:739:GLU:HA	2:A:979:HOH:O	2.17	0.45
1:A:21:HIS:NE2	1:A:123:ARG:O	2.50	0.45
1:A:68:SER:OG	1:A:69:LYS:N	2.50	0.45
1:A:665:VAL:C	1:A:669:VAL:HG23	2.32	0.45
1:A:883:ILE:CA	1:A:883:ILE:CG2	2.84	0.45
1:A:604:ASN:HD22	1:A:604:ASN:N	2.14	0.45
1:A:411:LEU:C	1:A:411:LEU:HD23	2.37	0.45
1:B:828:PHE:HZ	1:B:862:ASP:OD1	2.00	0.45
1:B:557:THR:HG22	1:B:558:ILE:N	2.32	0.45
1:A:743:THR:O	1:A:744:GLU:C	2.55	0.45
1:A:571:THR:HG22	1:A:572:ASN:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:LYS:HA	1:A:760:LYS:HE3	1.99	0.45
1:B:871:LEU:N	1:B:871:LEU:HD12	2.31	0.45
1:A:828:PHE:CD1	1:A:828:PHE:N	2.85	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:B:676:LYS:O	1:B:677:ILE:C	2.55	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:A:352:THR:OG1	1:A:352:THR:O	2.34	0.45
1:A:656:GLU:O	1:A:657:LEU:CB	2.65	0.45
1:B:696:TRP:CE3	1:B:700:SER:HB3	2.52	0.45
1:A:878:GLN:HE21	1:A:878:GLN:HB3	1.52	0.45
1:B:651:ARG:CZ	1:B:670:ARG:HH22	2.23	0.45
1:B:328:PHE:CD2	1:B:331:PHE:CZ	3.04	0.45
1:A:32:TYR:HB2	1:A:153:VAL:HG23	1.98	0.45
1:B:461:ALA:C	1:B:462:GLN:CG	2.83	0.45
1:B:404:GLU:C	1:B:405:SER:OG	2.56	0.45
1:A:193:GLU:O	1:A:194:ALA:C	2.56	0.44
1:B:581:SER:C	1:B:583:VAL:H	2.21	0.44
1:B:21:HIS:CE1	1:B:123:ARG:NE	2.85	0.44
1:B:430:THR:H	1:B:494:LYS:HZ1	1.65	0.44
1:A:803:TYR:CD2	1:A:803:TYR:C	2.88	0.44
1:A:521:LEU:N	1:A:522:PRO:CD	2.79	0.44
1:B:598:GLU:H	1:B:598:GLU:CD	2.20	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:A:355:ASN:O	1:A:356:TRP:CB	2.63	0.44
1:A:78:PRO:HB3	1:A:176:PHE:CE2	2.52	0.44
1:A:10:LYS:HD2	1:A:10:LYS:N	2.32	0.44
1:B:156:ASP:N	1:B:156:ASP:OD2	2.49	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:618:LEU:H	1:A:618:LEU:HD23	1.82	0.44
1:A:682:ASP:HB2	1:A:689:ILE:HG22	1.99	0.44
1:B:628:GLU:O	1:B:631:MET:N	2.45	0.44
1:A:491:GLU:HG3	1:A:491:GLU:H	1.55	0.44
1:B:212:THR:CG2	1:B:212:THR:O	2.62	0.44
1:B:585:LEU:HB3	1:B:586:MET:H	1.54	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:642:CYS:O	1:B:643:GLN:C	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:867:ALA:C	1:B:869:ARG:H	2.19	0.44
1:A:389:ILE:HD11	1:A:485:VAL:HG11	1.99	0.44
1:A:284:MET:O	1:A:323:GLU:O	2.35	0.44
1:B:614:ARG:HD2	1:B:614:ARG:HA	1.56	0.44
1:A:135:TYR:OH	1:A:156:ASP:OD1	2.27	0.44
1:B:113:SER:HA	1:B:116:LEU:HD13	1.99	0.44
1:A:270:LYS:CB	1:A:325:TRP:CH2	2.89	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:B:651:ARG:CZ	1:B:891:MET:HA	2.48	0.44
1:B:453:PHE:O	1:B:457:ASN:OD1	2.35	0.44
1:A:759:LEU:CD1	1:A:812:GLY:HA2	2.46	0.44
1:A:433:PHE:CE2	1:A:463:SER:HB3	2.53	0.44
1:B:697:LEU:CA	1:B:700:SER:HG	2.29	0.44
1:B:459:SER:HB2	1:B:461:ALA:H	1.82	0.44
1:A:207:PHE:C	1:A:208:THR:HG23	2.37	0.44
1:A:355:ASN:O	1:A:356:TRP:HB2	2.18	0.44
1:A:505:GLU:O	1:A:505:GLU:CG	2.66	0.44
1:B:438:VAL:HG12	1:B:439:PRO:HD2	2.00	0.44
1:A:731:VAL:CG2	1:A:733:LEU:CG	2.88	0.44
1:B:613:PHE:CD2	1:B:613:PHE:C	2.91	0.44
1:B:861:LEU:O	1:B:862:ASP:C	2.50	0.44
1:B:80:GLU:O	1:B:81:LEU:CD2	2.61	0.44
1:A:386:GLN:HB2	1:A:513:LEU:O	2.18	0.44
1:A:23:ARG:HH11	1:A:23:ARG:CG	2.31	0.44
1:A:677:ILE:O	1:A:678:PHE:C	2.52	0.44
1:A:502:PHE:CD1	1:A:502:PHE:N	2.85	0.44
1:A:114:LEU:HD13	1:A:121:LEU:CD2	2.44	0.44
1:B:36:ARG:O	1:B:37:ASN:C	2.54	0.44
1:A:313:GLU:O	1:A:313:GLU:CG	2.63	0.44
1:B:584:ASN:HD22	1:B:584:ASN:HA	1.62	0.44
1:A:626:ALA:O	1:A:628:GLU:N	2.51	0.44
1:B:883:ILE:CA	1:B:883:ILE:CG1	2.82	0.44
1:B:28:LEU:C	1:B:30:GLN:N	2.71	0.44
1:A:553:LYS:C	1:A:555:LEU:H	2.21	0.44
1:A:208:THR:O	1:A:343:LEU:HD11	2.18	0.44
1:A:200:THR:CB	1:A:200:THR:N	2.69	0.44
1:B:582:MET:HG2	1:B:602:LEU:HD21	1.99	0.44
1:B:3:GLY:O	1:B:778:SER:OG	2.21	0.44
1:A:27:TYR:CE2	1:A:28:LEU:HG	2.53	0.44
1:B:382:TRP:O	1:B:448:HIS:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ASP:O	1:B:322:GLY:C	2.57	0.44
1:A:319:MET:SD	1:A:322:GLY:O	2.76	0.44
1:A:94:ARG:HD3	2:A:1049:HOH:O	2.13	0.44
1:A:281:LEU:HD21	1:A:297:TRP:CZ2	2.53	0.44
1:B:651:ARG:CD	1:B:893:SER:OXT	2.64	0.44
1:B:342:ASN:CG	1:B:346:ASP:OD2	2.56	0.44
1:B:277:GLN:HA	1:B:277:GLN:NE2	2.32	0.44
1:B:100:GLY:N	2:B:903:HOH:O	2.48	0.44
1:A:677:ILE:O	1:A:679:LYS:N	2.50	0.44
1:B:318:LYS:O	1:B:320:GLU:HG2	2.18	0.44
1:A:795:ASN:O	1:A:796:ILE:C	2.52	0.44
1:B:293:TRP:CD1	1:B:324:PHE:CD1	3.06	0.43
1:A:94:ARG:C	1:A:95:THR:OG1	2.56	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:13:GLU:O	1:A:16:GLU:CA	2.66	0.43
1:A:117:ASN:OD1	1:A:117:ASN:C	2.57	0.43
1:A:631:MET:HB2	1:A:631:MET:SD	2.57	0.43
1:B:837:MET:CG	1:B:837:MET:CE	2.93	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:697:LEU:CA	1:B:700:SER:OG	2.66	0.43
1:A:435:VAL:HG13	1:A:461:ALA:HB3	2.00	0.43
1:B:230:LYS:CE	1:B:230:LYS:CG	2.86	0.43
1:B:610:LEU:CD1	1:B:610:LEU:CD2	2.86	0.43
1:B:349:LYS:HG2	1:B:350:SER:N	2.34	0.43
1:B:792:LEU:HD12	1:B:792:LEU:HA	1.94	0.43
1:A:228:ILE:CG1	1:A:337:LYS:NZ	2.77	0.43
1:A:225:TYR:CZ	1:A:280:ASN:HB3	2.54	0.43
1:A:874:ASN:O	1:A:875:GLY:C	2.51	0.43
1:A:157:LEU:O	1:A:158:LEU:HG	2.17	0.43
1:A:255:PHE:CB	1:A:333:ARG:HG2	2.48	0.43
1:A:833:HIS:CD2	1:A:834:ILE:N	2.87	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:A:403:ARG:CG	1:A:477:ARG:NE	2.81	0.43
1:A:293:TRP:CH2	1:A:326:MET:CB	3.01	0.43
1:A:63:LEU:HD12	1:A:70:THR:HG21	1.88	0.43
1:B:312:ARG:NE	1:B:312:ARG:CG	2.74	0.43
1:B:312:ARG:HG2	1:B:313:GLU:OE1	2.19	0.43
1:B:729:LEU:CB	1:B:729:LEU:CD2	2.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:LEU:HD22	1:B:674:LEU:H	1.82	0.43
1:B:746:MET:HE3	2:B:965:HOH:O	2.18	0.43
1:A:411:LEU:CD1	1:A:485:VAL:HG21	2.45	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:701:VAL:CG1	1:B:860:ARG:CD	2.97	0.43
1:A:741:SER:O	1:A:742:ALA:C	2.56	0.43
1:A:484:ILE:CD1	1:A:486:VAL:CG2	2.97	0.43
1:A:291:VAL:HG23	1:A:292:GLU:H	1.83	0.43
1:A:824:GLU:CB	1:A:829:HIS:HA	2.48	0.43
1:A:75:TRP:CE3	1:A:159:PRO:HG3	2.48	0.43
1:A:309:PRO:C	1:A:311:GLU:N	2.72	0.43
1:A:69:LYS:HB2	1:A:69:LYS:HE3	1.76	0.43
1:A:51:PHE:N	1:A:52:PRO:CD	2.82	0.43
1:B:387:PHE:CD2	1:B:387:PHE:N	2.86	0.43
1:A:370:THR:O	1:A:384:ASN:HA	2.19	0.43
1:B:595:GLY:HA3	1:B:598:GLU:OE1	2.18	0.43
1:A:831:ASN:C	2:A:919:HOH:O	2.54	0.43
1:B:100:GLY:HA3	1:B:167:PHE:HA	2.01	0.43
1:B:646:GLN:O	1:B:647:VAL:C	2.56	0.43
1:A:293:TRP:CE3	1:A:295:GLY:O	2.71	0.43
1:B:200:THR:H	1:B:200:THR:HG22	1.28	0.43
1:B:285:ARG:HA	1:B:322:GLY:O	2.18	0.43
1:B:215:TYR:HB2	1:B:337:LYS:HZ3	1.83	0.43
1:A:633:ILE:O	1:A:636:ALA:HB3	2.18	0.43
1:B:282:ILE:HD13	1:B:282:ILE:HG21	1.72	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:B:115:THR:O	1:B:116:LEU:C	2.56	0.43
1:A:140:HIS:HB3	1:A:153:VAL:CG2	2.49	0.43
1:A:668:LEU:HD23	1:A:668:LEU:HA	1.72	0.43
1:A:393:GLU:HB2	1:A:506:LYS:HG2	2.01	0.43
1:B:617:ASP:CG	1:B:617:ASP:O	2.47	0.43
1:B:204:PHE:CB	1:B:340:ILE:HG13	2.44	0.42
1:B:21:HIS:CE1	2:B:945:HOH:O	2.71	0.42
1:A:517:ILE:HG23	1:A:640:LEU:HD23	2.00	0.42
1:A:693:LEU:O	1:A:697:LEU:HG	2.18	0.42
1:A:543:LEU:CB	1:A:596:LEU:CB	2.97	0.42
1:B:862:ASP:CG	1:B:866:ARG:HE	2.21	0.42
1:B:860:ARG:NH1	1:B:860:ARG:HG3	2.34	0.42
1:A:273:THR:H	1:A:312:ARG:NH2	2.14	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:GLN:CG	1:A:851:PHE:HE1	2.32	0.42
1:A:775:VAL:HG12	1:A:776:MET:N	2.29	0.42
1:B:8:LEU:C	1:B:10:LYS:N	2.73	0.42
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:18:LEU:HD12	1:B:18:LEU:HA	1.80	0.42
1:A:129:GLN:OE1	1:A:139:PHE:HB3	2.20	0.42
1:B:211:VAL:HG13	1:B:212:THR:N	2.26	0.42
1:A:98:CYS:O	1:A:99:GLN:C	2.58	0.42
1:B:585:LEU:CD2	1:B:586:MET:HE3	2.49	0.42
1:A:758:ASP:O	1:A:759:LEU:O	2.37	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:A:599:PHE:HD2	1:A:599:PHE:C	2.17	0.42
1:B:242:ILE:HD13	1:B:243:ASN:CB	2.49	0.42
1:A:386:GLN:HG2	1:A:484:ILE:HD11	2.02	0.42
1:A:240:CYS:SG	1:A:266:VAL:HG23	2.60	0.42
1:A:329:ARG:HH21	1:A:333:ARG:NH1	2.17	0.42
1:A:97:ILE:O	1:A:98:CYS:CB	2.64	0.42
1:A:237:LEU:HB2	1:A:340:ILE:HG12	2.01	0.42
1:A:174:ASN:CG	1:A:174:ASN:H	2.23	0.42
1:B:613:PHE:HZ	1:B:623:SER:CA	2.33	0.42
1:B:485:VAL:HG11	1:B:502:PHE:HZ	1.84	0.42
1:A:599:PHE:CG	1:A:599:PHE:O	2.67	0.42
1:A:109:ALA:HB2	1:A:262:HIS:O	2.19	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:578:SER:C	1:A:582:MET:HG3	2.40	0.42
1:B:626:ALA:C	1:B:628:GLU:H	2.23	0.42
1:A:614:ARG:NH1	1:A:620:LYS:HB3	2.31	0.42
1:B:858:LEU:C	1:B:860:ARG:N	2.70	0.42
1:B:558:ILE:O	1:B:559:LEU:C	2.58	0.42
1:A:503:PHE:N	1:A:503:PHE:CD1	2.87	0.42
1:B:340:ILE:HG23	1:B:340:ILE:CD1	2.50	0.42
1:A:311:GLU:C	1:A:313:GLU:H	2.22	0.42
1:A:327:SER:N	1:A:329:ARG:HH11	1.99	0.42
1:A:59:GLY:HA3	1:A:193:GLU:OE2	2.19	0.42
1:A:429:GLU:CD	1:A:494:LYS:HE3	2.40	0.42
1:A:678:PHE:CE2	1:A:689:ILE:HG12	2.54	0.42
1:B:525:LYS:HG2	1:B:525:LYS:H	1.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:827:GLY:O	1:B:828:PHE:CD2	2.72	0.42
1:A:100:GLY:C	1:A:103:GLY:H	2.23	0.42
1:A:84:ASN:C	1:A:84:ASN:OD1	2.58	0.42
1:A:204:PHE:HE2	1:A:237:LEU:CD1	2.33	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
1:B:663:ASN:O	1:B:664:PHE:C	2.58	0.42
1:B:2:ALA:CB	2:B:999:HOH:O	2.67	0.42
1:B:579:CYS:HA	1:B:582:MET:HB2	2.00	0.42
1:A:403:ARG:HB3	1:A:477:ARG:CD	2.50	0.42
1:B:492:PRO:C	1:B:494:LYS:H	2.21	0.42
1:A:680:GLN:C	1:A:682:ASP:N	2.71	0.42
1:A:256:LYS:CA	1:A:258:LEU:CD1	2.97	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:696:TRP:O	1:B:700:SER:N	2.53	0.42
1:A:349:LYS:CG	1:A:349:LYS:O	2.68	0.42
1:A:77:ARG:HG3	1:A:157:LEU:HD12	2.02	0.42
1:B:503:PHE:CD1	1:B:503:PHE:N	2.88	0.42
1:B:313:GLU:CG	1:B:313:GLU:HA	2.47	0.42
1:B:681:LEU:C	1:B:683:PRO:CD	2.88	0.42
1:B:677:ILE:HG22	1:B:681:LEU:CD1	2.50	0.42
1:B:487:PRO:O	1:B:488:SER:CB	2.58	0.42
1:B:766:ILE:HG23	1:B:767:ASP:N	2.34	0.42
1:A:77:ARG:CG	1:A:156:ASP:OD2	2.53	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: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:625:SER:O	1:B:626:ALA:C	2.55	0.42
1:A:256:LYS:C	1:A:258:LEU:HD13	2.41	0.42
1:A:32:TYR:O	1:A:36:ARG:N	2.53	0.42
1:A:874:ASN:C	1:A:876:THR:N	2.72	0.42
1:B:197:GLY:C	1:B:198:GLY:O	2.58	0.42
1:B:33:GLU:OE1	1:B:37:ASN:OD1	2.38	0.42
1:A:809:ASP:O	1:A:810:ARG:C	2.58	0.42
1:A:715:ILE:HD12	1:A:715:ILE:HA	1.60	0.42
1:A:93:THR:CB	1:A:321:ASP:OD2	2.67	0.41
1:A:236:SER:C	1:A:238:LEU:HD12	2.40	0.41
1:B:100:GLY:HA3	1:B:167:PHE:CA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ARG:O	1:B:15:ALA:HB3	2.20	0.41
1:A:688:THR:N	1:A:688:THR:CG2	2.82	0.41
1:A:256:LYS:HD3	1:A:258:LEU:CD2	2.34	0.41
1:A:745:LEU:HD12	1:A:749:LEU:HD23	2.01	0.41
1:A:374:CYS:C	1:A:381:PHE:CD1	2.94	0.41
1:B:692:ASP:C	1:B:692:ASP:OD1	2.57	0.41
1:B:113:SER:OG	1:B:204:PHE:HE2	2.04	0.41
1:B:206:ASP:CG	1:B:470:ARG:HH22	2.24	0.41
1:B:610:LEU:HA	1:B:661:PHE:HE2	1.84	0.41
1:A:517:ILE:HG12	1:A:641:PRO:CD	2.50	0.41
1:A:229:LEU:O	1:A:230:LYS:C	2.57	0.41
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:A:364:THR:CG2	1:A:497:ASP:OD1	2.65	0.41
1:B:179:ALA:O	1:B:182:GLU:HB3	2.19	0.41
1:A:632:ALA:O	1:A:633:ILE:C	2.58	0.41
1:A:663:ASN:O	1:A:664:PHE:O	2.38	0.41
1:A:285:ARG:O	1:A:287:PRO:HD3	2.19	0.41
1:B:174:ASN:HD22	1:B:174:ASN:HA	1.41	0.41
1:B:321:ASP:O	1:B:323:GLU:N	2.54	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:67:SER:O	1:A:70:THR:N	2.51	0.41
1:A:600:ASN:C	1:A:602:LEU:H	2.22	0.41
1:A:223:ASP:CG	1:A:227:ILE:HD11	2.41	0.41
1:B:453:PHE:CE1	1:B:457:ASN:OD1	2.73	0.41
1:A:224:LEU:HD21	1:A:337:LYS:HZ1	1.86	0.41
1:B:644:LEU:HA	1:B:647:VAL:CG2	2.49	0.41
1:A:380:THR:C	1:A:382:TRP:N	2.73	0.41
1:A:856:SER:O	1:A:860:ARG:HG3	2.20	0.41
1:A:823:PHE:O	1:A:826:ALA:N	2.52	0.41
1:B:673:ILE:O	1:B:676:LYS:N	2.53	0.41
1:B:449:LEU:HD13	1:B:453:PHE:CD1	2.55	0.41
1:B:456:ALA:CA	1:B:457:ASN:N	2.66	0.41
1:B:856:SER:C	1:B:858:LEU:H	2.24	0.41
1:B:35:LEU:HD13	1:B:46:PHE:HE1	1.80	0.41
1:A:349:LYS:O	1:A:349:LYS:HG3	2.20	0.41
1:B:78:PRO:CD	1:B:156:ASP:HB2	2.51	0.41
1:B:211:VAL:HG11	1:B:410:LEU:HD23	2.02	0.41
1:B:294:LYS:CE	1:B:294:LYS:CG	2.87	0.41
1:A:616:PHE:HD2	1:A:628:GLU:HG2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:THR:N	1:B:468:ASN:HB2	2.35	0.41
1:A:224:LEU:O	1:A:228:ILE:N	2.49	0.41
1:A:172:GLN:O	1:A:174:ASN:N	2.53	0.41
1:A:689:ILE:O	1:A:689:ILE:HD12	2.19	0.41
1:B:581:SER:O	1:B:583:VAL:N	2.54	0.41
1:A:415:GLN:HE22	1:A:428:MET:HB3	1.86	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:B:632:ALA:O	1:B:635:ALA:HB3	2.20	0.41
1:B:256:LYS:CD	1:B:256:LYS:CB	2.80	0.41
1:B:95:THR:HG23	1:B:288:TRP:CD1	2.56	0.41
1:A:61:LYS:O	1:A:62:GLU:HB2	2.21	0.41
1:B:429:GLU:OE2	1:B:494:LYS:HB3	2.21	0.41
1:A:435:VAL:CG1	1:A:461:ALA:O	2.69	0.41
1:A:196:SER:O	1:A:197:GLY:O	2.38	0.41
1:A:775:VAL:O	1:A:775:VAL:CG1	2.62	0.41
1:A:571:THR:CG2	1:A:572:ASN:N	2.84	0.41
1:B:141:PHE:CD2	1:B:181:LEU:HD12	2.56	0.41
1:A:479:PRO:O	1:A:480:PRO:C	2.51	0.41
1:A:824:GLU:C	1:A:826:ALA:N	2.74	0.41
1:B:284:MET:HB2	1:B:324:PHE:CE2	2.56	0.41
1:B:113:SER:HA	1:B:116:LEU:CD1	2.51	0.41
1:A:88:ILE:HD13	1:A:88:ILE:HG21	1.40	0.41
1:B:335:PHE:CG	1:B:335:PHE:C	2.94	0.41
1:B:574:PHE:CZ	1:B:606:ILE:HD13	2.55	0.41
1:A:640:LEU:O	1:A:645:HIS:CD2	2.74	0.41
1:B:456:ALA:O	1:B:457:ASN:C	2.58	0.41
1:A:756:HIS:O	1:A:757:PRO:O	2.39	0.41
1:B:131:PHE:HA	1:B:135:TYR:CD1	2.56	0.41
1:B:40:LEU:CD1	1:B:136:ALA:HB2	2.50	0.41
1:A:677:ILE:C	1:A:679:LYS:N	2.74	0.41
1:B:647:VAL:HG23	1:B:648:ILE:N	2.36	0.41
1:A:697:LEU:HD23	1:A:697:LEU:HA	1.66	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:B:499:LEU:O	2:B:948:HOH:O	2.22	0.41
1:A:328:PHE:C	1:A:330:ASP:H	2.24	0.41
1:A:10:LYS:HE3	2:A:1021:HOH:O	2.21	0.41
1:B:37:ASN:HA	1:B:37:ASN:HD22	1.56	0.41
1:A:449:LEU:H	1:A:449:LEU:HG	1.55	0.41
1:A:852:ASP:C	1:A:852:ASP:OD2	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:ARG:HH12	1:B:670:ARG:NH1	2.09	0.41
1:A:628:GLU:C	1:A:630:ARG:N	2.73	0.41
1:A:388:LYS:HZ2	1:A:482:GLU:HG2	1.86	0.41
1:B:413:LEU:O	1:B:471:GLU:HA	2.21	0.41
1:A:620:LYS:HB3	1:A:620:LYS:HE3	1.67	0.41
1:B:853:ASN:HB3	1:B:854:PHE:H	1.71	0.41
1:A:64:GLY:HA3	1:A:65:PRO:HD3	1.89	0.40
1:B:583:VAL:HG23	1:B:594:LEU:HD13	2.02	0.40
1:B:120:ILE:HD11	1:B:342:ASN:HD21	1.86	0.40
1:A:625:SER:O	1:A:626:ALA:C	2.54	0.40
1:A:223:ASP:CG	1:A:227:ILE:CD1	2.90	0.40
1:B:456:ALA:O	1:B:457:ASN:O	2.38	0.40
1:B:492:PRO:HB2	1:B:493:ASN:CG	2.42	0.40
1:A:353:LEU:C	1:A:354:ARG:HG2	2.42	0.40
1:B:438:VAL:CG2	1:B:484:ILE:HD11	2.47	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:B:696:TRP:CD2	1:B:700:SER:HB3	2.56	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:409:PHE:N	1:B:409:PHE:CD2	2.88	0.40
1:A:829:HIS:HE1	2:A:917:HOH:O	2.04	0.40
1:B:97:ILE:HD13	1:B:97:ILE:HG23	1.72	0.40
1:B:790:LYS:O	1:B:792:LEU:N	2.51	0.40
1:B:487:PRO:O	1:B:487:PRO:HG2	2.20	0.40
1:B:76:LYS:HD2	1:B:81:LEU:HD21	2.02	0.40
1:B:875:GLY:C	1:B:877:GLY:H	2.22	0.40
1:B:719:GLU:N	1:B:719:GLU:CD	2.75	0.40
1:A:159:PRO:C	1:A:160:THR:CG2	2.89	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:A:268:ASP:CG	1:A:269:ALA:H	2.19	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:390:ARG:NH1	1:B:392:GLU:OE1	2.53	0.40
1:B:440:ARG:N	1:B:440:ARG:CD	2.85	0.40
1:B:369:SER:OG	1:B:646:GLN:HG2	2.21	0.40
1:A:674:LEU:O	1:A:675:PHE:C	2.57	0.40
1:B:27:TYR:CE2	1:B:28:LEU:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:VAL:H	1:B:291:VAL:HG22	1.30	0.40
1:A:89:VAL:N	1:A:175:GLU:CD	2.68	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:B:468:ASN:O	1:B:468:ASN:CG	2.58	0.40
1:B:492:PRO:O	1:B:494:LYS:N	2.55	0.40
1:B:413:LEU:HD22	1:B:487:PRO:HB2	2.02	0.40
1:B:648:ILE:HG22	1:B:649:VAL:N	2.37	0.40
1:A:766:ILE:HD13	1:A:766:ILE:HG21	1.52	0.40
1:A:263:ALA:HB2	1:A:288:TRP:CZ3	2.56	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	1
1	B	748/900 (83%)	497 (66%)	146 (20%)	105 (14%)	0	1
All	All	1495/1800 (83%)	997 (67%)	289 (19%)	209 (14%)	0	1

All (209) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	VAL

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	459 (76%)	147 (24%)	1	2
1	B	584/782 (75%)	429 (74%)	155 (26%)	0	1
All	All	1190/1564 (76%)	888 (75%)	302 (25%)	1	2

All (302) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	MET
1	A	7	LYS
1	A	10	LYS
1	A	12	ARG
1	A	13	GLU
1	A	22	GLU
1	A	29	ASN
1	A	30	GLN
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	98	CYS
1	A	108	LEU

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Mol	Chain	Res	Type
1	A	115	THR
1	A	116	LEU
1	A	121	LEU
1	A	132	GLN
1	A	144	TRP
1	A	151	ASP
1	A	153	VAL
1	A	155	ASP
1	A	162	ASP
1	A	165	LEU
1	A	174	ASN
1	A	191	SER
1	A	201	SER
1	A	204	PHE
1	A	211	VAL
1	A	218	GLN
1	A	219	LYS
1	A	224	LEU
1	A	229	LEU
1	A	230	LYS
1	A	242	ILE
1	A	258	LEU
1	A	264	TYR
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	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

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Mol	Chain	Res	Type
1	A	352	THR
1	A	354	ARG
1	A	355	ASN
1	A	356	TRP
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	442	LEU
1	A	447	VAL
1	A	465	HIS
1	A	467	ILE
1	A	468	ASN
1	A	470	ARG
1	A	484	ILE
1	A	487	PRO
1	A	497	ASP
1	A	499	LEU
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	605	ARG
1	A	610	LEU
1	A	612	ILE
1	A	620	LYS
1	A	625	SER
1	A	628	GLU
1	A	630	ARG
1	A	639	LYS
1	A	643	GLN
1	A	647	VAL
1	A	656	GLU
1	A	658	ILE

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Mol	Chain	Res	Type
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	711	HIS
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
1	A	775	VAL
1	A	777	ASP
1	A	788	GLU
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	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

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Mol	Chain	Res	Type
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
1	B	84	ASN
1	B	86	GLN
1	B	90	ASP
1	B	97	ILE
1	B	111	ILE
1	B	113	SER
1	B	118	GLU
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	200	THR
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	265	SER
1	B	277	GLN
1	B	278	ARG
1	B	279	VAL
1	B	291	VAL

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Mol	Chain	Res	Type
1	B	296	PRO
1	B	298	SER
1	B	303	GLU
1	B	304	TRP
1	B	305	ASN
1	B	308	ASP
1	B	313	GLU
1	B	315	LEU
1	B	321	ASP
1	B	329	ARG
1	B	331	PHE
1	B	335	PHE
1	B	337	LYS
1	B	339	GLU
1	B	343	LEU
1	B	346	ASP
1	B	348	LEU
1	B	350	SER
1	B	359	THR
1	B	364	THR
1	B	375	ARG
1	B	376	ASN
1	B	378	PRO
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	399	ASP
1	B	401	ASP
1	B	405	SER
1	B	409	PHE
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	450	LYS
1	B	451	ARG

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Mol	Chain	Res	Type
1	B	455	LEU
1	B	457	ASN
1	B	462	GLN
1	B	464	GLU
1	B	468	ASN
1	B	472	VAL
1	B	490	PHE
1	B	493	ASN
1	B	494	LYS
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	580	ARG
1	B	584	ASN
1	B	598	GLU
1	B	607	ARG
1	B	614	ARG
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	670	ARG
1	B	674	LEU
1	B	684	GLU
1	B	688	THR
1	B	690	GLN
1	B	691	LEU
1	B	699	PHE

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Mol	Chain	Res	Type
1	B	701	VAL
1	B	702	LEU
1	B	724	ARG
1	B	726	PHE
1	B	739	GLU
1	B	741	SER
1	B	775	VAL
1	B	779	ASP
1	B	781	THR
1	B	784	LEU
1	B	789	PHE
1	B	790	LYS
1	B	797	LYS
1	B	806	PHE
1	B	831	ASN
1	B	837	MET
1	B	851	PHE
1	B	853	ASN
1	B	854	PHE
1	B	857	CYS
1	B	860	ARG
1	B	866	ARG
1	B	893	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	37	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

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Mol	Chain	Res	Type
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	878	GLN
1	A	884	GLN
1	A	888	GLN
1	B	21	HIS
1	B	37	ASN
1	B	47	GLN
1	B	66	ASN
1	B	99	GLN
1	B	140	HIS
1	B	142	GLN
1	B	174	ASN
1	B	243	ASN
1	B	257	ASN
1	B	277	GLN
1	B	280	ASN
1	B	286	ASN
1	B	342	ASN
1	B	437	GLN
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	874	ASN

5.3.3 RNA ⓘ

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 carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.35	5 (0%) 90 86	16, 49, 81, 98	0
1	B	788/900 (87%)	-0.32	11 (1%) 78 69	17, 51, 84, 102	0
All	All	1571/1800 (87%)	-0.33	16 (1%) 84 77	16, 50, 83, 102	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	587	ASP	3.8
1	B	596	LEU	3.8
1	A	596	LEU	3.4
1	B	712	TYR	3.3
1	B	402	SER	3.3
1	A	595	GLY	3.1
1	A	550	ILE	3.0
1	B	843	SER	3.0
1	A	70	THR	2.9
1	B	400	TYR	2.7
1	B	714	ASN	2.7
1	B	594	LEU	2.5
1	B	398	ASP	2.2
1	B	823	PHE	2.2
1	B	695	SER	2.1
1	A	522	PRO	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 carbohydrates 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.