



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 12:03 am BST

PDB ID : 1TWG
Title : RNA polymerase II complexed with CTP
Authors : Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2004-06-30
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

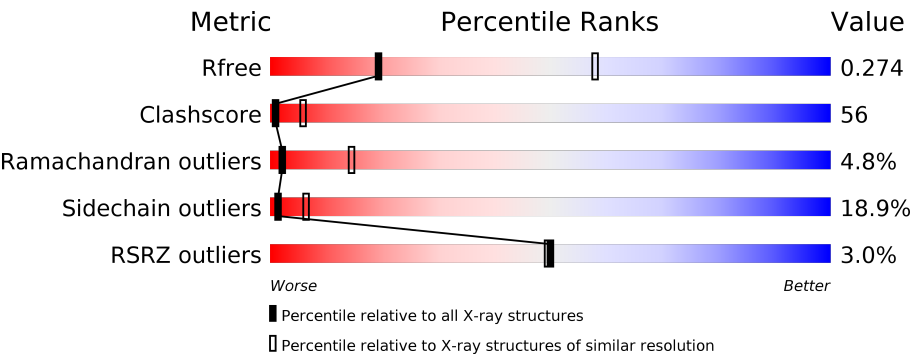
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	<div><div>2%</div><div>5%</div><div>34%</div><div>28%</div><div>11%</div><div>22%</div></div>
2	B	1224	<div><div>4%</div><div>6%</div><div>36%</div><div>33%</div><div>14%</div><div>11%</div></div>
3	C	318	<div><div>%</div><div>•</div><div>27%</div><div>39%</div><div>13%</div><div>16%</div></div>
4	E	215	<div><div>2%</div><div>7%</div><div>29%</div><div>46%</div><div>18%</div></div>
5	F	155	<div><div>%</div><div>•</div><div>24%</div><div>20%</div><div>6%</div><div>46%</div></div>
6	H	146	<div><div>4%</div><div>•</div><div>24%</div><div>30%</div><div>34%</div><div>9%</div></div>

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Mol	Chain	Length	Quality of chain
7	I	122	
8	J	70	
9	K	120	
10	L	70	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	ZN	J	3001	-	-	X	-
12	ZN	L	3005	-	-	X	-
13	CTP	B	3008	X	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 27731 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 DNA-directed RNA polymerase II largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1349	Total	C	N	O	S	0	0	0
			10606	6692	1839	2017	58			

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1091	Total	C	N	O	S	0	0	0
			8690	5511	1516	1610	53			

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	215	Total	C	N	O	S	0	0	0
			1760	1116	310	322	12			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	83	Total	C	N	O	S	0	0	0
			670	428	114	125	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II 14.2 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	121	Total	C	N	O	S	0	0	0
			990	610	181	188	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	64	Total	C	N	O	S	0	0	0
			525	334	92	93	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 11 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total	Mn	0	0
			2	2		

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

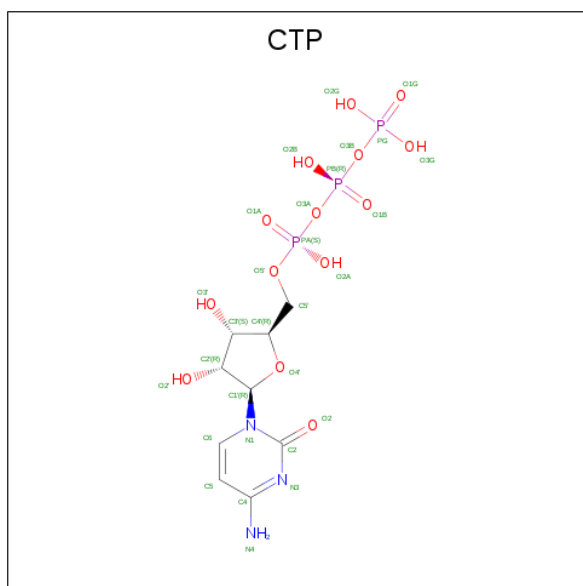
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	J	1	Total	Zn	0	0
			1	1		
12	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	I	2	Total	Zn	0	0
			2	2		
12	C	1	Total	Zn	0	0
			1	1		
12	A	2	Total	Zn	0	0
			2	2		
12	L	1	Total	Zn	0	0
			1	1		

- Molecule 13 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	N	O	P	0	0
			29	9	3	14	3		

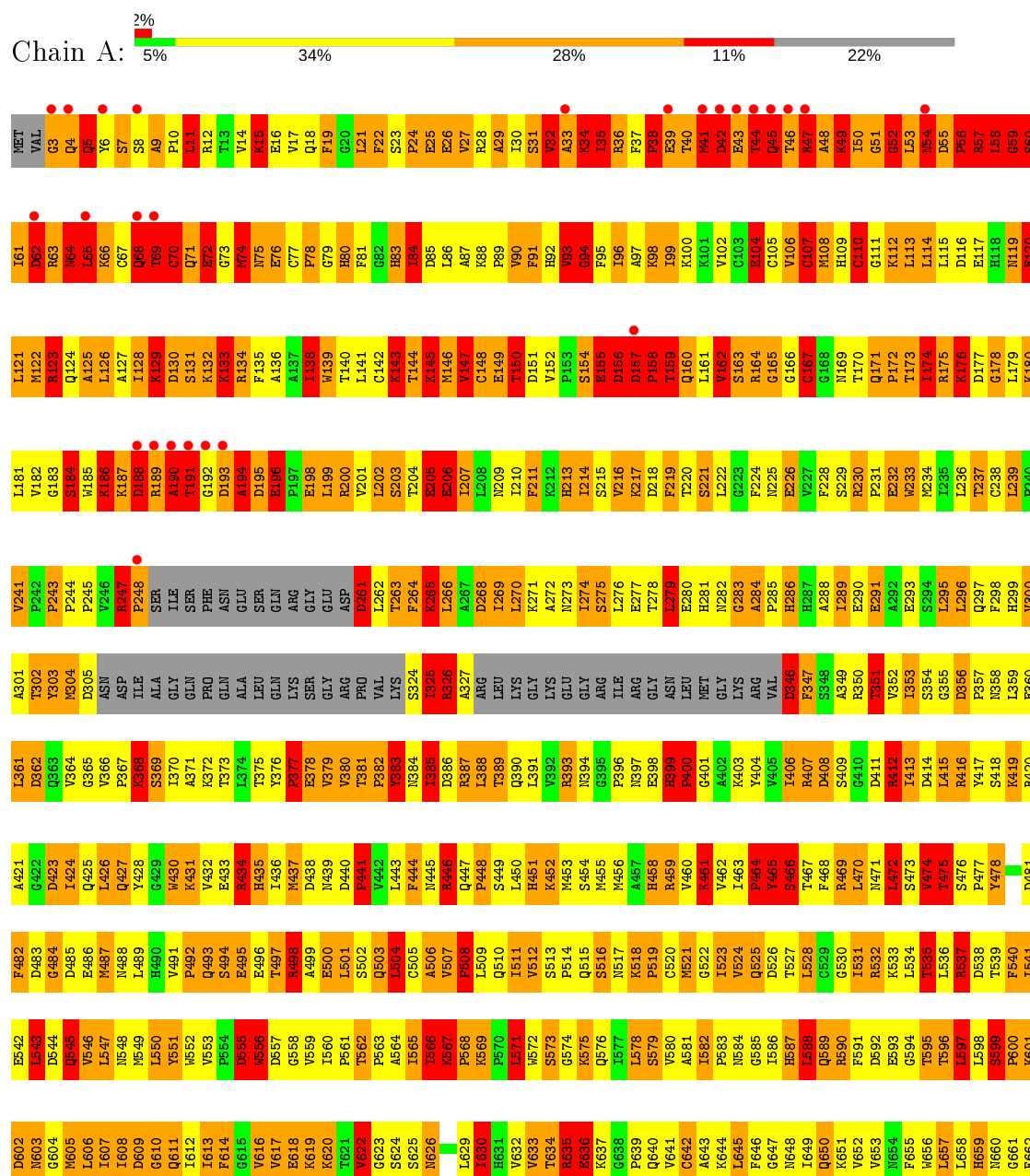
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	2	Total	O	0	0
			2	2		
14	B	3	Total	O	0	0
			3	3		

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

- Molecule 1: DNA-directed RNA polymerase II largest subunit



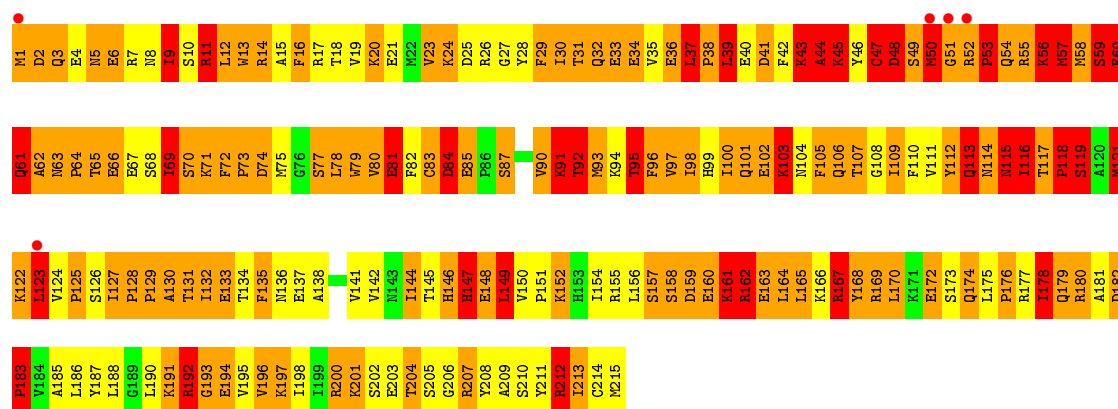
TYR	SER	THR	GLY	GLY	THR	ARG	R1326	T1266	K1205	S1145	PHE	R1023	I963	N903	K843	T783	N723	S663
PRO	THR	PRO	GLY	THR	GLY	HIS	I1327	M1267	D1206	V1146	HIS	S1024	I964	T904	A844	L784	E724	T664
THR	SER	THR	PHE	THR	PHE	PHE	Y1328	E1268	L1207	T1147	PHE	L1026	I965	D905	L845	P785	A725	G665
SER	SER	TYR	ALA	ASN	ALA	ALA	T1329	E1269	M1208	T1148	ALA	L1026	I966	R906	E846	H786	R726	G666
PRO	PRO	SER	S1330	T1270	ASN	ASN	S1331	I1271	M1209	S1149	GLY	A1027	A967	T907	D847	S788	K728	G667
SER	SER	PRO	T1332	T1272	ARG	ARG	T1332	T1272	Q1210	S1150	VAL	T1028	Q968	L908	L848	K789	A729	D668
TYR	THR	THR	T1333	T1273	ASN	ASN	T1333	T1273	Q1211	E1151	SER	R1029	Q969	D909	M849	D790	G730	A670
SER	SER	THR	D1334	R1274	THR	THR	D1334	R1274	K1213	T1152	K1092	V1031	F971	S911	H851	R731	R731	L671
PRO	PRO	PRO	T1335	G1275	GLY	GLY	T1335	G1275	R1214	E1153	K1093	L1032	H972	L912	Y852	L732	L732	D672
THR	THR	THR	M1336	G1276	ALA	ALA	R1215	G1276	R1215	D1154	V1094	Q1033	S793	S793	D853	A733	A733	G673
SER	SER	TYR	E1337	E1277	LEU	LEU	E1337	E1277	L1216	P1156	T1095	E1034	D974	E914	M854	P784	E734	P674
PRO	PRO	SER	V1338	I1278	MET	MET	V1338	I1278	K1217	D1157	T1096	L1035	H975	S915	T855	V735	V735	T675
SER	SER	PRO	L1339	I1279	ARG	ARG	L1339	I1279	K1217	P1158	G1097	R1036	T976	G916	T856	M736	M736	M676
TYR	TYR	THR	G1340	E1280	CYS	CYS	G1340	E1280	F1220	R1159	V1098	L1037	K977	S917	R857	K737	L737	R677
SER	SER	THR	T1341	E1281	SER	SER	T1341	E1281	K1221	S1160	V1098	T1038	P978	E918	M858	K738	K738	E678
PRO	PRO	PRO	E1342	V1282	PHE	PHE	E1342	V1282	M1222	T1161	K1099	Q1039	S979	L919	S859	F799	D739	R679
THR	THR	THR	L1343	G1283	GLY	GLY	L1343	G1283	D1223	E1162	L1101	R1040	D980	L920	L860	V800	L740	T680
SER	SER	TYR	G1344	M1284	GLY	GLY	G1344	M1284	L1224	T1163	K1102	A1041	L981	G921	G861	E801	K741	E681
PRO	PRO	SER	R1345	M1285	ALA	ALA	R1345	M1285	F1225	P1164	E1103	F1042	T982	D922	M862	M802	M742	T682
SER	SER	PRO	A1346	T1286	GLN	GLN	A1346	T1286	V1226	E1165	E1104	D1043	L983	L923	S863	S803	V743	T683
TYR	TYR	THR	E1407	Y1287	GLY	GLY	E1407	Y1287	I1227	D1166	L1105	D1044	K984	K924	M864	K744	K744	A684
SER	SER	SER	I1408	D1288	GLY	GLY	I1408	D1288	W1228	E1167	N1106	W1045	D985	L925	Q865	L805	Q745	E685
PRO	PRO	PRO	Y1409	R1289	ALA	ALA	Y1409	R1289	S1229	E1168	V1107	L1046	I986	Q926	F866	R806	M746	A686
THR	THR	THR	F1410	K1290	GLY	GLY	F1410	K1290	E1230	I1169	V1107	S1047	V987	V927	T867	G807	V747	K687
SER	SER	TYR	E1411	V1291	THR	THR	E1411	V1291	D1231	T1170	K1108	M1048	L988	L928	M868	L808	M748	K688
PRO	PRO	SER	V1352	P1292	SER	SER	V1352	P1292	M1232	L1171	M1110	I1049	G989	L929	G869	T809	A749	K689
SER	SER	PRO	G1413	S1293	GLY	GLY	G1413	S1293	D1233	Q1172	M1111	O1050	V990	D930	E870	P810	G750	V690
TYR	TYR	THR	A1414	T1294	ALA	ALA	A1414	T1294	E1234	R1173	K1112	A1051	K991	E931	D871	Q811	K751	L691
SER	SER	SER	S1415	T1295	ASN	ASN	S1415	T1295	K1235	PHE	T1113	Q1052	D992	E932	G872	E812	K752	D692
PRO	PRO	PRO	A1416	G1296	GLY	GLY	A1416	G1296	L1236	GLY	P1114	F1053	L993	V933	M873	F813	G753	V693
THR	THR	SER	E1417	E1297	SER	SER	E1417	E1297	I1237	L1176	S1115	L1054	Q994	K934	D874	F814	S754	T694
SER	SER	TYR	L1418	Y1298	LEU	LEU	L1418	Y1298	I1238	LEU	L1116	L1055	E995	Q935	A875	F815	F755	K695
PRO	PRO	SER	D1419	T1299	GLY	GLY	D1419	T1299	R1239	ASP	T1117	S1056	N996	L936	A876	H816	I756	K696
ALA	ALA	PRO	G1360	K1300	GLY	GLY	G1360	K1300	C1240	GLY	V1118	V1057	L997	V937	H877	M818	M757	A697
TYR	TYR	THR	E1361	E1301	GLY	GLY	E1361	E1301	R1241	ALA	Y1119	V1058	L998	K938	I878	G819	I758	Q698
SER	SER	SER	Y1362	P1302	ALA	ALA	Y1362	P1302	V1242	GLY	L1120	H1059	V999	D939	E879	G819	A759	A699
PRO	PRO	PRO	V1363	E1303	GLY	GLY	V1363	E1303	V1243	GLY	E1121	P1060	L1000	R940	K880	G820	Q760	I700
THR	THR	SER	M1364	W1304	GLN	GLN	M1364	W1304	ARG	GLN	P1122	G1061	K1001	F942	Q881	R821	M761	L701
SER	SER	TYR	E1365	V1305	SER	SER	E1365	V1305	PRO	SER	G1123	E1062	G1002	P942	S882	E822	S762	L702
PRO	PRO	PRO	R1366	L1306	PHE	PHE	R1366	L1306	LYS	ASP	G1123	M1063	K1003	L943	L883	G823	A763	T703
TYR	TYR	THR	N1427	E1307	SER	SER	N1427	E1307	SER	ASP	A1126	V1064	N1004	R944	D884	L824	V765	K705
SER	SER	SER	V1428	T1308	LEU	LEU	V1428	T1308	LEU	Q1187	D1127	G1065	E1005	E945	T885	I825	V765	K706
PRO	PRO	PRO	E1429	D1309	ASP	ASP	E1429	D1309	ASP	Q1188	Q1128	V1066	I1006	V946	I886	D826	Q766	G707
THR	THR	SER	L1370	G1310	ALA	ALA	L1370	G1310	ALA	S1189	E1129	L1067	I1007	F947	G887	T827	Q767	
PRO	PRO	SER	T1371	V1311	GLY	GLY	T1371	V1311	GLY	P1190	Q1130	A1068	Q1008	V948	G888	A828	Q768	
SER	SER	TYR	V1372	N1312	THR	THR	V1372	N1312	THR	W1191	A1131	A1069	N1009	D949	S889	V829	S769	T709
PRO	PRO	SER	D1373	L1313	GLY	GLY	D1373	L1313	GLY	L1192	K1132	A1010	G950	E951	D890	K830	V770	L710
SER	SER	PRO	V1374	S1314	GLY	GLY	V1374	S1314	GLY	L1193	Q1071	Q1070	A1011	E951	A891	T831	E771	R711
TYR	TYR	TYR	M1375	E1315	GLY	GLY	M1375	E1315	GLY	R1194	I1134	I1072	R1012	A952	A892	A832	G772	E712
SER	SER	SER	T1376	V1316	E1256	E1256	T1376	V1316	E1256	L1195	I1134	G1073	D1013	N953	F893	E833	K773	S713
PRO	PRO	PRO	T1377	M1317	D1257	D1257	T1377	M1317	D1257	L1196	S1136	A1014	N954	W954	E894	T834	R774	F714
THR	THR	THR	Q1378	T1318	H1258	H1258	Q1378	T1318	H1258	E1197	E1137	T1077	T1015	P955	K895	G835	I775	E715
SER	SER	TYR	G1379	V1319	M1259	M1259	G1379	V1319	M1259	D1198	I1138	Q1078	T1016	L956	R896	V836	A776	F716
PRO	PRO	SER	E1380	G1320	GLY	GLY	E1380	G1320	GLY	R1199	E1139	M1079	F1017	P957	Y887	I837	F777	N717
SER	SER	PRO	G1381	P1321	K1261	K1261	G1381	P1321	K1261	A1200	H1140	M1079	F1018	Y858	Y888	Q838	G778	
TYR	TYR	THR	T1382	I1322	K1262	K1262	T1382	I1322	K1262	A1201	H1140	T1080	C1019	N959	V899	R839	F779	
SER	SER	PRO	S1383	T1323	E1263	E1263	S1383	T1323	E1263	M1202	T1142	T1081	C1020	I960	D900	R840	V780	R720
PRO	PRO	PRO	V1384	P1324	I1264	I1264	V1384	P1324	I1264	M1203	T1142	ASN	L1143	R961	L901	L841	D781	F721
THR	THR	SER	T1385	T1325	N1265	N1265	T1385	T1325	N1265	D1204	K1144	THR	L1022	R962	L902	V842	R782	L722

SER	PRO	SER	SER	TYR	LEU	SER	PRO	THR	SER	PRO	ASN	ASN	ARG
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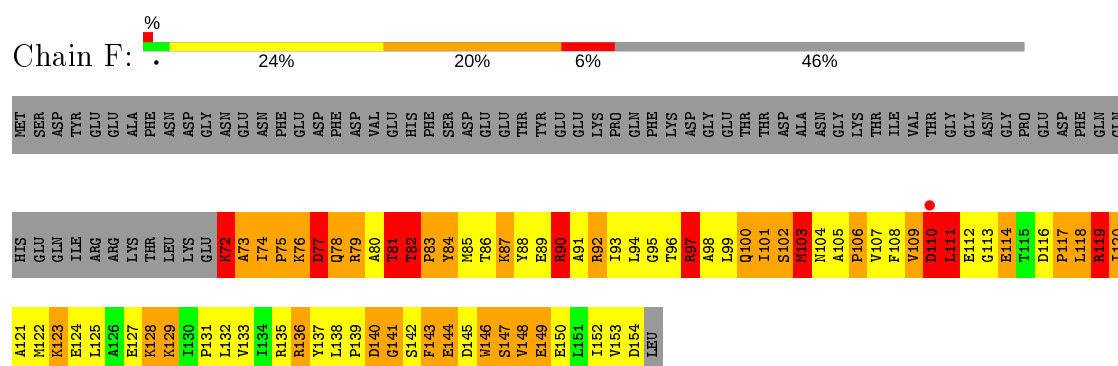
• Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide



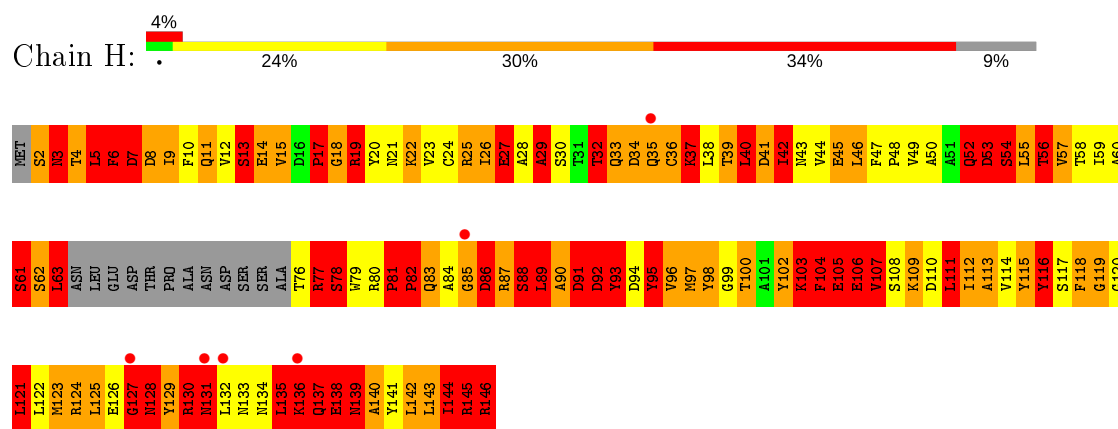
L663	L603	S543	L483	K423	H363	C302	S242	L181	M121	D61	MET
T664	R604	C544	M484	L424	T364	Y303	A243	S182	L122	I62	SER
T665	R605	T545	R485	L425	T365	D304	A244	S183	T244	I63	ASP
T666	K606	S546	Y486	K426	D366	Y305	K246	A184	Y124	C64	LEU
T667	G607	S547	T487	D427	L367	D307	K245	T185	K245	E65	ALA
T668	G548	G548	Y488	I428	E368	K308	G247	E186	S126	D66	ASN
I669	L609	T549	S489	F429	G369	K309	R249	S187	G127	S67	SER
GLU	M610	D540	S490	R430	F370	Q309	R248	D188	R248	T68	GLU
GLY	P611	P551	T491	Y431	E371	L311	F250	L189	F129	L69	LVS
GLY	E612	M552	L492	M432	S372	L312	T251	Y190	Y130	I70	TYR
PHE	V613	P553	S493	Q433	R373	E312	S252	K191	D131	LEU	TYR
GLU	S614	P554	H494	R434	K374	K313	T253	L192	Y132	GLU	ASP
ASP	M615	I555	L495	T435	A375	L314	L254	K193	K133	GLN	GLU
VAL	L616	T556	R496	V436	F376	K315	Q255	K194	K134	LEU	ASP
GLU	R617	F557	R497	E437	F377	P316	V256	C195	R135	ALA	PRO
E678	D618	L558	T498	GLU	L378	C317	K257	P196	T136	GLN	GLY
V679	L619	S559	M499	ALA	G379	V318	L258	F197	Y137	HIS	TYR
T680	R620	E560	T500	HIS	Y380	E319	Y259	D198	E138	THR	F18
M681	E621	M561	P501	ASP	K381	ASP	G260	M199	ALA	THR	E19
E742	E622	G562	I502	PHE	I382	G321	R261	G200	I1E	GLU	E19
E743	E623	M563	GLY	ASN	N383	G322	E262	Y201	ILE	SER	E21
H744	L624	E564	ARG	MTT	R384	V323	G263	G202	VAL	ASP	E22
P745	K625	P565	ASP	LVS	L385	L324	S264	F203	PRD	ASN	A23
M686	K626	L566	GLY	L446	L386	Q325	S265	I204	GLY	ILE	P24
E687	F627	E567	LVS	A447	L387	R326	A266	I205	ARG	SER	T25
M688	T628	D568	LEU	L448	C388	R327	R267	M206	GLU	ARG	T26
L689	D629	Y569	A509	M449	A389	E328	T268	GLU	LEU	LVS	A27
Y690	A630	W570	K510	A450	L390	T329	L269	S208	LVS	TYR	E28
E691	G631	P571	P511	K451	D391	A330	K270	E209	TYR	E29	D29
T692	R632	H572	R512	T452	R392	L331	A271	K210	GLU	I90	S30
L693	P633	Q573	Q513	T453	K393	D332	T272	V211	LEU	S91	K31
D694	Y634	S574	L514	T454	D394	L273	T273	L213	ILE	P92	A32
A695	R635	P575	H515	S455	K395	K213	P274	A124	ALA	G93	V33
E696	P636	D576	N516	G456	D396	R336	Y275	A214	GLU	K94	I34
E697	L637	A577	T517	L457	R397	R337	I276	Q215	GLU	I95	S35
E698	P638	T578	H518	K458	R398	G338	K277	E216	SER	Y96	A36
R699	G820	R579	M519	Y459	D399	T339	Q278	R217	GLU	F97	F37
W700	P640	V580	G520	A460	H400	A340	D279	ASP	ASP	T98	F38
L701	E641	F581	L521	A461	F401	L341	I280	ASP	ASP	K99	R39
L702	D642	V582	V522	A462	G402	G342	P281	N221	SER	P100	E40
L703	D643	M583	C523	T463	K403	I343	I282	L222	GLU	M101	K41
A704	E644	G584	P524	G464	K404	K344	R283	V223	SER	Y102	G42
M705	S645	V585	A525	M465	L405	K345	I284	Q224	GLY	M103	L43
T706	L646	M586	E526	V466	L406	E346	F286	V225	K164	E104	V44
E707	G647	H587	T527	G467	D407	K347	R287	K227	S45	S105	F45
T708	H648	G588	P528	GLU	L408	R348	K287	F166	F166	D106	A46
D709	K649	V589	E529	GLU	A409	I349	A288	K228	I167	G107	A47
T710	E650	H590	G530	LVS	G410	Q350	L289	E238	I167	T108	L48
L711	L651	R591	Q531	LVS	F411	K351	G290	K230	R169	T109	D49
P712	K652	A532	A532	ALA	L412	I291	G291	E231	R169	H110	S50
ALA	V653	P593	C533	MTT	L413	K353	I292	S232	P171	A111	F51
GLU	R654	A594	G534	ALA	A414	D354	P293	P233	M172	L112	N52
ALA	K655	R595	L535	SER	D415	I355	D294	T234	M173	Y113	O53
ASN	G656	L596	V536	ARG	L416	L356	G295	S235	L174	P114	F54
GLU	H657	M597	K537	A477	F417	Q357	E296	H236	R175	Q115	V55
GLU	T658	E598	N538	G478	K418	K358	I297	V237	S176	E116	D56
ASN	R659	T599	L539	V479	T419	E359	L298	K177	K177	A117	T57
ASP	K660	L600	S540	A480	L420	F360	E299	E238	M178	R118	S58
L761	L661	R601	Q481	A481	F421	L361	H300	E239	H300	L179	T59
L762	M662	T602	M642	V492	F422	P262	T301	E240	C159	E120	D60
L763	R663	H603	L643	V493	F423	P263	T302	E241	C160	E121	D61
L764	R664	H604	L644	V494	F424	P264	T303	E242	C161	E122	D62
L765	R665	H605	L645	V495	F425	P265	T304	E243	C162	E123	D63
L766	R666	H606	L646	V496	F426	P266	T305	E244	C163	E124	D64
L767	R667	H607	L647	V497	F427	P267	T306	E245	C164	E125	D65
L768	R668	H608	L648	V498	F428	P268	T307	E246	C165	E126	D66
L769	R669	H609	L649	V499	F429	P269	T308	E247	C166	E127	D67
L770	R670	H610	L650	V500	F430	P270	T309	E248	C167	E128	D68
L771	R671	H611	L651	V501	F431	P271	T310	E249	C168	E129	D69
L772	R672	H612	L652	V502	F432	P272	T311	E250	C169	E130	D70
L773	R673	H613	L653	V503	F433	P273	T312	E251	C170	E131	D71
L774	R674	H614	L654	V504	F434	P274	T313	E252	C171	E132	D72
L775	R675	H615	L655	V505	F435	P275	T314	E253	C172	E133	D73
L776	R676	H616	L656	V506	F436	P276	T315	E254	C173	E134	D74
L777	R677	H617	L657	V507	F437	P277	T316	E255	C174	E135	D75
L778	R678	H618	L658	V508	F438	P278	T317	E256	C175	E136	D76
L779	R679	H619	L659	V509	F439	P279	T318	E257	C176	E137	D77
L780	R680	H620	L660	V510	F440	P280	T319	E258	C177	E138	D78
L781	R681	H621	L661	V511	F441	P281	T320	E259	C178	E139	D79
L782	R682	H622	L662	V512	F442	P282	T321	E260	C179	E140	D80
L783	R683	H623	L663	V513	F443	P283	T322	E261	C180	E141	D81
L784	R684	H624	L664	V514	F444	P284	T323	E262	C181	E142	D82
L785	R685	H625	L665	V515	F445	P285	T324	E263	C182	E143	D83
L786	R686	H626	L666	V516	F446	P286	T325	E264	C183	E144	D84
L787	R687	H627	L667	V517	F447	P287	T326	E265	C184	E145	D85
L788	R688	H628	L668	V518	F448	P288	T327	E266	C185	E146	D86
L789	R689	H629	L669	V519	F449	P289	T328	E267	C186	E147	D87
L790	R690	H630	L670	V520	F450	P290	T329	E268	C187	E148	D88
L791	R691	H631	L671	V521	F451	P291	T330	E269	C188	E149	D89
L792	R692	H632	L672	V522	F452	P292	T331	E270	C189	E150	D90
L793	R693	H633	L673	V523	F453	P293	T332	E271	C190	E151	D91
L794	R694	H634	L674	V524	F454	P294	T333	E272	C191	E152	D92
L795	R695	H635	L675	V525	F455	P295	T334	E273	C192	E153	D93
L796	R696	H636	L676	V526	F456	P296	T335	E274	C193	E154	D94
L797	R697	H637	L677	V527	F457	P297	T336	E275	C194	E155	D95
L798	R698	H638	L678	V528	F458	P298	T337	E276	C195	E156	D96
L799	R699	H639	L679	V529	F459	P299	T338	E277	C196	E157	D97
Q800	R807	S746	M886	P745	T738	G800	F746	T739	F738	T737	GLY
A808	R808	S747	M887	P746	T739	G801	F747	T740	F739	T738	GLY
M809	R809	S748	M888	P747	T740	G802	F748	T741	F740	T739	GLY
E810	R810	S749	M889	P748	T741	G803	F749	T742	F741	T740	GLY
Y811	R811	G750	Y811	W751	T751	G804	F750	T752	F742	T741	GLY
L812	R812	H751	P812	K451	D391	A330	K270	E209	TYR	E29	D29
K813	R813	H572	R512	T452	R392	L331	A271	K210	GLU	I90	S30
R814	R814	S573	Q513	T453	K393	D332	T272	V211	LEU	S91	K31
F815	R815	S574	L514	T454	D394	L273	T273	L213	ILE	P92	A32
T816	R816	P575	H515	S455	K395	K213	P274	A124	ALA	G93	V33
L817	R817	T566	N516	G456	D396	R336	Y275	A214	GLU	K94	I34
P818	R818	E697	T517	L457	R397	R337	I276	Q215	GLU	I95	S35
A819	R819	T578	H518	K458	R398	G338	K277	E216	SER	Y96	A36
G820	R820	R579	M519	Y459	D399	T339	Q278	R217	GLU	F97	F37
E821	R821	W700	P640	V580	G520	A340	D279	ASP	ASP	T98	F38
F822	R822	L701	E641	F581	L521	A461	I280	ASP	ASP	K99	R39
L823	R823	L702	D642	V582	V522	A462	P281	N221	SER	P100	E40
T824	R824	L703	D643	M583	C523	T463	I282	L222	GLU	M101	K41
R825	R825	S764	E644	G584	P524	K344	R283	V223	SER	Y102	G42
P765	R765	M705	S645	V585	A525	K345	I284	Q224	GLY	M103	L43
L827	R766	T706	L646	M586	E526	K346	F286	V225	K164	E104	V44
A828	R767	E707	G647	H587	T527	D407	R287	K227	S45	S105	F45
C829	R768	T708	H648	G588	P528	R348	K287	F166	F166	D106	A46
Y830	R769	D709	K649	V589	E529	I349	A288	K228	I167	G107	A47
S831	R770	T710	E650	H590	G530	Q350	L289	E238	I167	T108	L48
G832	R771	L711	L651	R591	Q531	LVS	G290	K230	R169	T109	D49
A772	R772	P712	K652	A532	A532	ALA	G291	E231	R169	H110	S50
K834	R773	ALA	V653	P593	C533	MTT	I292	S232	P171	A111	F51
Q835	R774	GLU	R654	A594	G534	ALA	P293	P233	M172	L112	N52
K836	R775	ALA	K655	R595	L535	SER	D294	T234			



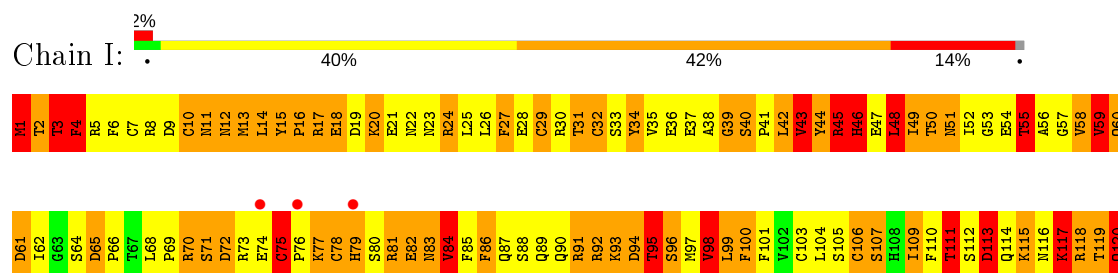
- Molecule 5: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



- Molecule 6: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



- Molecule 7: DNA-directed RNA polymerase II 14.2 kDa polypeptide



F121
SER

- Molecule 8: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide

Chain J: 

R1 I2 V3 P4 B5 C7 F8 S9 C10 G11 K12 V13 V14 G15 K17 W18 E19 S20 L22 N23 L24 L25 Q26 E27 D28 E29 L30 D31 E32 G33 T34 A35 L36 S37 E38 L39 G40 L41 K42 R43 Y44 C45 C46 R47 R48 Y49 I50 L51 T52 H53 V54 D55 L56 I57 E58 K59 F60

L61 R62 Y63 P64 P65 LEU GLU LYS ARG ASP

- Molecule 9: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K: 

R1 R2 A3 P4 D5 R6 F7 E8 L9 L11 L12 G13 E14 G15 E16 S17 K18 L19 K20 I21 D22 P23 D24 T25 K26 A27 P28 N29 A30 V31 V32 I33 T34 F35 N36 E37 K37 E38 D39 H40 T41 L42 G43 N44 L45 I46 R47 A48 E49 N50 L51 N52 D53 R54 K55 V56 L57 F58 Y61

K62 V63 E64 H65 P66 F67 F68 A69 R70 F71 F72 L73 R74 I75 Q76 T77 T78 E79 G80 Y81 D82 P83 K84 D85 A86 L87 K88 P89 A90 N91 S92 I93 I94 N95 N96 K97 L98 G99 A100 L101 K102 T103 N104 F105 E106 T107 E108 N109 N110 L111 Q112 T113 L114 ALA ALA ASP ASP ALA PHE

- Molecule 10: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide

Chain L: 

MET SER ARG GLU GLY PHE GLN ILE PRO THR ASN LEU ASP ALA ALA ALA ALA THR SER GLN ALA ARG THR A25 T26 L27 F28 Y29 I30 C31 A32 E33 C34 S35 S36 K37 L38 S39 L40 S41 R42 T43 D44 A45 V46 R47 C48 K49 D50 C51 G52 H53 R54 I55 L56 L57 K58 A59 R60

T61 R62 R63 L64 Y65 Q66 F67 E68 A69 R70

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.00Å 223.00Å 374.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30 39.42 – 3.29	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.30) 93.0 (39.42-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.32Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.263 , 0.281 0.214 , 0.274	Depositor DCC
R_{free} test set	2324 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	27731	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MN, CTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	4.63	2498/10792 (23.1%)	3.14	1255/14601 (8.6%)
2	B	4.65	2069/8860 (23.4%)	3.12	1000/11945 (8.4%)
3	C	4.80	513/2133 (24.1%)	3.12	254/2891 (8.8%)
4	E	4.70	404/1796 (22.5%)	3.05	209/2416 (8.7%)
5	F	4.16	139/682 (20.4%)	2.87	60/922 (6.5%)
6	H	4.56	229/1086 (21.1%)	3.04	130/1470 (8.8%)
7	I	5.31	288/1009 (28.5%)	3.40	147/1357 (10.8%)
8	J	4.28	125/533 (23.5%)	3.41	78/715 (10.9%)
9	K	4.50	226/937 (24.1%)	3.21	126/1265 (10.0%)
10	L	5.07	98/366 (26.8%)	3.32	59/485 (12.2%)
All	All	4.66	6589/28194 (23.4%)	3.14	3318/38067 (8.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	69
2	B	0	59
3	C	0	19
4	E	0	9
6	H	0	15
7	I	0	9
8	J	0	2
9	K	0	5
10	L	0	4
All	All	0	191

All (6589) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	564	GLU	CD-OE1	30.56	1.59	1.25
7	I	34	TYR	CD1-CE1	-29.71	0.94	1.39
1	A	1234	GLU	CD-OE1	29.21	1.57	1.25
7	I	34	TYR	CE2-CZ	-28.02	1.02	1.38
1	A	728	LYS	CD-CE	27.41	2.19	1.51
2	B	598	GLU	CG-CD	26.74	1.92	1.51
2	B	194	GLU	CD-OE1	26.64	1.54	1.25
4	E	162	ARG	NE-CZ	26.42	1.67	1.33
1	A	364	VAL	CB-CG1	-26.20	0.97	1.52
10	L	68	GLU	CG-CD	26.02	1.91	1.51
4	E	66	GLU	CD-OE2	25.40	1.53	1.25
2	B	529	GLU	CD-OE2	24.95	1.53	1.25
2	B	194	GLU	CD-OE2	24.81	1.52	1.25
3	C	166	GLU	CD-OE2	24.80	1.52	1.25
1	A	1277	GLU	CD-OE2	24.25	1.52	1.25
2	B	641	GLU	CG-CD	24.14	1.88	1.51
1	A	1280	GLU	CD-OE2	23.93	1.51	1.25
6	H	104	PHE	CE2-CZ	23.73	1.82	1.37
7	I	34	TYR	CE1-CZ	-23.66	1.07	1.38
1	A	932	GLU	CD-OE2	23.59	1.51	1.25
2	B	552	MET	CG-SD	23.35	2.41	1.81
2	B	305	VAL	CB-CG1	23.17	2.01	1.52
1	A	496	GLU	CD-OE1	23.02	1.50	1.25
3	C	209	TYR	CD2-CE2	22.93	1.73	1.39
2	B	346	GLU	CG-CD	22.66	1.85	1.51
1	A	1277	GLU	CG-CD	22.48	1.85	1.51
1	A	932	GLU	CD-OE1	22.36	1.50	1.25
1	A	16	GLU	CD-OE2	22.24	1.50	1.25
2	B	650	GLU	CD-OE2	21.73	1.49	1.25
1	A	1230	GLU	CD-OE1	21.62	1.49	1.25
1	A	1358	SER	CB-OG	21.62	1.70	1.42
1	A	734	GLU	CD-OE2	21.50	1.49	1.25
1	A	752	LYS	CE-NZ	21.29	2.02	1.49
2	B	690	VAL	CB-CG1	-21.29	1.08	1.52
1	A	162	VAL	CB-CG2	21.24	1.97	1.52
1	A	771	GLU	CD-OE2	21.19	1.49	1.25
1	A	1307	GLU	CD-OE1	21.15	1.49	1.25
2	B	239	GLU	CD-OE2	20.80	1.48	1.25
3	C	122	SER	CB-OG	20.77	1.69	1.42
4	E	20	LYS	CE-NZ	20.72	2.00	1.49
6	H	19	ARG	CG-CD	20.55	2.03	1.51
3	C	50	GLU	CG-CD	20.54	1.82	1.51
1	A	801	GLU	CD-OE1	20.50	1.48	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	133	GLU	CD-OE1	20.48	1.48	1.25
2	B	346	GLU	CD-OE1	20.31	1.48	1.25
1	A	705	LYS	CB-CG	20.15	2.06	1.52
7	I	54	GLU	CD-OE1	20.12	1.47	1.25
2	B	723	VAL	CB-CG1	20.08	1.95	1.52
4	E	57	MET	SD-CE	19.84	2.88	1.77
2	B	598	GLU	CD-OE2	19.83	1.47	1.25
1	A	681	GLU	CD-OE2	19.78	1.47	1.25
2	B	1023	VAL	CB-CG1	-19.70	1.11	1.52
2	B	870	ILE	CA-CB	19.69	2.00	1.54
1	A	205	GLU	CD-OE1	19.67	1.47	1.25
1	A	1230	GLU	CD-OE2	19.66	1.47	1.25
2	B	39	ARG	NE-CZ	19.65	1.58	1.33
1	A	555	ASP	CB-CG	19.62	1.93	1.51
9	K	61	TYR	CE1-CZ	-19.56	1.13	1.38
1	A	934	LYS	CD-CE	19.46	2.00	1.51
1	A	1015	VAL	CB-CG2	-19.39	1.12	1.52
2	B	370	PHE	CD1-CE1	19.37	1.77	1.39
1	A	1135	ARG	CG-CD	19.35	2.00	1.51
1	A	620	LYS	CD-CE	19.26	1.99	1.51
3	C	154	LYS	CD-CE	19.23	1.99	1.51
2	B	226	PHE	CD1-CE1	19.21	1.77	1.39
3	C	210	GLU	CD-OE1	19.16	1.46	1.25
6	H	139	ASN	CB-CG	19.15	1.95	1.51
1	A	895	LYS	CD-CE	19.14	1.99	1.51
2	B	621	GLU	CD-OE2	19.10	1.46	1.25
1	A	291	GLU	CG-CD	19.10	1.80	1.51
2	B	436	VAL	CA-CB	19.10	1.94	1.54
1	A	81	PHE	CE2-CZ	-19.02	1.01	1.37
1	A	149	GLU	CD-OE1	18.99	1.46	1.25
1	A	1119	TYR	CE2-CZ	-18.98	1.13	1.38
1	A	593	GLU	C-O	18.97	1.59	1.23
1	A	653	VAL	CB-CG2	-18.97	1.13	1.52
1	A	196	GLU	CG-CD	18.95	1.80	1.51
2	B	996	ARG	CZ-NH1	18.91	1.57	1.33
2	B	239	GLU	CG-CD	18.83	1.80	1.51
7	I	34	TYR	CB-CG	18.80	1.79	1.51
7	I	28	GLU	CD-OE1	18.77	1.46	1.25
1	A	1304	TRP	CE3-CZ3	-18.73	1.06	1.38
2	B	368	GLU	CG-CD	18.66	1.79	1.51
1	A	518	LYS	CD-CE	18.63	1.97	1.51
1	A	734	GLU	CD-OE1	18.61	1.46	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1083	ALA	CA-CB	-18.61	1.13	1.52
2	B	186	GLU	CD-OE2	18.56	1.46	1.25
1	A	941	LYS	CD-CE	18.56	1.97	1.51
1	A	1446	ASP	CB-CG	18.52	1.90	1.51
2	B	1153	GLU	CD-OE2	18.42	1.46	1.25
9	K	61	TYR	CE2-CZ	-18.37	1.14	1.38
1	A	117	GLU	CD-OE1	18.35	1.45	1.25
7	I	22	ASN	C-O	18.28	1.58	1.23
2	B	312	GLU	CD-OE2	18.16	1.45	1.25
2	B	945	GLU	CD-OE1	18.15	1.45	1.25
8	J	42	LYS	CD-CE	18.14	1.96	1.51
7	I	37	GLU	CD-OE1	18.10	1.45	1.25
1	A	1337	GLU	CD-OE1	17.98	1.45	1.25
1	A	464	PRO	C-O	-17.98	0.87	1.23
1	A	752	LYS	CD-CE	17.96	1.96	1.51
2	B	303	TYR	CE1-CZ	-17.96	1.15	1.38
6	H	129	TYR	CE2-CZ	17.92	1.61	1.38
4	E	162	ARG	CZ-NH1	17.76	1.56	1.33
6	H	131	ASN	CB-CG	17.76	1.91	1.51
4	E	106	GLN	CG-CD	17.75	1.91	1.51
5	F	129	LYS	CD-CE	17.75	1.95	1.51
1	A	618	GLU	CD-OE2	17.74	1.45	1.25
2	B	352	ALA	CA-CB	-17.71	1.15	1.52
2	B	986	GLN	CG-CD	17.71	1.91	1.51
2	B	137	TYR	CB-CG	17.70	1.78	1.51
1	A	423	ASP	CB-CG	17.66	1.88	1.51
3	C	3	GLU	CD-OE1	17.62	1.45	1.25
1	A	695	LYS	CD-CE	17.60	1.95	1.51
3	C	154	LYS	CB-CG	17.49	1.99	1.52
7	I	34	TYR	CZ-OH	17.48	1.67	1.37
2	B	775	LYS	CB-CG	17.48	1.99	1.52
6	H	104	PHE	CG-CD1	17.44	1.65	1.38
1	A	346	ASP	CB-CG	17.43	1.88	1.51
1	A	478	TYR	CD1-CE1	-17.42	1.13	1.39
1	A	1280	GLU	CG-CD	17.37	1.78	1.51
1	A	1135	ARG	CZ-NH2	17.36	1.55	1.33
2	B	371	GLU	CD-OE1	17.36	1.44	1.25
1	A	264	PHE	CB-CG	17.34	1.80	1.51
3	C	12	GLU	CD-OE1	17.32	1.44	1.25
6	H	93	TYR	CG-CD1	17.30	1.61	1.39
1	A	1297	GLU	CD-OE2	17.29	1.44	1.25
1	A	498	ARG	NE-CZ	-17.27	1.10	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1214	GLU	CD-OE1	17.25	1.44	1.25
3	C	165	LYS	CE-NZ	17.23	1.92	1.49
2	B	216	GLU	CD-OE2	17.18	1.44	1.25
1	A	123	ARG	NE-CZ	17.15	1.55	1.33
1	A	938	LYS	CD-CE	17.10	1.94	1.51
1	A	1277	GLU	CD-OE1	17.08	1.44	1.25
2	B	477	ALA	CA-CB	16.97	1.88	1.52
9	K	55	LYS	CD-CE	16.92	1.93	1.51
4	E	40	GLU	CD-OE1	16.89	1.44	1.25
7	I	84	VAL	CB-CG2	-16.88	1.17	1.52
2	B	183	GLU	CD-OE1	16.86	1.44	1.25
1	A	290	GLU	CD-OE2	16.85	1.44	1.25
2	B	1219	ASP	CB-CG	16.81	1.87	1.51
6	H	77	ARG	NE-CZ	16.80	1.54	1.33
1	A	681	GLU	CG-CD	16.79	1.77	1.51
3	C	114	TYR	CE2-CZ	-16.77	1.16	1.38
1	A	1232	ASN	CB-CG	16.77	1.89	1.51
2	B	691	GLU	CD-OE1	16.70	1.44	1.25
2	B	96	TYR	CG-CD1	16.69	1.60	1.39
7	I	17	ARG	CG-CD	16.66	1.93	1.51
4	E	28	TYR	CE2-CZ	-16.65	1.17	1.38
1	A	806	ARG	CZ-NH2	16.63	1.54	1.33
1	A	1411	GLU	CD-OE1	16.62	1.44	1.25
4	E	211	TYR	CE1-CZ	-16.56	1.17	1.38
7	I	34	TYR	CG-CD2	-16.56	1.17	1.39
10	L	45	ALA	CA-CB	16.56	1.87	1.52
2	B	895	ASP	CB-CG	16.49	1.86	1.51
3	C	209	TYR	CE2-CZ	16.45	1.59	1.38
1	A	1411	GLU	CG-CD	16.43	1.76	1.51
1	A	383	TYR	CD1-CE1	16.42	1.64	1.39
9	K	108	GLU	CD-OE2	16.40	1.43	1.25
1	A	1005	GLU	CD-OE1	16.38	1.43	1.25
7	I	55	THR	CB-CG2	16.36	2.06	1.52
3	C	102	GLN	CB-CG	16.35	1.96	1.52
1	A	889	SER	CA-CB	16.34	1.77	1.52
7	I	82	GLU	CD-OE1	16.34	1.43	1.25
1	A	226	GLU	CD-OE2	16.30	1.43	1.25
2	B	1153	GLU	CG-CD	16.29	1.76	1.51
2	B	18	PHE	CB-CG	16.27	1.79	1.51
1	A	1118	VAL	CB-CG2	-16.25	1.18	1.52
2	B	275	TYR	CG-CD1	-16.25	1.18	1.39
2	B	1163	CYS	CA-CB	16.24	1.89	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	124	TYR	CD2-CE2	16.17	1.63	1.39
1	A	833	GLU	CD-OE1	16.16	1.43	1.25
1	A	1110	ASN	CB-CG	16.13	1.88	1.51
6	H	45	GLU	CD-OE1	16.13	1.43	1.25
1	A	486	GLU	CD-OE2	-16.12	1.07	1.25
10	L	63	ARG	NE-CZ	16.12	1.54	1.33
2	B	1087	PHE	CE1-CZ	-16.11	1.06	1.37
1	A	724	GLU	CD-OE2	16.10	1.43	1.25
2	B	681	TRP	CG-CD1	-16.07	1.14	1.36
1	A	205	GLU	CG-CD	16.04	1.76	1.51
2	B	1086	PHE	CE2-CZ	-16.04	1.06	1.37
1	A	795	GLU	CG-CD	16.03	1.76	1.51
2	B	650	GLU	CD-OE1	16.03	1.43	1.25
2	B	337	ARG	NE-CZ	-15.99	1.12	1.33
2	B	96	TYR	CE1-CZ	15.98	1.59	1.38
9	K	102	LYS	CD-CE	15.97	1.91	1.51
10	L	46	VAL	CB-CG2	15.96	1.86	1.52
10	L	68	GLU	CD-OE2	15.95	1.43	1.25
1	A	155	GLU	CD-OE2	15.95	1.43	1.25
2	B	1156	ASP	CB-CG	15.95	1.85	1.51
1	A	553	VAL	CB-CG1	-15.92	1.19	1.52
1	A	954	TRP	CG-CD1	-15.91	1.14	1.36
1	A	1222	ASN	CB-CG	15.90	1.87	1.51
2	B	1050	ILE	C-O	-15.85	0.93	1.23
2	B	351	TYR	CG-CD2	-15.84	1.18	1.39
2	B	975	GLN	CD-NE2	15.83	1.72	1.32
1	A	724	GLU	CD-OE1	15.83	1.43	1.25
1	A	1042	PHE	CG-CD2	-15.83	1.15	1.38
1	A	520	CYS	CB-SG	-15.82	1.55	1.82
1	A	801	GLU	CD-OE2	15.82	1.43	1.25
3	C	174	ALA	CA-CB	-15.81	1.19	1.52
10	L	62	LYS	CD-CE	15.79	1.90	1.51
1	A	186	LYS	CG-CD	15.79	2.06	1.52
4	E	79	TRP	CB-CG	15.78	1.78	1.50
2	B	1021	MET	N-CA	-15.76	1.14	1.46
1	A	842	VAL	CB-CG2	-15.76	1.19	1.52
1	A	1272	THR	CB-CG2	15.75	2.04	1.52
6	H	146	ARG	NE-CZ	15.68	1.53	1.33
3	C	28	ALA	C-O	15.66	1.53	1.23
1	A	232	GLU	CD-OE1	15.64	1.42	1.25
3	C	137	LYS	CB-CG	15.60	1.94	1.52
2	B	666	TYR	CE1-CZ	15.57	1.58	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	592	ASN	CG-OD1	15.56	1.58	1.24
3	C	35	ARG	CB-CG	15.55	1.94	1.52
4	E	187	TYR	CG-CD1	-15.55	1.19	1.39
2	B	202	TYR	CG-CD2	-15.52	1.19	1.39
2	B	175	ARG	CZ-NH1	15.52	1.53	1.33
2	B	1097	HIS	CA-CB	15.49	1.88	1.53
1	A	952	ALA	CA-CB	15.48	1.84	1.52
2	B	1061	GLU	CB-CG	15.47	1.81	1.52
7	I	118	ARG	NE-CZ	15.45	1.53	1.33
4	E	41	ASP	CB-CG	15.44	1.84	1.51
1	A	66	LYS	CB-CG	15.44	1.94	1.52
1	A	1381	LEU	C-O	-15.44	0.94	1.23
2	B	502	ILE	CA-CB	15.41	1.90	1.54
3	C	87	PHE	CE2-CZ	-15.41	1.08	1.37
2	B	227	LYS	CD-CE	15.39	1.89	1.51
1	A	1259	MET	CG-SD	15.38	2.21	1.81
1	A	572	TRP	CB-CG	-15.35	1.22	1.50
2	B	106	ASP	CB-CG	15.35	1.83	1.51
1	A	148	CYS	CB-SG	-15.35	1.56	1.82
1	A	961	ARG	NE-CZ	15.31	1.52	1.33
1	A	933	TYR	CG-CD1	-15.30	1.19	1.39
1	A	1130	GLN	CG-CD	15.30	1.86	1.51
1	A	572	TRP	CZ3-CH2	-15.30	1.15	1.40
1	A	1132	LYS	CD-CE	15.29	1.89	1.51
1	A	16	GLU	CD-OE1	15.29	1.42	1.25
1	A	49	LYS	CD-CE	15.29	1.89	1.51
2	B	101	MET	SD-CE	15.28	2.63	1.77
2	B	866	TYR	CE2-CZ	15.28	1.58	1.38
2	B	347	LYS	CG-CD	15.26	2.04	1.52
2	B	652	LYS	CE-NZ	15.25	1.87	1.49
4	E	161	LYS	CD-CE	15.22	1.89	1.51
9	K	16	GLU	CG-CD	15.22	1.74	1.51
2	B	243	ALA	CA-CB	15.20	1.84	1.52
2	B	164	LYS	CD-CE	15.20	1.89	1.51
2	B	169	ARG	NE-CZ	15.20	1.52	1.33
1	A	1094	VAL	CB-CG1	15.19	1.84	1.52
1	A	1337	GLU	CD-OE2	15.18	1.42	1.25
2	B	137	TYR	CG-CD1	15.16	1.58	1.39
2	B	1041	GLU	CD-OE2	15.16	1.42	1.25
1	A	61	ILE	CA-CB	15.14	1.89	1.54
1	A	681	GLU	CD-OE1	15.12	1.42	1.25
1	A	1144	LYS	CD-CE	15.12	1.89	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	GLU	CD-OE2	15.10	1.42	1.25
4	E	162	ARG	CZ-NH2	15.09	1.52	1.33
1	A	1225	PHE	CE1-CZ	15.09	1.66	1.37
1	A	601	LYS	CD-CE	15.08	1.89	1.51
2	B	1134	GLU	CD-OE1	15.05	1.42	1.25
1	A	836	TYR	CG-CD2	15.04	1.58	1.39
1	A	1103	GLU	CD-OE2	15.02	1.42	1.25
2	B	692	TYR	CG-CD2	-15.01	1.19	1.39
4	E	17	ARG	NE-CZ	15.01	1.52	1.33
1	A	1187	GLN	CG-CD	14.99	1.85	1.51
4	E	152	LYS	CD-CE	14.98	1.88	1.51
1	A	728	LYS	CG-CD	14.97	2.03	1.52
1	A	1035	TYR	CE2-CZ	-14.97	1.19	1.38
4	E	157	SER	CA-CB	14.94	1.75	1.52
1	A	383	TYR	CD2-CE2	14.94	1.61	1.39
7	I	54	GLU	CD-OE2	14.91	1.42	1.25
2	B	319	GLU	CD-OE1	14.90	1.42	1.25
4	E	102	GLU	CD-OE1	14.89	1.42	1.25
1	A	1280	GLU	CD-OE1	14.88	1.42	1.25
7	I	58	VAL	CB-CG1	-14.89	1.21	1.52
3	C	116	LYS	CD-CE	14.87	1.88	1.51
3	C	209	TYR	CE1-CZ	14.83	1.57	1.38
7	I	75	CYS	CB-SG	-14.83	1.57	1.82
1	A	1414	ALA	CA-CB	-14.83	1.21	1.52
2	B	103	ASN	CB-CG	14.82	1.85	1.51
4	E	192	ARG	CZ-NH2	14.81	1.52	1.33
3	C	233	GLU	CD-OE1	14.81	1.42	1.25
3	C	260	LEU	CG-CD2	14.81	2.06	1.51
3	C	82	TYR	CZ-OH	14.80	1.63	1.37
3	C	179	GLU	CD-OE2	-14.80	1.09	1.25
1	A	643	ALA	CA-CB	-14.76	1.21	1.52
2	B	962	LYS	CD-CE	14.75	1.88	1.51
1	A	293	GLU	CD-OE2	14.74	1.41	1.25
2	B	1150	ARG	CZ-NH1	14.73	1.52	1.33
3	C	73	GLN	CG-CD	14.73	1.84	1.51
2	B	697	GLU	CD-OE2	14.71	1.41	1.25
1	A	1326	ARG	CG-CD	-14.71	1.15	1.51
10	L	26	THR	CA-CB	14.68	1.91	1.53
6	H	141	TYR	CE1-CZ	-14.67	1.19	1.38
1	A	1349	TYR	C-O	-14.64	0.95	1.23
4	E	43	LYS	CD-CE	14.58	1.87	1.51
5	F	146	TRP	CB-CG	-14.57	1.24	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	754	SER	CB-OG	14.56	1.61	1.42
1	A	416	ARG	CZ-NH2	-14.53	1.14	1.33
3	C	50	GLU	CD-OE1	14.53	1.41	1.25
5	F	114	GLU	CD-OE1	14.52	1.41	1.25
1	A	196	GLU	CD-OE1	14.52	1.41	1.25
1	A	368	LYS	CG-CD	14.52	2.01	1.52
2	B	235	SER	CB-OG	-14.50	1.23	1.42
2	B	987	LYS	CE-NZ	14.50	1.85	1.49
2	B	312	GLU	CD-OE1	14.48	1.41	1.25
9	K	20	LYS	CB-CG	14.47	1.91	1.52
2	B	1192	TYR	CG-CD1	-14.45	1.20	1.39
7	I	43	VAL	CB-CG1	-14.43	1.22	1.52
1	A	1328	TYR	CG-CD1	-14.41	1.20	1.39
2	B	668	ASP	CB-CG	14.41	1.82	1.51
3	C	215	GLU	CG-CD	14.40	1.73	1.51
1	A	291	GLU	CD-OE1	14.40	1.41	1.25
7	I	4	PHE	CE2-CZ	14.35	1.64	1.37
6	H	104	PHE	CE1-CZ	14.34	1.64	1.37
2	B	595	ARG	CG-CD	14.31	1.87	1.51
2	B	202	TYR	CE1-CZ	-14.29	1.20	1.38
2	B	736	THR	CB-CG2	14.29	1.99	1.52
5	F	129	LYS	CE-NZ	14.28	1.84	1.49
1	A	992	ASP	CB-CG	14.26	1.81	1.51
9	K	110	ASN	CB-CG	14.25	1.83	1.51
2	B	211	VAL	CB-CG1	-14.25	1.23	1.52
2	B	814	PHE	CE2-CZ	-14.25	1.10	1.37
1	A	1225	PHE	CB-CG	14.24	1.75	1.51
2	B	344	LYS	CD-CE	14.22	1.86	1.51
2	B	552	MET	SD-CE	14.20	2.57	1.77
2	B	70	ILE	CA-CB	14.19	1.87	1.54
1	A	1261	LYS	CD-CE	14.18	1.86	1.51
1	A	1264	GLU	CD-OE1	-14.18	1.10	1.25
3	C	117	ASP	C-O	14.17	1.50	1.23
1	A	1047	SER	CB-OG	14.16	1.60	1.42
2	B	962	LYS	CG-CD	14.15	2.00	1.52
1	A	1417	GLU	CD-OE2	14.15	1.41	1.25
4	E	82	PHE	CE1-CZ	-14.14	1.10	1.37
4	E	24	LYS	CE-NZ	14.13	1.84	1.49
1	A	1303	GLU	CD-OE1	14.11	1.41	1.25
2	B	226	PHE	CG-CD2	14.09	1.59	1.38
4	E	162	ARG	CB-CG	14.08	1.90	1.52
2	B	811	TYR	CE2-CZ	-14.05	1.20	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	129	TYR	CG-CD1	14.04	1.57	1.39
7	I	83	ASN	CB-CG	-14.04	1.18	1.51
2	B	328	GLU	CD-OE2	14.03	1.41	1.25
3	C	252	GLN	CD-OE1	14.02	1.54	1.24
2	B	1057	LYS	CD-CE	13.95	1.86	1.51
1	A	911	SER	CA-CB	13.95	1.73	1.52
2	B	531	GLN	CG-CD	13.94	1.83	1.51
1	A	157	ASP	CB-CG	13.93	1.81	1.51
2	B	620	ARG	CZ-NH2	13.92	1.51	1.33
10	L	36	SER	CB-OG	13.92	1.60	1.42
3	C	78	GLU	CG-CD	13.92	1.72	1.51
2	B	18	PHE	CG-CD2	13.90	1.59	1.38
1	A	393	ARG	CG-CD	13.88	1.86	1.51
1	A	731	ARG	CZ-NH2	13.86	1.51	1.33
1	A	37	PHE	CG-CD2	13.86	1.59	1.38
6	H	116	TYR	CG-CD1	13.85	1.57	1.39
2	B	488	TYR	CG-CD2	-13.84	1.21	1.39
2	B	65	GLU	CD-OE2	13.83	1.40	1.25
2	B	798	TYR	CG-CD1	-13.83	1.21	1.39
4	E	35	VAL	CB-CG1	-13.83	1.23	1.52
1	A	626	ASN	CG-ND2	13.82	1.67	1.32
1	A	983	ILE	CB-CG2	-13.82	1.10	1.52
2	B	665	GLU	CD-OE2	13.82	1.40	1.25
1	A	205	GLU	CD-OE2	13.82	1.40	1.25
9	K	54	ARG	NE-CZ	13.80	1.50	1.33
1	A	724	GLU	CG-CD	13.80	1.72	1.51
4	E	179	GLN	CA-CB	-13.80	1.23	1.53
2	B	21	GLU	CD-OE2	13.79	1.40	1.25
2	B	370	PHE	CE1-CZ	13.78	1.63	1.37
2	B	853	SER	CB-OG	13.78	1.60	1.42
1	A	705	LYS	CA-CB	13.77	1.84	1.53
1	A	5	GLN	CB-CG	13.75	1.89	1.52
1	A	941	LYS	CG-CD	13.75	1.99	1.52
1	A	293	GLU	CD-OE1	13.74	1.40	1.25
1	A	1235	LYS	CE-NZ	13.74	1.83	1.49
1	A	610	GLY	C-O	13.72	1.45	1.23
3	C	201	TRP	CE2-CZ2	-13.71	1.16	1.39
1	A	1109	LYS	CB-CG	13.70	1.89	1.52
7	I	93	LYS	CD-CE	13.69	1.85	1.51
1	A	1281	ARG	CG-CD	13.69	1.86	1.51
2	B	866	TYR	CD1-CE1	13.68	1.59	1.39
2	B	531	GLN	CB-CG	13.66	1.89	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	162	ARG	CG-CD	13.66	1.86	1.51
1	A	1326	ARG	NE-CZ	13.65	1.50	1.33
1	A	44	THR	CA-CB	13.62	1.88	1.53
7	I	21	GLU	CD-OE1	13.61	1.40	1.25
1	A	572	TRP	CG-CD1	-13.61	1.17	1.36
2	B	115	GLN	CB-CG	13.60	1.89	1.52
1	A	9	ALA	CA-CB	13.58	1.80	1.52
7	I	42	LEU	C-O	-13.56	0.97	1.23
2	B	315	LYS	CE-NZ	13.55	1.82	1.49
7	I	18	GLU	CD-OE2	13.51	1.40	1.25
2	B	838	SER	CB-OG	-13.50	1.24	1.42
3	C	32	SER	CB-OG	-13.48	1.24	1.42
1	A	1029	ARG	NE-CZ	-13.46	1.15	1.33
4	E	137	GLU	CD-OE1	13.45	1.40	1.25
9	K	1	MET	SD-CE	13.44	2.53	1.77
1	A	673	GLY	C-O	-13.43	1.02	1.23
1	A	941	LYS	CE-NZ	13.42	1.82	1.49
3	C	208	GLU	CD-OE2	13.40	1.40	1.25
6	H	9	ILE	CA-CB	13.38	1.85	1.54
1	A	1338	VAL	CA-CB	-13.37	1.26	1.54
2	B	1070	GLU	C-O	-13.37	0.97	1.23
3	C	209	TYR	CD1-CE1	13.37	1.59	1.39
2	B	1019	SER	CB-OG	-13.37	1.24	1.42
1	A	623	GLY	CA-C	-13.37	1.30	1.51
2	B	51	PHE	CB-CG	-13.36	1.28	1.51
2	B	57	TYR	CE1-CZ	-13.35	1.21	1.38
3	C	191	TYR	CB-CG	13.34	1.71	1.51
1	A	1098	VAL	CB-CG1	-13.33	1.24	1.52
2	B	536	VAL	CB-CG2	-13.32	1.24	1.52
2	B	384	ARG	CG-CD	13.30	1.85	1.51
3	C	166	GLU	CB-CG	13.30	1.77	1.52
2	B	346	GLU	CD-OE2	13.29	1.40	1.25
1	A	866	PHE	CE1-CZ	-13.28	1.12	1.37
3	C	78	GLU	CD-OE1	13.28	1.40	1.25
9	K	54	ARG	CD-NE	13.26	1.69	1.46
1	A	1407	GLU	CG-CD	13.25	1.71	1.51
1	A	1212	VAL	CB-CG1	-13.25	1.25	1.52
1	A	1232	ASN	C-O	13.25	1.48	1.23
2	B	1078	GLY	C-O	13.24	1.44	1.23
2	B	250	PHE	CG-CD2	13.23	1.58	1.38
2	B	1140	ALA	CA-CB	-13.22	1.24	1.52
2	B	1001	PHE	CD2-CE2	13.21	1.65	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	959	ASP	CB-CG	13.20	1.79	1.51
2	B	299	GLU	CD-OE1	13.19	1.40	1.25
3	C	86	CYS	CA-CB	13.18	1.82	1.53
7	I	82	GLU	CG-CD	13.16	1.71	1.51
2	B	1070	GLU	CD-OE2	13.15	1.40	1.25
2	B	1061	GLU	CD-OE1	13.14	1.40	1.25
2	B	811	TYR	CG-CD1	-13.11	1.22	1.39
1	A	1005	GLU	CD-OE2	13.10	1.40	1.25
9	K	91	CYS	C-O	13.10	1.48	1.23
2	B	1132	GLU	CD-OE1	13.10	1.40	1.25
1	A	899	VAL	CB-CG1	-13.10	1.25	1.52
2	B	286	PHE	CG-CD2	-13.09	1.19	1.38
1	A	766	GLY	C-O	-13.09	1.02	1.23
1	A	1363	VAL	CB-CG1	13.08	1.80	1.52
4	E	208	TYR	CE1-CZ	-13.07	1.21	1.38
6	H	3	ASN	CB-CG	13.06	1.81	1.51
1	A	677	ARG	CZ-NH1	13.05	1.50	1.33
4	E	66	GLU	CG-CD	13.05	1.71	1.51
2	B	434	ARG	CG-CD	13.05	1.84	1.51
1	A	1234	GLU	CG-CD	13.04	1.71	1.51
3	C	23	SER	CA-CB	13.03	1.72	1.52
3	C	12	GLU	CD-OE2	13.00	1.40	1.25
4	E	81	GLU	CA-C	-12.99	1.19	1.52
2	B	1020	ARG	CZ-NH2	12.98	1.50	1.33
2	B	537	LYS	C-O	-12.98	0.98	1.23
6	H	126	GLU	CD-OE1	12.97	1.40	1.25
7	I	83	ASN	C-O	12.97	1.48	1.23
2	B	1130	PHE	CG-CD2	-12.97	1.19	1.38
1	A	516	SER	CB-OG	12.97	1.59	1.42
9	K	99	GLY	C-O	12.95	1.44	1.23
7	I	110	PHE	CG-CD2	-12.95	1.19	1.38
2	B	1165	ILE	C-O	-12.93	0.98	1.23
1	A	379	VAL	CB-CG2	12.93	1.79	1.52
1	A	398	GLU	CD-OE2	12.92	1.39	1.25
7	I	120	GLN	CG-CD	12.92	1.80	1.51
3	C	163	ILE	CA-CB	-12.91	1.25	1.54
2	B	1193	GLN	C-O	-12.90	0.98	1.23
1	A	487	MET	SD-CE	-12.90	1.05	1.77
1	A	1349	TYR	CG-CD2	-12.90	1.22	1.39
1	A	1152	ILE	CA-CB	-12.90	1.25	1.54
2	B	546	SER	CB-OG	12.89	1.59	1.42
4	E	210	SER	CA-CB	-12.89	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	564	GLU	CD-OE2	12.88	1.39	1.25
2	B	726	ALA	CA-CB	12.86	1.79	1.52
2	B	792	MET	SD-CE	12.86	2.49	1.77
2	B	698	GLU	CD-OE1	12.85	1.39	1.25
5	F	87	LYS	CD-CE	12.84	1.83	1.51
3	C	113	VAL	CA-CB	-12.84	1.27	1.54
1	A	676	MET	CG-SD	12.82	2.14	1.81
2	B	466	TRP	CE3-CZ3	-12.79	1.16	1.38
2	B	963	PHE	CE1-CZ	12.79	1.61	1.37
3	C	135	GLN	CG-CD	12.79	1.80	1.51
4	E	84	ASP	CB-CG	12.78	1.78	1.51
2	B	1132	GLU	CB-CG	12.77	1.76	1.52
2	B	124	TYR	CE2-CZ	-12.77	1.22	1.38
4	E	192	ARG	NE-CZ	12.75	1.49	1.33
2	B	96	TYR	CG-CD2	12.75	1.55	1.39
2	B	945	GLU	CG-CD	12.74	1.71	1.51
1	A	995	GLU	CD-OE2	12.72	1.39	1.25
1	A	1099	PRO	C-O	-12.71	0.97	1.23
3	C	205	LYS	CB-CG	12.71	1.86	1.52
2	B	723	VAL	CB-CG2	12.70	1.79	1.52
1	A	69	THR	CA-C	12.70	1.85	1.52
3	C	104	PHE	CD2-CE2	12.70	1.64	1.39
2	B	415	GLN	CB-CG	12.69	1.86	1.52
2	B	1132	GLU	CG-CD	12.69	1.71	1.51
1	A	420	ARG	CZ-NH2	-12.68	1.16	1.33
1	A	556	TRP	CB-CG	-12.67	1.27	1.50
1	A	1355	VAL	CB-CG1	-12.67	1.26	1.52
1	A	198	GLU	CD-OE2	12.66	1.39	1.25
4	E	212	ARG	CZ-NH1	-12.66	1.16	1.33
1	A	298	PHE	CG-CD2	12.66	1.57	1.38
6	H	129	TYR	CE1-CZ	12.66	1.55	1.38
3	C	209	TYR	CG-CD2	12.65	1.55	1.39
2	B	238	ALA	CA-CB	12.63	1.78	1.52
4	E	168	TYR	CD2-CE2	12.62	1.58	1.39
1	A	1149	ALA	C-O	12.62	1.47	1.23
1	A	1129	GLU	CG-CD	12.60	1.70	1.51
3	C	35	ARG	CG-CD	12.59	1.83	1.51
4	E	17	ARG	CZ-NH1	12.59	1.49	1.33
4	E	211	TYR	CD2-CE2	-12.59	1.20	1.39
8	J	50	ILE	C-O	12.59	1.47	1.23
3	C	23	SER	CB-OG	12.58	1.58	1.42
2	B	263	GLY	C-O	12.57	1.43	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	412	ARG	NE-CZ	-12.57	1.16	1.33
2	B	1064	TYR	CG-CD2	-12.55	1.22	1.39
6	H	104	PHE	CD2-CE2	12.55	1.64	1.39
7	I	89	GLN	C-O	-12.54	0.99	1.23
2	B	529	GLU	CG-CD	12.54	1.70	1.51
3	C	127	ARG	C-O	12.53	1.47	1.23
1	A	961	ARG	CZ-NH2	12.53	1.49	1.33
7	I	44	TYR	CG-CD1	-12.52	1.22	1.39
6	H	104	PHE	CA-C	12.51	1.85	1.52
2	B	31	TRP	CE3-CZ3	12.51	1.59	1.38
6	H	126	GLU	CG-CD	12.49	1.70	1.51
1	A	618	GLU	CD-OE1	12.49	1.39	1.25
2	B	231	PRO	CB-CG	12.49	2.12	1.50
7	I	91	ARG	NE-CZ	12.48	1.49	1.33
1	A	1214	GLU	CG-CD	12.47	1.70	1.51
1	A	1227	ILE	C-O	-12.47	0.99	1.23
2	B	758	PHE	CE2-CZ	-12.46	1.13	1.37
3	C	146	LYS	CB-CG	12.46	1.86	1.52
1	A	656	TRP	CD2-CE3	-12.44	1.21	1.40
2	B	242	SER	CB-OG	12.44	1.58	1.42
7	I	35	VAL	CA-CB	-12.44	1.28	1.54
9	K	79	GLU	CG-CD	12.44	1.70	1.51
3	C	181	ASP	C-O	-12.44	0.99	1.23
1	A	874	ASP	CG-OD2	12.44	1.53	1.25
6	H	116	TYR	CE2-CZ	12.44	1.54	1.38
1	A	478	TYR	CD2-CE2	-12.44	1.20	1.39
2	B	27	ALA	CA-CB	-12.43	1.26	1.52
6	H	104	PHE	CD1-CE1	12.43	1.64	1.39
1	A	1422	ARG	NE-CZ	12.43	1.49	1.33
9	K	61	TYR	CG-CD2	-12.43	1.23	1.39
7	I	93	LYS	CE-NZ	12.42	1.80	1.49
2	B	980	PHE	CE1-CZ	12.42	1.60	1.37
4	E	194	GLU	CD-OE1	-12.41	1.11	1.25
2	B	711	GLU	CG-CD	12.41	1.70	1.51
1	A	474	VAL	CB-CG2	-12.40	1.26	1.52
3	C	171	GLY	C-O	12.39	1.43	1.23
2	B	592	ASN	CB-CG	12.38	1.79	1.51
2	B	1198	TYR	CE2-CZ	-12.37	1.22	1.38
2	B	632	ARG	NE-CZ	-12.37	1.17	1.33
1	A	496	GLU	CD-OE2	12.36	1.39	1.25
1	A	459	ARG	CD-NE	-12.35	1.25	1.46
2	B	883	LEU	CA-CB	12.35	1.82	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	915	THR	CA-CB	12.35	1.85	1.53
1	A	371	ALA	CA-CB	-12.34	1.26	1.52
2	B	1061	GLU	CG-CD	12.34	1.70	1.51
3	C	219	PHE	CD1-CE1	12.34	1.64	1.39
5	F	112	GLU	CG-CD	12.34	1.70	1.51
2	B	811	TYR	CZ-OH	-12.34	1.16	1.37
1	A	552	TRP	CD2-CE2	-12.34	1.26	1.41
4	E	102	GLU	CG-CD	12.34	1.70	1.51
7	I	34	TYR	CD2-CE2	-12.32	1.20	1.39
2	B	418	LYS	CD-CE	12.31	1.82	1.51
2	B	875	GLU	CG-CD	12.31	1.70	1.51
2	B	678	GLU	CD-OE1	12.31	1.39	1.25
3	C	152	GLU	CD-OE1	12.31	1.39	1.25
1	A	991	LYS	CE-NZ	12.30	1.79	1.49
2	B	1087	PHE	CD2-CE2	-12.29	1.14	1.39
9	K	16	GLU	CD-OE2	12.29	1.39	1.25
1	A	1055	ARG	CG-CD	12.28	1.82	1.51
2	B	866	TYR	CD2-CE2	12.27	1.57	1.39
1	A	37	PHE	CD1-CE1	12.25	1.63	1.39
1	A	698	GLN	CG-CD	12.25	1.79	1.51
1	A	822	GLU	CD-OE2	12.25	1.39	1.25
2	B	465	ASN	CB-CG	12.25	1.79	1.51
6	H	107	VAL	CA-CB	12.25	1.80	1.54
4	E	181	ALA	CA-CB	-12.24	1.26	1.52
1	A	755	PHE	CD2-CE2	12.23	1.63	1.39
4	E	31	THR	CA-CB	12.23	1.85	1.53
3	C	180	TYR	CD2-CE2	12.23	1.57	1.39
3	C	265	MET	SD-CE	12.23	2.46	1.77
9	K	16	GLU	CD-OE1	12.22	1.39	1.25
2	B	434	ARG	CB-CG	12.22	1.85	1.52
1	A	1362	TYR	CD1-CE1	12.22	1.57	1.39
2	B	249	ARG	CG-CD	12.20	1.82	1.51
1	A	718	VAL	CB-CG2	-12.20	1.27	1.52
3	C	199	LYS	CD-CE	12.20	1.81	1.51
4	E	72	PHE	CD1-CE1	-12.20	1.14	1.39
4	E	194	GLU	CB-CG	12.20	1.75	1.52
1	A	1361	SER	CB-OG	12.17	1.58	1.42
2	B	692	TYR	CG-CD1	-12.17	1.23	1.39
6	H	41	ASP	CB-CG	12.17	1.77	1.51
1	A	155	GLU	CG-CD	12.15	1.70	1.51
7	I	20	LYS	CD-CE	12.15	1.81	1.51
1	A	911	SER	CB-OG	12.15	1.58	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	221	ASN	C-O	12.14	1.46	1.23
4	E	194	GLU	C-O	-12.14	1.00	1.23
2	B	641	GLU	CD-OE2	12.14	1.39	1.25
3	C	108	GLU	C-O	12.14	1.46	1.23
1	A	1132	LYS	CE-NZ	12.13	1.79	1.49
6	H	19	ARG	CB-CG	12.13	1.85	1.52
4	E	152	LYS	CB-CG	12.12	1.85	1.52
2	B	1020	ARG	CA-C	12.12	1.84	1.52
3	C	228	PHE	N-CA	-12.12	1.22	1.46
2	B	896	ASP	CA-C	-12.10	1.21	1.52
2	B	200	GLY	C-O	-12.09	1.04	1.23
7	I	1	MET	CB-CG	12.08	1.90	1.51
5	F	108	PHE	CE2-CZ	12.08	1.60	1.37
8	J	38	ARG	CB-CG	12.07	1.85	1.52
1	A	291	GLU	CD-OE2	12.07	1.39	1.25
3	C	180	TYR	CG-CD1	-12.07	1.23	1.39
3	C	108	GLU	CD-OE2	12.07	1.39	1.25
1	A	947	PHE	CG-CD1	-12.06	1.20	1.38
1	A	1063	MET	CG-SD	-12.06	1.49	1.81
3	C	89	GLU	C-O	12.06	1.46	1.23
1	A	1315	GLU	CB-CG	12.05	1.75	1.52
7	I	72	ASP	CB-CG	12.05	1.77	1.51
2	B	201	GLY	C-O	12.05	1.43	1.23
1	A	264	PHE	CG-CD2	12.05	1.56	1.38
1	A	217	LYS	CD-CE	12.03	1.81	1.51
6	H	139	ASN	CA-CB	12.02	1.84	1.53
1	A	1328	TYR	CD1-CE1	-12.02	1.21	1.39
1	A	277	GLU	CD-OE2	12.02	1.38	1.25
1	A	1187	GLN	CB-CG	12.01	1.84	1.52
1	A	546	VAL	CB-CG2	-12.01	1.27	1.52
1	A	703	THR	CB-CG2	12.01	1.92	1.52
1	A	1303	GLU	CD-OE2	12.01	1.38	1.25
3	C	127	ARG	NE-CZ	12.00	1.48	1.33
1	A	537	ARG	CZ-NH2	12.00	1.48	1.33
10	L	68	GLU	CD-OE1	12.00	1.38	1.25
2	B	319	GLU	CG-CD	11.99	1.70	1.51
1	A	1153	TYR	CG-CD1	-11.99	1.23	1.39
1	A	1316	VAL	CB-CG2	-11.98	1.27	1.52
1	A	1290	LYS	CD-CE	11.97	1.81	1.51
2	B	797	TYR	CD1-CE1	11.97	1.57	1.39
7	I	120	GLN	CB-CG	11.97	1.84	1.52
2	B	1148	LYS	CD-CE	11.96	1.81	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	994	TYR	CE2-CZ	-11.96	1.23	1.38
2	B	1020	ARG	CZ-NH1	11.95	1.48	1.33
1	A	656	TRP	CG-CD2	-11.93	1.23	1.43
2	B	618	ASP	CG-OD1	11.93	1.52	1.25
2	B	619	ILE	CA-CB	-11.93	1.27	1.54
3	C	64	ALA	CA-CB	-11.93	1.27	1.52
1	A	1280	GLU	C-O	-11.93	1.00	1.23
2	B	707	PRO	N-CD	-11.92	1.31	1.47
3	C	20	PHE	CE2-CZ	11.92	1.60	1.37
2	B	191	LYS	CB-CG	11.92	1.84	1.52
3	C	78	GLU	CD-OE2	11.91	1.38	1.25
2	B	327	ARG	CZ-NH2	11.90	1.48	1.33
2	B	1154	ALA	CA-CB	11.90	1.77	1.52
1	A	1045	VAL	CB-CG1	-11.89	1.27	1.52
6	H	129	TYR	CG-CD2	11.89	1.54	1.39
1	A	1001	ARG	CZ-NH2	11.89	1.48	1.33
2	B	337	ARG	CD-NE	-11.87	1.26	1.46
1	A	990	VAL	CB-CG1	-11.86	1.27	1.52
1	A	407	ARG	CZ-NH1	11.86	1.48	1.33
2	B	961	LEU	CG-CD1	11.86	1.95	1.51
1	A	806	ARG	CZ-NH1	11.85	1.48	1.33
3	C	81	GLU	C-O	11.85	1.45	1.23
6	H	52	GLN	CG-CD	11.84	1.78	1.51
1	A	1319	VAL	CB-CG1	11.84	1.77	1.52
9	K	89	ASN	CB-CG	11.84	1.78	1.51
9	K	105	PHE	CE2-CZ	11.84	1.59	1.37
6	H	117	SER	C-O	11.83	1.45	1.23
1	A	188	ASP	CA-C	11.82	1.83	1.52
2	B	246	LYS	CA-C	11.80	1.83	1.52
1	A	1362	TYR	CE2-CZ	11.80	1.53	1.38
1	A	1289	ARG	NE-CZ	-11.79	1.17	1.33
7	I	15	TYR	CD1-CE1	11.79	1.57	1.39
1	A	110	CYS	CB-SG	11.77	2.02	1.82
3	C	191	TYR	CE2-CZ	11.76	1.53	1.38
2	B	497	ARG	C-O	-11.76	1.01	1.23
1	A	1196	GLU	CD-OE2	11.75	1.38	1.25
1	A	303	TYR	CG-CD2	-11.75	1.23	1.39
1	A	677	ARG	NE-CZ	11.75	1.48	1.33
2	B	1155	SER	CA-CB	11.75	1.70	1.52
2	B	581	PHE	CG-CD1	-11.74	1.21	1.38
1	A	1437	GLY	C-O	-11.74	1.04	1.23
1	A	718	VAL	CB-CG1	-11.73	1.28	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	89	GLU	CG-CD	11.73	1.69	1.51
2	B	90	ILE	N-CA	11.73	1.69	1.46
2	B	459	TYR	CG-CD2	11.72	1.54	1.39
2	B	1087	PHE	CE2-CZ	11.71	1.59	1.37
2	B	904	ARG	NE-CZ	-11.70	1.17	1.33
2	B	1165	ILE	CA-CB	11.71	1.81	1.54
1	A	678	GLU	CD-OE2	11.69	1.38	1.25
7	I	32	CYS	CB-SG	-11.69	1.62	1.82
2	B	319	GLU	CB-CG	11.69	1.74	1.52
6	H	136	LYS	CA-C	11.69	1.83	1.52
5	F	149	GLU	C-O	11.68	1.45	1.23
2	B	166	PHE	CE1-CZ	11.68	1.59	1.37
3	C	15	LYS	CB-CG	11.68	1.84	1.52
1	A	228	PHE	CG-CD1	-11.67	1.21	1.38
8	J	48	ARG	CZ-NH1	-11.67	1.17	1.33
3	C	115	SER	CA-CB	-11.66	1.35	1.52
3	C	171	GLY	CA-C	11.66	1.70	1.51
1	A	303	TYR	CD2-CE2	-11.66	1.21	1.39
2	B	866	TYR	CG-CD1	11.66	1.54	1.39
3	C	253	LYS	C-O	11.66	1.45	1.23
2	B	249	ARG	NE-CZ	11.65	1.48	1.33
1	A	1415	SER	CB-OG	-11.63	1.27	1.42
1	A	1315	GLU	CD-OE2	11.63	1.38	1.25
9	K	20	LYS	CG-CD	11.63	1.92	1.52
7	I	45	ARG	CG-CD	11.63	1.81	1.51
2	B	1002	THR	CA-C	11.63	1.83	1.52
4	E	65	THR	C-O	11.62	1.45	1.23
1	A	465	TYR	CG-CD2	-11.62	1.24	1.39
1	A	1368	MET	CG-SD	-11.62	1.50	1.81
2	B	851	PHE	CD1-CE1	11.61	1.62	1.39
1	A	1225	PHE	CA-CB	11.61	1.79	1.53
3	C	15	LYS	CD-CE	11.61	1.80	1.51
2	B	951	GLN	CG-CD	11.61	1.77	1.51
2	B	1224	PHE	CG-CD1	11.60	1.56	1.38
1	A	662	PHE	CG-CD2	-11.60	1.21	1.38
1	A	104	GLU	C-O	11.60	1.45	1.23
2	B	519	TRP	CE3-CZ3	11.59	1.58	1.38
1	A	387	ARG	CG-CD	11.58	1.80	1.51
2	B	108	VAL	CB-CG2	11.58	1.77	1.52
3	C	128	ASN	CG-OD1	11.58	1.49	1.24
3	C	257	SER	C-O	-11.58	1.01	1.23
2	B	31	TRP	CG-CD1	-11.58	1.20	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	27	PHE	C-O	-11.58	1.01	1.23
2	B	851	PHE	CD2-CE2	11.57	1.62	1.39
3	C	219	PHE	CE2-CZ	11.56	1.59	1.37
6	H	57	VAL	CB-CG1	-11.56	1.28	1.52
1	A	866	PHE	CE2-CZ	-11.56	1.15	1.37
6	H	121	LEU	C-O	11.55	1.45	1.23
2	B	19	GLU	CG-CD	11.55	1.69	1.51
1	A	1162	VAL	CB-CG1	11.55	1.77	1.52
1	A	123	ARG	CD-NE	11.55	1.66	1.46
2	B	567	GLU	CG-CD	11.55	1.69	1.51
1	A	499	ALA	CA-CB	-11.54	1.28	1.52
2	B	275	TYR	CE2-CZ	-11.52	1.23	1.38
7	I	91	ARG	CZ-NH1	11.52	1.48	1.33
1	A	671	ALA	CA-CB	-11.51	1.28	1.52
10	L	26	THR	CB-CG2	11.51	1.90	1.52
3	C	221	TYR	CB-CG	-11.50	1.34	1.51
4	E	178	ILE	C-O	11.49	1.45	1.23
1	A	744	LYS	CD-CE	11.49	1.79	1.51
1	A	171	GLN	C-O	-11.48	1.01	1.23
2	B	97	VAL	CB-CG1	-11.48	1.28	1.52
1	A	1282	VAL	CB-CG2	11.48	1.76	1.52
6	H	105	GLU	CG-CD	11.48	1.69	1.51
1	A	635	ARG	CG-CD	11.47	1.80	1.51
2	B	344	LYS	CB-CG	11.47	1.83	1.52
2	B	459	TYR	CD2-CE2	11.47	1.56	1.39
1	A	942	PHE	CG-CD2	-11.46	1.21	1.38
1	A	870	GLU	CD-OE2	11.46	1.38	1.25
1	A	656	TRP	CE3-CZ3	11.46	1.57	1.38
1	A	1262	LYS	CG-CD	11.45	1.91	1.52
6	H	79	TRP	CE3-CZ3	11.45	1.57	1.38
4	E	201	LYS	CG-CD	11.45	1.91	1.52
1	A	290	GLU	CD-OE1	11.43	1.38	1.25
4	E	168	TYR	CD1-CE1	11.43	1.56	1.39
2	B	1062	HIS	CA-CB	-11.43	1.28	1.53
1	A	469	ARG	CZ-NH2	-11.43	1.18	1.33
1	A	1126	ALA	CA-CB	-11.42	1.28	1.52
2	B	349	ILE	CB-CG2	-11.42	1.17	1.52
1	A	1304	TRP	CE2-CZ2	-11.42	1.20	1.39
1	A	948	VAL	C-O	-11.42	1.01	1.23
10	L	33	GLU	CD-OE2	11.42	1.38	1.25
3	C	6	PRO	C-O	11.41	1.46	1.23
4	E	8	ASN	CG-OD1	11.41	1.49	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	137	TYR	CG-CD2	11.41	1.53	1.39
1	A	1005	GLU	CG-CD	11.41	1.69	1.51
1	A	566	ILE	CB-CG2	11.41	1.88	1.52
1	A	1012	ARG	C-O	11.40	1.45	1.23
2	B	905	VAL	CB-CG1	-11.39	1.28	1.52
2	B	224	GLN	C-O	-11.39	1.01	1.23
2	B	781	PHE	CG-CD2	-11.39	1.21	1.38
2	B	780	VAL	CA-CB	-11.39	1.30	1.54
4	E	198	ILE	CB-CG2	-11.38	1.17	1.52
1	A	123	ARG	CG-CD	11.38	1.80	1.51
2	B	37	PHE	CE1-CZ	11.38	1.58	1.37
1	A	196	GLU	CD-OE2	11.37	1.38	1.25
2	B	983	ARG	NE-CZ	-11.37	1.18	1.33
1	A	198	GLU	CG-CD	11.36	1.69	1.51
1	A	949	ASP	CB-CG	-11.36	1.27	1.51
1	A	1225	PHE	CE2-CZ	11.36	1.58	1.37
3	C	26	ASP	C-O	11.36	1.45	1.23
3	C	181	ASP	CA-C	-11.35	1.23	1.52
2	B	39	ARG	CZ-NH2	11.35	1.47	1.33
3	C	191	TYR	CD1-CE1	11.35	1.56	1.39
6	H	2	SER	CA-C	11.35	1.82	1.52
2	B	874	PHE	CD1-CE1	-11.34	1.16	1.39
2	B	1155	SER	CB-OG	11.34	1.56	1.42
5	F	108	PHE	CG-CD1	11.34	1.55	1.38
2	B	124	TYR	CA-CB	-11.33	1.29	1.53
2	B	746	SER	C-O	11.33	1.44	1.23
1	A	1345	ARG	CZ-NH1	-11.33	1.18	1.33
3	C	192	TRP	CB-CG	11.33	1.70	1.50
1	A	938	LYS	CG-CD	11.32	1.91	1.52
1	A	866	PHE	CG-CD1	-11.31	1.21	1.38
1	A	1350	LYS	CD-CE	11.30	1.79	1.51
1	A	705	LYS	CE-NZ	11.30	1.77	1.49
1	A	117	GLU	CG-CD	11.30	1.68	1.51
1	A	796	SER	CB-OG	-11.29	1.27	1.42
2	B	556	THR	CB-CG2	11.29	1.89	1.52
1	A	685	GLU	CD-OE1	11.28	1.38	1.25
2	B	586	TRP	C-O	-11.28	1.01	1.23
10	L	27	LEU	CA-CB	11.27	1.79	1.53
1	A	1417	GLU	CG-CD	11.27	1.68	1.51
1	A	725	ALA	CA-CB	-11.27	1.28	1.52
1	A	433	GLU	CD-OE1	11.26	1.38	1.25
1	A	1297	GLU	CG-CD	11.26	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1151	GLU	C-O	11.26	1.44	1.23
4	E	79	TRP	C-O	-11.26	1.01	1.23
1	A	1222	ASN	CA-CB	11.25	1.82	1.53
1	A	412	ARG	CZ-NH2	-11.25	1.18	1.33
10	L	54	ARG	CG-CD	11.25	1.80	1.51
1	A	120	GLU	CD-OE1	11.24	1.38	1.25
2	B	65	GLU	CG-CD	11.24	1.68	1.51
4	E	46	TYR	CD2-CE2	11.24	1.56	1.39
6	H	98	TYR	CG-CD1	-11.24	1.24	1.39
8	J	14	VAL	CA-CB	-11.24	1.31	1.54
1	A	787	PHE	CG-CD1	-11.22	1.22	1.38
2	B	365	THR	CB-CG2	-11.22	1.15	1.52
1	A	814	PHE	CE1-CZ	11.22	1.58	1.37
8	J	18	TRP	CA-CB	-11.21	1.29	1.53
1	A	1410	PHE	CD1-CE1	-11.21	1.16	1.39
2	B	509	ALA	CA-CB	11.21	1.75	1.52
2	B	1185	CYS	CA-CB	11.21	1.78	1.53
2	B	115	GLN	CG-CD	11.19	1.76	1.51
7	I	37	GLU	CD-OE2	11.18	1.38	1.25
1	A	1108	ALA	CA-CB	-11.17	1.28	1.52
7	I	98	VAL	CB-CG2	-11.17	1.29	1.52
2	B	646	LEU	CG-CD2	11.16	1.93	1.51
1	A	614	PHE	CE2-CZ	-11.16	1.16	1.37
7	I	36	GLU	CD-OE2	11.16	1.38	1.25
1	A	209	ASN	CG-OD1	11.15	1.48	1.24
1	A	1367	HIS	C-O	-11.15	1.02	1.23
2	B	885	MET	SD-CE	11.14	2.40	1.77
2	B	1073	TYR	CB-CG	11.13	1.68	1.51
5	F	96	THR	N-CA	-11.13	1.24	1.46
9	K	32	VAL	CB-CG2	-11.12	1.29	1.52
1	A	875	ALA	CA-CB	-11.12	1.29	1.52
1	A	1235	LYS	CB-CG	11.12	1.82	1.52
1	A	830	LYS	CD-CE	11.11	1.79	1.51
1	A	219	PHE	CD2-CE2	-11.10	1.17	1.39
3	C	245	VAL	CB-CG2	-11.10	1.29	1.52
2	B	250	PHE	CE1-CZ	11.10	1.58	1.37
1	A	304	MET	SD-CE	11.10	2.40	1.77
2	B	692	TYR	CE2-CZ	-11.10	1.24	1.38
2	B	1101	ASP	CB-CG	11.10	1.75	1.51
1	A	186	LYS	CB-CG	11.09	1.82	1.52
4	E	121	MET	CG-SD	11.09	2.10	1.81
2	B	816	GLU	CD-OE2	-11.09	1.13	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	VAL	CB-CG1	11.09	1.76	1.52
1	A	247	ARG	C-O	11.09	1.44	1.23
2	B	96	TYR	CE2-CZ	11.09	1.52	1.38
3	C	260	LEU	CG-CD1	11.08	1.92	1.51
1	A	836	TYR	CZ-OH	11.07	1.56	1.37
1	A	1034	GLU	C-O	11.07	1.44	1.23
2	B	969	ARG	CZ-NH1	11.07	1.47	1.33
1	A	37	PHE	CE1-CZ	11.06	1.58	1.37
3	C	164	ALA	CA-CB	-11.06	1.29	1.52
2	B	994	TYR	CG-CD2	-11.06	1.24	1.39
3	C	55	THR	C-O	11.06	1.44	1.23
2	B	856	PHE	CD2-CE2	-11.06	1.17	1.39
4	E	44	ALA	CA-CB	11.05	1.75	1.52
2	B	999	MET	SD-CE	-11.05	1.16	1.77
7	I	6	PHE	CE1-CZ	-11.05	1.16	1.37
1	A	931	GLU	CD-OE1	11.05	1.37	1.25
6	H	11	GLN	CB-CG	11.05	1.82	1.52
1	A	1302	PRO	C-O	11.04	1.45	1.23
2	B	704	ALA	CA-CB	-11.04	1.29	1.52
3	C	88	CYS	CB-SG	-11.04	1.63	1.82
3	C	150	GLY	N-CA	11.04	1.62	1.46
1	A	1411	GLU	CB-CG	11.04	1.73	1.52
7	I	48	LEU	CG-CD2	-11.03	1.11	1.51
1	A	1322	ILE	CB-CG2	-11.03	1.18	1.52
2	B	975	GLN	CD-OE1	11.03	1.48	1.24
4	E	163	GLU	CG-CD	11.03	1.68	1.51
2	B	299	GLU	CB-CG	11.03	1.73	1.52
4	E	50	MET	CG-SD	11.02	2.09	1.81
3	C	245	VAL	CB-CG1	11.02	1.75	1.52
1	A	872	GLY	CA-C	-11.01	1.34	1.51
2	B	1215	ARG	C-O	-11.01	1.02	1.23
4	E	29	PHE	CE2-CZ	11.00	1.58	1.37
4	E	150	VAL	CB-CG2	-11.00	1.29	1.52
2	B	582	VAL	CB-CG1	-10.99	1.29	1.52
2	B	732	SER	CA-CB	10.99	1.69	1.52
2	B	952	VAL	CA-CB	-10.99	1.31	1.54
1	A	164	ARG	CB-CG	-10.99	1.22	1.52
1	A	326	ARG	NE-CZ	10.98	1.47	1.33
2	B	230	ALA	CA-CB	10.98	1.75	1.52
1	A	474	VAL	CA-CB	-10.98	1.31	1.54
9	K	26	LYS	CD-CE	10.98	1.78	1.51
5	F	100	GLN	CG-CD	10.98	1.76	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	PRO	CA-C	10.97	1.74	1.52
4	E	43	LYS	CE-NZ	10.97	1.76	1.49
1	A	1268	LEU	N-CA	-10.96	1.24	1.46
3	C	177	GLU	CD-OE2	10.96	1.37	1.25
1	A	178	GLY	C-O	-10.95	1.06	1.23
4	E	155	ARG	NE-CZ	10.95	1.47	1.33
2	B	598	GLU	CD-OE1	10.95	1.37	1.25
7	I	84	VAL	CA-CB	-10.95	1.31	1.54
2	B	313	MET	C-O	10.94	1.44	1.23
9	K	58	PHE	CD2-CE2	-10.94	1.17	1.39
2	B	735	ALA	N-CA	10.94	1.68	1.46
1	A	1038	THR	CA-C	-10.93	1.24	1.52
3	C	106	GLU	CD-OE1	10.93	1.37	1.25
1	A	1067	LEU	C-O	10.92	1.44	1.23
2	B	1080	LYS	CE-NZ	10.92	1.76	1.49
1	A	833	GLU	CG-CD	10.92	1.68	1.51
10	L	29	TYR	CD2-CE2	-10.90	1.23	1.39
3	C	20	PHE	CB-CG	-10.90	1.32	1.51
1	A	810	PRO	C-O	10.90	1.45	1.23
2	B	180	TYR	CA-C	10.90	1.81	1.52
1	A	1353	TYR	CD1-CE1	10.89	1.55	1.39
1	A	983	ILE	N-CA	10.89	1.68	1.46
1	A	393	ARG	CZ-NH2	10.89	1.47	1.33
1	A	1220	PHE	CG-CD2	-10.89	1.22	1.38
2	B	243	ALA	C-O	10.88	1.44	1.23
1	A	1053	PHE	CB-CG	-10.88	1.32	1.51
2	B	250	PHE	CG-CD1	10.88	1.55	1.38
3	C	68	GLY	C-O	10.88	1.41	1.23
3	C	62	PHE	CD1-CE1	-10.88	1.17	1.39
2	B	392	ARG	NE-CZ	-10.88	1.19	1.33
1	A	1092	LYS	C-O	10.87	1.44	1.23
1	A	1235	LYS	CD-CE	10.87	1.78	1.51
1	A	635	ARG	CZ-NH2	10.87	1.47	1.33
2	B	1137	CYS	C-O	-10.87	1.02	1.23
1	A	814	PHE	CD2-CE2	10.87	1.60	1.39
6	H	91	ASP	CA-C	10.86	1.81	1.52
4	E	137	GLU	CD-OE2	10.86	1.37	1.25
2	B	935	ARG	CG-CD	10.86	1.79	1.51
2	B	130	VAL	CB-CG2	-10.85	1.30	1.52
3	C	143	LEU	C-O	-10.85	1.02	1.23
1	A	1443	VAL	CB-CG1	-10.85	1.30	1.52
1	A	730	GLY	CA-C	-10.83	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	57	TYR	CG-CD1	-10.83	1.25	1.39
2	B	250	PHE	CB-CG	10.83	1.69	1.51
3	C	126	GLY	C-O	10.82	1.41	1.23
2	B	245	GLU	CG-CD	10.82	1.68	1.51
2	B	1189	ILE	CB-CG2	10.82	1.86	1.52
9	K	64	GLU	CD-OE1	10.82	1.37	1.25
2	B	377	PHE	CG-CD2	-10.81	1.22	1.38
2	B	949	VAL	CA-CB	-10.81	1.32	1.54
1	A	1225	PHE	CD1-CE1	10.81	1.60	1.39
1	A	873	MET	C-O	-10.80	1.02	1.23
1	A	1359	ASP	CB-CG	10.80	1.74	1.51
1	A	1102	LYS	CG-CD	10.79	1.89	1.52
1	A	944	ARG	CZ-NH2	-10.79	1.19	1.33
1	A	1365	TYR	CD1-CE1	10.79	1.55	1.39
3	C	214	ASN	CB-CG	10.79	1.75	1.51
1	A	397	ASN	C-O	10.78	1.43	1.23
4	E	52	ARG	C-O	10.78	1.43	1.23
2	B	486	TYR	CZ-OH	10.78	1.56	1.37
2	B	578	THR	C-O	-10.78	1.02	1.23
3	C	138	GLU	CD-OE1	10.78	1.37	1.25
10	L	65	VAL	C-O	10.77	1.43	1.23
2	B	586	TRP	CE3-CZ3	-10.77	1.20	1.38
1	A	1096	SER	CB-OG	10.77	1.56	1.42
2	B	916	THR	CA-C	10.75	1.80	1.52
1	A	516	SER	N-CA	-10.75	1.24	1.46
2	B	1018	PRO	CA-C	-10.75	1.31	1.52
3	C	124	LEU	CG-CD1	10.75	1.91	1.51
2	B	937	ALA	CA-CB	10.74	1.75	1.52
2	B	1135	ARG	CG-CD	-10.74	1.25	1.51
9	K	71	PHE	C-O	10.74	1.43	1.23
1	A	1154	TYR	CG-CD1	-10.73	1.25	1.39
1	A	417	TYR	CB-CG	10.73	1.67	1.51
3	C	49	VAL	CB-CG2	-10.73	1.30	1.52
8	J	44	TYR	CG-CD2	-10.73	1.25	1.39
2	B	138	GLU	CD-OE2	-10.73	1.13	1.25
2	B	181	LEU	C-O	10.72	1.43	1.23
5	F	102	SER	CB-OG	10.72	1.56	1.42
4	E	45	LYS	CD-CE	10.71	1.78	1.51
1	A	656	TRP	CD2-CE2	10.71	1.54	1.41
2	B	662	MET	SD-CE	10.71	2.37	1.77
2	B	848	ARG	C-O	10.71	1.43	1.23
2	B	394	ASP	CG-OD2	10.71	1.50	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	PHE	CE2-CZ	-10.70	1.17	1.37
1	A	853	ASP	CB-CG	-10.70	1.29	1.51
1	A	1154	TYR	CD1-CE1	10.70	1.55	1.39
2	B	1007	VAL	CB-CG2	-10.70	1.30	1.52
1	A	498	ARG	CZ-NH2	-10.68	1.19	1.33
1	A	933	TYR	CD1-CE1	10.68	1.55	1.39
6	H	136	LYS	CA-CB	10.68	1.77	1.53
1	A	155	GLU	CD-OE1	10.66	1.37	1.25
1	A	16	GLU	CG-CD	10.66	1.68	1.51
6	H	104	PHE	C-O	10.65	1.43	1.23
9	K	6	ARG	CB-CG	-10.65	1.23	1.52
2	B	370	PHE	CD2-CE2	10.65	1.60	1.39
2	B	705	MET	SD-CE	-10.64	1.18	1.77
2	B	226	PHE	CE2-CZ	10.63	1.57	1.37
2	B	313	MET	SD-CE	-10.63	1.18	1.77
1	A	1176	LEU	CB-CG	10.62	1.83	1.52
1	A	289	ILE	CA-CB	10.62	1.79	1.54
1	A	496	GLU	CG-CD	10.62	1.67	1.51
1	A	1191	TRP	CG-CD2	-10.62	1.25	1.43
9	K	17	SER	C-O	-10.62	1.03	1.23
2	B	1057	LYS	CG-CD	10.61	1.88	1.52
1	A	1023	ARG	CZ-NH1	-10.61	1.19	1.33
5	F	97	ARG	CZ-NH1	10.60	1.46	1.33
2	B	1070	GLU	CD-OE1	10.60	1.37	1.25
2	B	699	GLU	N-CA	-10.59	1.25	1.46
2	B	124	TYR	CE1-CZ	-10.59	1.24	1.38
2	B	622	LYS	CB-CG	10.58	1.81	1.52
1	A	1153	TYR	CD2-CE2	-10.58	1.23	1.39
1	A	19	PHE	CD1-CE1	-10.57	1.18	1.39
2	B	190	TYR	CD2-CE2	10.57	1.55	1.39
1	A	95	PHE	CD1-CE1	10.56	1.60	1.39
4	E	25	ASP	CB-CG	10.56	1.74	1.51
4	E	105	PHE	CE2-CZ	10.56	1.57	1.37
1	A	1093	LYS	CG-CD	10.56	1.88	1.52
7	I	36	GLU	CG-CD	10.56	1.67	1.51
2	B	766	ARG	CZ-NH1	10.56	1.46	1.33
2	B	39	ARG	C-O	-10.55	1.03	1.23
4	E	187	TYR	CZ-OH	10.55	1.55	1.37
2	B	745	PRO	C-O	-10.55	1.02	1.23
1	A	888	GLY	C-O	-10.55	1.06	1.23
7	I	57	GLY	CA-C	-10.54	1.34	1.51
1	A	218	ASP	CG-OD2	10.54	1.49	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	129	PRO	CG-CD	10.53	1.85	1.50
8	J	56	LEU	N-CA	-10.52	1.25	1.46
2	B	591	ARG	NE-CZ	10.52	1.46	1.33
4	E	72	PHE	CD2-CE2	-10.51	1.18	1.39
2	B	874	PHE	CD2-CE2	-10.51	1.18	1.39
1	A	747	VAL	CA-CB	-10.51	1.32	1.54
2	B	811	TYR	CD2-CE2	10.51	1.55	1.39
1	A	931	GLU	CG-CD	10.51	1.67	1.51
6	H	77	ARG	CB-CG	10.50	1.80	1.52
7	I	20	LYS	CE-NZ	10.50	1.75	1.49
2	B	723	VAL	CA-CB	10.50	1.76	1.54
8	J	60	PHE	CE1-CZ	-10.50	1.17	1.37
1	A	427	GLN	CB-CG	10.49	1.80	1.52
1	A	711	ARG	CB-CG	10.49	1.80	1.52
1	A	1358	SER	CA-CB	10.49	1.68	1.52
2	B	333	PHE	CG-CD2	-10.49	1.23	1.38
1	A	867	ILE	CB-CG2	10.49	1.85	1.52
3	C	85	ASP	CB-CG	10.49	1.73	1.51
1	A	378	GLU	CD-OE1	-10.47	1.14	1.25
3	C	3	GLU	CG-CD	10.47	1.67	1.51
4	E	79	TRP	CG-CD1	10.47	1.51	1.36
1	A	4	GLN	CB-CG	10.47	1.80	1.52
2	B	217	ARG	CZ-NH1	-10.46	1.19	1.33
2	B	1004	GLU	CD-OE1	10.46	1.37	1.25
1	A	1314	SER	C-O	10.45	1.43	1.23
1	A	1419	ASP	CG-OD1	10.44	1.49	1.25
9	K	54	ARG	CG-CD	10.44	1.78	1.51
2	B	303	TYR	CD2-CE2	-10.43	1.23	1.39
9	K	68	PHE	CG-CD1	-10.43	1.23	1.38
1	A	620	LYS	CE-NZ	10.42	1.75	1.49
2	B	307	ASP	CB-CG	-10.42	1.29	1.51
2	B	217	ARG	NE-CZ	-10.42	1.19	1.33
4	E	119	SER	C-O	10.42	1.43	1.23
2	B	343	ILE	CB-CG2	-10.41	1.20	1.52
4	E	44	ALA	C-O	10.41	1.43	1.23
3	C	87	PHE	CG-CD1	-10.41	1.23	1.38
1	A	1350	LYS	CE-NZ	10.41	1.75	1.49
1	A	965	GLN	CG-CD	10.41	1.75	1.51
2	B	617	ARG	CG-CD	10.40	1.77	1.51
1	A	1270	ASN	C-O	10.40	1.43	1.23
1	A	720	ARG	NE-CZ	10.40	1.46	1.33
2	B	52	ASN	CG-ND2	10.39	1.58	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	370	PHE	CE2-CZ	10.39	1.57	1.37
1	A	852	TYR	CE2-CZ	-10.39	1.25	1.38
3	C	214	ASN	N-CA	10.39	1.67	1.46
3	C	75	MET	SD-CE	10.38	2.35	1.77
1	A	851	HIS	CA-CB	-10.38	1.31	1.53
2	B	371	GLU	CG-CD	10.38	1.67	1.51
1	A	459	ARG	C-O	-10.37	1.03	1.23
7	I	75	CYS	C-O	-10.37	1.03	1.23
10	L	37	LYS	CB-CG	-10.37	1.24	1.52
6	H	118	PHE	CE1-CZ	-10.37	1.17	1.37
3	C	140	ASN	CG-OD1	10.36	1.46	1.24
1	A	173	THR	CB-CG2	10.36	1.86	1.52
1	A	1426	GLU	CD-OE2	10.36	1.37	1.25
1	A	389	THR	CB-CG2	10.36	1.86	1.52
2	B	787	VAL	CB-CG1	10.36	1.74	1.52
2	B	646	LEU	CG-CD1	10.35	1.90	1.51
2	B	994	TYR	CE1-CZ	-10.35	1.25	1.38
2	B	643	ASP	CB-CG	10.34	1.73	1.51
2	B	632	ARG	CG-CD	10.34	1.77	1.51
1	A	846	GLU	CG-CD	10.34	1.67	1.51
3	C	11	ARG	C-O	10.34	1.43	1.23
9	K	26	LYS	CE-NZ	10.34	1.74	1.49
2	B	377	PHE	CB-CG	-10.34	1.33	1.51
7	I	45	ARG	CD-NE	10.33	1.64	1.46
2	B	545	ILE	N-CA	-10.32	1.25	1.46
2	B	996	ARG	CG-CD	10.32	1.77	1.51
4	E	196	VAL	CB-CG1	-10.31	1.31	1.52
6	H	80	ARG	NE-CZ	10.31	1.46	1.33
1	A	1136	SER	CB-OG	10.30	1.55	1.42
2	B	848	ARG	N-CA	-10.30	1.25	1.46
2	B	1129	ARG	CZ-NH1	10.30	1.46	1.33
10	L	50	ASP	CB-CG	10.30	1.73	1.51
2	B	1198	TYR	CG-CD1	-10.30	1.25	1.39
2	B	895	ASP	CA-CB	10.29	1.76	1.53
6	H	129	TYR	CB-CG	10.29	1.67	1.51
1	A	1160	SER	CB-OG	10.29	1.55	1.42
2	B	666	TYR	CB-CG	-10.29	1.36	1.51
1	A	1003	LYS	CB-CG	10.28	1.80	1.52
2	B	994	TYR	CD1-CE1	-10.29	1.24	1.39
8	J	62	ARG	CZ-NH1	10.28	1.46	1.33
1	A	879	GLU	CD-OE1	10.26	1.36	1.25
1	A	1018	PHE	CE2-CZ	10.26	1.56	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	700	SER	CA-CB	-10.26	1.37	1.52
5	F	87	LYS	CE-NZ	10.26	1.74	1.49
7	I	46	HIS	CA-CB	10.25	1.76	1.53
1	A	830	LYS	CG-CD	10.25	1.87	1.52
1	A	1157	ASP	CB-CG	10.25	1.73	1.51
3	C	218	PRO	CA-C	10.24	1.73	1.52
1	A	74	MET	CB-CG	10.24	1.84	1.51
3	C	183	TRP	CE3-CZ3	10.23	1.55	1.38
1	A	774	ARG	CZ-NH2	-10.23	1.19	1.33
2	B	399	ASP	CB-CG	10.22	1.73	1.51
2	B	764	SER	CB-OG	-10.22	1.28	1.42
4	E	28	TYR	CD1-CE1	10.22	1.54	1.39
9	K	68	PHE	CB-CG	-10.22	1.33	1.51
1	A	234	MET	C-O	10.22	1.42	1.23
1	A	514	PRO	CG-CD	-10.22	1.17	1.50
2	B	527	THR	CB-OG1	10.22	1.63	1.43
1	A	1349	TYR	CD2-CE2	10.21	1.54	1.39
9	K	79	GLU	CD-OE1	10.22	1.36	1.25
3	C	50	GLU	CD-OE2	10.21	1.36	1.25
4	E	50	MET	C-O	10.21	1.42	1.23
6	H	105	GLU	CD-OE2	10.21	1.36	1.25
1	A	502	SER	C-O	-10.21	1.03	1.23
1	A	1328	TYR	CE1-CZ	-10.20	1.25	1.38
4	E	131	THR	CB-CG2	10.21	1.86	1.52
2	B	240	ILE	C-O	-10.20	1.03	1.23
1	A	129	LYS	CB-CG	10.20	1.80	1.52
3	C	42	PRO	CA-CB	-10.19	1.33	1.53
8	J	5	VAL	CB-CG2	10.18	1.74	1.52
7	I	27	PHE	CA-CB	-10.18	1.31	1.53
4	E	150	VAL	CB-CG1	-10.18	1.31	1.52
2	B	96	TYR	CD2-CE2	10.18	1.54	1.39
5	F	153	VAL	CB-CG1	10.18	1.74	1.52
10	L	47	ARG	NE-CZ	10.18	1.46	1.33
1	A	193	ASP	N-CA	10.17	1.66	1.46
2	B	983	ARG	CZ-NH2	-10.17	1.19	1.33
2	B	496	ARG	C-O	10.16	1.42	1.23
6	H	104	PHE	CG-CD2	10.16	1.53	1.38
2	B	733	HIS	C-O	10.15	1.42	1.23
1	A	549	MET	CA-C	-10.15	1.26	1.52
9	K	96	ASN	C-O	10.15	1.42	1.23
2	B	996	ARG	CD-NE	10.15	1.63	1.46
1	A	567	LYS	CE-NZ	10.14	1.74	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	GLN	CD-NE2	10.14	1.58	1.32
2	B	859	TYR	CB-CG	-10.14	1.36	1.51
4	E	138	ALA	C-O	-10.14	1.04	1.23
7	I	70	ARG	NE-CZ	-10.14	1.19	1.33
2	B	359	GLU	CD-OE1	10.13	1.36	1.25
2	B	622	LYS	CE-NZ	10.13	1.74	1.49
1	A	782	ARG	CZ-NH1	10.12	1.46	1.33
1	A	1239	ARG	CZ-NH2	-10.12	1.19	1.33
3	C	163	ILE	CB-CG2	10.12	1.84	1.52
1	A	468	PHE	CD1-CE1	10.12	1.59	1.39
2	B	916	THR	CB-CG2	10.12	1.85	1.52
3	C	175	ALA	CA-CB	-10.12	1.31	1.52
1	A	213	HIS	CA-CB	10.11	1.76	1.53
1	A	460	VAL	CB-CG2	-10.11	1.31	1.52
1	A	1349	TYR	CA-C	-10.11	1.26	1.52
7	I	3	THR	CB-CG2	10.11	1.85	1.52
5	F	84	TYR	CD1-CE1	10.11	1.54	1.39
1	A	1119	TYR	CG-CD1	-10.10	1.26	1.39
1	A	15	LYS	CB-CG	10.10	1.79	1.52
1	A	839	ARG	NE-CZ	10.10	1.46	1.33
4	E	202	SER	CB-OG	-10.10	1.29	1.42
3	C	172	PRO	C-O	10.09	1.43	1.23
2	B	615	MET	N-CA	-10.08	1.26	1.46
3	C	106	GLU	CD-OE2	10.08	1.36	1.25
1	A	1221	LYS	CB-CG	10.08	1.79	1.52
3	C	90	ASP	N-CA	10.08	1.66	1.46
1	A	1298	TYR	CE2-CZ	-10.08	1.25	1.38
2	B	785	TYR	CB-CG	-10.07	1.36	1.51
1	A	622	VAL	CB-CG1	-10.07	1.31	1.52
1	A	713	SER	N-CA	-10.07	1.26	1.46
2	B	479	VAL	CB-CG1	-10.06	1.31	1.52
7	I	8	ARG	CZ-NH1	10.06	1.46	1.33
2	B	1029	CYS	CA-C	10.06	1.79	1.52
1	A	1417	GLU	CD-OE1	10.06	1.36	1.25
7	I	59	VAL	CB-CG1	-10.05	1.31	1.52
1	A	1112	LYS	CB-CG	10.05	1.79	1.52
2	B	459	TYR	CD1-CE1	10.05	1.54	1.39
5	F	72	LYS	CD-CE	10.05	1.76	1.51
2	B	746	SER	CB-OG	-10.05	1.29	1.42
2	B	18	PHE	CG-CD1	10.04	1.53	1.38
2	B	41	LYS	CD-CE	10.05	1.76	1.51
7	I	44	TYR	C-O	10.04	1.42	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	845	SER	CB-OG	10.04	1.55	1.42
5	F	111	LEU	CG-CD2	10.04	1.89	1.51
9	K	30	ALA	CA-CB	-10.04	1.31	1.52
2	B	666	TYR	CD2-CE2	10.03	1.54	1.39
9	K	64	GLU	C-O	-10.03	1.04	1.23
1	A	972	HIS	C-O	-10.03	1.04	1.23
2	B	209	GLU	CA-CB	-10.03	1.31	1.53
2	B	357	GLN	C-O	-10.02	1.04	1.23
2	B	1183	LYS	CB-CG	10.02	1.79	1.52
1	A	1017	LEU	C-O	10.02	1.42	1.23
2	B	519	TRP	CB-CG	10.02	1.68	1.50
3	C	139	GLY	C-O	10.01	1.39	1.23
1	A	368	LYS	CD-CE	10.01	1.76	1.51
4	E	28	TYR	CG-CD1	-10.01	1.26	1.39
1	A	1176	LEU	CA-CB	10.00	1.76	1.53
1	A	971	PHE	CD1-CE1	-10.00	1.19	1.39
10	L	48	CYS	CA-C	10.00	1.78	1.52
1	A	734	GLU	CG-CD	10.00	1.67	1.51
1	A	806	ARG	CB-CG	10.00	1.79	1.52
10	L	29	TYR	CE1-CZ	-9.99	1.25	1.38
2	B	659	ALA	CA-CB	9.99	1.73	1.52
3	C	242	GLN	C-O	9.97	1.42	1.23
2	B	384	ARG	CZ-NH1	-9.95	1.20	1.33
2	B	655	LYS	CG-CD	9.95	1.86	1.52
1	A	572	TRP	CE2-CZ2	-9.95	1.22	1.39
1	A	464	PRO	C-N	-9.95	1.11	1.34
6	H	20	TYR	CD1-CE1	-9.94	1.24	1.39
6	H	84	ALA	CA-CB	9.94	1.73	1.52
4	E	215	MET	N-CA	9.94	1.66	1.46
1	A	1165	GLU	CD-OE1	9.92	1.36	1.25
1	A	1236	LEU	C-O	-9.92	1.04	1.23
2	B	850	LEU	CA-CB	-9.92	1.30	1.53
8	J	52	THR	C-O	9.92	1.42	1.23
1	A	465	TYR	CG-CD1	-9.92	1.26	1.39
2	B	1065	GLN	C-O	9.92	1.42	1.23
2	B	1109	GLY	CA-C	9.92	1.67	1.51
1	A	860	LEU	CG-CD1	9.92	1.88	1.51
1	A	268	ASP	CB-CG	9.92	1.72	1.51
3	C	125	MET	SD-CE	9.91	2.33	1.77
2	B	787	VAL	N-CA	-9.91	1.26	1.46
1	A	404	TYR	CG-CD1	-9.91	1.26	1.39
1	A	393	ARG	CZ-NH1	9.90	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	72	LYS	CD-CE	9.90	1.75	1.51
1	A	3	GLY	N-CA	9.89	1.60	1.46
7	I	74	GLU	CB-CG	9.89	1.71	1.52
1	A	842	VAL	C-O	-9.89	1.04	1.23
2	B	561	TRP	CD2-CE3	9.88	1.55	1.40
2	B	116	GLU	CD-OE2	9.88	1.36	1.25
2	B	875	GLU	CD-OE2	9.88	1.36	1.25
7	I	88	SER	CA-C	-9.88	1.27	1.52
5	F	121	ALA	C-O	-9.87	1.04	1.23
3	C	229	TYR	CE1-CZ	-9.87	1.25	1.38
1	A	432	VAL	C-O	-9.86	1.04	1.23
1	A	714	PHE	CE2-CZ	9.86	1.56	1.37
3	C	56	THR	CB-CG2	-9.86	1.19	1.52
2	B	137	TYR	CA-CB	9.86	1.75	1.53
3	C	193	TYR	CE2-CZ	-9.85	1.25	1.38
1	A	808	LEU	C-O	-9.85	1.04	1.23
1	A	1135	ARG	NE-CZ	9.85	1.45	1.33
2	B	519	TRP	CD2-CE2	-9.84	1.29	1.41
1	A	712	GLU	CD-OE2	9.83	1.36	1.25
1	A	1338	VAL	CB-CG2	-9.83	1.32	1.52
2	B	21	GLU	CG-CD	9.83	1.66	1.51
6	H	19	ARG	NE-CZ	9.83	1.45	1.33
1	A	1243	VAL	CB-CG2	9.82	1.73	1.52
1	A	1365	TYR	CG-CD2	9.82	1.51	1.39
5	F	103	MET	SD-CE	9.82	2.32	1.77
1	A	1345	ARG	NE-CZ	-9.82	1.20	1.33
4	E	50	MET	SD-CE	9.82	2.32	1.77
6	H	94	ASP	CB-CG	-9.82	1.31	1.51
2	B	136	THR	CA-CB	9.81	1.78	1.53
2	B	381	MET	SD-CE	-9.81	1.22	1.77
3	C	78	GLU	C-O	-9.81	1.04	1.23
1	A	969	GLN	CD-NE2	9.81	1.57	1.32
3	C	26	ASP	CG-OD1	9.81	1.48	1.25
1	A	428	TYR	CD1-CE1	9.81	1.54	1.39
3	C	106	GLU	C-O	9.81	1.42	1.23
1	A	843	LYS	CG-CD	9.80	1.85	1.52
1	A	1031	VAL	CA-CB	-9.80	1.34	1.54
1	A	1098	VAL	C-O	-9.80	1.04	1.23
3	C	205	LYS	CG-CD	9.80	1.85	1.52
8	J	26	GLN	CG-CD	9.80	1.73	1.51
4	E	11	ARG	C-O	9.80	1.42	1.23
3	C	215	GLU	CD-OE1	9.79	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	585	GLY	C-O	9.79	1.39	1.23
4	E	136	ASN	C-O	-9.79	1.04	1.23
4	E	212	ARG	CG-CD	9.79	1.76	1.51
1	A	804	TYR	CE1-CZ	-9.79	1.25	1.38
2	B	203	PHE	CG-CD2	-9.78	1.24	1.38
7	I	107	SER	CB-OG	-9.78	1.29	1.42
1	A	209	ASN	CG-ND2	9.78	1.57	1.32
1	A	660	ASN	N-CA	-9.78	1.26	1.46
1	A	1191	TRP	CZ3-CH2	-9.78	1.24	1.40
7	I	101	PHE	CB-CG	-9.78	1.34	1.51
2	B	531	GLN	CD-OE1	9.78	1.45	1.24
2	B	459	TYR	CE2-CZ	9.77	1.51	1.38
9	K	26	LYS	CB-CG	9.77	1.78	1.52
1	A	1064	VAL	CB-CG1	-9.77	1.32	1.52
6	H	22	LYS	CB-CG	9.77	1.78	1.52
1	A	396	PRO	CA-C	-9.77	1.33	1.52
1	A	897	TYR	CG-CD2	-9.77	1.26	1.39
2	B	286	PHE	CE1-CZ	-9.77	1.18	1.37
2	B	965	LYS	CD-CE	9.77	1.75	1.51
1	A	593	GLU	CD-OE2	9.76	1.36	1.25
4	E	103	LYS	CE-NZ	9.76	1.73	1.49
2	B	975	GLN	C-O	-9.76	1.04	1.23
1	A	180	LYS	CG-CD	9.76	1.85	1.52
2	B	871	THR	CA-CB	9.76	1.78	1.53
3	C	40	GLU	CD-OE2	9.75	1.36	1.25
4	E	105	PHE	CG-CD1	9.75	1.53	1.38
2	B	1069	PHE	C-O	9.75	1.41	1.23
2	B	182	SER	CB-OG	9.74	1.54	1.42
2	B	332	ASP	CB-CG	-9.74	1.31	1.51
4	E	28	TYR	CZ-OH	-9.74	1.21	1.37
5	F	79	ARG	NE-CZ	-9.74	1.20	1.33
1	A	1080	THR	CA-CB	9.73	1.78	1.53
1	A	804	TYR	CA-CB	-9.73	1.32	1.53
8	J	63	TYR	CB-CG	9.73	1.66	1.51
2	B	322	PHE	CG-CD1	-9.73	1.24	1.38
1	A	433	GLU	CD-OE2	9.72	1.36	1.25
2	B	305	VAL	C-O	9.72	1.41	1.23
4	E	110	PHE	CG-CD2	-9.72	1.24	1.38
2	B	216	GLU	C-O	-9.72	1.04	1.23
2	B	848	ARG	NE-CZ	-9.72	1.20	1.33
1	A	954	TRP	CD2-CE2	-9.72	1.29	1.41
2	B	1220	ARG	NE-CZ	9.72	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	118	ARG	CD-NE	9.72	1.62	1.46
2	B	259	TYR	CG-CD2	9.71	1.51	1.39
1	A	1269	GLU	CD-OE2	9.71	1.36	1.25
2	B	416	LEU	CG-CD2	9.71	1.87	1.51
4	E	75	MET	C-O	9.71	1.41	1.23
3	C	166	GLU	CG-CD	9.71	1.66	1.51
2	B	299	GLU	CD-OE2	9.70	1.36	1.25
7	I	16	PRO	C-O	9.70	1.42	1.23
1	A	625	SER	CA-CB	-9.70	1.38	1.52
2	B	780	VAL	C-O	-9.69	1.04	1.23
1	A	813	PHE	CG-CD1	-9.69	1.24	1.38
1	A	777	PHE	CE2-CZ	-9.69	1.19	1.37
1	A	1074	GLU	CD-OE2	9.69	1.36	1.25
3	C	173	ALA	CA-CB	-9.69	1.32	1.52
1	A	124	GLN	CD-NE2	9.68	1.57	1.32
2	B	992	ILE	CB-CG2	-9.68	1.22	1.52
1	A	46	THR	CA-CB	9.68	1.78	1.53
1	A	478	TYR	CE1-CZ	-9.68	1.25	1.38
1	A	484	GLY	C-O	9.68	1.39	1.23
1	A	931	GLU	CD-OE2	9.68	1.36	1.25
2	B	1032	SER	CB-OG	9.68	1.54	1.42
1	A	357	PRO	C-O	9.68	1.42	1.23
2	B	908	GLU	CG-CD	9.67	1.66	1.51
7	I	6	PHE	CG-CD2	-9.67	1.24	1.38
10	L	29	TYR	CE2-CZ	-9.67	1.25	1.38
2	B	37	PHE	CG-CD2	9.67	1.53	1.38
1	A	465	TYR	CE1-CZ	-9.67	1.25	1.38
1	A	1137	ALA	C-O	9.67	1.41	1.23
4	E	43	LYS	CB-CG	9.67	1.78	1.52
1	A	995	GLU	C-O	-9.66	1.04	1.23
1	A	1366	ARG	CZ-NH1	9.66	1.45	1.33
1	A	52	GLY	C-O	-9.66	1.08	1.23
2	B	123	THR	CA-CB	-9.66	1.28	1.53
4	E	74	ASP	CB-CG	-9.66	1.31	1.51
6	H	49	VAL	CA-CB	-9.66	1.34	1.54
2	B	845	SER	C-O	9.65	1.41	1.23
2	B	1204	PHE	CE2-CZ	-9.65	1.19	1.37
1	A	478	TYR	CG-CD2	-9.65	1.26	1.39
2	B	303	TYR	CG-CD2	-9.65	1.26	1.39
1	A	139	TRP	CB-CG	-9.64	1.32	1.50
2	B	408	LEU	CG-CD1	9.64	1.87	1.51
7	I	34	TYR	CG-CD1	-9.64	1.26	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1071	SER	CB-OG	9.64	1.54	1.42
2	B	785	TYR	CE1-CZ	9.64	1.51	1.38
2	B	1081	LEU	CA-C	-9.64	1.27	1.52
1	A	975	HIS	CA-CB	9.64	1.75	1.53
2	B	41	LYS	C-O	9.63	1.41	1.23
2	B	245	GLU	CB-CG	9.63	1.70	1.52
2	B	231	PRO	CA-C	9.63	1.72	1.52
1	A	469	ARG	CD-NE	-9.62	1.30	1.46
2	B	1069	PHE	CE1-CZ	-9.61	1.19	1.37
2	B	1102	LYS	CB-CG	9.62	1.78	1.52
6	H	131	ASN	CA-CB	9.61	1.78	1.53
1	A	400	PRO	C-O	-9.61	1.04	1.23
1	A	852	TYR	CG-CD1	-9.61	1.26	1.39
2	B	606	LYS	CD-CE	9.61	1.75	1.51
8	J	42	LYS	CG-CD	9.60	1.85	1.52
4	E	40	GLU	CG-CD	9.60	1.66	1.51
1	A	558	GLY	C-O	-9.60	1.08	1.23
1	A	684	ALA	CA-CB	9.60	1.72	1.52
8	J	24	LEU	C-O	-9.60	1.05	1.23
5	F	77	ASP	CG-OD1	9.59	1.47	1.25
7	I	96	SER	CB-OG	9.59	1.54	1.42
2	B	414	ALA	CA-CB	-9.58	1.32	1.52
7	I	31	THR	C-O	-9.58	1.05	1.23
2	B	1020	ARG	CD-NE	-9.57	1.30	1.46
3	C	127	ARG	N-CA	9.57	1.65	1.46
4	E	91	LYS	CB-CG	9.57	1.78	1.52
4	E	200	ARG	CB-CG	-9.57	1.26	1.52
1	A	417	TYR	CG-CD2	9.57	1.51	1.39
2	B	729	ILE	CA-CB	-9.57	1.32	1.54
2	B	1109	GLY	C-O	9.57	1.39	1.23
2	B	1106	ARG	NE-CZ	9.57	1.45	1.33
3	C	252	GLN	CG-CD	9.57	1.73	1.51
3	C	34	ARG	CZ-NH1	-9.56	1.20	1.33
5	F	83	PRO	C-O	9.56	1.42	1.23
1	A	1019	CYS	CB-SG	-9.56	1.66	1.82
2	B	370	PHE	CG-CD2	9.56	1.53	1.38
1	A	190	ALA	C-O	9.55	1.41	1.23
9	K	111	LEU	C-O	9.55	1.41	1.23
1	A	544	ASP	CB-CG	9.54	1.71	1.51
2	B	208	SER	CA-CB	-9.54	1.38	1.52
10	L	34	CYS	CB-SG	-9.54	1.66	1.82
8	J	43	ARG	CG-CD	9.54	1.75	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	654	ARG	CA-CB	-9.53	1.32	1.53
1	A	992	ASP	N-CA	-9.53	1.27	1.46
1	A	720	ARG	CZ-NH1	-9.52	1.20	1.33
3	C	205	LYS	CD-CE	9.52	1.75	1.51
3	C	241	ASP	CB-CG	9.52	1.71	1.51
2	B	733	HIS	CA-C	9.51	1.77	1.52
9	K	1	MET	N-CA	9.51	1.65	1.46
1	A	468	PHE	CB-CG	-9.51	1.35	1.51
2	B	394	ASP	CB-CG	9.51	1.71	1.51
6	H	146	ARG	CZ-NH1	9.51	1.45	1.33
1	A	550	LEU	C-O	-9.50	1.05	1.23
1	A	640	GLN	CD-OE1	9.50	1.44	1.24
2	B	118	ARG	CA-CB	9.50	1.74	1.53
3	C	233	GLU	CD-OE2	9.50	1.36	1.25
1	A	1367	HIS	CA-CB	-9.49	1.33	1.53
2	B	529	GLU	C-O	9.49	1.41	1.23
2	B	1198	TYR	CA-CB	9.49	1.74	1.53
1	A	1228	TRP	CD2-CE2	-9.49	1.29	1.41
2	B	1206	GLU	CD-OE1	9.49	1.36	1.25
7	I	84	VAL	CB-CG1	-9.49	1.32	1.52
1	A	999	VAL	CB-CG1	-9.48	1.32	1.52
2	B	1183	LYS	C-O	9.48	1.41	1.23
3	C	166	GLU	N-CA	-9.48	1.27	1.46
1	A	291	GLU	C-O	-9.47	1.05	1.23
1	A	614	PHE	CG-CD1	-9.47	1.24	1.38
2	B	1075	GLY	CA-C	9.47	1.67	1.51
10	L	62	LYS	CE-NZ	9.47	1.72	1.49
7	I	115	LYS	CE-NZ	9.47	1.72	1.49
2	B	691	GLU	CG-CD	9.47	1.66	1.51
3	C	195	GLN	CD-OE1	9.47	1.44	1.24
3	C	15	LYS	CG-CD	9.47	1.84	1.52
3	C	194	GLU	CD-OE1	9.46	1.36	1.25
1	A	203	SER	CA-CB	9.46	1.67	1.52
4	E	180	ARG	CZ-NH2	9.46	1.45	1.33
1	A	1420	ASP	CG-OD2	9.46	1.47	1.25
2	B	866	TYR	CE1-CZ	9.46	1.50	1.38
2	B	63	ILE	CA-C	9.45	1.77	1.52
2	B	882	THR	CB-CG2	9.46	1.83	1.52
7	I	52	ILE	CB-CG2	-9.46	1.23	1.52
1	A	1191	TRP	CB-CG	-9.45	1.33	1.50
4	E	98	ILE	CA-CB	9.45	1.76	1.54
1	A	748	MET	CG-SD	9.45	2.05	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1139	GLU	C-O	9.44	1.41	1.23
2	B	188	ASP	C-O	9.44	1.41	1.23
2	B	485	ARG	CZ-NH1	-9.44	1.20	1.33
2	B	1004	GLU	C-O	9.44	1.41	1.23
2	B	607	GLY	C-O	-9.43	1.08	1.23
7	I	93	LYS	C-O	9.43	1.41	1.23
1	A	123	ARG	CB-CG	9.43	1.78	1.52
3	C	192	TRP	CE3-CZ3	-9.43	1.22	1.38
1	A	1356	ILE	C-O	-9.43	1.05	1.23
7	I	56	ALA	C-O	-9.43	1.05	1.23
3	C	70	ILE	CB-CG2	9.42	1.82	1.52
1	A	200	ARG	C-O	-9.42	1.05	1.23
2	B	266	ALA	C-O	9.42	1.41	1.23
1	A	498	ARG	CB-CG	-9.42	1.27	1.52
1	A	1012	ARG	NE-CZ	9.41	1.45	1.33
4	E	109	ILE	CB-CG2	-9.41	1.23	1.52
1	A	224	PHE	CG-CD1	-9.41	1.24	1.38
2	B	1194	ILE	N-CA	-9.41	1.27	1.46
6	H	7	ASP	CB-CG	9.41	1.71	1.51
3	C	94	LYS	CB-CG	9.40	1.77	1.52
1	A	902	LEU	CG-CD2	-9.39	1.17	1.51
1	A	1328	TYR	CD2-CE2	-9.39	1.25	1.39
1	A	1450	LEU	CG-CD2	9.39	1.86	1.51
2	B	226	PHE	C-O	-9.39	1.05	1.23
1	A	110	CYS	CA-CB	9.39	1.74	1.53
4	E	82	PHE	CD2-CE2	-9.39	1.20	1.39
1	A	826	ASP	CG-OD2	9.38	1.47	1.25
1	A	1206	ASP	CB-CG	9.38	1.71	1.51
1	A	590	ARG	CZ-NH2	-9.38	1.20	1.33
2	B	811	TYR	CB-CG	-9.37	1.37	1.51
2	B	320	ASP	CG-OD1	9.37	1.47	1.25
1	A	466	SER	CB-OG	-9.37	1.30	1.42
2	B	592	ASN	CG-ND2	9.37	1.56	1.32
3	C	192	TRP	CZ3-CH2	9.37	1.55	1.40
7	I	4	PHE	CE1-CZ	9.37	1.55	1.37
2	B	208	SER	CB-OG	-9.36	1.30	1.42
1	A	552	TRP	CG-CD1	-9.36	1.23	1.36
2	B	250	PHE	CE2-CZ	9.36	1.55	1.37
1	A	1426	GLU	CD-OE1	9.36	1.35	1.25
2	B	711	GLU	C-O	9.36	1.41	1.23
3	C	97	VAL	C-O	-9.36	1.05	1.23
5	F	148	VAL	C-O	9.36	1.41	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	510	LYS	CE-NZ	9.36	1.72	1.49
2	B	1091	TYR	CB-CG	-9.36	1.37	1.51
10	L	29	TYR	CG-CD1	-9.36	1.26	1.39
2	B	322	PHE	CD2-CE2	-9.35	1.20	1.39
4	E	180	ARG	CG-CD	9.35	1.75	1.51
9	K	71	PHE	CA-CB	-9.35	1.33	1.53
4	E	42	PHE	CD1-CE1	9.35	1.57	1.39
4	E	202	SER	CA-CB	-9.35	1.39	1.52
1	A	551	TYR	CE1-CZ	-9.34	1.26	1.38
2	B	353	LYS	CG-CD	9.34	1.84	1.52
2	B	620	ARG	CG-CD	9.34	1.75	1.51
7	I	1	MET	CA-CB	9.34	1.74	1.53
1	A	984	LYS	CE-NZ	9.34	1.72	1.49
5	F	142	SER	C-O	-9.34	1.05	1.23
1	A	1128	GLN	CA-C	9.34	1.77	1.52
1	A	515	GLN	CD-OE1	9.33	1.44	1.24
1	A	699	ALA	CA-CB	-9.33	1.32	1.52
7	I	91	ARG	CA-C	-9.33	1.28	1.52
10	L	38	LEU	CG-CD1	9.33	1.86	1.51
7	I	110	PHE	CB-CG	-9.33	1.35	1.51
1	A	16	GLU	C-O	9.32	1.41	1.23
1	A	120	GLU	CD-OE2	9.32	1.35	1.25
1	A	843	LYS	CD-CE	9.32	1.74	1.51
1	A	1154	TYR	CG-CD2	-9.32	1.27	1.39
1	A	487	MET	CB-CG	-9.32	1.21	1.51
2	B	325	GLN	CG-CD	9.31	1.72	1.51
2	B	536	VAL	CB-CG1	-9.31	1.33	1.52
2	B	995	ARG	CD-NE	-9.31	1.30	1.46
2	B	1140	ALA	C-O	9.31	1.41	1.23
1	A	548	ASN	CG-OD1	9.30	1.44	1.24
2	B	875	GLU	CD-OE1	9.31	1.35	1.25
1	A	217	LYS	CG-CD	9.30	1.84	1.52
1	A	653	VAL	CB-CG1	-9.30	1.33	1.52
1	A	1010	ALA	CA-C	-9.30	1.28	1.52
1	A	41	MET	SD-CE	9.29	2.29	1.77
1	A	366	VAL	CB-CG1	-9.29	1.33	1.52
1	A	821	ARG	CD-NE	-9.29	1.30	1.46
2	B	666	TYR	CD1-CE1	9.29	1.53	1.39
2	B	987	LYS	C-O	-9.29	1.05	1.23
2	B	368	GLU	CB-CG	9.29	1.69	1.52
2	B	409	ALA	CA-CB	-9.29	1.32	1.52
3	C	180	TYR	CE2-CZ	-9.29	1.26	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	529	GLU	CD-OE1	9.29	1.35	1.25
9	K	22	ASP	CB-CG	9.29	1.71	1.51
1	A	1362	TYR	CB-CG	-9.29	1.37	1.51
2	B	1216	LEU	C-O	9.29	1.41	1.23
1	A	1129	GLU	CA-CB	9.28	1.74	1.53
2	B	481	GLN	C-O	9.28	1.41	1.23
1	A	390	GLN	C-O	9.28	1.41	1.23
1	A	556	TRP	CZ3-CH2	9.28	1.54	1.40
1	A	390	GLN	CD-OE1	9.28	1.44	1.24
1	A	411	ASP	N-CA	9.28	1.65	1.46
1	A	464	PRO	CA-C	-9.28	1.34	1.52
1	A	560	ILE	C-O	-9.28	1.05	1.23
2	B	203	PHE	C-O	9.28	1.41	1.23
4	E	34	GLU	CD-OE2	9.27	1.35	1.25
9	K	81	TYR	CE2-CZ	9.27	1.50	1.38
1	A	593	GLU	CB-CG	9.27	1.69	1.52
1	A	1140	HIS	C-O	-9.27	1.05	1.23
1	A	1277	GLU	N-CA	9.26	1.64	1.46
3	C	8	VAL	CB-CG2	-9.26	1.33	1.52
3	C	249	ASP	CA-CB	9.26	1.74	1.53
1	A	1301	GLU	CD-OE1	9.26	1.35	1.25
2	B	1096	ARG	CZ-NH1	9.26	1.45	1.33
3	C	154	LYS	CG-CD	9.26	1.83	1.52
2	B	1150	ARG	CZ-NH2	9.26	1.45	1.33
1	A	205	GLU	C-O	9.25	1.41	1.23
1	A	358	ASN	CG-ND2	9.25	1.55	1.32
1	A	1434	ALA	CA-CB	-9.25	1.33	1.52
8	J	5	VAL	C-O	-9.25	1.05	1.23
1	A	1281	ARG	NE-CZ	9.25	1.45	1.33
2	B	241	ARG	CG-CD	9.24	1.75	1.51
2	B	311	LEU	C-O	9.24	1.41	1.23
4	E	28	TYR	CD2-CE2	9.24	1.53	1.39
2	B	458	LYS	CG-CD	9.24	1.83	1.52
1	A	386	ASP	CB-CG	9.23	1.71	1.51
1	A	1103	GLU	CB-CG	-9.23	1.34	1.52
6	H	2	SER	CA-CB	9.23	1.66	1.52
2	B	18	PHE	CD1-CE1	9.23	1.57	1.39
2	B	51	PHE	CE2-CZ	9.23	1.54	1.37
7	I	47	GLU	CD-OE2	9.23	1.35	1.25
1	A	121	LEU	CG-CD1	9.23	1.85	1.51
2	B	137	TYR	CE1-CZ	9.23	1.50	1.38
2	B	866	TYR	CG-CD2	9.23	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	786	HIS	CA-CB	-9.22	1.33	1.53
4	E	80	VAL	C-O	9.22	1.40	1.23
8	J	18	TRP	CE2-CZ2	-9.22	1.24	1.39
2	B	980	PHE	C-O	-9.22	1.05	1.23
4	E	99	HIS	C-O	9.21	1.40	1.23
1	A	7	SER	N-CA	9.21	1.64	1.46
1	A	815	PHE	CG-CD2	-9.21	1.25	1.38
2	B	654	ARG	CB-CG	9.21	1.77	1.52
1	A	214	ILE	C-O	9.20	1.40	1.23
1	A	458	HIS	C-O	9.20	1.40	1.23
1	A	228	PHE	CD2-CE2	-9.20	1.20	1.39
1	A	1417	GLU	CA-CB	9.20	1.74	1.53
4	E	7	ARG	NE-CZ	9.20	1.45	1.33
7	I	70	ARG	CA-CB	-9.20	1.33	1.53
1	A	193	ASP	CA-CB	9.20	1.74	1.53
2	B	586	TRP	CG-CD1	-9.20	1.23	1.36
3	C	267	GLN	CA-C	9.20	1.76	1.52
1	A	219	PHE	CG-CD1	-9.19	1.25	1.38
1	A	469	ARG	CZ-NH1	-9.19	1.21	1.33
1	A	524	VAL	CB-CG1	9.19	1.72	1.52
1	A	1056	SER	CA-CB	-9.19	1.39	1.52
3	C	49	VAL	CB-CG1	9.19	1.72	1.52
3	C	199	LYS	CA-C	-9.19	1.29	1.52
1	A	811	GLN	CB-CG	-9.19	1.27	1.52
2	B	217	ARG	CG-CD	9.19	1.75	1.51
6	H	32	THR	CA-CB	9.19	1.77	1.53
1	A	847	ASP	CG-OD2	9.18	1.46	1.25
1	A	1256	GLU	N-CA	9.18	1.64	1.46
1	A	1290	LYS	CE-NZ	9.18	1.72	1.49
7	I	36	GLU	CA-CB	-9.18	1.33	1.53
1	A	739	ASP	CB-CG	9.18	1.71	1.51
2	B	853	SER	C-O	-9.18	1.05	1.23
2	B	1064	TYR	CB-CG	-9.18	1.37	1.51
5	F	88	TYR	CD2-CE2	-9.18	1.25	1.39
3	C	179	GLU	C-O	-9.17	1.05	1.23
6	H	111	LEU	N-CA	9.17	1.64	1.46
1	A	1034	GLU	CG-CD	9.16	1.65	1.51
1	A	720	ARG	CG-CD	9.16	1.74	1.51
3	C	17	ASN	CG-ND2	9.16	1.55	1.32
1	A	264	PHE	CE1-CZ	9.16	1.54	1.37
1	A	1378	GLN	CD-OE1	9.16	1.44	1.24
2	B	175	ARG	CZ-NH2	9.16	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	882	THR	CA-C	9.16	1.76	1.52
4	E	209	ALA	C-O	-9.16	1.05	1.23
1	A	37	PHE	CB-CG	9.15	1.67	1.51
1	A	1285	MET	SD-CE	9.15	2.29	1.77
1	A	1199	ARG	C-O	9.15	1.40	1.23
2	B	180	TYR	CG-CD1	9.15	1.51	1.39
2	B	733	HIS	N-CA	9.14	1.64	1.46
2	B	785	TYR	C-O	9.14	1.40	1.23
2	B	319	GLU	C-O	9.14	1.40	1.23
9	K	20	LYS	CD-CE	9.14	1.74	1.51
2	B	41	LYS	CE-NZ	9.14	1.71	1.49
2	B	99	LYS	CD-CE	9.14	1.74	1.51
6	H	93	TYR	CE1-CZ	9.14	1.50	1.38
10	L	29	TYR	CG-CD2	-9.14	1.27	1.39
1	A	423	ASP	CG-OD1	9.13	1.46	1.25
1	A	549	MET	SD-CE	-9.13	1.26	1.77
1	A	1114	PRO	N-CD	-9.13	1.35	1.47
2	B	451	LYS	CD-CE	9.13	1.74	1.51
4	E	130	ALA	CA-CB	9.13	1.71	1.52
8	J	8	PHE	CE1-CZ	9.13	1.54	1.37
2	B	365	THR	C-O	9.12	1.40	1.23
9	K	65	HIS	C-N	-9.12	1.17	1.34
2	B	307	ASP	C-O	-9.12	1.06	1.23
3	C	193	TYR	CG-CD1	-9.12	1.27	1.39
1	A	199	LEU	CG-CD1	9.11	1.85	1.51
2	B	270	LYS	CE-NZ	9.11	1.71	1.49
1	A	519	PRO	N-CA	-9.11	1.31	1.47
2	B	1028	GLU	CG-CD	9.11	1.65	1.51
1	A	206	GLU	CD-OE2	9.11	1.35	1.25
1	A	1214	GLU	CB-CG	9.11	1.69	1.52
2	B	595	ARG	NE-CZ	9.11	1.44	1.33
5	F	143	PHE	CB-CG	-9.11	1.35	1.51
8	J	58	GLU	CD-OE1	-9.11	1.15	1.25
1	A	44	THR	N-CA	9.10	1.64	1.46
1	A	1145	SER	C-O	-9.10	1.06	1.23
1	A	1303	GLU	C-O	-9.10	1.06	1.23
4	E	131	THR	CA-CB	9.10	1.77	1.53
4	E	113	GLN	CA-CB	9.09	1.74	1.53
1	A	1443	VAL	C-O	-9.09	1.06	1.23
2	B	810	GLU	CD-OE2	9.09	1.35	1.25
2	B	393	LYS	CD-CE	9.09	1.74	1.51
2	B	640	VAL	CA-CB	-9.09	1.35	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	60	PHE	CB-CG	9.09	1.66	1.51
1	A	171	GLN	CD-OE1	9.08	1.44	1.24
2	B	598	GLU	N-CA	9.08	1.64	1.46
4	E	187	TYR	CD1-CE1	-9.08	1.25	1.39
2	B	31	TRP	CD2-CE2	-9.08	1.30	1.41
6	H	26	ILE	C-O	9.08	1.40	1.23
7	I	49	ILE	CB-CG2	9.08	1.81	1.52
9	K	27	ALA	CA-CB	9.08	1.71	1.52
1	A	863	VAL	N-CA	-9.08	1.28	1.46
3	C	89	GLU	CD-OE1	9.08	1.35	1.25
1	A	274	ILE	CA-CB	9.07	1.75	1.54
1	A	821	ARG	NE-CZ	-9.07	1.21	1.33
2	B	322	PHE	CD1-CE1	-9.07	1.21	1.39
1	A	1191	TRP	CE3-CZ3	9.07	1.53	1.38
2	B	523	CYS	CA-C	-9.07	1.29	1.52
9	K	26	LYS	CG-CD	9.06	1.83	1.52
1	A	468	PHE	CG-CD1	-9.06	1.25	1.38
1	A	1102	LYS	CB-CG	9.06	1.77	1.52
1	A	1315	GLU	CG-CD	9.05	1.65	1.51
2	B	622	LYS	CG-CD	9.05	1.83	1.52
2	B	810	GLU	CA-CB	9.05	1.73	1.53
2	B	968	VAL	CB-CG2	-9.05	1.33	1.52
3	C	267	GLN	CG-CD	9.05	1.71	1.51
2	B	951	GLN	CB-CG	9.05	1.76	1.52
10	L	65	VAL	CB-CG2	9.05	1.71	1.52
3	C	208	GLU	CD-OE1	9.05	1.35	1.25
2	B	208	SER	C-O	9.05	1.40	1.23
2	B	486	TYR	CE1-CZ	9.04	1.50	1.38
1	A	1194	ARG	CD-NE	-9.04	1.31	1.46
2	B	534	GLY	N-CA	-9.04	1.32	1.46
1	A	104	GLU	CA-C	9.04	1.76	1.52
2	B	1201	LYS	CB-CG	-9.04	1.28	1.52
3	C	62	PHE	CB-CG	9.03	1.66	1.51
2	B	567	GLU	CB-CG	9.03	1.69	1.52
2	B	526	GLU	CG-CD	9.03	1.65	1.51
8	J	23	ASN	CB-CG	9.03	1.71	1.51
1	A	193	ASP	CB-CG	9.03	1.70	1.51
5	F	76	LYS	CE-NZ	9.03	1.71	1.49
2	B	231	PRO	N-CD	9.02	1.60	1.47
2	B	245	GLU	CA-C	9.02	1.76	1.52
1	A	1198	ASP	N-CA	9.02	1.64	1.46
2	B	1153	GLU	CD-OE1	9.02	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	56	THR	CA-CB	9.02	1.76	1.53
1	A	163	SER	CA-CB	9.02	1.66	1.52
2	B	364	ILE	CA-CB	-9.02	1.34	1.54
1	A	1268	LEU	CA-CB	-9.02	1.33	1.53
2	B	612	GLU	N-CA	-9.02	1.28	1.46
4	E	67	GLU	CB-CG	9.01	1.69	1.52
1	A	716	ASP	CG-OD1	9.01	1.46	1.25
1	A	918	GLU	CG-CD	9.01	1.65	1.51
8	J	51	LEU	C-O	9.01	1.40	1.23
2	B	706	GLN	CB-CG	9.00	1.76	1.52
2	B	883	LEU	CB-CG	9.00	1.78	1.52
1	A	484	GLY	N-CA	-9.00	1.32	1.46
1	A	508	PRO	CG-CD	9.00	1.80	1.50
2	B	373	ARG	CZ-NH1	9.00	1.44	1.33
2	B	1047	PHE	CE1-CZ	8.99	1.54	1.37
7	I	60	GLN	C-O	8.99	1.40	1.23
1	A	144	THR	CA-CB	8.99	1.76	1.53
1	A	729	ALA	CA-CB	-8.99	1.33	1.52
8	J	7	CYS	CA-CB	8.99	1.73	1.53
2	B	1178	ASN	CB-CG	-8.99	1.30	1.51
1	A	614	PHE	CG-CD2	-8.99	1.25	1.38
2	B	167	ILE	C-O	8.99	1.40	1.23
2	B	797	TYR	CG-CD1	-8.99	1.27	1.39
1	A	1066	VAL	CB-CG2	8.98	1.71	1.52
2	B	89	GLU	CB-CG	8.98	1.69	1.52
2	B	596	LEU	CG-CD1	-8.98	1.18	1.51
2	B	116	GLU	CD-OE1	8.98	1.35	1.25
2	B	797	TYR	CE1-CZ	-8.98	1.26	1.38
2	B	1071	VAL	C-O	8.98	1.40	1.23
3	C	132	PRO	CA-C	-8.98	1.34	1.52
1	A	461	LYS	CD-CE	8.97	1.73	1.51
1	A	1149	ALA	CA-CB	-8.97	1.33	1.52
1	A	1003	LYS	C-O	8.97	1.40	1.23
2	B	803	LEU	C-O	8.97	1.40	1.23
1	A	591	PHE	CE1-CZ	-8.97	1.20	1.37
2	B	1102	LYS	CA-CB	8.96	1.73	1.53
2	B	579	ARG	NE-CZ	-8.96	1.21	1.33
1	A	1226	VAL	CA-CB	-8.96	1.35	1.54
2	B	1221	SER	CA-CB	8.96	1.66	1.52
4	E	133	GLU	CD-OE2	8.96	1.35	1.25
8	J	47	ARG	CG-CD	8.95	1.74	1.51
1	A	896	ARG	N-CA	-8.95	1.28	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	516	ASN	C-O	-8.95	1.06	1.23
2	B	785	TYR	CA-C	-8.95	1.29	1.52
3	C	244	VAL	CB-CG1	-8.95	1.34	1.52
4	E	7	ARG	CD-NE	8.95	1.61	1.46
2	B	310	MET	N-CA	-8.94	1.28	1.46
6	H	115	TYR	C-O	-8.94	1.06	1.23
1	A	188	ASP	N-CA	8.94	1.64	1.46
1	A	1372	VAL	CB-CG1	-8.93	1.34	1.52
1	A	12	ARG	C-O	-8.93	1.06	1.23
1	A	469	ARG	CB-CG	8.93	1.76	1.52
1	A	551	TYR	C-O	8.93	1.40	1.23
4	E	20	LYS	CD-CE	8.93	1.73	1.51
1	A	1003	LYS	CG-CD	8.92	1.82	1.52
1	A	34	LYS	CB-CG	8.92	1.76	1.52
1	A	1080	THR	CA-C	8.92	1.76	1.52
2	B	197	PHE	CG-CD1	-8.92	1.25	1.38
4	E	152	LYS	CG-CD	8.92	1.82	1.52
6	H	63	LEU	C-O	8.92	1.40	1.23
1	A	943	LEU	C-O	-8.92	1.06	1.23
1	A	1239	ARG	CG-CD	8.92	1.74	1.51
2	B	908	GLU	CB-CG	8.92	1.69	1.52
1	A	756	ILE	C-O	8.91	1.40	1.23
2	B	415	GLN	CA-CB	8.91	1.73	1.53
3	C	128	ASN	CG-ND2	8.91	1.55	1.32
4	E	2	ASP	CB-CG	8.91	1.70	1.51
5	F	147	SER	CA-CB	8.91	1.66	1.52
9	K	71	PHE	CE1-CZ	-8.91	1.20	1.37
2	B	106	ASP	CA-C	8.91	1.76	1.52
2	B	258	LEU	CA-CB	-8.91	1.33	1.53
3	C	22	LEU	C-O	-8.91	1.06	1.23
9	K	94	ILE	CA-CB	8.91	1.75	1.54
1	A	840	ARG	NE-CZ	8.91	1.44	1.33
1	A	1289	ARG	CB-CG	-8.91	1.28	1.52
4	E	208	TYR	CZ-OH	8.91	1.52	1.37
4	E	21	GLU	CD-OE2	8.91	1.35	1.25
1	A	1001	ARG	C-O	8.90	1.40	1.23
2	B	830	TYR	CD1-CE1	8.90	1.52	1.39
2	B	1130	PHE	CE1-CZ	-8.90	1.20	1.37
3	C	180	TYR	CD1-CE1	8.90	1.52	1.39
1	A	569	LYS	C-O	-8.90	1.06	1.23
1	A	655	PHE	CG-CD2	-8.90	1.25	1.38
4	E	204	THR	CB-CG2	-8.90	1.23	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	712	PRO	CG-CD	8.89	1.80	1.50
6	H	123	MET	CG-SD	8.89	2.04	1.81
7	I	8	ARG	CZ-NH2	8.89	1.44	1.33
1	A	1130	GLN	CD-OE1	8.89	1.43	1.24
2	B	519	TRP	N-CA	-8.89	1.28	1.46
3	C	242	GLN	N-CA	-8.89	1.28	1.46
6	H	19	ARG	CA-CB	8.89	1.73	1.53
9	K	55	LYS	CG-CD	8.89	1.82	1.52
2	B	183	GLU	CG-CD	8.89	1.65	1.51
1	A	143	LYS	CE-NZ	8.88	1.71	1.49
2	B	1052	VAL	CB-CG2	-8.88	1.34	1.52
4	E	148	GLU	CA-C	-8.88	1.29	1.52
1	A	571	LEU	CG-CD2	8.88	1.84	1.51
4	E	46	TYR	CD1-CE1	8.88	1.52	1.39
2	B	137	TYR	N-CA	8.87	1.64	1.46
1	A	1293	SER	CB-OG	-8.87	1.30	1.42
7	I	35	VAL	CB-CG2	-8.87	1.34	1.52
10	L	64	LEU	CG-CD1	8.86	1.84	1.51
1	A	36	ARG	NE-CZ	8.86	1.44	1.33
6	H	23	VAL	CA-CB	-8.86	1.36	1.54
1	A	1035	TYR	CG-CD1	-8.86	1.27	1.39
1	A	967	ALA	CA-CB	-8.85	1.33	1.52
2	B	401	PHE	CG-CD1	-8.85	1.25	1.38
2	B	561	TRP	CE2-CZ2	8.85	1.54	1.39
2	B	99	LYS	CE-NZ	8.85	1.71	1.49
2	B	347	LYS	CD-CE	8.85	1.73	1.51
1	A	1214	GLU	CD-OE2	8.85	1.35	1.25
1	A	720	ARG	CB-CG	8.84	1.76	1.52
1	A	1103	GLU	CA-CB	-8.84	1.34	1.53
4	E	113	GLN	CD-NE2	8.84	1.54	1.32
1	A	836	TYR	CB-CG	8.84	1.65	1.51
2	B	42	GLY	C-O	8.84	1.37	1.23
2	B	890	TYR	CE1-CZ	8.84	1.50	1.38
2	B	1204	PHE	CB-CG	8.84	1.66	1.51
2	B	377	PHE	CE2-CZ	-8.84	1.20	1.37
2	B	124	TYR	CD1-CE1	8.83	1.52	1.39
2	B	380	TYR	CD2-CE2	-8.83	1.26	1.39
1	A	775	ILE	CA-CB	-8.83	1.34	1.54
2	B	1040	ASN	CG-ND2	8.83	1.54	1.32
1	A	639	PRO	CA-C	8.82	1.70	1.52
2	B	191	LYS	CD-CE	8.82	1.73	1.51
2	B	557	PHE	CG-CD2	8.82	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	589	GLN	CD-NE2	8.82	1.54	1.32
1	A	371	ALA	CA-C	-8.82	1.30	1.52
2	B	123	THR	C-O	8.82	1.40	1.23
6	H	118	PHE	CD1-CE1	8.82	1.56	1.39
10	L	47	ARG	CB-CG	8.82	1.76	1.52
1	A	699	ALA	C-O	-8.81	1.06	1.23
2	B	38	PHE	CE2-CZ	8.81	1.54	1.37
1	A	1212	VAL	CA-CB	-8.81	1.36	1.54
7	I	110	PHE	CE2-CZ	-8.81	1.20	1.37
2	B	375	ALA	CA-CB	-8.81	1.33	1.52
7	I	7	CYS	CA-CB	8.81	1.73	1.53
1	A	1221	LYS	C-O	8.80	1.40	1.23
3	C	186	LEU	CB-CG	-8.80	1.27	1.52
2	B	752	ALA	CA-CB	8.80	1.71	1.52
4	E	63	ASN	CB-CG	8.80	1.71	1.51
1	A	37	PHE	CD2-CE2	8.79	1.56	1.39
1	A	839	ARG	CZ-NH1	8.79	1.44	1.33
3	C	170	TRP	CD2-CE3	-8.79	1.27	1.40
1	A	1011	GLN	CD-OE1	-8.79	1.04	1.24
2	B	336	ARG	NE-CZ	-8.79	1.21	1.33
2	B	1191	ILE	CA-CB	-8.79	1.34	1.54
3	C	79	GLN	CD-NE2	8.79	1.54	1.32
3	C	48	SER	CB-OG	8.79	1.53	1.42
1	A	237	THR	CB-CG2	8.79	1.81	1.52
1	A	942	PHE	CE2-CZ	-8.79	1.20	1.37
1	A	1349	TYR	CE1-CZ	-8.79	1.27	1.38
1	A	84	ILE	C-O	-8.78	1.06	1.23
1	A	1383	SER	CA-CB	-8.78	1.39	1.52
2	B	108	VAL	CA-CB	8.78	1.73	1.54
1	A	965	GLN	CD-NE2	8.77	1.54	1.32
9	K	110	ASN	CG-OD1	8.77	1.43	1.24
2	B	776	GLN	CB-CG	-8.77	1.28	1.52
1	A	685	GLU	CD-OE2	8.77	1.35	1.25
1	A	1410	PHE	CD2-CE2	-8.77	1.21	1.39
1	A	1441	PHE	C-O	-8.76	1.06	1.23
1	A	1220	PHE	CG-CD1	-8.76	1.25	1.38
9	K	61	TYR	CG-CD1	-8.76	1.27	1.39
6	H	134	ASN	CB-CG	8.75	1.71	1.51
1	A	591	PHE	CB-CG	8.75	1.66	1.51
1	A	754	SER	CA-CB	-8.75	1.39	1.52
1	A	377	PRO	N-CA	-8.75	1.32	1.47
1	A	1191	TRP	CD2-CE3	-8.75	1.27	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	863	VAL	CB-CG2	8.74	1.71	1.52
2	B	113	TYR	CD1-CE1	-8.74	1.26	1.39
1	A	430	TRP	CZ3-CH2	-8.74	1.26	1.40
1	A	1237	ILE	N-CA	-8.74	1.28	1.46
1	A	264	PHE	CE2-CZ	8.73	1.53	1.37
4	E	155	ARG	CG-CD	8.73	1.73	1.51
1	A	12	ARG	CZ-NH1	8.73	1.44	1.33
1	A	175	ARG	CG-CD	8.72	1.73	1.51
1	A	1050	GLU	N-CA	-8.72	1.28	1.46
1	A	1189	SER	CA-C	-8.72	1.30	1.52
2	B	111	ALA	CA-CB	8.72	1.70	1.52
1	A	1092	LYS	CB-CG	8.72	1.76	1.52
2	B	540	SER	CA-CB	8.71	1.66	1.52
2	B	986	GLN	CD-OE1	8.71	1.43	1.24
4	E	54	GLN	CB-CG	8.71	1.76	1.52
4	E	165	LEU	CG-CD1	8.71	1.84	1.51
1	A	81	PHE	CG-CD1	-8.71	1.25	1.38
2	B	1027	ILE	N-CA	-8.71	1.28	1.46
9	K	106	GLU	CD-OE1	8.71	1.35	1.25
1	A	6	TYR	CG-CD1	8.71	1.50	1.39
1	A	843	LYS	CB-CG	8.70	1.76	1.52
1	A	1224	LEU	CA-CB	-8.70	1.33	1.53
3	C	159	ALA	C-O	-8.70	1.06	1.23
6	H	127	GLY	CA-C	8.70	1.65	1.51
1	A	1351	GLU	CD-OE2	8.70	1.35	1.25
2	B	172	ILE	C-O	8.70	1.39	1.23
2	B	1129	ARG	NE-CZ	8.70	1.44	1.33
2	B	1133	MET	CA-CB	-8.70	1.34	1.53
1	A	670	ILE	CB-CG2	8.70	1.79	1.52
1	A	1168	GLU	CA-CB	8.70	1.73	1.53
2	B	780	VAL	CB-CG2	-8.69	1.34	1.52
1	A	1194	ARG	CB-CG	8.69	1.76	1.52
1	A	1294	PRO	CB-CG	8.69	1.93	1.50
8	J	47	ARG	CB-CG	-8.69	1.29	1.52
1	A	1240	CYS	C-O	-8.69	1.06	1.23
1	A	946	VAL	CB-CG1	-8.69	1.34	1.52
1	A	26	GLU	CD-OE2	-8.68	1.16	1.25
1	A	302	THR	C-O	8.68	1.39	1.23
10	L	69	ALA	N-CA	8.68	1.63	1.46
1	A	933	TYR	CE2-CZ	-8.68	1.27	1.38
1	A	836	TYR	CE1-CZ	8.68	1.49	1.38
5	F	80	ALA	N-CA	-8.68	1.28	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	30	ARG	CG-CD	8.68	1.73	1.51
1	A	709	THR	CA-CB	-8.68	1.30	1.53
4	E	56	LYS	N-CA	-8.67	1.29	1.46
2	B	1143	ALA	CA-CB	-8.67	1.34	1.52
2	B	706	GLN	CG-CD	8.67	1.71	1.51
2	B	935	ARG	CD-NE	8.67	1.61	1.46
7	I	17	ARG	C-O	-8.67	1.06	1.23
1	A	133	LYS	CE-NZ	8.66	1.70	1.49
7	I	37	GLU	N-CA	-8.66	1.29	1.46
2	B	846	ILE	C-O	8.66	1.39	1.23
6	H	13	SER	CB-OG	8.66	1.53	1.42
2	B	451	LYS	CB-CG	8.65	1.75	1.52
7	I	50	THR	CA-C	-8.65	1.30	1.52
2	B	267	ARG	CZ-NH1	8.65	1.44	1.33
4	E	129	PRO	CB-CG	8.65	1.93	1.50
1	A	804	TYR	CD2-CE2	8.65	1.52	1.39
2	B	1052	VAL	CB-CG1	-8.65	1.34	1.52
2	B	1224	PHE	CE2-CZ	8.65	1.53	1.37
2	B	237	VAL	C-O	8.64	1.39	1.23
3	C	79	GLN	CG-CD	8.64	1.71	1.51
2	B	741	CYS	CA-CB	-8.64	1.34	1.53
9	K	113	THR	CB-CG2	8.64	1.80	1.52
1	A	894	GLU	CG-CD	8.63	1.65	1.51
2	B	255	GLN	C-O	-8.64	1.06	1.23
2	B	25	ILE	N-CA	8.63	1.63	1.46
1	A	911	SER	C-O	8.63	1.39	1.23
2	B	546	SER	CA-CB	8.63	1.65	1.52
9	K	47	ARG	CZ-NH1	8.63	1.44	1.33
7	I	34	TYR	CA-CB	-8.63	1.34	1.53
1	A	601	LYS	CG-CD	8.63	1.81	1.52
7	I	70	ARG	CZ-NH2	-8.62	1.21	1.33
6	H	115	TYR	CG-CD1	-8.62	1.27	1.39
1	A	71	GLN	CG-CD	8.62	1.70	1.51
1	A	1282	VAL	C-O	-8.62	1.06	1.23
2	B	547	VAL	CA-CB	-8.62	1.36	1.54
1	A	389	THR	C-O	8.61	1.39	1.23
1	A	945	GLU	CD-OE2	8.61	1.35	1.25
3	C	86	CYS	CB-SG	8.61	1.96	1.82
2	B	384	ARG	CZ-NH2	-8.61	1.21	1.33
6	H	115	TYR	CZ-OH	8.61	1.52	1.37
1	A	475	THR	N-CA	-8.61	1.29	1.46
1	A	731	ARG	CZ-NH1	8.61	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	958	VAL	CA-CB	-8.61	1.36	1.54
3	C	172	PRO	CA-C	-8.61	1.35	1.52
1	A	976	THR	CA-CB	8.60	1.75	1.53
1	A	1030	ARG	CB-CG	-8.60	1.29	1.52
1	A	1099	PRO	CA-C	-8.60	1.35	1.52
2	B	113	TYR	CZ-OH	8.60	1.52	1.37
2	B	901	PRO	CG-CD	8.60	1.79	1.50
2	B	227	LYS	CE-NZ	8.60	1.70	1.49
1	A	1443	VAL	CA-C	-8.60	1.30	1.52
3	C	193	TYR	CD1-CE1	-8.60	1.26	1.39
2	B	1075	GLY	N-CA	-8.60	1.33	1.46
2	B	1075	GLY	C-O	8.60	1.37	1.23
2	B	1192	TYR	CE1-CZ	-8.60	1.27	1.38
1	A	686	ALA	CA-CB	-8.59	1.34	1.52
1	A	404	TYR	C-O	-8.59	1.07	1.23
2	B	479	VAL	C-O	-8.59	1.07	1.23
1	A	893	PHE	CE2-CZ	-8.59	1.21	1.37
7	I	41	PRO	C-O	-8.59	1.06	1.23
2	B	561	TRP	CG-CD1	-8.58	1.24	1.36
2	B	690	VAL	CB-CG2	-8.58	1.34	1.52
2	B	205	ILE	CB-CG2	-8.58	1.26	1.52
2	B	1033	LYS	CB-CG	-8.57	1.29	1.52
3	C	212	PRO	C-O	-8.57	1.06	1.23
2	B	347	LYS	CA-CB	-8.57	1.35	1.53
2	B	368	GLU	CA-CB	8.57	1.72	1.53
2	B	976	ILE	C-O	8.57	1.39	1.23
8	J	21	TYR	CD2-CE2	8.57	1.52	1.39
3	C	223	ALA	CA-CB	-8.57	1.34	1.52
1	A	1221	LYS	CG-CD	8.56	1.81	1.52
9	K	88	LYS	CG-CD	8.56	1.81	1.52
2	B	623	GLU	CD-OE2	8.56	1.35	1.25
2	B	736	THR	CB-OG1	-8.56	1.26	1.43
3	C	7	GLN	CD-NE2	8.56	1.54	1.32
7	I	111	THR	CA-CB	-8.56	1.31	1.53
1	A	521	MET	SD-CE	-8.56	1.29	1.77
2	B	833	TYR	CE1-CZ	-8.56	1.27	1.38
2	B	235	SER	CA-CB	-8.56	1.40	1.52
5	F	92	ARG	CG-CD	-8.56	1.30	1.51
1	A	95	PHE	CG-CD1	8.55	1.51	1.38
2	B	641	GLU	CB-CG	8.55	1.68	1.52
2	B	275	TYR	CD1-CE1	-8.55	1.26	1.39
1	A	367	PRO	CG-CD	-8.55	1.22	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1019	SER	C-O	-8.55	1.07	1.23
1	A	604	GLY	CA-C	-8.55	1.38	1.51
2	B	617	ARG	CD-NE	8.54	1.60	1.46
2	B	1100	ASP	C-O	8.55	1.39	1.23
2	B	666	TYR	CG-CD2	8.54	1.50	1.39
2	B	380	TYR	CE2-CZ	8.54	1.49	1.38
2	B	811	TYR	N-CA	-8.54	1.29	1.46
8	J	29	GLU	C-O	8.54	1.39	1.23
9	K	54	ARG	CB-CG	8.54	1.75	1.52
2	B	390	LEU	C-O	8.54	1.39	1.23
1	A	1203	ASN	CA-C	8.54	1.75	1.52
1	A	1430	LEU	C-O	8.54	1.39	1.23
1	A	61	ILE	C-O	8.53	1.39	1.23
2	B	667	GLN	C-O	8.53	1.39	1.23
9	K	111	LEU	CG-CD1	8.53	1.83	1.51
10	L	49	LYS	CE-NZ	8.53	1.70	1.49
1	A	1120	LEU	C-O	-8.53	1.07	1.23
3	C	193	TYR	CB-CG	8.53	1.64	1.51
10	L	63	ARG	CD-NE	8.53	1.60	1.46
7	I	28	GLU	CG-CD	8.53	1.64	1.51
7	I	91	ARG	CA-CB	-8.53	1.35	1.53
1	A	1044	TRP	CG-CD2	-8.52	1.29	1.43
9	K	11	LEU	CG-CD1	8.52	1.83	1.51
1	A	347	PHE	CG-CD2	8.52	1.51	1.38
1	A	1286	LYS	CB-CG	8.52	1.75	1.52
3	C	138	GLU	CG-CD	8.52	1.64	1.51
1	A	295	LEU	CG-CD2	8.52	1.83	1.51
4	E	169	ARG	CZ-NH1	8.52	1.44	1.33
5	F	136	ARG	CZ-NH1	-8.52	1.22	1.33
9	K	105	PHE	C-O	8.52	1.39	1.23
1	A	205	GLU	CB-CG	8.52	1.68	1.52
1	A	829	VAL	CB-CG2	8.51	1.70	1.52
1	A	1018	PHE	CE1-CZ	-8.51	1.21	1.37
1	A	1359	ASP	N-CA	8.51	1.63	1.46
7	I	89	GLN	CG-CD	-8.51	1.31	1.51
10	L	44	ASP	C-O	8.51	1.39	1.23
1	A	188	ASP	CA-CB	8.51	1.72	1.53
4	E	133	GLU	C-O	8.51	1.39	1.23
1	A	646	PHE	CD1-CE1	-8.51	1.22	1.39
2	B	1168	LEU	CA-C	-8.51	1.30	1.52
5	F	119	ARG	C-O	8.51	1.39	1.23
1	A	1228	TRP	CG-CD1	-8.50	1.24	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1057	VAL	CB-CG2	-8.50	1.35	1.52
2	B	511	PRO	CA-CB	-8.49	1.36	1.53
2	B	1047	PHE	CB-CG	-8.49	1.36	1.51
1	A	690	VAL	C-O	-8.49	1.07	1.23
2	B	851	PHE	CG-CD2	8.49	1.51	1.38
2	B	131	ASP	CB-CG	8.49	1.69	1.51
2	B	738	PHE	CD2-CE2	-8.49	1.22	1.39
7	I	90	GLN	CG-CD	-8.49	1.31	1.51
4	E	85	GLU	CD-OE2	8.48	1.34	1.25
1	A	31	SER	CA-C	8.48	1.75	1.52
1	A	693	VAL	CA-C	-8.48	1.30	1.52
8	J	46	CYS	CB-SG	8.47	1.96	1.82
1	A	586	ILE	CB-CG2	-8.47	1.26	1.52
1	A	960	ILE	CB-CG2	-8.47	1.26	1.52
1	A	94	GLY	C-O	8.47	1.37	1.23
6	H	109	LYS	N-CA	8.47	1.63	1.46
2	B	271	ALA	C-O	-8.46	1.07	1.23
1	A	454	SER	CB-OG	-8.46	1.31	1.42
1	A	967	ALA	C-O	-8.46	1.07	1.23
4	E	112	TYR	CE1-CZ	-8.46	1.27	1.38
2	B	543	SER	N-CA	8.45	1.63	1.46
4	E	60	PHE	CG-CD1	8.46	1.51	1.38
4	E	61	GLN	CB-CG	8.45	1.75	1.52
1	A	396	PRO	CA-CB	-8.45	1.36	1.53
1	A	1234	GLU	CD-OE2	8.45	1.34	1.25
2	B	1091	TYR	CD2-CE2	8.45	1.52	1.39
3	C	179	GLU	CB-CG	8.45	1.68	1.52
5	F	145	ASP	CB-CG	-8.45	1.34	1.51
1	A	858	ASN	CB-CG	-8.44	1.31	1.51
6	H	19	ARG	CZ-NH1	8.44	1.44	1.33
1	A	1049	ILE	CA-CB	-8.43	1.35	1.54
1	A	721	PHE	C-O	8.43	1.39	1.23
1	A	1447	GLU	CG-CD	8.43	1.64	1.51
2	B	92	PHE	N-CA	8.42	1.63	1.46
3	C	50	GLU	CB-CG	8.42	1.68	1.52
7	I	6	PHE	CE2-CZ	8.42	1.53	1.37
3	C	82	TYR	CE2-CZ	8.42	1.49	1.38
7	I	103	CYS	C-O	-8.42	1.07	1.23
8	J	58	GLU	CG-CD	8.42	1.64	1.51
6	H	95	TYR	CD1-CE1	8.42	1.51	1.39
2	B	39	ARG	CZ-NH1	8.41	1.44	1.33
1	A	806	ARG	CA-C	-8.41	1.31	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1230	GLU	CG-CD	8.41	1.64	1.51
2	B	174	LEU	C-O	-8.41	1.07	1.23
7	I	99	LEU	CG-CD1	-8.41	1.20	1.51
2	B	337	ARG	CZ-NH1	-8.41	1.22	1.33
9	K	81	TYR	CE1-CZ	-8.41	1.27	1.38
6	H	49	VAL	CB-CG1	-8.40	1.35	1.52
9	K	63	VAL	CB-CG2	8.40	1.70	1.52
8	J	10	CYS	CB-SG	-8.40	1.68	1.82
2	B	537	LYS	CE-NZ	-8.39	1.28	1.49
7	I	32	CYS	C-O	8.39	1.39	1.23
2	B	933	SER	CA-C	8.38	1.74	1.52
1	A	708	MET	SD-CE	8.38	2.24	1.77
2	B	448	ILE	CA-CB	8.38	1.74	1.54
2	B	902	GLY	N-CA	-8.38	1.33	1.46
1	A	555	ASP	C-O	-8.38	1.07	1.23
1	A	1061	GLY	N-CA	-8.38	1.33	1.46
2	B	651	LEU	CG-CD2	-8.38	1.20	1.51
4	E	71	LYS	CD-CE	8.38	1.72	1.51
1	A	850	VAL	C-O	-8.37	1.07	1.23
2	B	249	ARG	CA-C	8.37	1.74	1.52
1	A	151	ASP	C-O	-8.37	1.07	1.23
2	B	47	GLN	CA-CB	-8.37	1.35	1.53
1	A	737	LEU	C-O	8.37	1.39	1.23
1	A	1410	PHE	CG-CD1	-8.37	1.26	1.38
2	B	1180	PHE	CE1-CZ	8.37	1.53	1.37
4	E	50	MET	CA-C	8.37	1.74	1.52
1	A	1154	TYR	CE1-CZ	-8.37	1.27	1.38
3	C	170	TRP	CZ3-CH2	-8.37	1.26	1.40
2	B	934	LYS	CB-CG	8.36	1.75	1.52
3	C	16	ASP	CB-CG	8.37	1.69	1.51
5	F	120	ILE	C-O	-8.36	1.07	1.23
1	A	988	LEU	C-O	-8.36	1.07	1.23
10	L	67	PHE	CG-CD2	-8.36	1.26	1.38
1	A	220	THR	CB-OG1	8.36	1.59	1.43
9	K	79	GLU	CB-CG	8.36	1.68	1.52
2	B	25	ILE	CB-CG2	8.36	1.78	1.52
1	A	1012	ARG	CG-CD	8.36	1.72	1.51
2	B	411	PRO	CA-C	8.36	1.69	1.52
2	B	1217	TYR	CG-CD2	8.36	1.50	1.39
1	A	367	PRO	CA-CB	-8.35	1.36	1.53
1	A	495	GLU	CD-OE1	8.35	1.34	1.25
1	A	813	PHE	CE1-CZ	-8.35	1.21	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	136	THR	C-O	8.35	1.39	1.23
2	B	339	THR	N-CA	8.35	1.63	1.46
2	B	1020	ARG	CG-CD	-8.35	1.31	1.51
2	B	138	GLU	N-CA	8.35	1.63	1.46
9	K	107	THR	C-O	8.35	1.39	1.23
1	A	564	ALA	C-O	-8.35	1.07	1.23
1	A	1351	GLU	CG-CD	8.35	1.64	1.51
2	B	192	LEU	CG-CD2	8.35	1.82	1.51
1	A	1138	ILE	C-O	8.34	1.39	1.23
2	B	882	THR	N-CA	8.34	1.63	1.46
4	E	177	ARG	C-O	-8.34	1.07	1.23
2	B	1206	GLU	CG-CD	8.34	1.64	1.51
1	A	194	ALA	CA-CB	8.34	1.70	1.52
1	A	777	PHE	CD1-CE1	8.33	1.55	1.39
1	A	1202	MET	CG-SD	-8.33	1.59	1.81
1	A	1199	ARG	CG-CD	-8.33	1.31	1.51
3	C	82	TYR	CD1-CE1	-8.33	1.26	1.39
2	B	265	SER	CA-CB	8.33	1.65	1.52
10	L	49	LYS	CB-CG	8.32	1.75	1.52
1	A	884	ASP	N-CA	8.32	1.62	1.46
1	A	1220	PHE	CE2-CZ	-8.32	1.21	1.37
1	A	593	GLU	C-N	8.32	1.48	1.33
2	B	1221	SER	CA-C	8.32	1.74	1.52
1	A	942	PHE	CG-CD1	-8.31	1.26	1.38
1	A	1432	GLN	CB-CG	8.31	1.75	1.52
7	I	15	TYR	CG-CD2	-8.31	1.28	1.39
2	B	18	PHE	CD2-CE2	8.31	1.55	1.39
5	F	79	ARG	CZ-NH1	-8.31	1.22	1.33
9	K	28	PRO	CG-CD	-8.31	1.23	1.50
1	A	1131	ALA	CA-CB	-8.30	1.35	1.52
5	F	86	THR	C-O	-8.30	1.07	1.23
1	A	132	LYS	CG-CD	8.30	1.80	1.52
1	A	1103	GLU	CG-CD	8.30	1.64	1.51
1	A	1328	TYR	CE2-CZ	-8.30	1.27	1.38
2	B	808	ALA	CA-CB	-8.30	1.35	1.52
1	A	832	ALA	CA-CB	-8.29	1.35	1.52
3	C	130	GLY	C-O	8.29	1.36	1.23
3	C	204	SER	C-O	8.29	1.39	1.23
1	A	190	ALA	CA-CB	8.29	1.69	1.52
1	A	215	SER	CB-OG	-8.29	1.31	1.42
2	B	57	TYR	CE2-CZ	-8.29	1.27	1.38
4	E	172	GLU	CD-OE2	8.29	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	619	ILE	CB-CG2	-8.29	1.27	1.52
1	A	852	TYR	CE1-CZ	-8.29	1.27	1.38
3	C	81	GLU	CD-OE2	8.29	1.34	1.25
1	A	1202	MET	SD-CE	8.28	2.24	1.77
1	A	1341	ILE	CA-CB	-8.28	1.35	1.54
2	B	89	GLU	C-O	8.28	1.39	1.23
2	B	556	THR	C-O	8.28	1.39	1.23
4	E	97	VAL	CB-CG1	8.28	1.70	1.52
2	B	1193	GLN	CD-OE1	8.27	1.42	1.24
1	A	283	GLY	C-O	8.27	1.36	1.23
2	B	135	ARG	C-O	8.27	1.39	1.23
3	C	132	PRO	N-CA	-8.27	1.33	1.47
4	E	175	LEU	C-N	-8.27	1.18	1.34
10	L	33	GLU	CG-CD	8.27	1.64	1.51
1	A	582	ILE	C-O	8.26	1.39	1.23
2	B	315	LYS	CD-CE	8.26	1.72	1.51
2	B	811	TYR	CD1-CE1	8.26	1.51	1.39
4	E	169	ARG	CB-CG	-8.26	1.30	1.52
1	A	491	VAL	CB-CG2	-8.26	1.35	1.52
2	B	250	PHE	CD1-CE1	8.26	1.55	1.39
2	B	1085	ILE	CA-CB	-8.26	1.35	1.54
2	B	448	ILE	N-CA	8.26	1.62	1.46
3	C	194	GLU	CB-CG	8.26	1.67	1.52
2	B	98	THR	CA-CB	8.26	1.74	1.53
2	B	203	PHE	CE1-CZ	-8.25	1.21	1.37
1	A	775	ILE	C-O	-8.25	1.07	1.23
2	B	660	LYS	CD-CE	-8.25	1.30	1.51
1	A	1065	GLY	C-O	8.25	1.36	1.23
1	A	1199	ARG	CZ-NH1	8.25	1.43	1.33
10	L	34	CYS	C-O	-8.25	1.07	1.23
3	C	219	PHE	CG-CD1	8.25	1.51	1.38
1	A	880	LYS	C-O	-8.25	1.07	1.23
4	E	20	LYS	CB-CG	8.25	1.74	1.52
1	A	69	THR	CA-CB	8.24	1.74	1.53
2	B	49	ASP	CB-CG	8.24	1.69	1.51
2	B	629	ASP	CB-CG	8.24	1.69	1.51
1	A	1209	MET	SD-CE	-8.24	1.31	1.77
1	A	1374	VAL	C-O	8.24	1.39	1.23
2	B	1099	VAL	CA-CB	-8.24	1.37	1.54
2	B	296	GLU	CD-OE1	8.24	1.34	1.25
2	B	383	ASN	CB-CG	8.24	1.70	1.51
2	B	1224	PHE	CE1-CZ	8.24	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	995	GLU	CD-OE1	8.23	1.34	1.25
2	B	18	PHE	CE1-CZ	8.23	1.52	1.37
4	E	46	TYR	CG-CD2	8.23	1.49	1.39
6	H	118	PHE	CE2-CZ	8.23	1.52	1.37
1	A	1419	ASP	CG-OD2	8.23	1.44	1.25
1	A	171	GLN	CD-NE2	8.23	1.53	1.32
1	A	1286	LYS	C-O	-8.23	1.07	1.23
2	B	961	LEU	CG-CD2	8.23	1.82	1.51
2	B	1102	LYS	N-CA	8.23	1.62	1.46
2	B	360	PHE	CG-CD1	-8.22	1.26	1.38
2	B	578	THR	CB-OG1	8.22	1.59	1.43
2	B	959	ASP	C-O	8.22	1.39	1.23
1	A	1357	ALA	C-O	-8.22	1.07	1.23
1	A	1362	TYR	CG-CD2	-8.22	1.28	1.39
1	A	1419	ASP	CB-CG	8.22	1.69	1.51
2	B	892	LYS	CD-CE	8.22	1.71	1.51
1	A	1385	THR	CB-CG2	8.21	1.79	1.52
4	E	180	ARG	CB-CG	8.21	1.74	1.52
4	E	57	MET	CB-CG	8.21	1.77	1.51
2	B	136	THR	N-CA	8.21	1.62	1.46
1	A	1209	MET	N-CA	-8.20	1.29	1.46
2	B	1183	LYS	CA-C	8.20	1.74	1.52
10	L	41	SER	N-CA	8.20	1.62	1.46
1	A	94	GLY	CA-C	8.20	1.65	1.51
1	A	942	PHE	CB-CG	-8.20	1.37	1.51
4	E	157	SER	CB-OG	8.20	1.52	1.42
2	B	212	LEU	C-O	-8.20	1.07	1.23
2	B	617	ARG	CZ-NH2	-8.20	1.22	1.33
2	B	758	PHE	CG-CD1	-8.20	1.26	1.38
8	J	13	VAL	C-O	-8.20	1.07	1.23
4	E	40	GLU	CB-CG	8.19	1.67	1.52
9	K	109	TRP	N-CA	-8.19	1.29	1.46
10	L	49	LYS	CG-CD	8.19	1.80	1.52
1	A	899	VAL	CA-CB	-8.19	1.37	1.54
5	F	79	ARG	CZ-NH2	-8.19	1.22	1.33
9	K	34	THR	C-O	8.19	1.39	1.23
9	K	56	VAL	C-O	-8.19	1.07	1.23
1	A	695	LYS	CG-CD	8.18	1.80	1.52
2	B	1074	ASN	C-O	-8.18	1.07	1.23
1	A	524	VAL	CB-CG2	-8.18	1.35	1.52
8	J	13	VAL	CA-CB	-8.18	1.37	1.54
1	A	572	TRP	CD2-CE2	-8.18	1.31	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1210	MET	CG-SD	-8.18	1.59	1.81
6	H	85	GLY	CA-C	8.18	1.65	1.51
8	J	44	TYR	CZ-OH	8.17	1.51	1.37
1	A	616	VAL	CA-CB	-8.17	1.37	1.54
1	A	755	PHE	CE2-CZ	-8.17	1.21	1.37
9	K	10	PHE	CE2-CZ	-8.17	1.21	1.37
1	A	382	PRO	CA-C	-8.17	1.36	1.52
3	C	114	TYR	CG-CD1	-8.17	1.28	1.39
3	C	126	GLY	CA-C	8.17	1.65	1.51
1	A	1238	ILE	C-O	-8.16	1.07	1.23
1	A	1285	MET	CG-SD	8.16	2.02	1.81
2	B	807	ARG	CZ-NH2	-8.16	1.22	1.33
6	H	50	ALA	CA-CB	8.16	1.69	1.52
2	B	579	ARG	CG-CD	8.16	1.72	1.51
2	B	1041	GLU	CD-OE1	8.16	1.34	1.25
1	A	1272	THR	C-O	8.16	1.38	1.23
1	A	1366	ARG	CA-CB	-8.16	1.35	1.53
2	B	854	LEU	C-O	-8.16	1.07	1.23
8	J	47	ARG	NE-CZ	-8.16	1.22	1.33
1	A	862	ASN	CB-CG	-8.16	1.32	1.51
3	C	246	ARG	N-CA	-8.15	1.30	1.46
1	A	1132	LYS	CG-CD	8.15	1.80	1.52
1	A	739	ASP	C-O	8.15	1.38	1.23
1	A	1116	LEU	CA-CB	-8.15	1.35	1.53
2	B	220	GLY	CA-C	-8.15	1.38	1.51
2	B	466	TRP	CE2-CZ2	-8.15	1.25	1.39
1	A	1198	ASP	C-O	8.14	1.38	1.23
2	B	908	GLU	C-O	8.14	1.38	1.23
7	I	106	CYS	CA-C	-8.14	1.31	1.52
1	A	66	LYS	CA-CB	8.14	1.71	1.53
2	B	655	LYS	CA-CB	-8.14	1.36	1.53
2	B	851	PHE	CB-CG	8.14	1.65	1.51
7	I	38	ALA	CA-CB	8.14	1.69	1.52
2	B	1062	HIS	C-O	8.14	1.38	1.23
3	C	40	GLU	CD-OE1	8.14	1.34	1.25
1	A	711	ARG	CZ-NH2	-8.14	1.22	1.33
2	B	857	ARG	NE-CZ	8.14	1.43	1.33
1	A	739	ASP	N-CA	-8.14	1.30	1.46
1	A	897	TYR	CE2-CZ	-8.13	1.27	1.38
2	B	1137	CYS	CB-SG	-8.13	1.68	1.82
2	B	245	GLU	CD-OE1	8.13	1.34	1.25
7	I	59	VAL	CB-CG2	-8.13	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	91	LYS	C-O	8.13	1.38	1.23
1	A	106	VAL	CB-CG1	8.12	1.70	1.52
1	A	893	PHE	CD1-CE1	-8.12	1.23	1.39
1	A	384	ASN	N-CA	-8.12	1.30	1.46
2	B	113	TYR	CG-CD2	-8.12	1.28	1.39
2	B	255	GLN	CA-CB	-8.12	1.36	1.53
4	E	71	LYS	N-CA	8.12	1.62	1.46
7	I	7	CYS	CB-SG	-8.12	1.68	1.82
7	I	77	LYS	CG-CD	8.12	1.80	1.52
5	F	79	ARG	CD-NE	-8.12	1.32	1.46
1	A	502	SER	CB-OG	8.12	1.52	1.42
1	A	769	SER	CA-CB	-8.12	1.40	1.52
2	B	451	LYS	CG-CD	8.12	1.80	1.52
2	B	734	HIS	C-N	8.12	1.52	1.34
4	E	137	GLU	CG-CD	8.12	1.64	1.51
10	L	43	THR	CA-CB	8.12	1.74	1.53
9	K	82	ASP	C-N	-8.12	1.18	1.34
1	A	135	PHE	CG-CD1	-8.12	1.26	1.38
3	C	51	VAL	CB-CG2	-8.11	1.35	1.52
4	E	1	MET	CG-SD	8.11	2.02	1.81
1	A	117	GLU	CD-OE2	8.11	1.34	1.25
3	C	206	ASN	CB-CG	-8.11	1.32	1.51
1	A	404	TYR	CD2-CE2	8.10	1.51	1.39
10	L	66	GLN	C-O	-8.10	1.07	1.23
1	A	473	SER	CB-OG	8.10	1.52	1.42
8	J	44	TYR	CE2-CZ	8.10	1.49	1.38
2	B	1064	TYR	CZ-OH	8.10	1.51	1.37
6	H	138	GLU	CD-OE2	8.10	1.34	1.25
1	A	678	GLU	CG-CD	8.10	1.64	1.51
1	A	677	ARG	CD-NE	8.10	1.60	1.46
1	A	714	PHE	CD2-CE2	-8.10	1.23	1.39
1	A	1159	ARG	CG-CD	8.10	1.72	1.51
4	E	112	TYR	CE2-CZ	8.10	1.49	1.38
4	E	211	TYR	CE2-CZ	-8.10	1.28	1.38
1	A	1357	ALA	CA-CB	-8.09	1.35	1.52
2	B	434	ARG	CA-CB	8.09	1.71	1.53
1	A	896	ARG	CZ-NH1	8.09	1.43	1.33
5	F	136	ARG	CB-CG	-8.09	1.30	1.52
1	A	591	PHE	CG-CD2	-8.08	1.26	1.38
1	A	1276	VAL	CB-CG1	-8.08	1.35	1.52
7	I	119	THR	N-CA	8.08	1.62	1.46
3	C	236	GLY	N-CA	-8.08	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	93	LYS	CA-CB	8.08	1.71	1.53
4	E	55	ARG	CZ-NH1	-8.08	1.22	1.33
4	E	98	ILE	CA-C	8.07	1.74	1.52
2	B	459	TYR	CE1-CZ	8.07	1.49	1.38
1	A	160	GLN	CB-CG	8.07	1.74	1.52
1	A	350	ARG	C-O	-8.07	1.08	1.23
2	B	186	GLU	CD-OE1	8.07	1.34	1.25
2	B	194	GLU	C-O	-8.07	1.08	1.23
2	B	859	TYR	CD2-CE2	8.07	1.51	1.39
1	A	50	ILE	N-CA	8.07	1.62	1.46
1	A	803	SER	CA-CB	8.07	1.65	1.52
1	A	115	LEU	C-O	8.06	1.38	1.23
1	A	603	ASN	CB-CG	-8.06	1.32	1.51
1	A	49	LYS	CG-CD	8.06	1.79	1.52
2	B	216	GLU	CD-OE1	8.06	1.34	1.25
4	E	21	GLU	CG-CD	8.06	1.64	1.51
2	B	513	GLN	C-O	8.06	1.38	1.23
6	H	27	GLU	C-O	-8.06	1.08	1.23
7	I	28	GLU	CA-C	-8.06	1.31	1.52
1	A	523	ILE	N-CA	-8.06	1.30	1.46
1	A	1003	LYS	CD-CE	8.06	1.71	1.51
1	A	503	GLN	CD-OE1	8.05	1.41	1.24
1	A	1050	GLU	CG-CD	8.06	1.64	1.51
2	B	138	GLU	CD-OE1	-8.05	1.16	1.25
6	H	123	MET	C-O	-8.05	1.08	1.23
1	A	1056	SER	CB-OG	-8.05	1.31	1.42
1	A	962	ARG	CZ-NH1	8.04	1.43	1.33
1	A	722	LEU	C-O	-8.04	1.08	1.23
2	B	624	LEU	CG-CD1	-8.04	1.22	1.51
3	C	20	PHE	CD2-CE2	8.04	1.55	1.39
1	A	346	ASP	CA-CB	8.03	1.71	1.53
2	B	351	TYR	CE1-CZ	-8.03	1.28	1.38
4	E	212	ARG	CZ-NH2	8.03	1.43	1.33
10	L	42	ARG	NE-CZ	8.03	1.43	1.33
1	A	973	ILE	CA-CB	8.03	1.73	1.54
1	A	206	GLU	CD-OE1	8.03	1.34	1.25
3	C	14	SER	CB-OG	8.03	1.52	1.42
7	I	86	PHE	CD2-CE2	8.03	1.55	1.39
1	A	741	ASN	C-O	-8.02	1.08	1.23
1	A	737	LEU	CG-CD2	8.02	1.81	1.51
5	F	78	GLN	CB-CG	8.02	1.74	1.52
2	B	1224	PHE	CG-CD2	8.02	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	54	ARG	CZ-NH2	8.02	1.43	1.33
1	A	1364	ASN	C-O	8.02	1.38	1.23
5	F	92	ARG	NE-CZ	8.02	1.43	1.33
4	E	207	ARG	N-CA	-8.01	1.30	1.46
2	B	653	VAL	CB-CG2	-8.01	1.36	1.52
1	A	711	ARG	CA-C	-8.01	1.32	1.52
1	A	1332	PHE	N-CA	-8.01	1.30	1.46
2	B	663	ALA	CA-CB	8.01	1.69	1.52
2	B	1091	TYR	CD1-CE1	8.01	1.51	1.39
6	H	62	SER	CA-CB	8.00	1.65	1.52
1	A	1053	PHE	CE2-CZ	-8.00	1.22	1.37
7	I	9	ASP	CG-OD2	8.00	1.43	1.25
10	L	65	VAL	CA-C	-8.00	1.32	1.52
1	A	619	LYS	CE-NZ	8.00	1.69	1.49
1	A	1338	VAL	CB-CG1	-8.00	1.36	1.52
4	E	113	GLN	CG-CD	8.00	1.69	1.51
1	A	836	TYR	N-CA	-7.99	1.30	1.46
1	A	1211	GLN	CB-CG	7.99	1.74	1.52
2	B	250	PHE	CD2-CE2	7.99	1.55	1.39
4	E	211	TYR	CG-CD1	-7.99	1.28	1.39
2	B	893	LEU	CG-CD2	-7.99	1.22	1.51
2	B	488	TYR	CE1-CZ	-7.99	1.28	1.38
6	H	119	GLY	C-O	7.99	1.36	1.23
2	B	803	LEU	CA-CB	-7.99	1.35	1.53
2	B	259	TYR	CG-CD1	-7.99	1.28	1.39
1	A	1128	GLN	CD-OE1	-7.98	1.06	1.24
2	B	401	PHE	CB-CG	-7.98	1.37	1.51
4	E	141	VAL	C-O	7.98	1.38	1.23
7	I	117	LYS	CE-NZ	7.98	1.69	1.49
2	B	352	ALA	CA-C	-7.98	1.32	1.52
1	A	191	THR	CB-CG2	7.98	1.78	1.52
1	A	760	GLN	CG-CD	7.98	1.69	1.51
1	A	1448	GLU	N-CA	7.98	1.62	1.46
2	B	385	LEU	N-CA	-7.97	1.30	1.46
2	B	528	PRO	N-CD	-7.97	1.36	1.47
1	A	1225	PHE	CG-CD2	7.97	1.50	1.38
2	B	870	ILE	CB-CG2	7.97	1.77	1.52
8	J	24	LEU	CA-CB	-7.97	1.35	1.53
1	A	446	ARG	C-O	-7.97	1.08	1.23
2	B	296	GLU	CG-CD	7.96	1.63	1.51
3	C	96	SER	N-CA	-7.96	1.30	1.46
3	C	147	LEU	CB-CG	7.96	1.75	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	821	GLN	CD-OE1	-7.96	1.06	1.24
3	C	191	TYR	CE1-CZ	-7.96	1.28	1.38
6	H	13	SER	CA-CB	7.96	1.64	1.52
1	A	1278	ASN	CB-CG	-7.95	1.32	1.51
1	A	1242	VAL	CA-CB	-7.95	1.38	1.54
7	I	27	PHE	CE1-CZ	-7.95	1.22	1.37
1	A	1150	SER	C-O	-7.95	1.08	1.23
1	A	454	SER	CA-CB	-7.95	1.41	1.52
1	A	135	PHE	CB-CG	-7.94	1.37	1.51
1	A	971	PHE	CD2-CE2	-7.94	1.23	1.39
2	B	486	TYR	CG-CD1	7.94	1.49	1.39
5	F	90	ARG	CG-CD	-7.94	1.32	1.51
1	A	135	PHE	CD1-CE1	-7.94	1.23	1.39
2	B	230	ALA	CA-C	7.93	1.73	1.52
2	B	1196	ILE	C-O	7.93	1.38	1.23
3	C	24	ASN	C-O	7.93	1.38	1.23
5	F	123	LYS	CE-NZ	7.93	1.68	1.49
2	B	421	PHE	CG-CD1	-7.93	1.26	1.38
4	E	28	TYR	CE1-CZ	-7.93	1.28	1.38
4	E	164	LEU	CA-C	-7.93	1.32	1.52
1	A	1130	GLN	CD-NE2	7.93	1.52	1.32
2	B	667	GLN	CD-OE1	7.93	1.41	1.24
9	K	45	LEU	C-O	-7.93	1.08	1.23
1	A	477	PRO	N-CA	-7.92	1.33	1.47
1	A	798	GLY	C-O	7.92	1.36	1.23
4	E	53	PRO	CB-CG	7.92	1.89	1.50
2	B	635	ARG	CZ-NH2	-7.92	1.22	1.33
2	B	1091	TYR	CG-CD2	-7.92	1.28	1.39
3	C	7	GLN	CB-CG	7.92	1.74	1.52
1	A	576	GLN	CB-CG	-7.92	1.31	1.52
2	B	710	LEU	CG-CD1	-7.92	1.22	1.51
2	B	418	LYS	CG-CD	7.92	1.79	1.52
1	A	1303	GLU	N-CA	-7.91	1.30	1.46
7	I	21	GLU	CD-OE2	7.91	1.34	1.25
2	B	963	PHE	CB-CG	-7.91	1.37	1.51
1	A	651	LYS	C-O	7.91	1.38	1.23
2	B	485	ARG	CG-CD	-7.91	1.32	1.51
2	B	637	LEU	N-CA	-7.91	1.30	1.46
1	A	738	LYS	CD-CE	7.91	1.71	1.51
1	A	751	SER	CB-OG	7.91	1.52	1.42
2	B	226	PHE	CE1-CZ	7.91	1.52	1.37
1	A	216	VAL	CB-CG2	-7.90	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1164	PRO	CG-CD	7.90	1.76	1.50
1	A	889	SER	CA-C	-7.90	1.32	1.52
2	B	959	ASP	CA-CB	7.90	1.71	1.53
1	A	61	ILE	CB-CG2	7.89	1.77	1.52
1	A	1450	LEU	N-CA	7.89	1.62	1.46
2	B	271	ALA	CA-CB	-7.89	1.35	1.52
2	B	1190	ASP	CB-CG	-7.89	1.35	1.51
2	B	875	GLU	CB-CG	7.89	1.67	1.52
5	F	72	LYS	CG-CD	7.89	1.79	1.52
1	A	293	GLU	CG-CD	7.89	1.63	1.51
2	B	262	GLU	CB-CG	7.89	1.67	1.52
6	H	14	GLU	CD-OE2	7.89	1.34	1.25
7	I	92	ARG	CA-C	7.89	1.73	1.52
2	B	1134	GLU	CD-OE2	7.89	1.34	1.25
2	B	842	ASN	CG-ND2	-7.89	1.13	1.32
3	C	191	TYR	C-O	-7.88	1.08	1.23
6	H	102	TYR	CZ-OH	7.88	1.51	1.37
9	K	86	ALA	CA-CB	-7.88	1.35	1.52
7	I	50	THR	C-O	-7.88	1.08	1.23
1	A	835	GLY	C-O	-7.88	1.11	1.23
1	A	1293	SER	CA-CB	-7.88	1.41	1.52
2	B	1183	LYS	CA-CB	7.88	1.71	1.53
3	C	54	ASN	CB-CG	-7.88	1.32	1.51
4	E	14	ARG	CA-CB	-7.88	1.36	1.53
1	A	305	ASP	CB-CG	7.88	1.68	1.51
2	B	760	ASP	CG-OD2	7.88	1.43	1.25
1	A	28	ARG	NE-CZ	7.88	1.43	1.33
2	B	805	THR	CB-OG1	7.88	1.59	1.43
4	E	208	TYR	CE2-CZ	-7.88	1.28	1.38
5	F	100	GLN	CB-CG	7.88	1.73	1.52
2	B	893	LEU	CA-CB	-7.88	1.35	1.53
2	B	316	PRO	CA-CB	-7.87	1.37	1.53
4	E	13	TRP	CD2-CE2	7.87	1.50	1.41
2	B	513	GLN	CD-OE1	7.87	1.41	1.24
1	A	1121	GLU	CG-CD	7.87	1.63	1.51
2	B	1151	LEU	C-O	-7.87	1.08	1.23
2	B	499	ASN	C-O	-7.87	1.08	1.23
1	A	449	SER	CA-CB	-7.86	1.41	1.52
1	A	1227	ILE	N-CA	-7.86	1.30	1.46
2	B	18	PHE	CA-CB	7.86	1.71	1.53
3	C	177	GLU	CG-CD	7.86	1.63	1.51
1	A	1304	TRP	CA-C	-7.86	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1205	LYS	CD-CE	7.86	1.70	1.51
1	A	1326	ARG	CA-CB	7.86	1.71	1.53
1	A	39	GLU	CD-OE2	-7.86	1.17	1.25
1	A	917	SER	C-O	-7.86	1.08	1.23
2	B	554	ILE	CA-CB	-7.86	1.36	1.54
2	B	935	ARG	CB-CG	7.86	1.73	1.52
4	E	33	GLU	CD-OE1	7.86	1.34	1.25
2	B	1096	ARG	CB-CG	-7.85	1.31	1.52
2	B	456	GLY	CA-C	7.85	1.64	1.51
2	B	1095	LEU	CG-CD1	-7.85	1.22	1.51
3	C	122	SER	CA-CB	7.85	1.64	1.52
3	C	173	ALA	C-O	7.85	1.38	1.23
1	A	603	ASN	C-O	-7.85	1.08	1.23
1	A	1212	VAL	CB-CG2	-7.85	1.36	1.52
2	B	29	ASP	CB-CG	-7.84	1.35	1.51
1	A	359	LEU	C-O	7.84	1.38	1.23
1	A	852	TYR	C-O	7.84	1.38	1.23
1	A	864	ILE	N-CA	-7.84	1.30	1.46
1	A	107	CYS	CB-SG	7.84	1.95	1.82
2	B	639	ILE	CB-CG2	7.84	1.77	1.52
1	A	767	GLN	C-O	-7.83	1.08	1.23
1	A	849	MET	SD-CE	-7.83	1.33	1.77
2	B	822	ASN	CG-ND2	7.83	1.52	1.32
6	H	79	TRP	CG-CD1	-7.83	1.25	1.36
7	I	110	PHE	CD1-CE1	7.83	1.54	1.39
9	K	102	LYS	C-O	7.83	1.38	1.23
1	A	264	PHE	CA-CB	7.83	1.71	1.53
2	B	594	ALA	CA-C	-7.83	1.32	1.52
8	J	49	MET	CB-CG	-7.83	1.26	1.51
1	A	527	THR	C-O	-7.83	1.08	1.23
1	A	460	VAL	N-CA	-7.83	1.30	1.46
6	H	132	LEU	CA-CB	7.83	1.71	1.53
1	A	31	SER	C-O	7.83	1.38	1.23
1	A	718	VAL	CA-CB	-7.83	1.38	1.54
2	B	404	LYS	CB-CG	-7.83	1.31	1.52
2	B	825	VAL	CA-CB	-7.83	1.38	1.54
3	C	34	ARG	NE-CZ	-7.83	1.22	1.33
1	A	1274	ARG	NE-CZ	-7.82	1.22	1.33
3	C	249	ASP	C-O	7.82	1.38	1.23
4	E	208	TYR	C-O	7.82	1.38	1.23
1	A	180	LYS	CB-CG	7.82	1.73	1.52
2	B	855	PHE	CG-CD2	-7.82	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	152	VAL	CB-CG1	-7.82	1.36	1.52
1	A	1109	LYS	CD-CE	7.82	1.70	1.51
2	B	266	ALA	CA-CB	7.82	1.68	1.52
8	J	18	TRP	CG-CD2	-7.82	1.30	1.43
2	B	116	GLU	CB-CG	7.81	1.67	1.52
1	A	1081	LEU	N-CA	7.81	1.61	1.46
1	A	1351	GLU	C-O	-7.81	1.08	1.23
2	B	703	ILE	CA-CB	-7.81	1.36	1.54
5	F	108	PHE	CE1-CZ	7.81	1.52	1.37
1	A	1207	LEU	N-CA	7.81	1.61	1.46
10	L	40	LEU	CB-CG	7.81	1.75	1.52
1	A	297	GLN	C-O	-7.81	1.08	1.23
1	A	1216	ILE	CA-CB	-7.81	1.36	1.54
1	A	563	PRO	CA-C	-7.81	1.37	1.52
1	A	1196	GLU	CA-C	7.81	1.73	1.52
1	A	527	THR	CB-OG1	7.80	1.58	1.43
2	B	654	ARG	CZ-NH1	-7.80	1.23	1.33
9	K	16	GLU	CB-CG	7.80	1.67	1.52
2	B	542	MET	SD-CE	-7.80	1.34	1.77
10	L	59	ALA	CA-CB	7.80	1.68	1.52
2	B	862	GLN	CG-CD	7.80	1.69	1.51
6	H	111	LEU	CG-CD1	7.80	1.80	1.51
1	A	1012	ARG	CD-NE	7.79	1.59	1.46
1	A	1319	VAL	N-CA	-7.79	1.30	1.46
2	B	1080	LYS	CD-CE	7.79	1.70	1.51
1	A	721	PHE	CD2-CE2	-7.79	1.23	1.39
1	A	1145	SER	CB-OG	7.79	1.52	1.42
6	H	124	ARG	CB-CG	-7.79	1.31	1.52
1	A	188	ASP	CB-CG	7.79	1.68	1.51
3	C	11	ARG	CZ-NH2	-7.79	1.23	1.33
4	E	66	GLU	C-O	7.79	1.38	1.23
2	B	634	TYR	N-CA	-7.79	1.30	1.46
2	B	1012	ILE	CB-CG1	-7.79	1.32	1.54
1	A	1096	SER	CA-CB	7.78	1.64	1.52
1	A	1352	VAL	C-O	-7.78	1.08	1.23
3	C	249	ASP	CA-C	7.78	1.73	1.52
4	E	13	TRP	CZ3-CH2	7.78	1.52	1.40
3	C	104	PHE	CB-CG	-7.78	1.38	1.51
2	B	610	ASN	C-O	7.78	1.38	1.23
3	C	73	GLN	CA-CB	7.78	1.71	1.53
6	H	50	ALA	N-CA	7.78	1.61	1.46
2	B	734	HIS	C-O	7.78	1.38	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	67	PHE	C-O	-7.78	1.08	1.23
1	A	277	GLU	CG-CD	7.77	1.63	1.51
2	B	498	THR	CA-CB	7.77	1.73	1.53
1	A	580	VAL	CB-CG2	-7.77	1.36	1.52
2	B	681	TRP	CZ3-CH2	7.77	1.52	1.40
2	B	969	ARG	N-CA	-7.77	1.30	1.46
1	A	303	TYR	CD1-CE1	-7.77	1.27	1.39
1	A	1441	PHE	CB-CG	-7.77	1.38	1.51
2	B	493	SER	CA-CB	-7.77	1.41	1.52
2	B	970	THR	CA-CB	-7.77	1.33	1.53
4	E	151	PRO	C-O	-7.77	1.07	1.23
4	E	185	ALA	CA-CB	-7.77	1.36	1.52
2	B	679	TYR	CE1-CZ	-7.76	1.28	1.38
4	E	82	PHE	CG-CD2	-7.76	1.27	1.38
4	E	207	ARG	NE-CZ	7.76	1.43	1.33
1	A	885	THR	N-CA	-7.76	1.30	1.46
4	E	148	GLU	CG-CD	-7.76	1.40	1.51
2	B	51	PHE	CD1-CE1	7.76	1.54	1.39
1	A	586	ILE	CA-C	-7.76	1.32	1.52
2	B	774	GLY	CA-C	7.76	1.64	1.51
1	A	618	GLU	CB-CG	7.75	1.66	1.52
2	B	193	LYS	CG-CD	7.75	1.78	1.52
1	A	1093	LYS	CB-CG	7.75	1.73	1.52
1	A	441	PRO	CB-CG	-7.75	1.11	1.50
2	B	763	GLN	CD-NE2	-7.75	1.13	1.32
9	K	37	LYS	C-O	7.75	1.38	1.23
8	J	9	SER	CB-OG	7.75	1.52	1.42
7	I	91	ARG	CB-CG	7.75	1.73	1.52
2	B	1013	ASN	C-O	-7.75	1.08	1.23
3	C	222	LYS	CB-CG	7.75	1.73	1.52
1	A	1035	TYR	CE1-CZ	7.74	1.48	1.38
1	A	406	ILE	CA-C	-7.74	1.32	1.52
2	B	354	ASP	CA-CB	7.74	1.71	1.53
1	A	1410	PHE	CG-CD2	-7.74	1.27	1.38
2	B	248	SER	CA-CB	7.74	1.64	1.52
2	B	963	PHE	CE2-CZ	7.74	1.52	1.37
2	B	1002	THR	CB-CG2	7.74	1.77	1.52
10	L	63	ARG	CG-CD	7.74	1.71	1.51
2	B	184	ALA	CA-CB	-7.73	1.36	1.52
2	B	488	TYR	CD1-CE1	-7.73	1.27	1.39
2	B	767	ASN	CB-CG	-7.73	1.33	1.51
1	A	146	MET	CG-SD	7.73	2.01	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1278	ASN	CA-CB	7.73	1.73	1.53
4	E	58	MET	CB-CG	-7.73	1.26	1.51
2	B	1047	PHE	CG-CD1	-7.72	1.27	1.38
1	A	261	ASP	CB-CG	7.72	1.68	1.51
1	A	1119	TYR	CZ-OH	-7.72	1.24	1.37
3	C	231	ASN	CB-CG	7.72	1.68	1.51
3	C	134	ILE	N-CA	7.72	1.61	1.46
8	J	29	GLU	CD-OE2	7.72	1.34	1.25
2	B	567	GLU	CD-OE2	7.72	1.34	1.25
7	I	86	PHE	CB-CG	-7.71	1.38	1.51
1	A	1208	THR	CA-CB	7.71	1.73	1.53
2	B	1198	TYR	CE1-CZ	7.71	1.48	1.38
6	H	107	VAL	CB-CG1	7.71	1.69	1.52
2	B	699	GLU	CA-C	-7.71	1.32	1.52
2	B	1182	CYS	CA-C	7.71	1.73	1.52
4	E	191	LYS	CB-CG	7.71	1.73	1.52
5	F	88	TYR	CZ-OH	7.71	1.50	1.37
1	A	167	CYS	N-CA	7.71	1.61	1.46
2	B	581	PHE	C-O	7.71	1.38	1.23
1	A	360	GLU	CG-CD	7.70	1.63	1.51
2	B	1128	LEU	CA-C	7.70	1.73	1.52
3	C	4	GLU	CD-OE1	7.70	1.34	1.25
3	C	229	TYR	CE2-CZ	7.70	1.48	1.38
1	A	81	PHE	CE1-CZ	-7.70	1.22	1.37
1	A	1151	GLU	CD-OE1	7.69	1.34	1.25
2	B	980	PHE	CG-CD2	7.69	1.50	1.38
2	B	308	TRP	CE3-CZ3	-7.69	1.25	1.38
2	B	1085	ILE	N-CA	-7.69	1.30	1.46
2	B	1156	ASP	CA-CB	7.69	1.70	1.53
1	A	1093	LYS	N-CA	7.69	1.61	1.46
2	B	997	GLU	C-O	-7.69	1.08	1.23
9	K	81	TYR	CD2-CE2	-7.69	1.27	1.39
2	B	237	VAL	CA-CB	-7.69	1.38	1.54
7	I	13	MET	N-CA	-7.69	1.30	1.46
1	A	1078	GLN	CG-CD	7.69	1.68	1.51
2	B	420	LEU	CG-CD1	7.69	1.80	1.51
4	E	6	GLU	CD-OE2	7.69	1.34	1.25
9	K	62	LYS	CE-NZ	-7.69	1.29	1.49
1	A	238	CYS	C-O	-7.68	1.08	1.23
2	B	50	SER	C-O	7.68	1.38	1.23
2	B	245	GLU	CA-CB	7.68	1.70	1.53
2	B	589	VAL	CB-CG2	-7.68	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	12	LEU	CG-CD1	7.68	1.80	1.51
1	A	1448	GLU	CA-CB	7.68	1.70	1.53
2	B	228	LYS	CG-CD	7.68	1.78	1.52
2	B	214	ALA	N-CA	-7.68	1.30	1.46
2	B	296	GLU	CD-OE2	7.68	1.34	1.25
2	B	793	ALA	CA-CB	-7.68	1.36	1.52
2	B	1030	LEU	CA-CB	-7.68	1.36	1.53
10	L	27	LEU	CB-CG	7.68	1.74	1.52
2	B	961	LEU	CB-CG	7.67	1.74	1.52
1	A	891	ALA	CA-CB	7.67	1.68	1.52
1	A	1265	ASN	CA-C	7.67	1.72	1.52
6	H	136	LYS	N-CA	7.67	1.61	1.46
1	A	1030	ARG	NE-CZ	-7.67	1.23	1.33
2	B	425	THR	CB-CG2	7.67	1.77	1.52
3	C	121	VAL	CA-CB	7.67	1.70	1.54
1	A	1350	LYS	CG-CD	7.66	1.78	1.52
2	B	28	GLU	C-O	7.66	1.38	1.23
6	H	102	TYR	CD2-CE2	-7.66	1.27	1.39
9	K	4	PRO	CG-CD	7.66	1.75	1.50
1	A	1048	ASN	C-O	7.65	1.37	1.23
1	A	1166	ASP	CG-OD2	7.65	1.43	1.25
1	A	1141	THR	C-O	7.65	1.37	1.23
2	B	644	GLU	CD-OE2	7.65	1.34	1.25
1	A	567	LYS	CD-CE	7.65	1.70	1.51
2	B	532	ALA	CA-C	-7.65	1.33	1.52
1	A	648	ASN	C-O	-7.64	1.08	1.23
1	A	1194	ARG	CZ-NH2	7.64	1.43	1.33
7	I	73	ARG	NE-CZ	7.64	1.43	1.33
1	A	261	ASP	N-CA	7.64	1.61	1.46
1	A	551	TYR	CD2-CE2	-7.64	1.27	1.39
2	B	945	GLU	C-O	7.64	1.37	1.23
2	B	1077	THR	CA-C	7.64	1.72	1.52
2	B	1082	MET	CG-SD	7.64	2.01	1.81
1	A	326	ARG	CA-C	7.64	1.72	1.52
5	F	92	ARG	CA-C	-7.64	1.33	1.52
5	F	110	ASP	CG-OD1	7.64	1.43	1.25
2	B	134	LYS	CD-CE	7.64	1.70	1.51
8	J	7	CYS	CB-SG	-7.64	1.69	1.82
2	B	1069	PHE	CE2-CZ	-7.63	1.22	1.37
1	A	1445	ILE	CB-CG2	7.63	1.76	1.52
3	C	114	TYR	CE1-CZ	-7.63	1.28	1.38
4	E	136	ASN	CB-CG	7.63	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	27	VAL	CB-CG1	7.63	1.68	1.52
1	A	770	VAL	CB-CG1	-7.63	1.36	1.52
1	A	1277	GLU	CB-CG	7.63	1.66	1.52
2	B	519	TRP	CG-CD1	-7.63	1.26	1.36
5	F	83	PRO	N-CA	-7.63	1.34	1.47
1	A	839	ARG	CZ-NH2	7.63	1.43	1.33
1	A	1050	GLU	CD-OE1	7.63	1.34	1.25
2	B	384	ARG	C-N	-7.63	1.16	1.34
2	B	1053	GLU	CD-OE1	7.63	1.34	1.25
9	K	31	VAL	CB-CG1	-7.63	1.36	1.52
4	E	161	LYS	CG-CD	-7.62	1.26	1.52
1	A	1220	PHE	CE1-CZ	-7.62	1.22	1.37
3	C	180	TYR	CA-CB	-7.62	1.37	1.53
1	A	175	ARG	CZ-NH1	7.62	1.43	1.33
1	A	163	SER	N-CA	7.62	1.61	1.46
1	A	751	SER	C-O	7.62	1.37	1.23
1	A	835	GLY	N-CA	7.62	1.57	1.46
1	A	510	GLN	CG-CD	-7.62	1.33	1.51
1	A	381	THR	CB-OG1	-7.62	1.28	1.43
10	L	61	THR	CB-CG2	7.62	1.77	1.52
1	A	1449	SER	CB-OG	-7.61	1.32	1.42
3	C	148	ARG	CZ-NH1	7.61	1.43	1.33
3	C	187	LYS	C-O	-7.61	1.08	1.23
8	J	51	LEU	CA-CB	-7.61	1.36	1.53
8	J	63	TYR	CD1-CE1	-7.61	1.27	1.39
4	E	30	ILE	C-O	-7.61	1.08	1.23
1	A	217	LYS	CB-CG	7.60	1.73	1.52
1	A	1015	VAL	CB-CG1	-7.60	1.36	1.52
4	E	148	GLU	CD-OE1	-7.60	1.17	1.25
2	B	283	VAL	C-O	-7.60	1.08	1.23
1	A	592	ASP	C-O	-7.60	1.08	1.23
1	A	821	ARG	C-O	7.60	1.37	1.23
2	B	285	ILE	CA-CB	-7.60	1.37	1.54
2	B	465	ASN	CG-ND2	7.60	1.51	1.32
2	B	1050	ILE	CA-C	-7.60	1.33	1.52
2	B	1149	GLU	C-O	-7.60	1.08	1.23
6	H	81	PRO	CA-C	7.60	1.68	1.52
1	A	104	GLU	CG-CD	7.60	1.63	1.51
2	B	1174	LYS	N-CA	7.60	1.61	1.46
2	B	1039	GLY	CA-C	-7.59	1.39	1.51
9	K	79	GLU	CD-OE2	7.59	1.34	1.25
1	A	1071	SER	CA-CB	-7.59	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1153	GLU	CA-C	7.59	1.72	1.52
3	C	237	SER	CA-CB	7.59	1.64	1.52
10	L	25	ALA	CA-CB	7.59	1.68	1.52
2	B	328	GLU	CD-OE1	7.59	1.33	1.25
3	C	104	PHE	CD1-CE1	7.59	1.54	1.39
2	B	822	ASN	C-O	-7.59	1.08	1.23
8	J	3	VAL	CA-CB	-7.59	1.38	1.54
1	A	482	PHE	CA-CB	-7.58	1.37	1.53
2	B	227	LYS	CG-CD	7.58	1.78	1.52
2	B	265	SER	CA-C	7.58	1.72	1.52
2	B	583	ASN	CG-OD1	-7.58	1.07	1.24
1	A	1297	GLU	N-CA	-7.58	1.31	1.46
2	B	1011	ILE	C-O	-7.58	1.08	1.23
2	B	489	SER	C-O	-7.58	1.08	1.23
1	A	1368	MET	C-O	-7.58	1.08	1.23
2	B	531	GLN	CD-NE2	7.58	1.51	1.32
1	A	122	MET	CA-CB	-7.57	1.37	1.53
1	A	721	PHE	CB-CG	7.57	1.64	1.51
1	A	750	GLY	CA-C	-7.57	1.39	1.51
2	B	1030	LEU	N-CA	-7.57	1.31	1.46
1	A	411	ASP	CA-C	-7.57	1.33	1.52
2	B	42	GLY	N-CA	7.57	1.57	1.46
1	A	248	PRO	N-CD	7.57	1.58	1.47
3	C	17	ASN	CB-CG	7.56	1.68	1.51
9	K	7	PHE	CE2-CZ	7.56	1.51	1.37
2	B	1130	PHE	CE2-CZ	-7.56	1.23	1.37
10	L	38	LEU	CG-CD2	7.56	1.79	1.51
1	A	736	ASN	C-N	-7.55	1.16	1.34
1	A	1264	GLU	CD-OE2	-7.55	1.17	1.25
1	A	1421	CYS	C-O	-7.55	1.08	1.23
2	B	327	ARG	CZ-NH1	7.55	1.42	1.33
2	B	1086	PHE	CG-CD2	-7.55	1.27	1.38
7	I	15	TYR	CD2-CE2	7.55	1.50	1.39
2	B	115	GLN	CD-NE2	7.55	1.51	1.32
2	B	502	ILE	CB-CG2	7.55	1.76	1.52
2	B	809	MET	C-N	-7.55	1.16	1.34
6	H	82	PRO	CA-C	7.55	1.68	1.52
3	C	95	CYS	C-O	-7.54	1.09	1.23
3	C	153	LEU	C-O	7.54	1.37	1.23
1	A	1188	GLN	CA-C	7.54	1.72	1.52
2	B	746	SER	CA-CB	-7.54	1.41	1.52
2	B	380	TYR	N-CA	-7.54	1.31	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	404	TYR	CE2-CZ	-7.54	1.28	1.38
1	A	613	ILE	C-O	-7.54	1.09	1.23
1	A	689	LYS	CD-CE	7.54	1.70	1.51
1	A	1026	LEU	C-O	-7.54	1.09	1.23
2	B	225	VAL	CB-CG2	-7.54	1.37	1.52
2	B	227	LYS	CA-C	-7.54	1.33	1.52
2	B	350	GLN	CD-OE1	7.54	1.40	1.24
2	B	542	MET	N-CA	-7.54	1.31	1.46
3	C	160	LYS	CG-CD	7.53	1.78	1.52
1	A	383	TYR	CA-CB	7.53	1.70	1.53
2	B	57	TYR	CB-CG	7.53	1.62	1.51
2	B	1192	TYR	CG-CD2	-7.53	1.29	1.39
9	K	98	LEU	C-O	7.53	1.37	1.23
2	B	45	SER	CB-OG	7.53	1.52	1.42
2	B	816	GLU	CD-OE1	7.53	1.33	1.25
9	K	8	GLU	CD-OE2	-7.53	1.17	1.25
1	A	815	PHE	CE2-CZ	-7.52	1.23	1.37
1	A	1109	LYS	CG-CD	7.52	1.78	1.52
2	B	182	SER	CA-CB	7.52	1.64	1.52
10	L	28	LYS	CA-C	7.52	1.72	1.52
10	L	33	GLU	CA-C	7.52	1.72	1.52
3	C	5	GLY	C-O	-7.52	1.11	1.23
3	C	114	TYR	CD2-CE2	-7.52	1.28	1.39
4	E	103	LYS	C-O	7.52	1.37	1.23
1	A	491	VAL	CA-CB	-7.52	1.39	1.54
1	A	874	ASP	CG-OD1	7.52	1.42	1.25
2	B	227	LYS	C-O	-7.52	1.09	1.23
2	B	557	PHE	C-O	7.52	1.37	1.23
6	H	26	ILE	CA-CB	-7.52	1.37	1.54
8	J	62	ARG	CG-CD	-7.52	1.33	1.51
1	A	664	THR	N-CA	7.52	1.61	1.46
2	B	326	ASP	CB-CG	7.52	1.67	1.51
2	B	706	GLN	CD-NE2	7.51	1.51	1.32
3	C	174	ALA	N-CA	-7.51	1.31	1.46
1	A	1127	ASP	CB-CG	7.51	1.67	1.51
3	C	94	LYS	CG-CD	7.51	1.77	1.52
2	B	620	ARG	CB-CG	7.51	1.72	1.52
1	A	1077	THR	C-O	-7.51	1.09	1.23
3	C	41	ILE	C-O	7.51	1.37	1.23
5	F	84	TYR	CE2-CZ	7.51	1.48	1.38
2	B	1149	GLU	CA-C	-7.51	1.33	1.52
9	K	37	LYS	N-CA	-7.51	1.31	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	34	ILE	CA-CB	-7.50	1.37	1.54
4	E	60	PHE	CE2-CZ	7.50	1.51	1.37
1	A	393	ARG	CA-C	-7.50	1.33	1.52
2	B	268	THR	CA-CB	7.50	1.72	1.53
5	F	119	ARG	CB-CG	7.50	1.72	1.52
1	A	358	ASN	CA-C	-7.50	1.33	1.52
1	A	1283	VAL	CA-CB	-7.50	1.39	1.54
1	A	460	VAL	C-O	-7.50	1.09	1.23
2	B	303	TYR	CE2-CZ	-7.49	1.28	1.38
4	E	96	PHE	CD1-CE1	7.49	1.54	1.39
7	I	91	ARG	CG-CD	-7.49	1.33	1.51
1	A	89	PRO	C-O	-7.49	1.08	1.23
1	A	512	VAL	CB-CG1	-7.49	1.37	1.52
10	L	27	LEU	CG-CD2	7.49	1.79	1.51
2	B	1013	ASN	C-N	-7.49	1.20	1.34
7	I	25	LEU	C-O	-7.49	1.09	1.23
8	J	38	ARG	CA-C	-7.49	1.33	1.52
2	B	895	ASP	CG-OD1	7.49	1.42	1.25
1	A	1448	GLU	C-O	7.49	1.37	1.23
2	B	593	PRO	CB-CG	7.49	1.87	1.50
5	F	94	LEU	CA-C	-7.49	1.33	1.52
2	B	825	VAL	CB-CG1	-7.48	1.37	1.52
4	E	12	LEU	CG-CD1	7.48	1.79	1.51
6	H	105	GLU	CD-OE1	7.48	1.33	1.25
9	K	6	ARG	C-O	7.48	1.37	1.23
1	A	650	GLN	CD-OE1	-7.48	1.07	1.24
2	B	747	MET	SD-CE	-7.48	1.35	1.77
2	B	958	GLN	N-CA	7.48	1.61	1.46
9	K	112	GLN	CD-OE1	-7.48	1.07	1.24
1	A	828	ALA	CA-CB	-7.48	1.36	1.52
4	E	164	LEU	CA-CB	-7.48	1.36	1.53
1	A	645	LEU	C-O	-7.47	1.09	1.23
1	A	1025	ARG	CZ-NH2	7.47	1.42	1.33
1	A	213	HIS	CB-CG	7.47	1.63	1.50
2	B	277	LYS	CD-CE	7.47	1.70	1.51
3	C	96	SER	CB-OG	7.47	1.51	1.42
1	A	174	ILE	CA-CB	7.47	1.72	1.54
1	A	1056	SER	C-O	-7.47	1.09	1.23
2	B	552	MET	CA-CB	-7.47	1.37	1.53
2	B	581	PHE	CE2-CZ	-7.47	1.23	1.37
1	A	1354	ASN	C-O	-7.46	1.09	1.23
7	I	28	GLU	N-CA	-7.46	1.31	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	520	GLY	C-N	-7.46	1.16	1.34
3	C	5	GLY	CA-C	7.46	1.63	1.51
7	I	97	MET	C-O	7.46	1.37	1.23
10	L	26	THR	N-CA	7.46	1.61	1.46
2	B	184	ALA	C-O	-7.46	1.09	1.23
3	C	230	MET	C-O	-7.46	1.09	1.23
2	B	180	TYR	CZ-OH	-7.46	1.25	1.37
2	B	642	ASP	CB-CG	7.46	1.67	1.51
2	B	37	PHE	CG-CD1	-7.46	1.27	1.38
1	A	414	ASP	C-O	-7.45	1.09	1.23
2	B	691	GLU	CD-OE2	7.45	1.33	1.25
1	A	498	ARG	C-O	7.45	1.37	1.23
1	A	351	THR	C-O	-7.45	1.09	1.23
5	F	119	ARG	CA-C	-7.45	1.33	1.52
7	I	45	ARG	N-CA	7.45	1.61	1.46
7	I	68	LEU	C-O	-7.44	1.09	1.23
2	B	1149	GLU	CD-OE2	-7.44	1.17	1.25
1	A	929	LEU	CG-CD2	-7.44	1.24	1.51
2	B	367	LEU	CG-CD1	7.44	1.79	1.51
1	A	1156	PRO	CA-C	7.44	1.67	1.52
1	A	387	ARG	CD-NE	7.43	1.59	1.46
2	B	381	MET	CG-SD	7.43	2.00	1.81
2	B	466	TRP	CA-C	7.43	1.72	1.52
2	B	521	LEU	C-O	-7.43	1.09	1.23
3	C	166	GLU	C-O	7.43	1.37	1.23
7	I	73	ARG	C-O	-7.43	1.09	1.23
1	A	27	VAL	CA-CB	-7.43	1.39	1.54
1	A	850	VAL	CB-CG1	-7.43	1.37	1.52
1	A	1119	TYR	C-O	7.43	1.37	1.23
5	F	143	PHE	CG-CD2	-7.43	1.27	1.38
7	I	112	SER	CA-C	7.43	1.72	1.52
2	B	1057	LYS	C-O	7.43	1.37	1.23
2	B	278	GLN	CA-CB	-7.43	1.37	1.53
10	L	60	ARG	CD-NE	7.43	1.59	1.46
2	B	666	TYR	CE2-CZ	7.43	1.48	1.38
1	A	228	PHE	CG-CD2	-7.42	1.27	1.38
3	C	87	PHE	CD2-CE2	7.42	1.54	1.39
3	C	87	PHE	CB-CG	-7.42	1.38	1.51
1	A	815	PHE	CD1-CE1	-7.42	1.24	1.39
2	B	1110	PRO	CA-C	7.42	1.67	1.52
4	E	144	ILE	CB-CG1	-7.42	1.33	1.54
1	A	184	SER	CA-CB	7.42	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	425	GLN	CD-NE2	7.42	1.51	1.32
1	A	1062	GLU	CA-CB	-7.42	1.37	1.53
1	A	1122	PRO	C-O	7.42	1.38	1.23
4	E	138	ALA	CA-CB	-7.42	1.36	1.52
9	K	64	GLU	CD-OE2	-7.42	1.17	1.25
1	A	866	PHE	CG-CD2	-7.42	1.27	1.38
2	B	809	MET	CG-SD	7.42	2.00	1.81
3	C	89	GLU	CD-OE2	7.42	1.33	1.25
1	A	1420	ASP	CB-CG	7.42	1.67	1.51
2	B	398	ARG	CA-CB	-7.42	1.37	1.53
2	B	512	ARG	CD-NE	-7.42	1.33	1.46
6	H	85	GLY	C-O	7.42	1.35	1.23
1	A	578	LEU	CG-CD1	-7.41	1.24	1.51
2	B	368	GLU	C-O	7.41	1.37	1.23
2	B	541	LEU	CA-CB	-7.41	1.36	1.53
10	L	58	LYS	CE-NZ	7.41	1.67	1.49
1	A	1367	HIS	C-N	-7.41	1.17	1.34
5	F	118	LEU	CG-CD1	-7.41	1.24	1.51
9	K	50	LEU	C-O	-7.41	1.09	1.23
1	A	33	ALA	CA-CB	7.41	1.68	1.52
1	A	298	PHE	CD2-CE2	7.41	1.54	1.39
2	B	1016	ALA	CA-CB	7.41	1.68	1.52
4	E	188	LEU	CG-CD2	-7.41	1.24	1.51
1	A	1013	ASP	CG-OD2	7.40	1.42	1.25
2	B	954	VAL	CB-CG2	7.40	1.68	1.52
2	B	843	GLN	C-O	7.40	1.37	1.23
4	E	57	MET	CG-SD	7.40	2.00	1.81
2	B	603	LEU	N-CA	-7.40	1.31	1.46
2	B	879	ARG	CZ-NH1	7.40	1.42	1.33
9	K	51	LEU	CA-C	7.40	1.72	1.52
1	A	744	LYS	CA-C	-7.40	1.33	1.52
1	A	1325	THR	CA-CB	-7.40	1.34	1.53
2	B	452	THR	CA-CB	7.40	1.72	1.53
1	A	514	PRO	N-CA	-7.40	1.34	1.47
4	E	210	SER	CB-OG	7.39	1.51	1.42
4	E	46	TYR	CG-CD1	-7.39	1.29	1.39
1	A	761	MET	CA-C	-7.39	1.33	1.52
1	A	1435	PRO	CA-CB	-7.39	1.38	1.53
3	C	20	PHE	CG-CD1	7.39	1.49	1.38
1	A	378	GLU	CG-CD	-7.39	1.40	1.51
1	A	789	LYS	CE-NZ	-7.39	1.30	1.49
2	B	573	GLN	CG-CD	7.39	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	813	PHE	N-CA	-7.39	1.31	1.46
2	B	560	GLU	CD-OE2	7.39	1.33	1.25
1	A	24	PRO	CB-CG	7.38	1.86	1.50
2	B	60	GLN	C-O	-7.38	1.09	1.23
2	B	1053	GLU	CD-OE2	7.38	1.33	1.25
1	A	233	TRP	CZ3-CH2	7.38	1.51	1.40
2	B	241	ARG	CZ-NH1	7.38	1.42	1.33
2	B	722	ASP	CA-CB	7.38	1.70	1.53
2	B	1220	ARG	C-O	7.38	1.37	1.23
3	C	41	ILE	CA-CB	-7.38	1.37	1.54
6	H	104	PHE	CA-CB	7.38	1.70	1.53
7	I	99	LEU	CG-CD2	-7.38	1.24	1.51
1	A	838	GLN	CD-NE2	7.38	1.51	1.32
1	A	1209	MET	C-O	-7.38	1.09	1.23
2	B	846	ILE	CA-CB	7.38	1.71	1.54
1	A	81	PHE	CB-CG	7.37	1.63	1.51
1	A	107	CYS	CA-C	-7.37	1.33	1.52
9	K	102	LYS	CA-CB	7.37	1.70	1.53
1	A	280	GLU	CG-CD	7.37	1.63	1.51
2	B	1176	ASN	N-CA	7.37	1.61	1.46
9	K	58	PHE	CB-CG	7.37	1.63	1.51
2	B	1023	VAL	CA-CB	-7.37	1.39	1.54
1	A	1414	ALA	C-O	-7.37	1.09	1.23
2	B	514	LEU	CA-CB	-7.37	1.36	1.53
2	B	864	LYS	C-O	7.37	1.37	1.23
4	E	49	SER	CA-C	7.37	1.72	1.52
4	E	162	ARG	CA-CB	7.37	1.70	1.53
6	H	142	LEU	CA-CB	-7.37	1.36	1.53
1	A	28	ARG	C-O	7.37	1.37	1.23
1	A	776	ALA	C-O	-7.37	1.09	1.23
3	C	158	VAL	CB-CG2	-7.37	1.37	1.52
4	E	136	ASN	CG-OD1	7.37	1.40	1.24
7	I	80	SER	CB-OG	7.37	1.51	1.42
1	A	892	ALA	CA-C	-7.36	1.33	1.52
1	A	1020	CYS	C-O	7.36	1.37	1.23
2	B	859	TYR	CG-CD1	-7.36	1.29	1.39
2	B	1181	GLU	CD-OE1	-7.36	1.17	1.25
1	A	24	PRO	CG-CD	-7.36	1.26	1.50
1	A	624	SER	N-CA	7.36	1.61	1.46
1	A	813	PHE	CE2-CZ	-7.36	1.23	1.37
9	K	35	PHE	CE1-CZ	-7.36	1.23	1.37
2	B	45	SER	CA-CB	7.35	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	734	GLU	CB-CG	7.35	1.66	1.52
2	B	1129	ARG	CZ-NH2	7.35	1.42	1.33
1	A	1040	GLN	CD-NE2	7.35	1.51	1.32
1	A	817	ALA	CA-C	-7.35	1.33	1.52
1	A	461	LYS	CG-CD	-7.35	1.27	1.52
1	A	507	VAL	CB-CG1	-7.35	1.37	1.52
1	A	536	LEU	N-CA	-7.35	1.31	1.46
1	A	1236	LEU	CG-CD2	7.34	1.79	1.51
1	A	1317	MET	CG-SD	7.34	2.00	1.81
2	B	1219	ASP	CA-CB	7.34	1.70	1.53
1	A	1349	TYR	CB-CG	-7.34	1.40	1.51
2	B	340	ALA	C-O	-7.34	1.09	1.23
4	E	23	VAL	C-O	7.34	1.37	1.23
1	A	409	SER	CA-CB	7.34	1.64	1.52
2	B	255	GLN	N-CA	-7.34	1.31	1.46
1	A	1232	ASN	CG-OD1	7.34	1.40	1.24
3	C	32	SER	CA-CB	-7.34	1.42	1.52
5	F	110	ASP	CB-CG	7.34	1.67	1.51
9	K	41	THR	C-O	-7.34	1.09	1.23
1	A	430	TRP	CD2-CE3	-7.33	1.29	1.40
1	A	1353	TYR	CB-CG	-7.33	1.40	1.51
2	B	46	GLN	CG-CD	-7.33	1.34	1.51
1	A	859	SER	CA-CB	-7.33	1.42	1.52
2	B	1223	ASP	N-CA	7.33	1.61	1.46
4	E	18	THR	CB-OG1	7.33	1.57	1.43
3	C	177	GLU	C-O	-7.33	1.09	1.23
1	A	1323	ASP	CG-OD2	-7.33	1.08	1.25
2	B	935	ARG	NE-CZ	7.33	1.42	1.33
1	A	757	ASN	CA-CB	-7.33	1.34	1.53
6	H	19	ARG	CD-NE	7.33	1.58	1.46
4	E	90	VAL	CB-CG1	7.32	1.68	1.52
1	A	1297	GLU	CB-CG	7.32	1.66	1.52
2	B	280	ILE	CB-CG2	-7.32	1.30	1.52
2	B	352	ALA	C-O	7.32	1.37	1.23
1	A	76	GLU	CG-CD	7.32	1.62	1.51
1	A	1044	TRP	CB-CG	-7.32	1.37	1.50
1	A	1062	GLU	CG-CD	-7.32	1.41	1.51
1	A	1320	PRO	CA-C	-7.32	1.38	1.52
2	B	787	VAL	CA-C	-7.32	1.33	1.52
2	B	854	LEU	N-CA	-7.32	1.31	1.46
1	A	264	PHE	CG-CD1	7.31	1.49	1.38
1	A	1359	ASP	CG-OD1	7.31	1.42	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	209	GLU	CG-CD	7.31	1.62	1.51
2	B	595	ARG	CB-CG	7.31	1.72	1.52
2	B	1170	THR	C-O	7.31	1.37	1.23
3	C	166	GLU	CD-OE1	7.31	1.33	1.25
1	A	57	ARG	C-O	-7.31	1.09	1.23
2	B	312	GLU	CA-C	7.31	1.72	1.52
4	E	163	GLU	CD-OE1	7.31	1.33	1.25
1	A	277	GLU	CD-OE1	7.30	1.33	1.25
1	A	934	LYS	CG-CD	7.30	1.77	1.52
1	A	1096	SER	C-O	7.30	1.37	1.23
7	I	72	ASP	CG-OD1	7.30	1.42	1.25
1	A	865	GLN	CG-CD	7.30	1.67	1.51
4	E	172	GLU	CB-CG	7.30	1.66	1.52
1	A	948	VAL	CB-CG1	-7.30	1.37	1.52
2	B	958	GLN	CG-CD	7.30	1.67	1.51
1	A	87	ALA	N-CA	-7.29	1.31	1.46
3	C	141	GLY	N-CA	7.29	1.56	1.46
1	A	225	ASN	C-O	7.29	1.37	1.23
1	A	1206	ASP	C-O	7.29	1.37	1.23
2	B	376	PHE	C-O	-7.29	1.09	1.23
2	B	769	TYR	CB-CG	7.29	1.62	1.51
2	B	883	LEU	CG-CD1	7.29	1.78	1.51
6	H	146	ARG	CZ-NH2	7.29	1.42	1.33
1	A	229	SER	CB-OG	7.29	1.51	1.42
1	A	1256	GLU	CA-C	7.29	1.72	1.52
1	A	827	THR	C-O	-7.29	1.09	1.23
2	B	728	ARG	CB-CG	-7.29	1.32	1.52
2	B	899	ILE	CA-CB	-7.29	1.38	1.54
1	A	247	ARG	CA-C	7.29	1.71	1.52
1	A	782	ARG	CB-CG	-7.29	1.32	1.52
7	I	86	PHE	CA-CB	-7.29	1.38	1.53
1	A	1029	ARG	C-O	-7.29	1.09	1.23
1	A	360	GLU	CD-OE2	7.28	1.33	1.25
4	E	187	TYR	CD2-CE2	-7.28	1.28	1.39
2	B	1220	ARG	N-CA	7.28	1.60	1.46
3	C	47	ASP	C-O	-7.28	1.09	1.23
2	B	113	TYR	CE1-CZ	7.28	1.48	1.38
3	C	87	PHE	CD1-CE1	7.28	1.53	1.39
4	E	31	THR	CB-CG2	7.28	1.76	1.52
4	E	35	VAL	CB-CG2	-7.28	1.37	1.52
1	A	750	GLY	C-O	-7.28	1.12	1.23
1	A	821	ARG	N-CA	-7.28	1.31	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1153	TYR	CZ-OH	7.28	1.50	1.37
7	I	47	GLU	CG-CD	7.28	1.62	1.51
2	B	203	PHE	CD2-CE2	-7.27	1.24	1.39
2	B	870	ILE	CB-CG1	7.27	1.74	1.54
2	B	1047	PHE	C-O	-7.27	1.09	1.23
2	B	571	PRO	C-O	-7.27	1.08	1.23
2	B	1019	SER	C-N	-7.27	1.17	1.34
1	A	1339	LEU	N-CA	-7.27	1.31	1.46
2	B	52	ASN	N-CA	-7.27	1.31	1.46
2	B	665	GLU	CA-C	-7.27	1.34	1.52
2	B	284	ILE	CA-CB	-7.27	1.38	1.54
2	B	876	LYS	CD-CE	7.27	1.69	1.51
7	I	44	TYR	N-CA	7.26	1.60	1.46
7	I	118	ARG	CZ-NH2	7.26	1.42	1.33
1	A	404	TYR	CG-CD2	-7.26	1.29	1.39
1	A	583	PRO	N-CD	-7.26	1.37	1.47
2	B	682	SER	CB-OG	7.26	1.51	1.42
1	A	792	TYR	C-O	-7.26	1.09	1.23
1	A	900	ASP	N-CA	7.26	1.60	1.46
1	A	632	VAL	CB-CG1	-7.26	1.37	1.52
1	A	998	LEU	C-O	-7.26	1.09	1.23
2	B	751	VAL	CA-CB	-7.26	1.39	1.54
3	C	221	TYR	CD1-CE1	7.26	1.50	1.39
9	K	77	THR	C-O	7.26	1.37	1.23
1	A	205	GLU	N-CA	-7.25	1.31	1.46
2	B	366	GLN	CB-CG	-7.25	1.32	1.52
3	C	220	ASP	CA-CB	7.25	1.70	1.53
2	B	660	LYS	N-CA	-7.25	1.31	1.46
2	B	888	GLY	N-CA	7.25	1.56	1.46
1	A	383	TYR	CB-CG	7.25	1.62	1.51
2	B	1224	PHE	CD2-CE2	7.25	1.53	1.39
1	A	419	LYS	CE-NZ	-7.24	1.30	1.49
1	A	447	GLN	CD-OE1	7.24	1.39	1.24
2	B	337	ARG	C-O	7.24	1.37	1.23
4	E	3	GLN	CB-CG	7.24	1.72	1.52
1	A	1042	PHE	CB-CG	-7.24	1.39	1.51
6	H	27	GLU	CG-CD	7.24	1.62	1.51
1	A	1305	VAL	CB-CG1	-7.24	1.37	1.52
1	A	583	PRO	CA-C	7.24	1.67	1.52
4	E	4	GLU	CG-CD	7.24	1.62	1.51
4	E	16	PHE	CD2-CE2	7.24	1.53	1.39
1	A	191	THR	N-CA	7.24	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1209	MET	CA-C	-7.24	1.34	1.52
2	B	1159	ARG	CG-CD	7.24	1.70	1.51
1	A	98	LYS	CD-CE	7.24	1.69	1.51
1	A	219	PHE	CE1-CZ	-7.24	1.23	1.37
2	B	138	GLU	CA-CB	7.24	1.69	1.53
1	A	247	ARG	C-N	7.23	1.48	1.34
1	A	655	PHE	CA-C	-7.23	1.34	1.52
1	A	1259	MET	SD-CE	7.23	2.18	1.77
4	E	162	ARG	CD-NE	7.23	1.58	1.46
8	J	2	ILE	C-O	-7.23	1.09	1.23
1	A	65	LEU	C-O	7.23	1.37	1.23
1	A	218	ASP	CG-OD1	7.23	1.42	1.25
2	B	264	SER	CB-OG	7.23	1.51	1.42
2	B	755	ILE	C-O	7.23	1.37	1.23
1	A	139	TRP	CZ3-CH2	-7.22	1.28	1.40
1	A	513	SER	C-O	-7.22	1.09	1.23
1	A	993	LEU	C-O	-7.22	1.09	1.23
1	A	1170	ILE	CA-CB	7.22	1.71	1.54
2	B	797	TYR	CG-CD2	-7.22	1.29	1.39
1	A	1350	LYS	CB-CG	-7.21	1.33	1.52
7	I	14	LEU	CG-CD1	-7.21	1.25	1.51
2	B	629	ASP	C-O	-7.21	1.09	1.23
1	A	532	ARG	C-O	-7.21	1.09	1.23
2	B	191	LYS	CE-NZ	7.21	1.67	1.49
7	I	85	PHE	CG-CD2	-7.21	1.27	1.38
1	A	1158	PRO	CA-CB	7.21	1.68	1.53
1	A	1309	ASP	CA-C	-7.20	1.34	1.52
2	B	167	ILE	CB-CG2	7.20	1.75	1.52
6	H	131	ASN	CA-C	7.20	1.71	1.52
2	B	292	ILE	CB-CG1	-7.20	1.33	1.54
1	A	738	LYS	CE-NZ	7.20	1.67	1.49
4	E	63	ASN	CG-OD1	7.20	1.39	1.24
1	A	461	LYS	CE-NZ	7.20	1.67	1.49
1	A	825	ILE	C-O	-7.20	1.09	1.23
2	B	1224	PHE	CB-CG	7.19	1.63	1.51
5	F	142	SER	CA-CB	7.19	1.63	1.52
1	A	880	LYS	CE-NZ	7.19	1.67	1.49
5	F	95	GLY	CA-C	7.19	1.63	1.51
1	A	730	GLY	C-O	-7.19	1.12	1.23
2	B	274	PRO	CA-CB	7.19	1.68	1.53
2	B	454	THR	N-CA	7.19	1.60	1.46
6	H	62	SER	C-O	-7.19	1.09	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	63	TYR	C-O	-7.19	1.09	1.23
1	A	488	ASN	C-O	-7.19	1.09	1.23
1	A	899	VAL	CB-CG2	-7.19	1.37	1.52
2	B	1073	TYR	CD2-CE2	-7.19	1.28	1.39
2	B	69	LEU	CA-C	7.18	1.71	1.52
2	B	605	ARG	CG-CD	7.18	1.70	1.51
2	B	983	ARG	CG-CD	7.18	1.70	1.51
2	B	1097	HIS	CA-C	7.18	1.71	1.52
1	A	1228	TRP	CB-CG	7.18	1.63	1.50
4	E	96	PHE	CA-C	7.18	1.71	1.52
7	I	115	LYS	CD-CE	7.18	1.69	1.51
2	B	138	GLU	CB-CG	7.18	1.65	1.52
2	B	781	PHE	CB-CG	-7.18	1.39	1.51
7	I	92	ARG	CA-CB	7.18	1.69	1.53
1	A	415	LEU	CG-CD1	7.17	1.78	1.51
1	A	1171	GLN	CG-CD	7.17	1.67	1.51
2	B	249	ARG	CD-NE	7.17	1.58	1.46
1	A	969	GLN	CA-CB	7.17	1.69	1.53
2	B	232	SER	C-O	-7.17	1.09	1.23
2	B	1067	ARG	C-O	7.17	1.36	1.23
1	A	347	PHE	CD1-CE1	7.17	1.53	1.39
2	B	852	ARG	C-O	-7.17	1.09	1.23
7	I	109	ILE	CB-CG2	-7.17	1.30	1.52
1	A	1444	MET	N-CA	7.17	1.60	1.46
2	B	415	GLN	CD-OE1	7.17	1.39	1.24
1	A	1413	GLY	N-CA	-7.16	1.35	1.46
1	A	1237	ILE	CA-CB	-7.16	1.38	1.54
4	E	135	PHE	CG-CD2	-7.16	1.28	1.38
1	A	578	LEU	N-CA	7.16	1.60	1.46
1	A	394	ASN	CA-CB	-7.16	1.34	1.53
1	A	431	LYS	CG-CD	7.16	1.76	1.52
1	A	766	GLY	CA-C	-7.16	1.40	1.51
1	A	975	HIS	CB-CG	7.16	1.62	1.50
3	C	199	LYS	CG-CD	7.16	1.76	1.52
3	C	228	PHE	CE1-CZ	-7.16	1.23	1.37
9	K	81	TYR	CD1-CE1	-7.16	1.28	1.39
7	I	69	PRO	N-CA	-7.15	1.35	1.47
2	B	236	HIS	C-O	-7.15	1.09	1.23
3	C	99	LEU	N-CA	-7.15	1.32	1.46
9	K	107	THR	N-CA	7.15	1.60	1.46
1	A	781	ASP	CG-OD1	7.15	1.41	1.25
3	C	220	ASP	CB-CG	7.15	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	41	ASP	CG-OD1	7.15	1.41	1.25
6	H	96	VAL	N-CA	-7.15	1.32	1.46
7	I	41	PRO	C-N	-7.15	1.17	1.34
1	A	771	GLU	CG-CD	7.15	1.62	1.51
5	F	84	TYR	C-O	-7.15	1.09	1.23
1	A	1433	MET	N-CA	7.14	1.60	1.46
1	A	755	PHE	C-O	7.14	1.36	1.23
2	B	165	VAL	CB-CG1	7.14	1.67	1.52
2	B	611	PRO	CB-CG	-7.14	1.14	1.50
4	E	51	GLY	N-CA	7.14	1.56	1.46
1	A	1276	VAL	CA-C	-7.14	1.34	1.52
4	E	99	HIS	CA-CB	7.14	1.69	1.53
1	A	559	VAL	CB-CG1	7.14	1.67	1.52
1	A	966	ASN	N-CA	-7.14	1.32	1.46
1	A	799	PHE	CB-CG	7.14	1.63	1.51
2	B	286	PHE	CD2-CE2	-7.14	1.25	1.39
1	A	646	PHE	CE1-CZ	7.14	1.50	1.37
1	A	1231	ASP	C-O	7.14	1.36	1.23
2	B	286	PHE	C-O	-7.13	1.09	1.23
1	A	108	MET	SD-CE	-7.13	1.38	1.77
1	A	778	GLY	C-O	-7.13	1.12	1.23
8	J	21	TYR	CE1-CZ	-7.13	1.29	1.38
2	B	962	LYS	CE-NZ	7.13	1.66	1.49
7	I	95	THR	CB-CG2	-7.13	1.28	1.52
1	A	1411	GLU	CA-CB	7.13	1.69	1.53
2	B	56	ASP	CB-CG	-7.13	1.36	1.51
1	A	1176	LEU	CG-CD1	7.13	1.78	1.51
3	C	71	PRO	CB-CG	-7.13	1.14	1.50
6	H	138	GLU	CG-CD	7.13	1.62	1.51
1	A	1008	GLN	CD-OE1	7.12	1.39	1.24
4	E	79	TRP	CA-CB	7.12	1.69	1.53
4	E	154	ILE	CB-CG2	-7.12	1.30	1.52
5	F	145	ASP	C-O	7.12	1.36	1.23
9	K	21	ILE	CB-CG2	-7.12	1.30	1.52
2	B	804	GLY	N-CA	7.12	1.56	1.46
3	C	142	VAL	CA-CB	-7.12	1.39	1.54
1	A	191	THR	CA-CB	7.12	1.71	1.53
2	B	376	PHE	CE2-CZ	-7.12	1.23	1.37
10	L	33	GLU	CD-OE1	7.12	1.33	1.25
1	A	347	PHE	CE1-CZ	7.12	1.50	1.37
1	A	590	ARG	C-O	-7.12	1.09	1.23
1	A	1188	GLN	N-CA	7.12	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	987	VAL	CB-CG1	-7.11	1.38	1.52
3	C	183	TRP	CD2-CE2	7.11	1.49	1.41
1	A	924	LYS	CA-C	7.11	1.71	1.52
6	H	25	ARG	NE-CZ	-7.11	1.23	1.33
8	J	49	MET	CG-SD	7.11	1.99	1.81
2	B	203	PHE	CE2-CZ	-7.11	1.23	1.37
1	A	1294	PRO	CA-C	7.11	1.67	1.52
2	B	89	GLU	CD-OE2	7.11	1.33	1.25
2	B	183	GLU	CD-OE2	7.11	1.33	1.25
2	B	792	MET	CA-CB	-7.11	1.38	1.53
2	B	865	LYS	CA-CB	7.11	1.69	1.53
2	B	1097	HIS	CD2-NE2	7.11	1.56	1.42
2	B	1182	CYS	CA-CB	7.11	1.69	1.53
3	C	170	TRP	CE3-CZ3	-7.11	1.26	1.38
9	K	85	ASP	CB-CG	7.11	1.66	1.51
1	A	646	PHE	C-O	-7.10	1.09	1.23
8	J	31	ASP	C-O	7.10	1.36	1.23
1	A	1133	LEU	CG-CD2	7.10	1.78	1.51
1	A	177	ASP	CG-OD2	7.10	1.41	1.25
2	B	870	ILE	N-CA	7.10	1.60	1.46
1	A	1450	LEU	CA-C	7.09	1.71	1.52
2	B	175	ARG	NE-CZ	7.09	1.42	1.33
2	B	182	SER	N-CA	7.09	1.60	1.46
7	I	18	GLU	CA-C	7.09	1.71	1.52
1	A	1311	VAL	CB-CG2	-7.09	1.38	1.52
2	B	524	PRO	CA-C	-7.09	1.38	1.52
2	B	408	LEU	C-O	-7.09	1.09	1.23
1	A	543	LEU	CG-CD1	-7.09	1.25	1.51
1	A	1167	GLU	CA-CB	7.09	1.69	1.53
3	C	159	ALA	CA-CB	7.08	1.67	1.52
1	A	62	ASP	N-CA	7.08	1.60	1.46
1	A	136	ALA	CA-CB	7.08	1.67	1.52
1	A	655	PHE	CE1-CZ	-7.08	1.23	1.37
7	I	4	PHE	C-O	7.08	1.36	1.23
2	B	684	LEU	CG-CD1	-7.08	1.25	1.51
2	B	883	LEU	CG-CD2	7.08	1.78	1.51
2	B	916	THR	N-CA	7.08	1.60	1.46
2	B	1176	ASN	CB-CG	7.08	1.67	1.51
1	A	167	CYS	CB-SG	-7.08	1.70	1.82
8	J	27	GLU	CG-CD	7.08	1.62	1.51
1	A	186	LYS	CD-CE	7.07	1.69	1.51
1	A	1052	GLN	CA-CB	-7.07	1.38	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1157	ASP	CA-CB	7.07	1.69	1.53
1	A	962	ARG	C-N	-7.07	1.17	1.34
1	A	1092	LYS	CD-CE	7.07	1.69	1.51
2	B	963	PHE	C-O	7.07	1.36	1.23
3	C	155	LEU	C-O	7.07	1.36	1.23
5	F	108	PHE	CD2-CE2	7.07	1.53	1.39
1	A	758	ILE	CA-CB	-7.07	1.38	1.54
1	A	868	TYR	CG-CD2	7.07	1.48	1.39
2	B	109	THR	CA-CB	7.07	1.71	1.53
1	A	196	GLU	CB-CG	7.06	1.65	1.52
1	A	304	MET	CG-SD	7.06	1.99	1.81
2	B	638	PHE	CG-CD2	-7.06	1.28	1.38
2	B	1103	ILE	N-CA	7.06	1.60	1.46
2	B	323	VAL	CB-CG2	7.06	1.67	1.52
9	K	95	ILE	CB-CG2	7.06	1.74	1.52
2	B	1174	LYS	CA-C	7.06	1.71	1.52
2	B	579	ARG	CA-CB	-7.06	1.38	1.53
1	A	1194	ARG	CG-CD	-7.06	1.34	1.51
2	B	51	PHE	CD2-CE2	7.06	1.53	1.39
2	B	520	GLY	C-O	-7.05	1.12	1.23
2	B	279	ASP	CB-CG	7.05	1.66	1.51
1	A	951	GLU	CA-CB	-7.05	1.38	1.53
1	A	979	SER	CA-CB	7.05	1.63	1.52
8	J	10	CYS	C-O	-7.05	1.09	1.23
2	B	1201	LYS	CD-CE	7.05	1.68	1.51
7	I	88	SER	C-O	-7.05	1.09	1.23
1	A	1381	LEU	C-N	-7.05	1.17	1.34
2	B	1146	PHE	CD2-CE2	-7.05	1.25	1.39
9	K	84	LYS	CD-CE	7.04	1.68	1.51
1	A	979	SER	CB-OG	7.04	1.51	1.42
1	A	1356	ILE	CB-CG2	-7.04	1.31	1.52
1	A	302	THR	CB-CG2	7.04	1.75	1.52
1	A	1344	GLY	CA-C	-7.04	1.40	1.51
2	B	1204	PHE	CG-CD1	-7.04	1.28	1.38
8	J	5	VAL	CA-CB	7.04	1.69	1.54
10	L	46	VAL	C-O	-7.04	1.09	1.23
1	A	1309	ASP	CG-OD1	7.04	1.41	1.25
2	B	694	ASP	CB-CG	7.04	1.66	1.51
2	B	776	GLN	CA-CB	-7.04	1.38	1.53
1	A	553	VAL	C-O	-7.04	1.09	1.23
1	A	818	MET	CG-SD	7.04	1.99	1.81
1	A	1433	MET	CA-C	-7.04	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	606	LEU	C-O	-7.04	1.09	1.23
2	B	723	VAL	N-CA	7.04	1.60	1.46
1	A	1116	LEU	N-CA	-7.03	1.32	1.46
2	B	284	ILE	N-CA	-7.03	1.32	1.46
3	C	219	PHE	CG-CD2	-7.03	1.28	1.38
7	I	24	ARG	CZ-NH2	-7.03	1.24	1.33
4	E	96	PHE	C-O	7.03	1.36	1.23
4	E	102	GLU	CD-OE2	7.03	1.33	1.25
1	A	594	GLY	N-CA	7.03	1.56	1.46
2	B	942	ARG	CZ-NH2	7.03	1.42	1.33
4	E	174	GLN	CD-OE1	7.03	1.39	1.24
6	H	21	ASN	C-O	-7.03	1.09	1.23
8	J	14	VAL	CA-C	7.03	1.71	1.52
8	J	22	LEU	N-CA	-7.03	1.32	1.46
9	K	105	PHE	CA-CB	7.03	1.69	1.53
2	B	680	THR	C-O	7.03	1.36	1.23
2	B	1074	ASN	C-N	-7.02	1.20	1.33
5	F	149	GLU	CG-CD	7.02	1.62	1.51
1	A	269	ILE	CA-CB	-7.02	1.38	1.54
2	B	965	LYS	CE-NZ	7.02	1.66	1.49
1	A	376	TYR	CD1-CE1	-7.02	1.28	1.39
1	A	1331	SER	CB-OG	7.02	1.51	1.42
1	A	1335	ILE	CB-CG2	-7.02	1.31	1.52
1	A	231	PRO	N-CD	-7.01	1.38	1.47
1	A	1063	MET	C-O	-7.01	1.10	1.23
6	H	138	GLU	C-O	-7.01	1.10	1.23
1	A	1332	PHE	CB-CG	-7.01	1.39	1.51
3	C	218	PRO	CG-CD	7.01	1.73	1.50
1	A	213	HIS	C-O	7.01	1.36	1.23
1	A	1428	VAL	CA-CB	-7.01	1.40	1.54
10	L	70	ARG	CA-CB	-7.00	1.38	1.53
2	B	770	GLN	CG-CD	-7.00	1.34	1.51
1	A	503	GLN	CB-CG	7.00	1.71	1.52
2	B	366	GLN	CA-C	7.00	1.71	1.52
1	A	566	ILE	CA-CB	7.00	1.71	1.54
1	A	647	GLY	N-CA	-7.00	1.35	1.46
2	B	1021	MET	C-O	7.00	1.36	1.23
8	J	44	TYR	CD1-CE1	-7.00	1.28	1.39
1	A	555	ASP	N-CA	-7.00	1.32	1.46
1	A	587	HIS	C-O	7.00	1.36	1.23
1	A	1239	ARG	NE-CZ	-7.00	1.24	1.33
6	H	80	ARG	CD-NE	7.00	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	18	VAL	CA-C	-7.00	1.34	1.52
1	A	521	MET	CG-SD	-6.99	1.62	1.81
1	A	1362	TYR	C-O	-6.99	1.10	1.23
6	H	88	SER	CA-CB	6.99	1.63	1.52
1	A	1438	THR	N-CA	-6.99	1.32	1.46
2	B	278	GLN	CB-CG	-6.99	1.33	1.52
4	E	27	GLY	CA-C	6.99	1.63	1.51
1	A	183	GLY	C-O	-6.99	1.12	1.23
1	A	792	TYR	CA-CB	-6.99	1.38	1.53
1	A	1287	TYR	CA-CB	6.99	1.69	1.53
2	B	518	HIS	CA-CB	-6.99	1.38	1.53
2	B	1008	PRO	CA-C	-6.99	1.38	1.52
9	K	38	GLU	CA-CB	-6.99	1.38	1.53
9	K	95	ILE	C-O	6.99	1.36	1.23
2	B	191	LYS	CA-C	-6.99	1.34	1.52
1	A	495	GLU	CD-OE2	-6.98	1.18	1.25
2	B	601	ARG	CZ-NH1	6.98	1.42	1.33
2	B	667	GLN	CD-NE2	6.98	1.50	1.32
3	C	232	VAL	C-O	6.98	1.36	1.23
6	H	109	LYS	CA-CB	6.98	1.69	1.53
1	A	934	LYS	CA-CB	6.98	1.69	1.53
1	A	954	TRP	CE2-CZ2	-6.98	1.27	1.39
3	C	43	THR	CB-OG1	-6.98	1.29	1.43
1	A	261	ASP	CA-C	6.98	1.71	1.52
1	A	979	SER	C-O	-6.98	1.10	1.23
1	A	130	ASP	CB-CG	6.98	1.66	1.51
1	A	1211	GLN	CA-C	-6.98	1.34	1.52
6	H	96	VAL	CA-CB	-6.98	1.40	1.54
3	C	208	GLU	CA-C	6.98	1.71	1.52
2	B	203	PHE	CG-CD1	-6.97	1.28	1.38
2	B	560	GLU	CG-CD	6.97	1.62	1.51
2	B	1154	ALA	N-CA	6.97	1.60	1.46
1	A	203	SER	CB-OG	6.97	1.51	1.42
7	I	117	LYS	CD-CE	6.97	1.68	1.51
1	A	170	THR	CA-CB	6.97	1.71	1.53
2	B	1166	CYS	CA-CB	6.97	1.69	1.53
1	A	221	SER	CB-OG	-6.97	1.33	1.42
2	B	309	GLN	CA-C	6.97	1.71	1.52
6	H	120	GLY	CA-C	6.97	1.62	1.51
1	A	839	ARG	CG-CD	6.97	1.69	1.51
1	A	1304	TRP	CG-CD1	6.97	1.46	1.36
2	B	817	LEU	CG-CD2	-6.97	1.26	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	28	GLU	CD-OE2	6.96	1.33	1.25
4	E	40	GLU	CA-CB	6.96	1.69	1.53
1	A	1331	SER	CA-CB	-6.96	1.42	1.52
2	B	58	THR	CA-CB	-6.96	1.35	1.53
1	A	846	GLU	CD-OE2	6.96	1.33	1.25
2	B	398	ARG	C-O	-6.96	1.10	1.23
2	B	810	GLU	N-CA	-6.96	1.32	1.46
7	I	4	PHE	CB-CG	-6.96	1.39	1.51
5	F	124	GLU	CD-OE1	-6.95	1.18	1.25
1	A	1068	ALA	CA-CB	-6.95	1.37	1.52
1	A	1051	ALA	CA-CB	6.95	1.67	1.52
1	A	97	ALA	CA-C	-6.95	1.34	1.52
2	B	180	TYR	CE1-CZ	-6.95	1.29	1.38
4	E	129	PRO	CA-CB	6.95	1.67	1.53
7	I	15	TYR	CG-CD1	-6.95	1.30	1.39
2	B	1160	VAL	CB-CG1	-6.95	1.38	1.52
3	C	230	MET	CB-CG	6.95	1.73	1.51
1	A	528	LEU	C-O	-6.95	1.10	1.23
1	A	712	GLU	CG-CD	6.95	1.62	1.51
1	A	659	HIS	C-O	-6.94	1.10	1.23
1	A	696	GLU	CB-CG	6.94	1.65	1.52
1	A	810	PRO	N-CA	-6.94	1.35	1.47
1	A	288	ALA	CA-CB	6.94	1.67	1.52
1	A	655	PHE	N-CA	6.94	1.60	1.46
3	C	87	PHE	CG-CD2	-6.94	1.28	1.38
8	J	54	VAL	N-CA	-6.94	1.32	1.46
1	A	518	LYS	CB-CG	-6.94	1.33	1.52
2	B	660	LYS	CG-CD	6.94	1.76	1.52
9	K	102	LYS	CE-NZ	6.94	1.66	1.49
1	A	909	ASP	CB-CG	-6.93	1.37	1.51
9	K	78	THR	C-O	6.93	1.36	1.23
1	A	1040	GLN	CD-OE1	6.93	1.39	1.24
1	A	1264	GLU	CG-CD	-6.93	1.41	1.51
1	A	1298	TYR	CA-CB	-6.93	1.38	1.53
5	F	90	ARG	NE-CZ	-6.93	1.24	1.33
1	A	579	SER	C-O	6.93	1.36	1.23
2	B	769	TYR	CD2-CE2	-6.93	1.28	1.39
1	A	6	TYR	CE1-CZ	6.93	1.47	1.38
7	I	100	PHE	CD2-CE2	6.93	1.53	1.39
1	A	248	PRO	CA-C	6.93	1.66	1.52
1	A	892	ALA	CA-CB	-6.93	1.38	1.52
1	A	90	VAL	CA-CB	-6.92	1.40	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	350	GLN	CA-CB	-6.92	1.38	1.53
2	B	397	ASP	C-O	6.92	1.36	1.23
2	B	753	ALA	CA-CB	-6.92	1.38	1.52
2	B	815	ARG	NE-CZ	-6.92	1.24	1.33
7	I	29	CYS	C-O	6.92	1.36	1.23
1	A	728	LYS	C-O	6.92	1.36	1.23
1	A	882	SER	CA-CB	6.92	1.63	1.52
2	B	1069	PHE	CG-CD2	-6.92	1.28	1.38
2	B	1133	MET	CG-SD	6.92	1.99	1.81
1	A	1031	VAL	C-O	6.92	1.36	1.23
4	E	32	GLN	CG-CD	6.92	1.67	1.51
1	A	1363	VAL	CA-CB	-6.92	1.40	1.54
10	L	50	ASP	C-O	6.92	1.36	1.23
1	A	180	LYS	CE-NZ	-6.92	1.31	1.49
2	B	238	ALA	C-O	-6.92	1.10	1.23
2	B	635	ARG	CZ-NH1	-6.92	1.24	1.33
2	B	1183	LYS	CD-CE	6.92	1.68	1.51
2	B	1188	LYS	CG-CD	6.92	1.75	1.52
1	A	613	ILE	CA-C	-6.92	1.34	1.52
1	A	419	LYS	CD-CE	6.91	1.68	1.51
2	B	746	SER	N-CA	-6.91	1.32	1.46
7	I	73	ARG	CZ-NH1	6.91	1.42	1.33
7	I	95	THR	N-CA	6.91	1.60	1.46
9	K	69	ALA	N-CA	6.91	1.60	1.46
2	B	695	ALA	N-CA	-6.91	1.32	1.46
2	B	966	VAL	CB-CG2	-6.91	1.38	1.52
5	F	94	LEU	C-N	-6.91	1.20	1.33
1	A	159	THR	CA-CB	6.91	1.71	1.53
1	A	1339	LEU	CA-CB	-6.91	1.37	1.53
2	B	762	ASN	C-O	-6.91	1.10	1.23
1	A	95	PHE	CE2-CZ	6.90	1.50	1.37
1	A	809	THR	C-O	-6.90	1.10	1.23
2	B	624	LEU	CA-CB	-6.90	1.37	1.53
1	A	608	ILE	CB-CG1	6.90	1.73	1.54
2	B	590	HIS	N-CA	-6.90	1.32	1.46
2	B	1028	GLU	CD-OE2	-6.90	1.18	1.25
9	K	91	CYS	CB-SG	-6.90	1.70	1.82
1	A	159	THR	C-O	-6.90	1.10	1.23
1	A	1223	ASP	CG-OD1	6.90	1.41	1.25
2	B	707	PRO	CA-C	6.90	1.66	1.52
3	C	15	LYS	CA-CB	6.90	1.69	1.53
1	A	940	ARG	CZ-NH2	-6.90	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	997	GLU	CB-CG	6.90	1.65	1.52
2	B	96	TYR	N-CA	6.90	1.60	1.46
4	E	134	THR	CB-CG2	-6.90	1.29	1.52
2	B	649	LYS	CB-CG	-6.89	1.33	1.52
4	E	52	ARG	CA-C	6.89	1.70	1.52
7	I	40	SER	CB-OG	6.89	1.51	1.42
2	B	403	LYS	CB-CG	6.89	1.71	1.52
2	B	569	TYR	CE1-CZ	6.89	1.47	1.38
1	A	652	VAL	CB-CG1	-6.89	1.38	1.52
2	B	833	TYR	CG-CD2	-6.89	1.30	1.39
2	B	380	TYR	CZ-OH	6.89	1.49	1.37
1	A	6	TYR	C-O	6.88	1.36	1.23
1	A	636	GLU	CG-CD	6.88	1.62	1.51
4	E	95	THR	CB-CG2	6.88	1.75	1.52
1	A	229	SER	CA-CB	-6.88	1.42	1.52
3	C	34	ARG	CD-NE	-6.88	1.34	1.46
5	F	93	ILE	C-O	-6.88	1.10	1.23
4	E	54	GLN	CG-CD	6.88	1.66	1.51
1	A	426	LEU	CA-C	-6.88	1.35	1.52
1	A	1234	GLU	CB-CG	6.88	1.65	1.52
2	B	626	ILE	CB-CG1	-6.88	1.34	1.54
2	B	963	PHE	CD2-CE2	6.88	1.53	1.39
6	H	117	SER	CB-OG	6.88	1.51	1.42
1	A	656	TRP	C-O	6.87	1.36	1.23
1	A	742	ASN	CB-CG	-6.87	1.35	1.51
1	A	1262	LYS	CD-CE	6.87	1.68	1.51
3	C	117	ASP	CA-C	6.87	1.70	1.52
3	C	222	LYS	C-O	6.87	1.36	1.23
9	K	49	GLU	CG-CD	-6.87	1.41	1.51
2	B	1101	ASP	CA-C	6.87	1.70	1.52
5	F	146	TRP	CA-C	6.87	1.70	1.52
1	A	1053	PHE	CD1-CE1	6.87	1.52	1.39
1	A	1257	ASP	CB-CG	-6.87	1.37	1.51
1	A	1446	ASP	CG-OD2	6.87	1.41	1.25
1	A	1448	GLU	CA-C	6.87	1.70	1.52
1	A	99	ILE	CA-CB	-6.86	1.39	1.54
1	A	466	SER	CA-CB	-6.86	1.42	1.52
2	B	312	GLU	C-O	-6.86	1.10	1.23
1	A	444	PHE	CD1-CE1	-6.86	1.25	1.39
2	B	235	SER	N-CA	-6.86	1.32	1.46
2	B	1135	ARG	CZ-NH2	6.86	1.42	1.33
1	A	1129	GLU	CD-OE1	6.86	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	512	ARG	CA-C	6.86	1.70	1.52
5	F	108	PHE	CD1-CE1	6.86	1.52	1.39
2	B	1137	CYS	CA-CB	-6.85	1.38	1.53
1	A	105	CYS	CB-SG	-6.85	1.70	1.82
1	A	238	CYS	CA-C	-6.85	1.35	1.52
1	A	1277	GLU	CA-C	-6.85	1.35	1.52
1	A	5	GLN	C-O	-6.84	1.10	1.23
4	E	191	LYS	C-O	-6.84	1.10	1.23
1	A	380	VAL	CB-CG2	-6.84	1.38	1.52
1	A	805	LEU	CA-C	-6.84	1.35	1.52
4	E	115	ASN	CB-CG	6.84	1.66	1.51
8	J	6	ARG	C-O	6.84	1.36	1.23
1	A	919	ILE	C-O	-6.84	1.10	1.23
1	A	1143	LEU	N-CA	6.84	1.60	1.46
2	B	644	GLU	CA-C	6.84	1.70	1.52
1	A	1243	VAL	CA-CB	6.83	1.69	1.54
1	A	57	ARG	NE-CZ	6.83	1.42	1.33
3	C	124	LEU	CG-CD2	6.83	1.77	1.51
2	B	617	ARG	NE-CZ	-6.83	1.24	1.33
4	E	180	ARG	C-O	6.83	1.36	1.23
1	A	611	GLN	CB-CG	6.83	1.71	1.52
2	B	135	ARG	CG-CD	6.83	1.69	1.51
1	A	1188	GLN	CD-OE1	6.83	1.39	1.24
2	B	1057	LYS	CE-NZ	6.83	1.66	1.49
5	F	135	ARG	N-CA	-6.83	1.32	1.46
1	A	1384	VAL	CB-CG2	6.82	1.67	1.52
2	B	874	PHE	CE1-CZ	-6.82	1.24	1.37
10	L	28	LYS	CE-NZ	6.82	1.66	1.49
2	B	661	LEU	C-O	-6.82	1.10	1.23
6	H	46	LEU	C-O	6.82	1.36	1.23
1	A	423	ASP	CG-OD2	6.82	1.41	1.25
2	B	315	LYS	CA-CB	-6.82	1.39	1.53
2	B	840	ILE	CA-CB	-6.82	1.39	1.54
2	B	381	MET	CA-CB	-6.82	1.39	1.53
1	A	711	ARG	C-O	-6.81	1.10	1.23
2	B	1212	ILE	CA-CB	-6.81	1.39	1.54
2	B	118	ARG	NE-CZ	6.81	1.42	1.33
4	E	197	LYS	CG-CD	6.81	1.75	1.52
6	H	132	LEU	CA-C	6.81	1.70	1.52
1	A	974	ASP	CA-C	-6.81	1.35	1.52
1	A	437	MET	SD-CE	6.80	2.15	1.77
1	A	852	TYR	CG-CD2	-6.80	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	173	SER	CA-CB	-6.80	1.42	1.52
5	F	137	TYR	CE1-CZ	-6.80	1.29	1.38
1	A	478	TYR	CG-CD1	-6.80	1.30	1.39
1	A	716	ASP	CG-OD2	6.80	1.41	1.25
3	C	196	ASP	CB-CG	6.80	1.66	1.51
2	B	548	GLY	N-CA	6.80	1.56	1.46
3	C	228	PHE	CG-CD2	-6.80	1.28	1.38
5	F	116	ASP	C-O	-6.80	1.10	1.23
6	H	35	GLN	CG-CD	6.80	1.66	1.51
1	A	777	PHE	C-O	6.80	1.36	1.23
2	B	323	VAL	CB-CG1	6.80	1.67	1.52
1	A	1069	ALA	C-O	6.80	1.36	1.23
8	J	31	ASP	CG-OD1	6.79	1.41	1.25
1	A	96	ILE	CB-CG2	-6.79	1.31	1.52
1	A	198	GLU	CB-CG	6.79	1.65	1.52
2	B	859	TYR	CD1-CE1	6.79	1.49	1.39
1	A	981	LEU	C-N	-6.79	1.18	1.34
5	F	124	GLU	CD-OE2	-6.79	1.18	1.25
6	H	129	TYR	CD1-CE1	6.79	1.49	1.39
2	B	522	VAL	CB-CG2	-6.79	1.38	1.52
1	A	862	ASN	CA-C	6.79	1.70	1.52
1	A	905	ASP	CB-CG	-6.79	1.37	1.51
2	B	1155	SER	N-CA	6.78	1.59	1.46
1	A	922	ASP	CB-CG	6.78	1.66	1.51
7	I	37	GLU	C-O	-6.78	1.10	1.23
8	J	30	LEU	CG-CD2	6.78	1.76	1.51
1	A	175	ARG	CD-NE	6.78	1.57	1.46
2	B	177	LYS	C-O	6.78	1.36	1.23
2	B	589	VAL	C-O	-6.78	1.10	1.23
2	B	646	LEU	CB-CG	6.78	1.72	1.52
1	A	1444	MET	CG-SD	-6.78	1.63	1.81
2	B	958	GLN	CD-NE2	6.78	1.49	1.32
1	A	1172	LEU	C-O	-6.78	1.10	1.23
8	J	26	GLN	CD-OE1	6.78	1.38	1.24
1	A	65	LEU	CA-CB	6.78	1.69	1.53
1	A	1443	VAL	CB-CG2	6.78	1.67	1.52
2	B	291	ILE	CB-CG2	-6.78	1.31	1.52
6	H	21	ASN	CG-OD1	6.78	1.38	1.24
6	H	56	THR	N-CA	-6.78	1.32	1.46
2	B	202	TYR	CD1-CE1	-6.77	1.29	1.39
9	K	102	LYS	CB-CG	6.77	1.70	1.52
1	A	919	ILE	N-CA	6.77	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	PHE	CG-CD2	-6.77	1.28	1.38
2	B	981	ALA	CA-CB	-6.77	1.38	1.52
9	K	105	PHE	CG-CD2	6.77	1.49	1.38
1	A	1297	GLU	CA-CB	-6.77	1.39	1.53
9	K	23	PRO	C-O	6.77	1.36	1.23
8	J	14	VAL	CB-CG1	-6.77	1.38	1.52
1	A	403	LYS	CE-NZ	6.76	1.66	1.49
1	A	905	ASP	CA-CB	-6.76	1.39	1.53
2	B	751	VAL	CB-CG1	-6.76	1.38	1.52
2	B	784	ASN	N-CA	-6.76	1.32	1.46
3	C	238	ILE	CB-CG1	-6.76	1.35	1.54
6	H	22	LYS	CG-CD	6.76	1.75	1.52
2	B	1073	TYR	CA-C	-6.76	1.35	1.52
4	E	49	SER	N-CA	6.76	1.59	1.46
3	C	234	SER	CB-OG	6.76	1.51	1.42
1	A	1292	PRO	N-CA	-6.76	1.35	1.47
2	B	242	SER	CA-CB	6.76	1.63	1.52
2	B	370	PHE	CG-CD1	6.76	1.48	1.38
4	E	92	THR	N-CA	6.75	1.59	1.46
3	C	82	TYR	CE1-CZ	6.75	1.47	1.38
2	B	94	LYS	CD-CE	6.75	1.68	1.51
1	A	451	HIS	CA-CB	-6.75	1.39	1.53
7	I	78	CYS	CA-CB	6.75	1.68	1.53
1	A	1226	VAL	CB-CG1	-6.74	1.38	1.52
1	A	1229	SER	CB-OG	-6.74	1.33	1.42
10	L	29	TYR	CD1-CE1	-6.74	1.29	1.39
1	A	769	SER	CB-OG	6.74	1.51	1.42
1	A	1223	ASP	CB-CG	6.74	1.65	1.51
7	I	88	SER	N-CA	-6.73	1.32	1.46
1	A	673	GLY	CA-C	-6.73	1.41	1.51
3	C	219	PHE	CD2-CE2	6.73	1.52	1.39
1	A	1273	LEU	C-O	6.73	1.36	1.23
2	B	630	ALA	CA-CB	6.73	1.66	1.52
1	A	165	GLY	N-CA	6.73	1.56	1.46
1	A	892	ALA	C-O	-6.73	1.10	1.23
2	B	19	GLU	N-CA	6.73	1.59	1.46
1	A	461	LYS	CB-CG	-6.72	1.34	1.52
1	A	1114	PRO	N-CA	-6.72	1.35	1.47
4	E	182	ASP	CB-CG	6.72	1.65	1.51
2	B	134	LYS	CB-CG	6.72	1.70	1.52
7	I	1	MET	SD-CE	6.72	2.15	1.77
7	I	99	LEU	C-O	-6.72	1.10	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	51	ASN	CB-CG	6.72	1.66	1.51
2	B	1008	PRO	N-CD	-6.72	1.38	1.47
1	A	248	PRO	CB-CG	6.71	1.83	1.50
2	B	193	LYS	CE-NZ	-6.71	1.32	1.49
1	A	443	LEU	CA-C	-6.71	1.35	1.52
2	B	421	PHE	CD1-CE1	-6.71	1.25	1.39
1	A	214	ILE	C-N	6.71	1.49	1.34
1	A	831	THR	N-CA	-6.71	1.32	1.46
2	B	223	VAL	C-O	-6.71	1.10	1.23
2	B	579	ARG	CZ-NH2	-6.71	1.24	1.33
2	B	857	ARG	CA-CB	-6.71	1.39	1.53
4	E	33	GLU	CG-CD	6.71	1.62	1.51
1	A	72	GLU	N-CA	6.71	1.59	1.46
2	B	360	PHE	CE1-CZ	-6.71	1.24	1.37
6	H	63	LEU	CG-CD2	6.71	1.76	1.51
1	A	69	THR	N-CA	6.71	1.59	1.46
1	A	895	LYS	CE-NZ	6.71	1.65	1.49
2	B	595	ARG	C-O	-6.71	1.10	1.23
1	A	43	GLU	C-O	6.71	1.36	1.23
6	H	89	LEU	CA-CB	6.71	1.69	1.53
1	A	303	TYR	CG-CD1	-6.70	1.30	1.39
1	A	500	GLU	CD-OE1	6.70	1.33	1.25
2	B	1186	ASP	CA-CB	6.70	1.68	1.53
1	A	1036	ARG	C-N	-6.70	1.18	1.34
2	B	904	ARG	CD-NE	-6.70	1.35	1.46
4	E	74	ASP	CG-OD2	-6.70	1.09	1.25
1	A	27	VAL	C-O	6.70	1.36	1.23
2	B	1046	PRO	CA-C	-6.70	1.39	1.52
4	E	14	ARG	C-O	6.70	1.36	1.23
2	B	262	GLU	CD-OE2	6.70	1.33	1.25
2	B	897	GLY	CA-C	6.70	1.62	1.51
2	B	556	THR	N-CA	-6.70	1.32	1.46
3	C	79	GLN	N-CA	-6.70	1.32	1.46
3	C	183	TRP	CG-CD2	-6.70	1.32	1.43
7	I	107	SER	CA-CB	-6.70	1.43	1.52
1	A	382	PRO	CG-CD	-6.69	1.28	1.50
1	A	819	GLY	C-O	6.69	1.34	1.23
2	B	1146	PHE	C-O	-6.69	1.10	1.23
2	B	434	ARG	CA-C	6.69	1.70	1.52
3	C	165	LYS	CD-CE	6.69	1.68	1.51
1	A	35	ILE	CA-C	6.69	1.70	1.52
1	A	302	THR	N-CA	-6.69	1.32	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	28	ASP	CG-OD1	6.69	1.40	1.25
1	A	560	ILE	C-N	-6.69	1.21	1.34
1	A	711	ARG	CA-CB	-6.69	1.39	1.53
1	A	738	LYS	C-O	-6.69	1.10	1.23
6	H	61	SER	C-O	6.69	1.36	1.23
7	I	98	VAL	C-O	-6.69	1.10	1.23
1	A	804	TYR	CG-CD1	6.68	1.47	1.39
2	B	577	ALA	CA-C	-6.68	1.35	1.52
7	I	29	CYS	CA-C	-6.68	1.35	1.52
1	A	617	VAL	CA-CB	-6.68	1.40	1.54
2	B	272	THR	CB-CG2	-6.68	1.30	1.52
3	C	209	TYR	CG-CD1	6.68	1.47	1.39
1	A	356	ASP	CG-OD1	6.68	1.40	1.25
4	E	60	PHE	CD1-CE1	6.68	1.52	1.39
2	B	705	MET	C-O	-6.67	1.10	1.23
2	B	649	LYS	C-O	6.67	1.36	1.23
3	C	252	GLN	CD-NE2	6.67	1.49	1.32
1	A	714	PHE	CE1-CZ	-6.67	1.24	1.37
3	C	28	ALA	CA-CB	-6.67	1.38	1.52
3	C	73	GLN	CD-OE1	-6.67	1.09	1.24
1	A	896	ARG	NE-CZ	-6.67	1.24	1.33
3	C	223	ALA	CA-C	-6.67	1.35	1.52
10	L	49	LYS	N-CA	6.67	1.59	1.46
1	A	918	GLU	CB-CG	6.67	1.64	1.52
2	B	103	ASN	CA-CB	6.67	1.70	1.53
3	C	196	ASP	C-O	6.67	1.36	1.23
1	A	1114	PRO	CA-CB	-6.66	1.40	1.53
2	B	509	ALA	N-CA	-6.66	1.33	1.46
2	B	604	ARG	N-CA	6.66	1.59	1.46
2	B	387	LEU	CG-CD1	-6.66	1.27	1.51
4	E	7	ARG	CG-CD	6.66	1.68	1.51
7	I	111	THR	CB-CG2	-6.66	1.30	1.52
2	B	612	GLU	CB-CG	6.66	1.64	1.52
2	B	230	ALA	N-CA	6.66	1.59	1.46
3	C	98	VAL	CB-CG1	-6.66	1.38	1.52
5	F	80	ALA	CA-CB	6.66	1.66	1.52
9	K	111	LEU	CG-CD2	6.66	1.76	1.51
2	B	813	LYS	CG-CD	6.66	1.75	1.52
7	I	100	PHE	CG-CD1	6.66	1.48	1.38
1	A	1308	THR	CB-CG2	-6.65	1.30	1.52
2	B	895	ASP	N-CA	6.65	1.59	1.46
1	A	855	THR	CB-CG2	-6.65	1.30	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	57	MET	CA-CB	6.65	1.68	1.53
1	A	780	VAL	C-O	6.65	1.35	1.23
1	A	987	VAL	CA-CB	-6.65	1.40	1.54
1	A	1233	ASP	CB-CG	6.65	1.65	1.51
1	A	1314	SER	N-CA	-6.65	1.33	1.46
2	B	362	PRO	N-CA	-6.65	1.35	1.47
9	K	39	ASP	CG-OD2	6.65	1.40	1.25
2	B	804	GLY	C-O	-6.65	1.13	1.23
1	A	169	ASN	CB-CG	-6.65	1.35	1.51
1	A	1146	VAL	N-CA	-6.65	1.33	1.46
2	B	1195	HIS	CA-CB	6.65	1.68	1.53
7	I	87	GLN	C-O	-6.65	1.10	1.23
2	B	112	LEU	CA-C	-6.64	1.35	1.52
7	I	9	ASP	CB-CG	6.64	1.65	1.51
3	C	199	LYS	CB-CG	6.64	1.70	1.52
1	A	226	GLU	C-O	-6.64	1.10	1.23
1	A	872	GLY	C-O	-6.64	1.13	1.23
2	B	1100	ASP	CA-C	6.64	1.70	1.52
2	B	1182	CYS	N-CA	6.64	1.59	1.46
3	C	183	TRP	CD2-CE3	-6.64	1.30	1.40
1	A	83	HIS	C-O	6.64	1.35	1.23
1	A	912	LEU	CA-C	-6.64	1.35	1.52
1	A	1164	PRO	CA-CB	6.64	1.66	1.53
3	C	249	ASP	CB-CG	6.64	1.65	1.51
2	B	19	GLU	CD-OE2	6.64	1.32	1.25
7	I	12	ASN	N-CA	-6.64	1.33	1.46
7	I	52	ILE	CA-C	-6.64	1.35	1.52
8	J	49	MET	N-CA	6.64	1.59	1.46
1	A	152	VAL	CA-CB	6.63	1.68	1.54
1	A	467	THR	CA-CB	-6.63	1.36	1.53
7	I	73	ARG	CZ-NH2	6.63	1.41	1.33
1	A	1130	GLN	N-CA	6.63	1.59	1.46
2	B	870	ILE	C-O	6.63	1.35	1.23
6	H	79	TRP	CA-CB	-6.63	1.39	1.53
4	E	151	PRO	CA-C	-6.63	1.39	1.52
1	A	761	MET	SD-CE	6.63	2.15	1.77
2	B	220	GLY	C-O	-6.63	1.13	1.23
3	C	144	ILE	CB-CG2	-6.62	1.32	1.52
1	A	748	MET	C-O	6.62	1.35	1.23
1	A	949	ASP	N-CA	-6.62	1.33	1.46
1	A	1231	ASP	CA-CB	-6.62	1.39	1.53
6	H	17	PRO	CA-C	6.62	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	85	PHE	CG-CD1	-6.62	1.28	1.38
1	A	284	ALA	CA-CB	6.62	1.66	1.52
2	B	267	ARG	CD-NE	6.62	1.57	1.46
1	A	434	ARG	CD-NE	-6.62	1.35	1.46
1	A	913	LEU	CA-CB	6.62	1.69	1.53
2	B	890	TYR	CD2-CE2	6.62	1.49	1.39
2	B	904	ARG	CZ-NH1	-6.62	1.24	1.33
10	L	37	LYS	CA-CB	-6.62	1.39	1.53
1	A	446	ARG	NE-CZ	-6.62	1.24	1.33
2	B	199	MET	CG-SD	6.62	1.98	1.81
2	B	821	GLN	N-CA	-6.62	1.33	1.46
2	B	1106	ARG	CA-CB	6.62	1.68	1.53
3	C	179	GLU	CD-OE1	-6.62	1.18	1.25
1	A	1199	ARG	CB-CG	6.61	1.70	1.52
1	A	898	ARG	N-CA	6.61	1.59	1.46
2	B	728	ARG	CZ-NH1	-6.61	1.24	1.33
5	F	78	GLN	C-O	-6.61	1.10	1.23
7	I	18	GLU	CA-CB	6.61	1.68	1.53
3	C	160	LYS	CE-NZ	6.61	1.65	1.49
4	E	183	PRO	N-CA	-6.61	1.36	1.47
1	A	349	ALA	C-O	-6.61	1.10	1.23
2	B	262	GLU	CD-OE1	6.61	1.32	1.25
1	A	388	LEU	N-CA	-6.61	1.33	1.46
1	A	813	PHE	C-O	6.61	1.35	1.23
3	C	165	LYS	CG-CD	6.60	1.75	1.52
1	A	1196	GLU	CA-CB	-6.60	1.39	1.53
2	B	96	TYR	CD1-CE1	6.60	1.49	1.39
6	H	129	TYR	CD2-CE2	6.60	1.49	1.39
1	A	123	ARG	CZ-NH2	6.60	1.41	1.33
2	B	680	THR	CB-CG2	-6.60	1.30	1.52
2	B	978	ASP	CG-OD2	6.60	1.40	1.25
1	A	815	PHE	CD2-CE2	-6.60	1.26	1.39
2	B	190	TYR	CD1-CE1	6.60	1.49	1.39
3	C	47	ASP	CB-CG	6.60	1.65	1.51
4	E	42	PHE	CB-CG	-6.60	1.40	1.51
7	I	118	ARG	CG-CD	6.60	1.68	1.51
9	K	106	GLU	CG-CD	6.60	1.61	1.51
1	A	198	GLU	CA-C	-6.59	1.35	1.52
2	B	1219	ASP	C-O	6.59	1.35	1.23
7	I	6	PHE	CB-CG	-6.59	1.40	1.51
1	A	1176	LEU	CG-CD2	6.59	1.76	1.51
2	B	819	ALA	N-CA	-6.59	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	61	LEU	CA-CB	-6.59	1.38	1.53
1	A	279	LEU	CG-CD2	6.59	1.76	1.51
1	A	211	PHE	CD2-CE2	6.59	1.52	1.39
1	A	286	HIS	CB-CG	6.59	1.61	1.50
1	A	783	THR	C-O	-6.59	1.10	1.23
1	A	187	LYS	C-O	6.59	1.35	1.23
2	B	249	ARG	CB-CG	6.58	1.70	1.52
1	A	190	ALA	CA-C	6.58	1.70	1.52
1	A	1012	ARG	N-CA	-6.58	1.33	1.46
3	C	113	VAL	CB-CG1	-6.58	1.39	1.52
2	B	249	ARG	CZ-NH1	6.58	1.41	1.33
4	E	192	ARG	CG-CD	6.58	1.68	1.51
1	A	22	PHE	CE1-CZ	6.58	1.49	1.37
1	A	969	GLN	CG-CD	6.58	1.66	1.51
10	L	48	CYS	C-O	6.58	1.35	1.23
1	A	747	VAL	CB-CG1	-6.58	1.39	1.52
3	C	170	TRP	CD2-CE2	-6.58	1.33	1.41
1	A	1237	ILE	C-O	6.58	1.35	1.23
4	E	59	SER	C-O	6.58	1.35	1.23
6	H	129	TYR	CZ-OH	6.58	1.49	1.37
2	B	325	GLN	C-O	-6.57	1.10	1.23
1	A	705	LYS	C-O	6.57	1.35	1.23
3	C	154	LYS	C-O	-6.57	1.10	1.23
1	A	985	ASP	CG-OD2	6.57	1.40	1.25
2	B	452	THR	N-CA	6.57	1.59	1.46
2	B	1092	TYR	CE2-CZ	-6.57	1.30	1.38
8	J	54	VAL	CA-CB	-6.57	1.41	1.54
1	A	957	PRO	CA-CB	-6.56	1.40	1.53
2	B	389	ALA	CA-CB	-6.56	1.38	1.52
2	B	369	GLY	CA-C	6.56	1.62	1.51
1	A	693	VAL	C-O	-6.56	1.10	1.23
1	A	934	LYS	CE-NZ	6.56	1.65	1.49
2	B	1213	THR	CA-CB	-6.56	1.36	1.53
1	A	993	LEU	N-CA	6.56	1.59	1.46
1	A	1211	GLN	CG-CD	6.56	1.66	1.51
1	A	440	ASP	CB-CG	-6.56	1.38	1.51
1	A	493	GLN	CA-CB	-6.55	1.39	1.53
2	B	711	GLU	CD-OE1	6.55	1.32	1.25
2	B	1093	GLN	CD-OE1	6.55	1.38	1.24
3	C	10	ILE	CB-CG2	6.55	1.73	1.52
8	J	21	TYR	CB-CG	6.55	1.61	1.51
9	K	74	ARG	NE-CZ	-6.55	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	632	VAL	C-O	-6.55	1.10	1.23
1	A	793	SER	C-O	-6.55	1.10	1.23
1	A	971	PHE	CG-CD2	-6.55	1.28	1.38
1	A	1169	ILE	CB-CG2	-6.55	1.32	1.52
2	B	310	MET	CA-CB	-6.55	1.39	1.53
2	B	66	ASP	CA-C	6.55	1.70	1.52
2	B	308	TRP	CZ2-CH2	-6.55	1.25	1.37
4	E	69	ILE	C-O	6.55	1.35	1.23
2	B	401	PHE	C-O	-6.55	1.10	1.23
8	J	27	GLU	CD-OE1	6.55	1.32	1.25
1	A	451	HIS	C-O	-6.54	1.10	1.23
2	B	27	ALA	N-CA	-6.54	1.33	1.46
1	A	546	VAL	CA-CB	-6.54	1.41	1.54
1	A	804	TYR	CB-CG	6.54	1.61	1.51
1	A	893	PHE	C-O	-6.54	1.10	1.23
2	B	984	HIS	C-O	-6.54	1.10	1.23
7	I	42	LEU	CG-CD1	6.54	1.76	1.51
1	A	371	ALA	C-O	-6.54	1.10	1.23
4	E	36	GLU	CD-OE1	6.54	1.32	1.25
1	A	568	PRO	CB-CG	-6.54	1.17	1.50
1	A	847	ASP	C-O	-6.54	1.10	1.23
7	I	110	PHE	CE1-CZ	-6.54	1.25	1.37
10	L	60	ARG	CG-CD	6.54	1.68	1.51
1	A	763	ALA	C-O	-6.54	1.10	1.23
2	B	336	ARG	CB-CG	-6.54	1.34	1.52
2	B	809	MET	SD-CE	-6.54	1.41	1.77
3	C	123	ASN	CA-CB	6.54	1.70	1.53
1	A	404	TYR	CB-CG	-6.54	1.41	1.51
1	A	446	ARG	CG-CD	-6.54	1.35	1.51
2	B	509	ALA	CA-C	6.54	1.70	1.52
1	A	551	TYR	CE2-CZ	6.53	1.47	1.38
1	A	644	LYS	CA-CB	-6.53	1.39	1.53
2	B	733	HIS	CA-CB	6.53	1.68	1.53
3	C	205	LYS	CE-NZ	6.53	1.65	1.49
1	A	7	SER	CB-OG	-6.53	1.33	1.42
2	B	937	ALA	N-CA	6.53	1.59	1.46
1	A	816	HIS	CB-CG	-6.53	1.38	1.50
1	A	1222	ASN	CA-C	6.53	1.70	1.52
4	E	98	ILE	C-O	6.53	1.35	1.23
4	E	66	GLU	CA-CB	6.53	1.68	1.53
9	K	17	SER	N-CA	6.53	1.59	1.46
1	A	383	TYR	CG-CD1	6.53	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	CYS	CA-C	-6.53	1.35	1.52
2	B	701	ILE	CA-CB	-6.53	1.39	1.54
2	B	839	MET	CG-SD	6.53	1.98	1.81
3	C	22	LEU	CA-C	-6.53	1.35	1.52
6	H	98	TYR	CG-CD2	-6.53	1.30	1.39
1	A	40	THR	CA-CB	6.52	1.70	1.53
1	A	644	LYS	CE-NZ	6.52	1.65	1.49
6	H	40	LEU	CG-CD1	-6.52	1.27	1.51
1	A	90	VAL	N-CA	-6.52	1.33	1.46
1	A	645	LEU	C-N	-6.52	1.19	1.34
2	B	1022	THR	CB-OG1	-6.52	1.30	1.43
3	C	163	ILE	CB-CG1	-6.52	1.35	1.54
1	A	506	ALA	C-O	-6.52	1.10	1.23
9	K	55	LYS	C-O	6.52	1.35	1.23
10	L	33	GLU	N-CA	6.52	1.59	1.46
1	A	983	ILE	C-O	-6.52	1.10	1.23
1	A	1214	GLU	C-O	6.52	1.35	1.23
2	B	589	VAL	N-CA	-6.52	1.33	1.46
1	A	202	LEU	CG-CD2	6.52	1.75	1.51
1	A	1123	GLY	CA-C	6.52	1.62	1.51
2	B	1033	LYS	CD-CE	6.52	1.67	1.51
5	F	106	PRO	CB-CG	6.52	1.82	1.50
1	A	411	ASP	CG-OD2	6.51	1.40	1.25
1	A	434	ARG	CB-CG	-6.51	1.34	1.52
1	A	1335	ILE	CA-C	-6.51	1.36	1.52
2	B	323	VAL	N-CA	-6.51	1.33	1.46
2	B	1002	THR	CB-OG1	-6.51	1.30	1.43
2	B	418	LYS	C-O	-6.51	1.10	1.23
2	B	497	ARG	CD-NE	-6.51	1.35	1.46
2	B	975	GLN	CB-CG	-6.51	1.34	1.52
5	F	83	PRO	CG-CD	-6.51	1.29	1.50
1	A	1154	TYR	CB-CG	-6.51	1.41	1.51
2	B	1106	ARG	CZ-NH2	6.51	1.41	1.33
7	I	28	GLU	CD-OE2	6.51	1.32	1.25
1	A	1094	VAL	CB-CG2	6.50	1.66	1.52
8	J	7	CYS	C-O	6.50	1.35	1.23
1	A	324	SER	CA-CB	6.50	1.62	1.52
1	A	601	LYS	CE-NZ	6.50	1.65	1.49
1	A	1057	VAL	CA-CB	6.50	1.68	1.54
2	B	488	TYR	C-O	6.50	1.35	1.23
2	B	621	GLU	CG-CD	6.50	1.61	1.51
2	B	773	MET	CG-SD	-6.50	1.64	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	8	ARG	CG-CD	6.50	1.68	1.51
9	K	62	LYS	C-O	6.50	1.35	1.23
1	A	241	VAL	CA-CB	6.50	1.68	1.54
1	A	973	ILE	C-O	6.50	1.35	1.23
1	A	1112	LYS	CD-CE	6.50	1.67	1.51
10	L	67	PHE	CA-CB	6.50	1.68	1.53
1	A	733	ALA	C-O	-6.50	1.11	1.23
5	F	110	ASP	C-O	6.50	1.35	1.23
2	B	887	HIS	CB-CG	6.50	1.61	1.50
1	A	852	TYR	CD2-CE2	-6.50	1.29	1.39
2	B	1048	THR	CA-C	-6.50	1.36	1.52
1	A	228	PHE	CE1-CZ	-6.49	1.25	1.37
1	A	420	ARG	CZ-NH1	-6.49	1.24	1.33
1	A	552	TRP	CE2-CZ2	-6.49	1.28	1.39
1	A	1118	VAL	N-CA	-6.49	1.33	1.46
2	B	241	ARG	NE-CZ	6.49	1.41	1.33
3	C	175	ALA	CA-C	-6.49	1.36	1.52
1	A	995	GLU	CA-C	-6.49	1.36	1.52
3	C	219	PHE	CE1-CZ	-6.49	1.25	1.37
2	B	341	LEU	CA-C	-6.49	1.36	1.52
1	A	452	LYS	CD-CE	-6.49	1.35	1.51
9	K	92	ASN	CB-CG	6.49	1.66	1.51
1	A	940	ARG	CA-CB	-6.48	1.39	1.53
1	A	1383	SER	CB-OG	6.48	1.50	1.42
1	A	34	LYS	C-O	-6.48	1.11	1.23
1	A	134	ARG	CB-CG	-6.48	1.35	1.52
1	A	135	PHE	CD2-CE2	-6.48	1.26	1.39
2	B	417	PHE	CD1-CE1	-6.48	1.26	1.39
2	B	564	GLU	CB-CG	6.48	1.64	1.52
2	B	644	GLU	CD-OE1	6.48	1.32	1.25
1	A	1231	ASP	CG-OD2	6.48	1.40	1.25
2	B	478	GLY	N-CA	6.48	1.55	1.46
1	A	471	ASN	N-CA	6.48	1.59	1.46
3	C	76	ASP	N-CA	6.48	1.59	1.46
3	C	108	GLU	CA-C	6.48	1.69	1.52
7	I	45	ARG	CZ-NH2	-6.48	1.24	1.33
1	A	43	GLU	CA-C	6.48	1.69	1.52
1	A	770	VAL	CB-CG2	6.48	1.66	1.52
9	K	26	LYS	CA-CB	6.48	1.68	1.53
1	A	280	GLU	CD-OE1	6.47	1.32	1.25
1	A	644	LYS	CD-CE	6.47	1.67	1.51
1	A	1256	GLU	CG-CD	6.47	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	351	TYR	CD1-CE1	6.47	1.49	1.39
3	C	215	GLU	CD-OE2	6.47	1.32	1.25
4	E	60	PHE	CG-CD2	6.47	1.48	1.38
1	A	656	TRP	CG-CD1	6.47	1.45	1.36
2	B	654	ARG	NE-CZ	-6.47	1.24	1.33
2	B	664	THR	CB-OG1	6.47	1.56	1.43
9	K	111	LEU	CA-C	6.47	1.69	1.52
2	B	171	PRO	CB-CG	6.47	1.82	1.50
4	E	40	GLU	CD-OE2	6.47	1.32	1.25
4	E	136	ASN	CG-ND2	6.47	1.49	1.32
4	E	191	LYS	CE-NZ	6.47	1.65	1.49
2	B	50	SER	CA-CB	-6.47	1.43	1.52
2	B	344	LYS	CA-C	6.47	1.69	1.52
2	B	1211	ASN	CB-CG	-6.47	1.36	1.51
5	F	91	ALA	CA-CB	-6.47	1.38	1.52
7	I	65	ASP	C-O	6.47	1.35	1.23
2	B	125	SER	CA-CB	-6.46	1.43	1.52
2	B	789	MET	SD-CE	6.46	2.14	1.77
1	A	879	GLU	C-O	-6.46	1.11	1.23
1	A	1136	SER	N-CA	-6.46	1.33	1.46
2	B	615	MET	CG-SD	6.46	1.98	1.81
1	A	677	ARG	CZ-NH2	6.46	1.41	1.33
2	B	426	LYS	CB-CG	6.46	1.70	1.52
1	A	935	GLN	C-O	-6.46	1.11	1.23
2	B	306	ASN	CB-CG	6.46	1.66	1.51
2	B	364	ILE	N-CA	-6.46	1.33	1.46
1	A	977	LYS	CG-CD	6.46	1.74	1.52
2	B	325	GLN	N-CA	6.46	1.59	1.46
3	C	111	THR	CB-OG1	6.46	1.56	1.43
6	H	120	GLY	C-O	6.46	1.33	1.23
2	B	1220	ARG	CD-NE	6.46	1.57	1.46
6	H	88	SER	CB-OG	6.45	1.50	1.42
1	A	189	ARG	N-CA	6.45	1.59	1.46
2	B	164	LYS	CG-CD	6.45	1.74	1.52
2	B	1204	PHE	CG-CD2	-6.45	1.29	1.38
3	C	253	LYS	CA-C	6.45	1.69	1.52
4	E	23	VAL	CB-CG2	6.45	1.66	1.52
7	I	110	PHE	CD2-CE2	6.45	1.52	1.39
1	A	135	PHE	N-CA	6.45	1.59	1.46
2	B	204	ILE	CA-CB	-6.45	1.40	1.54
2	B	1086	PHE	CG-CD1	-6.45	1.29	1.38
1	A	478	TYR	CZ-OH	6.45	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	731	ARG	CG-CD	6.45	1.68	1.51
1	A	864	ILE	C-O	6.45	1.35	1.23
6	H	100	THR	CB-CG2	6.45	1.73	1.52
2	B	1219	ASP	N-CA	6.44	1.59	1.46
2	B	557	PHE	CB-CG	-6.44	1.40	1.51
3	C	211	ASP	C-O	6.44	1.35	1.23
9	K	67	PHE	CG-CD1	-6.44	1.29	1.38
6	H	139	ASN	C-O	6.44	1.35	1.23
7	I	1	MET	CG-SD	6.44	1.97	1.81
7	I	93	LYS	CB-CG	6.44	1.70	1.52
2	B	384	ARG	CB-CG	6.44	1.70	1.52
2	B	1214	PRO	C-O	6.44	1.36	1.23
1	A	1382	THR	CA-CB	6.44	1.70	1.53
1	A	65	LEU	CB-CG	6.43	1.71	1.52
1	A	969	GLN	CD-OE1	6.43	1.38	1.24
2	B	1097	HIS	ND1-CE1	6.43	1.50	1.34
2	B	429	PHE	CE1-CZ	6.43	1.49	1.37
3	C	201	TRP	CE3-CZ3	-6.43	1.27	1.38
8	J	47	ARG	C-O	6.43	1.35	1.23
1	A	439	ASN	CG-ND2	-6.43	1.16	1.32
3	C	141	GLY	CA-C	6.43	1.62	1.51
7	I	87	GLN	CD-NE2	6.43	1.49	1.32
2	B	1099	VAL	CB-CG1	-6.43	1.39	1.52
1	A	1354	ASN	CB-CG	6.43	1.65	1.51
1	A	516	SER	C-O	6.42	1.35	1.23
1	A	864	ILE	CA-C	-6.42	1.36	1.52
1	A	1333	ILE	CB-CG2	-6.42	1.32	1.52
3	C	124	LEU	C-O	6.42	1.35	1.23
2	B	51	PHE	N-CA	6.42	1.59	1.46
2	B	135	ARG	C-N	6.42	1.48	1.34
1	A	1064	VAL	N-CA	-6.42	1.33	1.46
2	B	649	LYS	CD-CE	6.42	1.67	1.51
5	F	76	LYS	CD-CE	6.42	1.67	1.51
1	A	865	GLN	CA-CB	-6.42	1.39	1.53
5	F	125	LEU	CG-CD1	-6.42	1.28	1.51
2	B	1135	ARG	CZ-NH1	6.42	1.41	1.33
1	A	572	TRP	CD2-CE3	-6.41	1.30	1.40
2	B	241	ARG	CD-NE	6.41	1.57	1.46
3	C	177	GLU	CA-C	-6.41	1.36	1.52
2	B	281	PRO	C-O	-6.41	1.10	1.23
1	A	114	LEU	CG-CD1	-6.41	1.28	1.51
2	B	665	GLU	CD-OE1	6.41	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	26	ARG	CB-CG	-6.41	1.35	1.52
6	H	95	TYR	CE1-CZ	-6.41	1.30	1.38
1	A	206	GLU	CG-CD	6.41	1.61	1.51
1	A	37	PHE	C-O	-6.40	1.11	1.23
1	A	790	ASP	CA-CB	-6.40	1.39	1.53
4	E	14	ARG	CZ-NH2	-6.40	1.24	1.33
4	E	82	PHE	CD1-CE1	-6.40	1.26	1.39
4	E	108	GLY	C-O	-6.40	1.13	1.23
8	J	24	LEU	C-N	-6.40	1.19	1.34
1	A	198	GLU	CD-OE1	6.40	1.32	1.25
2	B	135	ARG	NE-CZ	6.40	1.41	1.33
4	E	172	GLU	CG-CD	6.40	1.61	1.51
8	J	5	VAL	CB-CG1	-6.40	1.39	1.52
2	B	282	ILE	N-CA	-6.40	1.33	1.46
2	B	1020	ARG	NE-CZ	-6.40	1.24	1.33
4	E	37	LEU	CG-CD1	6.40	1.75	1.51
4	E	83	CYS	CB-SG	6.40	1.93	1.82
6	H	141	TYR	CA-CB	-6.40	1.39	1.53
9	K	1	MET	CA-CB	6.40	1.68	1.53
5	F	112	GLU	CD-OE2	6.40	1.32	1.25
4	E	70	SER	C-O	6.39	1.35	1.23
1	A	15	LYS	CD-CE	6.39	1.67	1.51
1	A	482	PHE	CE1-CZ	-6.39	1.25	1.37
6	H	111	LEU	C-O	6.39	1.35	1.23
7	I	44	TYR	CZ-OH	6.39	1.48	1.37
2	B	608	ASP	CB-CG	6.39	1.65	1.51
9	K	106	GLU	C-O	6.39	1.35	1.23
1	A	614	PHE	CD1-CE1	-6.39	1.26	1.39
1	A	69	THR	C-O	6.39	1.35	1.23
1	A	183	GLY	CA-C	-6.39	1.41	1.51
2	B	822	ASN	CA-C	-6.39	1.36	1.52
2	B	245	GLU	CD-OE2	6.38	1.32	1.25
7	I	57	GLY	C-O	-6.38	1.13	1.23
2	B	191	LYS	CG-CD	6.38	1.74	1.52
1	A	947	PHE	CG-CD2	-6.38	1.29	1.38
1	A	1061	GLY	C-O	6.38	1.33	1.23
2	B	557	PHE	N-CA	-6.38	1.33	1.46
1	A	1092	LYS	CA-CB	6.38	1.68	1.53
8	J	54	VAL	CB-CG1	6.38	1.66	1.52
1	A	556	TRP	CZ2-CH2	-6.38	1.25	1.37
1	A	986	ILE	CB-CG2	6.38	1.72	1.52
2	B	620	ARG	CZ-NH1	6.38	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	256	VAL	CB-CG2	-6.38	1.39	1.52
1	A	781	ASP	CB-CG	6.37	1.65	1.51
1	A	1080	THR	N-CA	6.37	1.59	1.46
2	B	345	LYS	CB-CG	-6.37	1.35	1.52
4	E	149	LEU	CG-CD1	-6.37	1.28	1.51
6	H	39	THR	CB-CG2	6.37	1.73	1.52
9	K	91	CYS	CA-C	6.37	1.69	1.52
4	E	2	ASP	C-O	6.37	1.35	1.23
1	A	571	LEU	CG-CD1	-6.37	1.28	1.51
2	B	429	PHE	CG-CD2	6.37	1.48	1.38
2	B	738	PHE	CG-CD1	-6.37	1.29	1.38
3	C	218	PRO	C-O	6.37	1.35	1.23
1	A	1117	THR	N-CA	6.37	1.59	1.46
1	A	1204	ASP	CB-CG	6.37	1.65	1.51
2	B	368	GLU	CD-OE1	6.37	1.32	1.25
2	B	1186	ASP	CB-CG	6.37	1.65	1.51
1	A	603	ASN	N-CA	-6.36	1.33	1.46
2	B	780	VAL	N-CA	-6.36	1.33	1.46
2	B	1192	TYR	CD2-CE2	6.36	1.48	1.39
1	A	388	LEU	CA-C	6.36	1.69	1.52
1	A	563	PRO	C-O	-6.36	1.10	1.23
1	A	1420	ASP	CG-OD1	6.36	1.40	1.25
2	B	39	ARG	CA-CB	6.36	1.68	1.53
4	E	79	TRP	C-N	-6.36	1.19	1.34
1	A	808	LEU	CG-CD2	-6.36	1.28	1.51
2	B	1019	SER	N-CA	-6.36	1.33	1.46
1	A	58	LEU	C-O	6.35	1.35	1.23
1	A	66	LYS	N-CA	6.35	1.59	1.46
1	A	670	ILE	C-O	-6.35	1.11	1.23
1	A	827	THR	CB-CG2	6.35	1.73	1.52
2	B	421	PHE	C-O	-6.35	1.11	1.23
2	B	1035	ALA	CA-CB	-6.35	1.39	1.52
7	I	77	LYS	CB-CG	6.35	1.69	1.52
1	A	5	GLN	CA-CB	6.35	1.68	1.53
1	A	1159	ARG	C-O	-6.35	1.11	1.23
1	A	1196	GLU	N-CA	-6.35	1.33	1.46
1	A	560	ILE	CA-CB	-6.35	1.40	1.54
1	A	714	PHE	CB-CG	-6.35	1.40	1.51
1	A	508	PRO	CA-CB	6.35	1.66	1.53
1	A	614	PHE	CB-CG	-6.35	1.40	1.51
1	A	1425	SER	CB-OG	6.35	1.50	1.42
2	B	366	GLN	N-CA	6.35	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1030	ARG	CZ-NH2	-6.35	1.24	1.33
2	B	986	GLN	CA-C	6.35	1.69	1.52
4	E	69	ILE	CA-CB	-6.35	1.40	1.54
1	A	1450	LEU	CA-CB	6.34	1.68	1.53
7	I	55	THR	CA-CB	-6.34	1.36	1.53
2	B	212	LEU	CG-CD2	6.34	1.75	1.51
5	F	95	GLY	C-O	-6.34	1.13	1.23
1	A	1311	VAL	N-CA	-6.34	1.33	1.46
2	B	823	ALA	CA-C	-6.34	1.36	1.52
1	A	370	ILE	CB-CG2	-6.34	1.33	1.52
1	A	677	ARG	CG-CD	6.34	1.67	1.51
2	B	1106	ARG	CA-C	6.34	1.69	1.52
1	A	1420	ASP	N-CA	6.34	1.59	1.46
2	B	246	LYS	CA-CB	6.34	1.67	1.53
3	C	256	ALA	N-CA	-6.34	1.33	1.46
9	K	7	PHE	CD2-CE2	-6.34	1.26	1.39
1	A	435	HIS	CB-CG	-6.33	1.38	1.50
1	A	722	LEU	CA-CB	-6.33	1.39	1.53
1	A	860	LEU	C-O	-6.33	1.11	1.23
2	B	213	ILE	N-CA	-6.33	1.33	1.46
7	I	44	TYR	CG-CD2	6.33	1.47	1.39
1	A	1359	ASP	CG-OD2	6.33	1.40	1.25
2	B	371	GLU	C-O	-6.33	1.11	1.23
2	B	1211	ASN	C-O	6.33	1.35	1.23
1	A	838	GLN	CD-OE1	6.33	1.37	1.24
1	A	642	CYS	N-CA	-6.33	1.33	1.46
3	C	242	GLN	CG-CD	6.33	1.65	1.51
6	H	95	TYR	C-O	-6.33	1.11	1.23
1	A	110	CYS	C-N	6.33	1.44	1.33
2	B	634	TYR	CE2-CZ	-6.33	1.30	1.38
6	H	85	GLY	N-CA	6.33	1.55	1.46
2	B	1110	PRO	C-O	6.32	1.35	1.23
7	I	36	GLU	C-O	-6.32	1.11	1.23
1	A	814	PHE	CG-CD1	-6.32	1.29	1.38
8	J	27	GLU	CB-CG	6.32	1.64	1.52
1	A	1001	ARG	CA-C	6.32	1.69	1.52
1	A	1049	ILE	C-O	-6.32	1.11	1.23
2	B	608	ASP	CA-CB	6.32	1.67	1.53
1	A	106	VAL	N-CA	-6.32	1.33	1.46
1	A	383	TYR	N-CA	6.32	1.58	1.46
1	A	443	LEU	CG-CD1	-6.32	1.28	1.51
2	B	65	GLU	CD-OE1	6.32	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	186	LEU	N-CA	6.32	1.58	1.46
1	A	681	GLU	CB-CG	6.31	1.64	1.52
1	A	1255	GLU	CA-C	6.31	1.69	1.52
2	B	60	GLN	N-CA	-6.31	1.33	1.46
2	B	104	GLU	N-CA	6.31	1.58	1.46
2	B	1164	GLY	C-O	6.31	1.33	1.23
3	C	177	GLU	CB-CG	6.31	1.64	1.52
2	B	633	VAL	CB-CG2	6.31	1.66	1.52
2	B	654	ARG	CD-NE	-6.31	1.35	1.46
1	A	143	LYS	CB-CG	6.31	1.69	1.52
2	B	591	ARG	CB-CG	6.31	1.69	1.52
2	B	1085	ILE	C-N	-6.31	1.19	1.34
2	B	1176	ASN	CG-OD1	6.31	1.37	1.24
7	I	4	PHE	CG-CD2	6.31	1.48	1.38
1	A	111	GLY	C-O	6.30	1.33	1.23
1	A	382	PRO	CB-CG	6.30	1.81	1.50
1	A	1226	VAL	C-O	6.30	1.35	1.23
1	A	1134	ILE	CB-CG2	-6.30	1.33	1.52
1	A	1445	ILE	C-O	6.30	1.35	1.23
2	B	1018	PRO	C-O	-6.30	1.10	1.23
1	A	677	ARG	N-CA	6.30	1.58	1.46
9	K	36	GLU	CA-CB	-6.29	1.40	1.53
1	A	1033	GLN	CD-NE2	6.29	1.48	1.32
2	B	411	PRO	N-CA	-6.29	1.36	1.47
2	B	459	TYR	CG-CD1	6.29	1.47	1.39
2	B	1077	THR	C-O	-6.29	1.11	1.23
7	I	119	THR	CA-CB	6.29	1.69	1.53
1	A	482	PHE	C-O	-6.29	1.11	1.23
1	A	555	ASP	CG-OD1	6.29	1.39	1.25
2	B	519	TRP	CZ3-CH2	-6.29	1.29	1.40
2	B	997	GLU	CD-OE2	-6.29	1.18	1.25
6	H	59	ILE	C-O	-6.29	1.11	1.23
2	B	511	PRO	CA-C	-6.28	1.40	1.52
1	A	641	VAL	C-O	-6.28	1.11	1.23
1	A	954	TRP	NE1-CE2	-6.28	1.29	1.37
1	A	1025	ARG	NE-CZ	-6.28	1.24	1.33
9	K	24	ASP	CG-OD2	6.28	1.39	1.25
2	B	202	TYR	CD2-CE2	-6.28	1.29	1.39
1	A	372	LYS	CD-CE	-6.28	1.35	1.51
1	A	426	LEU	C-O	-6.28	1.11	1.23
1	A	699	ALA	CA-C	6.28	1.69	1.52
1	A	1127	ASP	CA-CB	6.28	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	209	GLU	C-O	-6.28	1.11	1.23
2	B	1106	ARG	CB-CG	6.28	1.69	1.52
2	B	745	PRO	CA-C	-6.27	1.40	1.52
2	B	815	ARG	C-O	-6.27	1.11	1.23
3	C	251	LEU	CG-CD2	-6.27	1.28	1.51
1	A	387	ARG	CB-CG	6.27	1.69	1.52
1	A	1207	LEU	CA-C	6.27	1.69	1.52
1	A	1275	GLY	C-O	6.27	1.33	1.23
2	B	626	ILE	CB-CG2	-6.27	1.33	1.52
2	B	1084	GLN	CG-CD	6.27	1.65	1.51
2	B	967	ARG	CB-CG	-6.27	1.35	1.52
3	C	129	ILE	CA-CB	6.27	1.69	1.54
1	A	810	PRO	CB-CG	-6.26	1.18	1.50
1	A	814	PHE	CE2-CZ	6.26	1.49	1.37
1	A	1159	ARG	NE-CZ	6.26	1.41	1.33
4	E	91	LYS	CA-CB	6.26	1.67	1.53
4	E	208	TYR	CB-CG	6.26	1.61	1.51
1	A	677	ARG	C-O	-6.26	1.11	1.23
1	A	1215	ARG	CB-CG	6.26	1.69	1.52
2	B	1093	GLN	N-CA	-6.26	1.33	1.46
4	E	93	MET	SD-CE	6.26	2.12	1.77
7	I	100	PHE	CG-CD2	-6.26	1.29	1.38
2	B	241	ARG	C-O	-6.26	1.11	1.23
2	B	260	GLY	C-O	6.26	1.33	1.23
1	A	1228	TRP	CA-C	-6.26	1.36	1.52
2	B	547	VAL	CB-CG1	-6.26	1.39	1.52
2	B	562	GLY	CA-C	-6.26	1.41	1.51
4	E	8	ASN	C-O	-6.26	1.11	1.23
9	K	58	PHE	C-O	6.26	1.35	1.23
1	A	983	ILE	C-N	-6.25	1.19	1.34
1	A	1043	ASP	CB-CG	6.25	1.64	1.51
2	B	417	PHE	CA-CB	-6.25	1.40	1.53
3	C	136	ASP	CG-OD1	-6.25	1.10	1.25
5	F	73	ALA	N-CA	6.25	1.58	1.46
1	A	1202	MET	C-O	6.25	1.35	1.23
2	B	903	VAL	CA-CB	-6.25	1.41	1.54
4	E	2	ASP	N-CA	6.25	1.58	1.46
7	I	8	ARG	NE-CZ	6.25	1.41	1.33
2	B	734	HIS	CA-CB	6.25	1.67	1.53
7	I	8	ARG	CB-CG	6.25	1.69	1.52
1	A	711	ARG	N-CA	-6.25	1.33	1.46
2	B	306	ASN	CA-CB	6.25	1.69	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	308	TRP	CZ3-CH2	6.25	1.50	1.40
3	C	37	MET	CG-SD	-6.25	1.65	1.81
5	F	101	ILE	CA-CB	-6.25	1.40	1.54
1	A	45	GLN	N-CA	6.25	1.58	1.46
1	A	475	THR	CB-OG1	6.24	1.55	1.43
2	B	34	ILE	CB-CG2	-6.24	1.33	1.52
2	B	423	LYS	CD-CE	6.24	1.66	1.51
1	A	147	VAL	CA-CB	6.24	1.67	1.54
1	A	867	ILE	CA-C	6.24	1.69	1.52
2	B	654	ARG	CA-C	-6.24	1.36	1.52
6	H	43	ASN	CB-CG	6.24	1.65	1.51
8	J	62	ARG	CZ-NH2	6.24	1.41	1.33
1	A	660	ASN	CA-C	-6.24	1.36	1.52
1	A	904	THR	C-O	6.24	1.35	1.23
3	C	244	VAL	CA-CB	-6.24	1.41	1.54
4	E	142	VAL	CB-CG2	-6.24	1.39	1.52
7	I	64	SER	CB-OG	6.24	1.50	1.42
8	J	16	ASP	CA-C	6.24	1.69	1.52
7	I	58	VAL	N-CA	6.24	1.58	1.46
1	A	1283	VAL	N-CA	-6.24	1.33	1.46
3	C	149	LYS	CD-CE	6.24	1.66	1.51
2	B	31	TRP	C-N	-6.23	1.19	1.34
2	B	934	LYS	CA-CB	6.23	1.67	1.53
2	B	1071	VAL	CB-CG1	-6.23	1.39	1.52
3	C	40	GLU	CG-CD	6.23	1.61	1.51
9	K	28	PRO	CA-CB	-6.23	1.41	1.53
1	A	72	GLU	CD-OE2	-6.23	1.18	1.25
1	A	1111	MET	CG-SD	6.23	1.97	1.81
1	A	1135	ARG	CZ-NH1	6.23	1.41	1.33
3	C	243	VAL	CA-C	-6.23	1.36	1.52
9	K	92	ASN	CA-CB	6.23	1.69	1.53
1	A	646	PHE	CG-CD1	-6.23	1.29	1.38
1	A	696	GLU	CD-OE2	-6.23	1.18	1.25
1	A	756	ILE	CA-CB	-6.23	1.40	1.54
3	C	107	SER	CB-OG	-6.23	1.34	1.42
1	A	652	VAL	N-CA	-6.23	1.33	1.46
1	A	721	PHE	CD1-CE1	-6.23	1.26	1.39
1	A	15	LYS	CE-NZ	6.23	1.64	1.49
1	A	435	HIS	N-CA	-6.23	1.33	1.46
1	A	919	ILE	CA-CB	6.23	1.69	1.54
1	A	955	PRO	CA-CB	-6.23	1.41	1.53
1	A	1422	ARG	CZ-NH1	6.23	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	267	ARG	C-O	-6.23	1.11	1.23
3	C	240	VAL	CB-CG2	6.23	1.66	1.52
2	B	308	TRP	N-CA	-6.23	1.33	1.46
2	B	794	ASN	N-CA	-6.23	1.33	1.46
1	A	10	PRO	CG-CD	6.22	1.71	1.50
2	B	217	ARG	CD-NE	-6.22	1.35	1.46
2	B	1094	ARG	CB-CG	-6.22	1.35	1.52
1	A	661	GLY	C-O	-6.22	1.13	1.23
2	B	106	ASP	CA-CB	6.22	1.67	1.53
1	A	848	ILE	CB-CG2	-6.22	1.33	1.52
1	A	1044	TRP	CE3-CZ3	6.22	1.49	1.38
3	C	53	THR	C-O	6.22	1.35	1.23
7	I	31	THR	CA-CB	-6.22	1.37	1.53
7	I	65	ASP	N-CA	6.22	1.58	1.46
10	L	40	LEU	CG-CD2	6.22	1.74	1.51
1	A	742	ASN	C-O	-6.22	1.11	1.23
2	B	581	PHE	CD2-CE2	-6.22	1.26	1.39
6	H	6	PHE	CA-CB	-6.22	1.40	1.53
9	K	72	LYS	CE-NZ	6.22	1.64	1.49
2	B	1170	THR	CB-CG2	6.22	1.72	1.52
2	B	120	ARG	CZ-NH2	6.21	1.41	1.33
6	H	95	TYR	C-N	-6.21	1.19	1.34
8	J	44	TYR	CG-CD1	6.21	1.47	1.39
1	A	660	ASN	C-O	6.21	1.35	1.23
2	B	627	PHE	CD2-CE2	-6.21	1.26	1.39
2	B	766	ARG	N-CA	-6.21	1.33	1.46
7	I	93	LYS	N-CA	-6.21	1.33	1.46
1	A	357	PRO	CA-CB	-6.21	1.41	1.53
2	B	275	TYR	CB-CG	6.21	1.60	1.51
1	A	93	VAL	CB-CG2	6.21	1.65	1.52
4	E	146	HIS	C-O	-6.21	1.11	1.23
1	A	4	GLN	CA-C	6.21	1.69	1.52
1	A	598	LEU	C-O	-6.21	1.11	1.23
2	B	662	MET	CG-SD	-6.21	1.65	1.81
9	K	36	GLU	CG-CD	6.21	1.61	1.51
1	A	1301	GLU	CD-OE2	6.20	1.32	1.25
4	E	67	GLU	CD-OE1	6.20	1.32	1.25
6	H	48	PRO	C-O	6.20	1.35	1.23
1	A	232	GLU	CD-OE2	6.20	1.32	1.25
1	A	806	ARG	C-O	6.20	1.35	1.23
2	B	502	ILE	N-CA	6.20	1.58	1.46
5	F	92	ARG	CZ-NH1	6.20	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	297	GLN	CA-C	-6.20	1.36	1.52
3	C	88	CYS	C-O	-6.20	1.11	1.23
6	H	2	SER	N-CA	6.20	1.58	1.46
1	A	853	ASP	CA-CB	-6.20	1.40	1.53
1	A	765	VAL	C-O	-6.20	1.11	1.23
2	B	246	LYS	N-CA	6.20	1.58	1.46
2	B	587	HIS	N-CA	-6.20	1.33	1.46
2	B	698	GLU	CB-CG	-6.20	1.40	1.52
2	B	858	SER	CA-CB	-6.20	1.43	1.52
2	B	1078	GLY	N-CA	-6.20	1.36	1.46
1	A	914	GLU	C-O	6.19	1.35	1.23
1	A	1017	LEU	CG-CD1	-6.19	1.28	1.51
2	B	1217	TYR	CG-CD1	-6.19	1.31	1.39
7	I	94	ASP	CA-CB	6.19	1.67	1.53
1	A	589	GLN	CG-CD	6.19	1.65	1.51
2	B	25	ILE	CA-CB	6.19	1.69	1.54
2	B	213	ILE	CB-CG2	-6.19	1.33	1.52
2	B	525	ALA	C-O	6.19	1.35	1.23
5	F	137	TYR	CA-CB	-6.19	1.40	1.53
1	A	1353	TYR	CD2-CE2	6.19	1.48	1.39
2	B	1224	PHE	CD1-CE1	6.19	1.51	1.39
1	A	723	ASN	N-CA	-6.19	1.33	1.46
1	A	1154	TYR	C-O	6.19	1.35	1.23
9	K	67	PHE	CD1-CE1	6.19	1.51	1.39
2	B	328	GLU	N-CA	6.19	1.58	1.46
2	B	1104	HIS	CB-CG	6.19	1.61	1.50
7	I	17	ARG	CD-NE	6.19	1.56	1.46
8	J	2	ILE	CA-CB	6.19	1.69	1.54
6	H	146	ARG	CB-CG	6.18	1.69	1.52
1	A	57	ARG	CG-CD	6.18	1.67	1.51
1	A	1092	LYS	CG-CD	6.18	1.73	1.52
3	C	51	VAL	CB-CG1	-6.18	1.39	1.52
9	K	14	GLU	CD-OE1	6.18	1.32	1.25
1	A	567	LYS	N-CA	6.18	1.58	1.46
3	C	135	GLN	CA-C	6.18	1.69	1.52
1	A	781	ASP	CA-C	-6.18	1.36	1.52
2	B	997	GLU	CD-OE1	6.18	1.32	1.25
4	E	183	PRO	CB-CG	-6.18	1.19	1.50
1	A	22	PHE	CB-CG	-6.18	1.40	1.51
2	B	302	CYS	CB-SG	-6.18	1.71	1.82
1	A	585	GLY	C-N	6.17	1.48	1.34
2	B	207	GLY	CA-C	6.17	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	26	ARG	CA-CB	-6.17	1.40	1.53
2	B	1223	ASP	CB-CG	-6.17	1.38	1.51
1	A	933	TYR	CB-CG	-6.17	1.42	1.51
3	C	94	LYS	CA-CB	6.17	1.67	1.53
1	A	1020	CYS	N-CA	-6.17	1.34	1.46
1	A	551	TYR	CB-CG	6.17	1.60	1.51
2	B	1148	LYS	CE-NZ	-6.17	1.33	1.49
2	B	1171	VAL	CB-CG2	-6.17	1.39	1.52
3	C	85	ASP	C-O	-6.17	1.11	1.23
2	B	517	THR	CB-OG1	-6.17	1.30	1.43
2	B	627	PHE	CD1-CE1	-6.17	1.26	1.39
7	I	105	SER	N-CA	6.17	1.58	1.46
9	K	7	PHE	CB-CG	-6.17	1.40	1.51
1	A	1023	ARG	NE-CZ	-6.17	1.25	1.33
2	B	1215	ARG	CG-CD	6.17	1.67	1.51
1	A	461	LYS	CA-CB	-6.16	1.40	1.53
1	A	471	ASN	CB-CG	6.16	1.65	1.51
1	A	519	PRO	CG-CD	-6.16	1.30	1.50
2	B	1021	MET	CG-SD	-6.16	1.65	1.81
3	C	94	LYS	N-CA	6.16	1.58	1.46
1	A	668	ASP	CB-CG	-6.16	1.38	1.51
2	B	978	ASP	CB-CG	6.16	1.64	1.51
1	A	1383	SER	N-CA	-6.16	1.34	1.46
1	A	1438	THR	CB-CG2	-6.16	1.32	1.52
2	B	1008	PRO	CG-CD	-6.16	1.30	1.50
3	C	250	THR	CB-OG1	6.16	1.55	1.43
1	A	1416	ALA	C-O	-6.16	1.11	1.23
4	E	68	SER	N-CA	6.16	1.58	1.46
1	A	1270	ASN	CB-CG	6.16	1.65	1.51
2	B	482	VAL	CA-C	-6.16	1.36	1.52
2	B	485	ARG	N-CA	-6.15	1.34	1.46
9	K	18	LYS	N-CA	6.15	1.58	1.46
1	A	935	GLN	CG-CD	-6.15	1.36	1.51
1	A	1432	GLN	CD-NE2	-6.15	1.17	1.32
4	E	148	GLU	CD-OE2	6.15	1.32	1.25
7	I	28	GLU	CB-CG	6.15	1.63	1.52
2	B	912	ILE	N-CA	-6.15	1.34	1.46
1	A	459	ARG	CA-CB	-6.15	1.40	1.53
9	K	34	THR	CA-CB	-6.15	1.37	1.53
1	A	1256	GLU	CB-CG	6.14	1.63	1.52
2	B	424	LEU	C-O	-6.14	1.11	1.23
1	A	247	ARG	CB-CG	6.14	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	410	GLY	C-N	-6.14	1.22	1.34
2	B	1185	CYS	CB-SG	-6.14	1.71	1.82
2	B	1194	ILE	C-O	6.14	1.35	1.23
1	A	728	LYS	CE-NZ	6.14	1.64	1.49
1	A	44	THR	CB-CG2	6.14	1.72	1.52
2	B	1070	GLU	N-CA	-6.14	1.34	1.46
3	C	127	ARG	CG-CD	-6.14	1.36	1.51
6	H	107	VAL	CB-CG2	-6.14	1.40	1.52
6	H	128	ASN	C-O	-6.14	1.11	1.23
1	A	74	MET	CA-CB	6.13	1.67	1.53
3	C	230	MET	N-CA	-6.13	1.34	1.46
6	H	144	ILE	C-O	6.13	1.35	1.23
1	A	426	LEU	CG-CD1	6.13	1.74	1.51
2	B	1217	TYR	CD1-CE1	-6.13	1.30	1.39
3	C	76	ASP	CB-CG	6.13	1.64	1.51
1	A	1001	ARG	CD-NE	-6.13	1.36	1.46
1	A	1409	LEU	CG-CD1	6.13	1.74	1.51
9	K	14	GLU	CA-C	6.13	1.68	1.52
1	A	1241	ARG	CZ-NH1	6.13	1.41	1.33
2	B	353	LYS	CD-CE	6.13	1.66	1.51
6	H	123	MET	CA-C	-6.13	1.37	1.52
1	A	129	LYS	C-O	6.13	1.34	1.23
2	B	785	TYR	CD2-CE2	-6.13	1.30	1.39
2	B	1137	CYS	C-N	-6.13	1.20	1.34
3	C	25	VAL	CB-CG2	-6.13	1.40	1.52
7	I	78	CYS	N-CA	6.13	1.58	1.46
8	J	8	PHE	CD2-CE2	6.13	1.51	1.39
2	B	267	ARG	CG-CD	6.12	1.67	1.51
2	B	489	SER	CA-C	-6.12	1.37	1.52
3	C	12	GLU	CG-CD	6.12	1.61	1.51
2	B	791	THR	N-CA	-6.12	1.34	1.46
4	E	122	LYS	C-O	6.12	1.34	1.23
1	A	913	LEU	CG-CD2	-6.12	1.29	1.51
1	A	1328	TYR	C-N	-6.12	1.20	1.34
2	B	224	GLN	C-N	-6.12	1.20	1.34
1	A	494	SER	CB-OG	6.12	1.50	1.42
1	A	1215	ARG	C-O	6.12	1.34	1.23
1	A	909	ASP	CG-OD1	6.11	1.39	1.25
2	B	112	LEU	CG-CD1	-6.11	1.29	1.51
2	B	799	PRO	CA-C	-6.11	1.40	1.52
8	J	60	PHE	CD2-CE2	-6.11	1.27	1.39
1	A	239	LEU	C-O	6.11	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	843	LYS	N-CA	-6.11	1.34	1.46
2	B	117	ALA	CA-C	-6.11	1.37	1.52
2	B	286	PHE	CG-CD1	-6.11	1.29	1.38
1	A	470	LEU	C-O	6.11	1.34	1.23
1	A	1119	TYR	CE1-CZ	6.11	1.46	1.38
2	B	542	MET	CB-CG	6.11	1.71	1.51
4	E	191	LYS	CD-CE	6.11	1.66	1.51
10	L	47	ARG	CG-CD	6.11	1.67	1.51
1	A	379	VAL	C-O	-6.11	1.11	1.23
2	B	173	MET	C-O	-6.11	1.11	1.23
1	A	1153	TYR	N-CA	-6.11	1.34	1.46
1	A	1347	ALA	C-O	-6.11	1.11	1.23
2	B	916	THR	CA-CB	6.11	1.69	1.53
1	A	452	LYS	CG-CD	6.10	1.73	1.52
1	A	175	ARG	CA-CB	-6.10	1.40	1.53
1	A	1024	SER	CA-C	-6.10	1.37	1.52
1	A	1441	PHE	CG-CD2	-6.10	1.29	1.38
2	B	1097	HIS	CG-CD2	6.10	1.46	1.35
5	F	152	ILE	N-CA	-6.10	1.34	1.46
3	C	261	ALA	C-O	-6.10	1.11	1.23
1	A	95	PHE	CE1-CZ	-6.10	1.25	1.37
1	A	1197	LEU	CA-C	-6.10	1.37	1.52
2	B	115	GLN	CD-OE1	6.10	1.37	1.24
1	A	1028	THR	CB-OG1	6.09	1.55	1.43
2	B	177	LYS	CD-CE	6.09	1.66	1.51
2	B	216	GLU	CG-CD	6.09	1.61	1.51
2	B	709	ASP	CA-C	-6.09	1.37	1.52
4	E	56	LYS	CA-CB	6.09	1.67	1.53
1	A	182	VAL	C-N	-6.09	1.22	1.33
3	C	15	LYS	N-CA	6.09	1.58	1.46
1	A	430	TRP	CE3-CZ3	-6.09	1.28	1.38
2	B	224	GLN	CB-CG	6.09	1.69	1.52
2	B	616	ILE	CB-CG2	6.09	1.71	1.52
2	B	712	PRO	CB-CG	6.09	1.80	1.50
8	J	41	LEU	CG-CD2	-6.09	1.29	1.51
1	A	117	GLU	CB-CG	6.09	1.63	1.52
1	A	419	LYS	C-O	-6.09	1.11	1.23
2	B	864	LYS	CA-C	6.09	1.68	1.52
2	B	945	GLU	CA-C	6.09	1.68	1.52
1	A	45	GLN	CA-C	6.08	1.68	1.52
1	A	942	PHE	C-O	-6.08	1.11	1.23
1	A	187	LYS	CA-C	6.08	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	517	THR	CA-CB	6.08	1.69	1.53
2	B	790	ASP	CA-CB	6.08	1.67	1.53
3	C	97	VAL	CA-CB	-6.08	1.42	1.54
6	H	20	TYR	CG-CD2	-6.08	1.31	1.39
1	A	211	PHE	CB-CG	-6.08	1.41	1.51
9	K	71	PHE	CD2-CE2	-6.08	1.27	1.39
1	A	662	PHE	CE1-CZ	-6.08	1.25	1.37
2	B	328	GLU	CA-CB	6.08	1.67	1.53
1	A	8	SER	CA-CB	6.08	1.62	1.52
1	A	719	VAL	CB-CG2	-6.08	1.40	1.52
1	A	1371	LEU	C-O	6.08	1.34	1.23
7	I	83	ASN	CG-OD1	6.08	1.37	1.24
1	A	796	SER	C-O	-6.08	1.11	1.23
2	B	436	VAL	CA-C	6.08	1.68	1.52
2	B	1049	ASP	C-O	-6.08	1.11	1.23
1	A	556	TRP	CE3-CZ3	-6.07	1.28	1.38
2	B	119	LEU	CA-CB	-6.07	1.39	1.53
2	B	372	SER	C-O	6.07	1.34	1.23
1	A	953	ASN	CG-ND2	-6.07	1.17	1.32
1	A	1034	GLU	CD-OE2	6.07	1.32	1.25
2	B	308	TRP	CA-C	-6.07	1.37	1.52
2	B	687	GLU	CD-OE2	-6.07	1.19	1.25
2	B	1145	SER	CA-CB	-6.07	1.43	1.52
8	J	6	ARG	NE-CZ	-6.07	1.25	1.33
1	A	149	GLU	CD-OE2	6.07	1.32	1.25
2	B	415	GLN	N-CA	6.07	1.58	1.46
8	J	49	MET	CA-CB	-6.07	1.40	1.53
1	A	1276	VAL	CB-CG2	6.07	1.65	1.52
2	B	1108	ARG	CA-C	6.07	1.68	1.52
1	A	1042	PHE	CA-C	-6.06	1.37	1.52
1	A	1100	ARG	CD-NE	-6.06	1.36	1.46
1	A	19	PHE	CE2-CZ	-6.06	1.25	1.37
1	A	149	GLU	CG-CD	6.06	1.61	1.51
2	B	20	ASP	N-CA	6.06	1.58	1.46
9	K	32	VAL	C-O	6.06	1.34	1.23
2	B	304	ASP	CB-CG	6.06	1.64	1.51
1	A	764	CYS	CA-CB	-6.06	1.40	1.53
1	A	762	SER	C-O	-6.05	1.11	1.23
2	B	181	LEU	CA-CB	-6.05	1.39	1.53
2	B	338	GLY	CA-C	-6.05	1.42	1.51
2	B	657	HIS	CA-CB	-6.05	1.40	1.53
1	A	1106	ASN	C-N	-6.05	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1040	ASN	CB-CG	-6.05	1.37	1.51
2	B	1073	TYR	CE1-CZ	-6.05	1.30	1.38
1	A	450	LEU	CA-CB	-6.05	1.39	1.53
2	B	31	TRP	N-CA	-6.05	1.34	1.46
2	B	446	LEU	CA-C	6.05	1.68	1.52
4	E	13	TRP	CG-CD1	6.05	1.45	1.36
2	B	656	GLY	CA-C	6.05	1.61	1.51
2	B	679	TYR	CG-CD2	-6.05	1.31	1.39
3	C	19	ASP	CG-OD2	6.05	1.39	1.25
8	J	54	VAL	CB-CG2	-6.05	1.40	1.52
2	B	120	ARG	CG-CD	6.05	1.67	1.51
5	F	94	LEU	CA-CB	-6.05	1.39	1.53
1	A	1022	LEU	CG-CD1	-6.05	1.29	1.51
1	A	1191	TRP	C-N	-6.05	1.20	1.34
1	A	1298	TYR	CG-CD1	-6.05	1.31	1.39
2	B	465	ASN	C-O	6.05	1.34	1.23
2	B	1083	ALA	N-CA	6.05	1.58	1.46
5	F	139	PRO	C-O	-6.05	1.11	1.23
9	K	114	LEU	CB-CG	6.04	1.70	1.52
1	A	882	SER	CB-OG	-6.04	1.34	1.42
2	B	496	ARG	N-CA	-6.04	1.34	1.46
2	B	649	LYS	CE-NZ	-6.04	1.33	1.49
1	A	792	TYR	CA-C	-6.04	1.37	1.52
3	C	204	SER	CA-C	6.04	1.68	1.52
1	A	1066	VAL	C-N	-6.04	1.20	1.34
2	B	879	ARG	N-CA	6.04	1.58	1.46
3	C	67	LEU	CA-CB	6.04	1.67	1.53
4	E	17	ARG	CD-NE	6.04	1.56	1.46
10	L	40	LEU	CA-CB	6.04	1.67	1.53
1	A	975	HIS	CA-C	6.03	1.68	1.52
2	B	722	ASP	CB-CG	6.03	1.64	1.51
10	L	47	ARG	CD-NE	6.03	1.56	1.46
1	A	175	ARG	CB-CG	6.03	1.68	1.52
1	A	503	GLN	C-O	-6.03	1.11	1.23
1	A	991	LYS	C-O	-6.03	1.11	1.23
1	A	816	HIS	N-CA	6.03	1.58	1.46
2	B	955	THR	CA-CB	6.03	1.69	1.53
3	C	227	THR	CA-CB	6.03	1.69	1.53
4	E	129	PRO	N-CD	6.03	1.56	1.47
6	H	34	ASP	CB-CG	6.03	1.64	1.51
2	B	664	THR	CB-CG2	6.03	1.72	1.52
1	A	1104	ILE	C-O	-6.02	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	17	ARG	CA-C	-6.02	1.37	1.52
2	B	763	GLN	CD-OE1	-6.02	1.10	1.24
1	A	1275	GLY	CA-C	-6.02	1.42	1.51
1	A	838	GLN	CG-CD	6.02	1.64	1.51
2	B	582	VAL	CB-CG2	-6.02	1.40	1.52
2	B	1014	PRO	N-CD	-6.02	1.39	1.47
2	B	849	GLY	N-CA	6.02	1.55	1.46
2	B	1107	ALA	CA-CB	-6.02	1.39	1.52
2	B	684	LEU	CG-CD2	6.02	1.74	1.51
5	F	79	ARG	CA-C	6.02	1.68	1.52
2	B	361	LEU	C-N	-6.01	1.22	1.34
2	B	542	MET	CA-CB	6.01	1.67	1.53
2	B	848	ARG	CA-CB	-6.01	1.40	1.53
1	A	176	LYS	CA-CB	-6.01	1.40	1.53
4	E	52	ARG	N-CA	6.01	1.58	1.46
1	A	911	SER	N-CA	6.01	1.58	1.46
1	A	1319	VAL	CB-CG2	-6.01	1.40	1.52
7	I	37	GLU	CG-CD	6.01	1.60	1.51
9	K	49	GLU	CB-CG	-6.01	1.40	1.52
2	B	104	GLU	CA-C	6.01	1.68	1.52
2	B	586	TRP	CD2-CE2	-6.01	1.34	1.41
5	F	119	ARG	N-CA	-6.01	1.34	1.46
8	J	6	ARG	CD-NE	6.01	1.56	1.46
1	A	296	LEU	C-O	-6.01	1.11	1.23
4	E	123	LEU	CA-C	6.01	1.68	1.52
1	A	226	GLU	CB-CG	6.00	1.63	1.52
1	A	376	TYR	CE2-CZ	-6.00	1.30	1.38
1	A	1368	MET	CB-CG	6.00	1.70	1.51
2	B	964	VAL	CA-CB	-6.00	1.42	1.54
7	I	42	LEU	CA-C	-6.00	1.37	1.52
1	A	389	THR	N-CA	-6.00	1.34	1.46
2	B	706	GLN	N-CA	6.00	1.58	1.46
1	A	359	LEU	N-CA	6.00	1.58	1.46
1	A	859	SER	N-CA	-6.00	1.34	1.46
2	B	708	GLU	N-CA	-6.00	1.34	1.46
4	E	169	ARG	N-CA	6.00	1.58	1.46
2	B	265	SER	N-CA	6.00	1.58	1.46
7	I	6	PHE	CA-CB	-6.00	1.40	1.53
1	A	1312	ASN	CB-CG	-6.00	1.37	1.51
3	C	83	SER	C-O	6.00	1.34	1.23
4	E	186	LEU	CA-CB	-6.00	1.40	1.53
1	A	663	SER	CB-OG	-5.99	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	85	GLU	CG-CD	5.99	1.60	1.51
1	A	862	ASN	N-CA	-5.99	1.34	1.46
1	A	907	THR	CA-CB	5.99	1.69	1.53
2	B	257	LYS	CA-C	-5.99	1.37	1.52
9	K	61	TYR	C-O	-5.99	1.11	1.23
1	A	109	HIS	CA-CB	5.99	1.67	1.53
1	A	382	PRO	CA-CB	-5.99	1.41	1.53
1	A	472	LEU	CB-CG	-5.99	1.35	1.52
1	A	589	GLN	CD-OE1	5.99	1.37	1.24
2	B	215	GLN	CB-CG	-5.99	1.36	1.52
1	A	1025	ARG	CD-NE	-5.99	1.36	1.46
1	A	1419	ASP	C-O	5.99	1.34	1.23
3	C	62	PHE	CG-CD2	5.99	1.47	1.38
3	C	229	TYR	CA-C	5.99	1.68	1.52
9	K	69	ALA	CA-C	-5.99	1.37	1.52
2	B	1027	ILE	C-O	-5.99	1.11	1.23
1	A	504	LEU	CG-CD1	-5.99	1.29	1.51
2	B	782	LEU	CG-CD2	-5.99	1.29	1.51
2	B	848	ARG	CG-CD	5.99	1.67	1.51
2	B	347	LYS	N-CA	-5.98	1.34	1.46
1	A	497	THR	CB-CG2	-5.98	1.32	1.52
1	A	876	ALA	CA-C	-5.98	1.37	1.52
2	B	486	TYR	C-N	-5.98	1.20	1.34
7	I	3	THR	CA-C	-5.98	1.37	1.52
2	B	466	TRP	C-N	5.98	1.43	1.33
2	B	586	TRP	CB-CG	-5.98	1.39	1.50
1	A	271	LYS	CE-NZ	5.97	1.64	1.49
1	A	783	THR	CA-CB	-5.97	1.37	1.53
2	B	121	ASN	C-O	5.97	1.34	1.23
5	F	114	GLU	CG-CD	5.97	1.60	1.51
9	K	24	ASP	CB-CG	5.97	1.64	1.51
2	B	995	ARG	CB-CG	5.97	1.68	1.52
7	I	21	GLU	C-O	-5.97	1.12	1.23
1	A	185	TRP	N-CA	-5.97	1.34	1.46
1	A	302	THR	CA-CB	5.97	1.68	1.53
2	B	860	MET	C-O	-5.97	1.12	1.23
6	H	60	ALA	CA-C	-5.97	1.37	1.52
1	A	368	LYS	CE-NZ	5.97	1.64	1.49
1	A	1163	ILE	CB-CG2	-5.97	1.34	1.52
1	A	1188	GLN	C-O	5.97	1.34	1.23
2	B	698	GLU	CA-C	5.97	1.68	1.52
4	E	43	LYS	C-O	5.97	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1099	PRO	CB-CG	5.96	1.79	1.50
2	B	327	ARG	CG-CD	5.96	1.66	1.51
2	B	1084	GLN	CB-CG	-5.96	1.36	1.52
2	B	1144	ALA	C-O	5.96	1.34	1.23
2	B	1183	LYS	CE-NZ	5.96	1.64	1.49
2	B	1192	TYR	CB-CG	-5.96	1.42	1.51
3	C	31	ASN	CG-ND2	5.96	1.47	1.32
9	K	77	THR	CB-CG2	5.96	1.72	1.52
2	B	451	LYS	N-CA	-5.96	1.34	1.46
6	H	98	TYR	CE1-CZ	-5.96	1.30	1.38
3	C	149	LYS	C-N	5.96	1.43	1.33
9	K	63	VAL	CA-C	-5.96	1.37	1.52
2	B	100	PRO	CB-CG	-5.96	1.20	1.50
3	C	21	ILE	C-O	5.96	1.34	1.23
3	C	110	THR	CA-C	-5.96	1.37	1.52
1	A	528	LEU	CA-C	-5.96	1.37	1.52
1	A	800	VAL	CA-CB	-5.96	1.42	1.54
1	A	1410	PHE	CE2-CZ	-5.96	1.26	1.37
2	B	771	SER	C-O	-5.96	1.12	1.23
5	F	90	ARG	CZ-NH1	5.96	1.40	1.33
1	A	461	LYS	C-O	5.95	1.34	1.23
1	A	696	GLU	CG-CD	5.95	1.60	1.51
1	A	1168	GLU	CB-CG	5.95	1.63	1.52
8	J	18	TRP	CB-CG	-5.95	1.39	1.50
1	A	1193	LEU	N-CA	5.95	1.58	1.46
7	I	27	PHE	CB-CG	5.95	1.61	1.51
1	A	462	VAL	CB-CG2	-5.95	1.40	1.52
1	A	1328	TYR	CZ-OH	5.95	1.48	1.37
2	B	105	SER	CA-CB	5.95	1.61	1.52
2	B	435	THR	CA-C	5.95	1.68	1.52
9	K	5	ASP	CG-OD2	5.95	1.39	1.25
1	A	95	PHE	CB-CG	5.95	1.61	1.51
1	A	929	LEU	N-CA	-5.95	1.34	1.46
1	A	1010	ALA	C-O	-5.95	1.12	1.23
2	B	694	ASP	C-O	5.95	1.34	1.23
3	C	67	LEU	N-CA	5.95	1.58	1.46
1	A	95	PHE	CG-CD2	5.95	1.47	1.38
1	A	217	LYS	CA-C	5.95	1.68	1.52
2	B	629	ASP	C-N	-5.95	1.20	1.34
6	H	103	LYS	CA-C	-5.95	1.37	1.52
1	A	125	ALA	N-CA	-5.95	1.34	1.46
3	C	80	LEU	CG-CD1	-5.95	1.29	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	203	GLU	CD-OE2	5.95	1.32	1.25
9	K	66	PRO	CA-C	-5.95	1.41	1.52
2	B	189	LEU	C-O	5.94	1.34	1.23
2	B	584	GLY	C-O	5.94	1.33	1.23
2	B	1218	THR	CA-CB	-5.94	1.37	1.53
2	B	48	LEU	CA-CB	-5.94	1.40	1.53
9	K	2	ASN	C-O	5.94	1.34	1.23
2	B	1068	GLY	CA-C	-5.94	1.42	1.51
5	F	136	ARG	NE-CZ	-5.94	1.25	1.33
6	H	140	ALA	N-CA	5.94	1.58	1.46
2	B	249	ARG	N-CA	5.94	1.58	1.46
2	B	513	GLN	CD-NE2	5.94	1.47	1.32
2	B	815	ARG	CD-NE	-5.94	1.36	1.46
3	C	241	ASP	CG-OD1	5.94	1.39	1.25
1	A	467	THR	C-O	-5.94	1.12	1.23
2	B	1193	GLN	C-N	-5.94	1.20	1.34
2	B	458	LYS	CB-CG	5.93	1.68	1.52
2	B	678	GLU	CA-CB	5.93	1.67	1.53
4	E	196	VAL	N-CA	5.93	1.58	1.46
1	A	276	LEU	CA-CB	-5.93	1.40	1.53
1	A	1287	TYR	CE2-CZ	5.93	1.46	1.38
7	I	79	HIS	C-O	5.93	1.34	1.23
1	A	87	ALA	CA-C	-5.93	1.37	1.52
1	A	658	LEU	C-O	5.93	1.34	1.23
2	B	1032	SER	CA-CB	5.93	1.61	1.52
1	A	666	ILE	CA-CB	-5.93	1.41	1.54
4	E	193	GLY	CA-C	5.93	1.61	1.51
2	B	284	ILE	C-O	5.93	1.34	1.23
7	I	20	LYS	C-O	5.93	1.34	1.23
1	A	192	GLY	CA-C	5.92	1.61	1.51
1	A	483	ASP	N-CA	5.92	1.58	1.46
2	B	456	GLY	C-O	5.92	1.33	1.23
2	B	581	PHE	CG-CD2	-5.92	1.29	1.38
2	B	581	PHE	CA-CB	5.92	1.67	1.53
2	B	627	PHE	C-O	-5.92	1.12	1.23
2	B	1106	ARG	N-CA	5.92	1.58	1.46
3	C	146	LYS	N-CA	-5.92	1.34	1.46
1	A	1142	THR	CA-CB	-5.92	1.38	1.53
2	B	380	TYR	CA-CB	-5.92	1.41	1.53
2	B	761	HIS	C-O	-5.92	1.12	1.23
7	I	17	ARG	NE-CZ	5.92	1.40	1.33
1	A	324	SER	N-CA	5.92	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	72	LYS	C-O	-5.92	1.12	1.23
1	A	19	PHE	CG-CD1	-5.92	1.29	1.38
3	C	92	CYS	CA-CB	5.92	1.67	1.53
1	A	630	ILE	CA-CB	-5.92	1.41	1.54
1	A	1440	ALA	C-O	5.92	1.34	1.23
2	B	732	SER	CB-OG	5.92	1.50	1.42
6	H	109	LYS	C-O	5.92	1.34	1.23
8	J	55	ASP	N-CA	5.92	1.58	1.46
9	K	97	LYS	C-N	-5.92	1.20	1.34
1	A	1298	TYR	CD2-CE2	-5.92	1.30	1.39
2	B	275	TYR	C-O	-5.92	1.12	1.23
2	B	1012	ILE	CA-CB	-5.92	1.41	1.54
7	I	61	ASP	C-O	-5.92	1.12	1.23
9	K	105	PHE	CG-CD1	5.92	1.47	1.38
1	A	945	GLU	CA-CB	5.92	1.67	1.53
2	B	905	VAL	CA-CB	-5.92	1.42	1.54
4	E	20	LYS	N-CA	-5.92	1.34	1.46
1	A	464	PRO	N-CA	-5.91	1.37	1.47
2	B	687	GLU	CB-CG	5.91	1.63	1.52
2	B	692	TYR	CD1-CE1	5.91	1.48	1.39
2	B	711	GLU	C-N	5.91	1.45	1.34
1	A	1336	MET	CG-SD	-5.91	1.65	1.81
2	B	1175	LEU	CG-CD1	5.91	1.73	1.51
1	A	1147	THR	C-O	-5.91	1.12	1.23
4	E	7	ARG	CZ-NH1	5.91	1.40	1.33
1	A	1162	VAL	CB-CG2	5.91	1.65	1.52
2	B	203	PHE	CD1-CE1	-5.91	1.27	1.39
7	I	107	SER	C-O	-5.91	1.12	1.23
9	K	49	GLU	CD-OE2	5.91	1.32	1.25
9	K	81	TYR	CZ-OH	5.91	1.47	1.37
3	C	120	ILE	CB-CG1	-5.90	1.37	1.54
3	C	135	GLN	C-O	-5.90	1.12	1.23
4	E	98	ILE	CB-CG2	5.90	1.71	1.52
2	B	1077	THR	C-N	-5.90	1.22	1.33
4	E	180	ARG	CD-NE	5.90	1.56	1.46
1	A	152	VAL	C-O	5.90	1.34	1.23
1	A	575	LYS	CD-CE	5.90	1.66	1.51
2	B	252	SER	N-CA	5.90	1.58	1.46
2	B	788	ARG	N-CA	5.90	1.58	1.46
4	E	118	PRO	C-O	5.90	1.35	1.23
1	A	688	LYS	C-O	-5.90	1.12	1.23
2	B	349	ILE	CA-CB	-5.90	1.41	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	LYS	CB-CG	5.89	1.68	1.52
2	B	682	SER	CA-C	-5.89	1.37	1.52
4	E	104	ASN	CG-OD1	5.89	1.36	1.24
6	H	78	SER	CB-OG	-5.89	1.34	1.42
1	A	38	PRO	CB-CG	-5.89	1.20	1.50
2	B	164	LYS	CE-NZ	5.89	1.63	1.49
2	B	634	TYR	CG-CD1	-5.89	1.31	1.39
5	F	104	ASN	CG-ND2	5.89	1.47	1.32
2	B	761	HIS	CG-CD2	5.89	1.45	1.35
2	B	812	LEU	C-O	-5.89	1.12	1.23
5	F	111	LEU	C-O	5.89	1.34	1.23
1	A	1363	VAL	CB-CG2	5.89	1.65	1.52
4	E	114	ASN	CB-CG	-5.89	1.37	1.51
4	E	145	THR	CA-CB	-5.89	1.38	1.53
8	J	48	ARG	CA-C	-5.89	1.37	1.52
1	A	63	ARG	CB-CG	5.88	1.68	1.52
1	A	528	LEU	CG-CD2	5.88	1.73	1.51
1	A	1045	VAL	CA-CB	-5.88	1.42	1.54
1	A	1191	TRP	CG-CD1	5.88	1.45	1.36
2	B	461	LEU	C-O	-5.88	1.12	1.23
2	B	880	THR	N-CA	5.88	1.58	1.46
8	J	28	ASP	CB-CG	5.88	1.64	1.51
1	A	1044	TRP	CZ2-CH2	5.88	1.48	1.37
2	B	228	LYS	CD-CE	5.88	1.66	1.51
1	A	1200	ALA	C-O	5.88	1.34	1.23
2	B	661	LEU	C-N	-5.88	1.20	1.34
1	A	1317	MET	C-O	5.88	1.34	1.23
1	A	42	ASP	C-O	5.88	1.34	1.23
1	A	489	LEU	N-CA	-5.88	1.34	1.46
1	A	1431	GLY	C-O	-5.88	1.14	1.23
2	B	348	ARG	CA-CB	-5.88	1.41	1.53
1	A	815	PHE	CG-CD1	-5.88	1.29	1.38
1	A	944	ARG	NE-CZ	-5.88	1.25	1.33
3	C	123	ASN	CB-CG	5.88	1.64	1.51
4	E	135	PHE	CE2-CZ	-5.88	1.26	1.37
9	K	12	LEU	CA-C	-5.88	1.37	1.52
2	B	687	GLU	CG-CD	5.88	1.60	1.51
2	B	1172	ILE	CB-CG2	5.88	1.71	1.52
1	A	1042	PHE	CD1-CE1	-5.87	1.27	1.39
2	B	1154	ALA	CA-C	5.87	1.68	1.52
5	F	96	THR	CA-CB	-5.87	1.38	1.53
7	I	85	PHE	C-O	-5.87	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	MET	SD-CE	-5.87	1.45	1.77
1	A	152	VAL	N-CA	5.87	1.58	1.46
1	A	839	ARG	CD-NE	5.87	1.56	1.46
2	B	910	VAL	C-O	-5.87	1.12	1.23
2	B	1109	GLY	C-N	5.87	1.45	1.34
3	C	20	PHE	CA-CB	-5.87	1.41	1.53
4	E	23	VAL	N-CA	-5.87	1.34	1.46
1	A	1195	LEU	CA-CB	-5.87	1.40	1.53
1	A	86	LEU	CG-CD1	-5.87	1.30	1.51
10	L	27	LEU	CA-C	5.87	1.68	1.52
1	A	809	THR	CA-CB	5.87	1.68	1.53
1	A	983	ILE	CA-C	-5.87	1.37	1.52
1	A	359	LEU	CG-CD2	-5.87	1.30	1.51
2	B	703	ILE	C-O	5.87	1.34	1.23
6	H	21	ASN	CG-ND2	5.87	1.47	1.32
1	A	352	VAL	CA-CB	-5.86	1.42	1.54
1	A	383	TYR	CZ-OH	-5.86	1.27	1.37
2	B	372	SER	C-N	-5.86	1.20	1.34
1	A	300	VAL	CA-C	5.86	1.68	1.52
2	B	320	ASP	C-O	-5.86	1.12	1.23
2	B	711	GLU	CA-CB	-5.86	1.41	1.53
2	B	1134	GLU	CA-CB	-5.86	1.41	1.53
2	B	1026	LEU	N-CA	-5.86	1.34	1.46
6	H	103	LYS	C-O	-5.86	1.12	1.23
3	C	20	PHE	CE1-CZ	5.86	1.48	1.37
2	B	65	GLU	C-O	5.86	1.34	1.23
2	B	69	LEU	C-O	5.86	1.34	1.23
3	C	68	GLY	N-CA	5.86	1.54	1.46
1	A	325	ILE	C-O	-5.86	1.12	1.23
5	F	143	PHE	CE1-CZ	5.86	1.48	1.37
4	E	201	LYS	C-O	5.85	1.34	1.23
1	A	364	VAL	CB-CG2	-5.85	1.40	1.52
1	A	689	LYS	CE-NZ	5.85	1.63	1.49
2	B	1108	ARG	CZ-NH1	5.85	1.40	1.33
8	J	2	ILE	CB-CG2	5.85	1.71	1.52
1	A	48	ALA	N-CA	5.85	1.58	1.46
2	B	479	VAL	CA-CB	-5.85	1.42	1.54
1	A	740	LEU	CA-CB	-5.85	1.40	1.53
3	C	49	VAL	CA-CB	-5.85	1.42	1.54
3	C	184	ASN	CA-CB	5.85	1.68	1.53
1	A	326	ARG	CD-NE	5.85	1.56	1.46
2	B	289	LEU	C-N	-5.85	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	PRO	CB-CG	-5.85	1.20	1.50
2	B	1197	PRO	CA-CB	-5.85	1.41	1.53
3	C	142	VAL	CB-CG1	5.85	1.65	1.52
9	K	32	VAL	CA-CB	-5.85	1.42	1.54
9	K	68	PHE	CE2-CZ	-5.85	1.26	1.37
1	A	93	VAL	CB-CG1	5.84	1.65	1.52
1	A	408	ASP	CB-CG	-5.84	1.39	1.51
2	B	233	PRO	CA-C	-5.84	1.41	1.52
2	B	355	ILE	CB-CG1	-5.84	1.37	1.54
2	B	1043	ASP	CG-OD2	5.84	1.38	1.25
3	C	261	ALA	CA-C	-5.84	1.37	1.52
6	H	80	ARG	CZ-NH2	5.84	1.40	1.33
4	E	151	PRO	N-CD	-5.84	1.39	1.47
1	A	154	SER	CA-CB	5.84	1.61	1.52
1	A	34	LYS	CD-CE	5.84	1.65	1.51
1	A	711	ARG	CZ-NH1	-5.84	1.25	1.33
2	B	845	SER	C-N	-5.84	1.20	1.34
4	E	79	TRP	CD2-CE3	5.84	1.49	1.40
4	E	110	PHE	CE1-CZ	-5.84	1.26	1.37
6	H	21	ASN	CA-C	-5.84	1.37	1.52
5	F	77	ASP	CG-OD2	5.84	1.38	1.25
6	H	80	ARG	CB-CG	5.84	1.68	1.52
6	H	116	TYR	CZ-OH	5.84	1.47	1.37
1	A	978	PRO	CB-CG	5.84	1.79	1.50
1	A	1103	GLU	C-O	5.84	1.34	1.23
4	E	187	TYR	CA-C	-5.84	1.37	1.52
6	H	15	VAL	C-O	5.84	1.34	1.23
7	I	41	PRO	CA-C	-5.84	1.41	1.52
2	B	591	ARG	CZ-NH1	5.83	1.40	1.33
1	A	42	ASP	CB-CG	5.83	1.64	1.51
1	A	291	GLU	CA-CB	5.83	1.66	1.53
1	A	821	ARG	CB-CG	5.83	1.68	1.52
2	B	65	GLU	CA-C	5.83	1.68	1.52
6	H	109	LYS	CB-CG	5.83	1.68	1.52
2	B	187	SER	C-O	5.83	1.34	1.23
2	B	522	VAL	CB-CG1	-5.83	1.40	1.52
2	B	131	ASP	C-O	5.83	1.34	1.23
2	B	197	PHE	N-CA	-5.83	1.34	1.46
1	A	488	ASN	N-CA	-5.83	1.34	1.46
1	A	659	HIS	CB-CG	-5.83	1.39	1.50
1	A	48	ALA	CA-C	5.83	1.68	1.52
1	A	467	THR	CB-CG2	-5.83	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	772	GLY	N-CA	-5.83	1.37	1.46
9	K	83	PRO	N-CA	-5.83	1.37	1.47
1	A	218	ASP	CA-C	5.82	1.68	1.52
1	A	705	LYS	CG-CD	5.82	1.72	1.52
1	A	1355	VAL	C-O	-5.82	1.12	1.23
7	I	58	VAL	CA-CB	-5.82	1.42	1.54
1	A	1298	TYR	CD1-CE1	5.82	1.48	1.39
2	B	550	ASP	C-O	5.82	1.34	1.23
2	B	602	THR	CB-CG2	-5.82	1.33	1.52
3	C	45	ALA	CA-CB	5.82	1.64	1.52
7	I	82	GLU	CB-CG	5.82	1.63	1.52
4	E	155	ARG	N-CA	5.82	1.57	1.46
1	A	624	SER	C-O	-5.82	1.12	1.23
1	A	795	GLU	CD-OE1	5.82	1.32	1.25
3	C	60	ASP	CB-CG	-5.82	1.39	1.51
3	C	125	MET	CA-C	5.82	1.68	1.52
1	A	702	LEU	CG-CD1	5.81	1.73	1.51
1	A	785	PRO	N-CD	-5.81	1.39	1.47
1	A	1208	THR	CA-C	5.81	1.68	1.52
1	A	1427	ASN	CA-CB	-5.81	1.38	1.53
2	B	278	GLN	CD-NE2	5.81	1.47	1.32
3	C	30	ALA	C-O	5.81	1.34	1.23
3	C	110	THR	CB-CG2	-5.81	1.33	1.52
2	B	629	ASP	CG-OD2	5.81	1.38	1.25
7	I	74	GLU	CG-CD	5.81	1.60	1.51
5	F	143	PHE	CE2-CZ	-5.81	1.26	1.37
9	K	44	ASN	CG-ND2	5.81	1.47	1.32
10	L	31	CYS	CA-CB	5.81	1.66	1.53
1	A	530	GLY	N-CA	-5.81	1.37	1.46
6	H	27	GLU	CD-OE1	5.81	1.32	1.25
6	H	29	ALA	CA-C	5.81	1.68	1.52
7	I	41	PRO	CG-CD	-5.81	1.31	1.50
1	A	840	ARG	CZ-NH2	5.81	1.40	1.33
4	E	129	PRO	N-CA	5.81	1.57	1.47
1	A	597	LEU	CG-CD1	5.80	1.73	1.51
2	B	497	ARG	CA-CB	-5.80	1.41	1.53
1	A	1266	THR	C-O	-5.80	1.12	1.23
2	B	113	TYR	CD2-CE2	-5.80	1.30	1.39
3	C	267	GLN	N-CA	5.80	1.57	1.46
6	H	113	ALA	CA-CB	-5.80	1.40	1.52
1	A	1374	VAL	CB-CG1	5.80	1.65	1.52
2	B	949	VAL	CB-CG1	-5.80	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1008	PRO	CA-CB	-5.80	1.42	1.53
4	E	106	GLN	CB-CG	5.80	1.68	1.52
1	A	845	LEU	CG-CD1	-5.80	1.30	1.51
2	B	422	LYS	CG-CD	5.80	1.72	1.52
3	C	235	VAL	CB-CG2	5.80	1.65	1.52
1	A	21	LEU	CA-C	5.80	1.68	1.52
1	A	243	PRO	CA-CB	-5.80	1.42	1.53
1	A	1066	VAL	CA-C	-5.80	1.37	1.52
2	B	373	ARG	CD-NE	5.80	1.56	1.46
1	A	539	THR	N-CA	-5.79	1.34	1.46
1	A	472	LEU	CG-CD2	-5.79	1.30	1.51
1	A	961	ARG	CD-NE	5.79	1.56	1.46
2	B	626	ILE	CA-CB	-5.79	1.41	1.54
2	B	826	ALA	C-O	-5.79	1.12	1.23
3	C	156	THR	CA-C	-5.79	1.37	1.52
9	K	108	GLU	CA-CB	-5.79	1.41	1.53
2	B	745	PRO	CG-CD	5.79	1.69	1.50
3	C	210	GLU	C-O	-5.79	1.12	1.23
9	K	96	ASN	CB-CG	5.79	1.64	1.51
1	A	854	ASN	C-O	-5.79	1.12	1.23
1	A	1140	HIS	CA-C	-5.79	1.37	1.52
2	B	190	TYR	CE2-CZ	5.79	1.46	1.38
2	B	462	ALA	CA-CB	5.79	1.64	1.52
5	F	102	SER	C-O	5.79	1.34	1.23
1	A	274	ILE	N-CA	5.79	1.57	1.46
1	A	531	ILE	CB-CG2	-5.79	1.34	1.52
2	B	983	ARG	CD-NE	-5.79	1.36	1.46
1	A	119	ASN	CG-OD1	-5.79	1.11	1.24
1	A	139	TRP	N-CA	5.79	1.57	1.46
2	B	994	TYR	N-CA	-5.79	1.34	1.46
2	B	317	CYS	CB-SG	-5.78	1.72	1.81
2	B	432	MET	CA-CB	5.78	1.66	1.53
3	C	253	LYS	N-CA	5.78	1.57	1.46
1	A	377	PRO	CB-CG	-5.78	1.21	1.50
1	A	1365	TYR	CG-CD1	-5.78	1.31	1.39
1	A	741	ASN	CG-OD1	5.78	1.36	1.24
2	B	904	ARG	C-O	-5.78	1.12	1.23
9	K	53	ASP	CB-CG	5.78	1.63	1.51
1	A	1092	LYS	CA-C	5.78	1.68	1.52
1	A	1169	ILE	CA-CB	5.78	1.68	1.54
1	A	6	TYR	CZ-OH	-5.78	1.28	1.37
1	A	546	VAL	N-CA	-5.78	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	344	LYS	C-O	5.78	1.34	1.23
5	F	137	TYR	CD1-CE1	5.78	1.48	1.39
2	B	593	PRO	CA-CB	5.78	1.65	1.53
1	A	239	LEU	N-CA	-5.77	1.34	1.46
2	B	712	PRO	N-CA	5.77	1.57	1.47
3	C	89	GLU	CA-C	-5.77	1.38	1.52
9	K	109	TRP	CG-CD2	5.77	1.53	1.43
1	A	1072	ILE	C-N	-5.77	1.22	1.33
2	B	1110	PRO	N-CD	5.77	1.55	1.47
1	A	109	HIS	CB-CG	5.77	1.60	1.50
1	A	1144	LYS	N-CA	-5.77	1.34	1.46
2	B	58	THR	C-O	5.77	1.34	1.23
2	B	742	GLU	N-CA	-5.77	1.34	1.46
1	A	965	GLN	CB-CG	-5.77	1.36	1.52
2	B	769	TYR	CE1-CZ	-5.77	1.31	1.38
4	E	213	ILE	C-O	-5.77	1.12	1.23
1	A	599	SER	CA-C	-5.76	1.38	1.52
2	B	965	LYS	C-O	-5.76	1.12	1.23
1	A	616	VAL	CB-CG2	-5.76	1.40	1.52
1	A	812	GLU	CD-OE2	-5.76	1.19	1.25
2	B	498	THR	C-O	-5.76	1.12	1.23
4	E	45	LYS	CG-CD	5.76	1.72	1.52
1	A	397	ASN	CG-ND2	5.76	1.47	1.32
1	A	1261	LYS	CE-NZ	5.76	1.63	1.49
2	B	793	ALA	C-O	-5.76	1.12	1.23
2	B	889	THR	CB-CG2	5.76	1.71	1.52
1	A	195	ASP	CB-CG	-5.76	1.39	1.51
3	C	161	LYS	CE-NZ	-5.76	1.34	1.49
1	A	1065	GLY	CA-C	5.76	1.61	1.51
10	L	42	ARG	CD-NE	5.76	1.56	1.46
1	A	271	LYS	CD-CE	5.75	1.65	1.51
2	B	999	MET	CA-C	-5.75	1.38	1.52
1	A	833	GLU	CD-OE2	5.75	1.31	1.25
2	B	47	GLN	CG-CD	5.75	1.64	1.51
2	B	938	SER	CA-C	-5.75	1.38	1.52
9	K	10	PHE	CG-CD1	-5.75	1.30	1.38
1	A	856	THR	N-CA	-5.75	1.34	1.46
1	A	1439	GLY	CA-C	5.75	1.61	1.51
2	B	239	GLU	N-CA	-5.75	1.34	1.46
4	E	46	TYR	CZ-OH	5.75	1.47	1.37
6	H	9	ILE	C-O	5.75	1.34	1.23
8	J	18	TRP	CE3-CZ3	-5.75	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	78	THR	CA-CB	-5.75	1.38	1.53
9	K	102	LYS	CA-C	5.75	1.68	1.52
2	B	1176	ASN	C-O	5.75	1.34	1.23
1	A	96	ILE	CA-C	5.75	1.67	1.52
1	A	393	ARG	CD-NE	5.75	1.56	1.46
1	A	944	ARG	CG-CD	5.75	1.66	1.51
2	B	994	TYR	CZ-OH	5.75	1.47	1.37
1	A	589	GLN	CA-C	-5.75	1.38	1.52
1	A	596	THR	C-O	-5.75	1.12	1.23
1	A	640	GLN	CD-NE2	5.75	1.47	1.32
2	B	1055	ILE	CA-C	-5.75	1.38	1.52
2	B	1092	TYR	CG-CD2	-5.75	1.31	1.39
2	B	1094	ARG	CA-CB	-5.75	1.41	1.53
1	A	171	GLN	CG-CD	5.75	1.64	1.51
2	B	1078	GLY	C-N	-5.75	1.20	1.34
1	A	22	PHE	CD2-CE2	-5.74	1.27	1.39
1	A	544	ASP	CG-OD1	5.74	1.38	1.25
1	A	665	GLY	CA-C	-5.74	1.42	1.51
1	A	1339	LEU	C-O	5.74	1.34	1.23
2	B	1204	PHE	CE1-CZ	-5.74	1.26	1.37
4	E	117	THR	CB-CG2	-5.74	1.33	1.52
1	A	926	GLN	CA-C	-5.74	1.38	1.52
2	B	876	LYS	C-O	-5.74	1.12	1.23
8	J	23	ASN	CG-ND2	5.74	1.47	1.32
2	B	25	ILE	C-O	-5.74	1.12	1.23
2	B	398	ARG	CG-CD	5.74	1.66	1.51
2	B	634	TYR	CA-C	-5.74	1.38	1.52
2	B	1149	GLU	CG-CD	5.74	1.60	1.51
3	C	36	VAL	CB-CG2	-5.74	1.40	1.52
5	F	146	TRP	CE3-CZ3	-5.74	1.28	1.38
1	A	129	LYS	CA-CB	5.74	1.66	1.53
1	A	507	VAL	C-N	-5.74	1.23	1.34
2	B	362	PRO	CB-CG	-5.74	1.21	1.50
2	B	602	THR	N-CA	5.74	1.57	1.46
3	C	147	LEU	C-O	-5.74	1.12	1.23
6	H	33	GLN	CB-CG	5.74	1.68	1.52
7	I	93	LYS	CG-CD	5.74	1.72	1.52
1	A	1028	THR	C-O	5.74	1.34	1.23
2	B	294	ASP	CG-OD2	5.74	1.38	1.25
3	C	45	ALA	CA-C	-5.74	1.38	1.52
3	C	170	TRP	CZ2-CH2	-5.74	1.26	1.37
3	C	216	GLY	C-O	5.74	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	105	PHE	CG-CD2	5.74	1.47	1.38
1	A	228	PHE	N-CA	5.73	1.57	1.46
6	H	87	ARG	CA-C	5.73	1.67	1.52
7	I	107	SER	N-CA	5.73	1.57	1.46
2	B	842	ASN	CB-CG	-5.73	1.37	1.51
6	H	146	ARG	C-OXT	5.73	1.34	1.23
1	A	1154	TYR	CA-CB	5.73	1.66	1.53
2	B	661	LEU	CG-CD1	-5.73	1.30	1.51
3	C	33	LEU	CG-CD2	-5.73	1.30	1.51
3	C	47	ASP	CG-OD2	5.73	1.38	1.25
3	C	231	ASN	CG-OD1	5.73	1.36	1.24
7	I	65	ASP	CG-OD1	5.73	1.38	1.25
4	E	11	ARG	CB-CG	5.73	1.68	1.52
4	E	215	MET	CG-SD	5.73	1.96	1.81
2	B	979	LYS	CB-CG	-5.73	1.37	1.52
2	B	662	MET	C-O	-5.73	1.12	1.23
3	C	137	LYS	CD-CE	5.73	1.65	1.51
2	B	1132	GLU	CA-CB	5.72	1.66	1.53
1	A	362	ASP	CB-CG	-5.72	1.39	1.51
1	A	409	SER	CB-OG	5.72	1.49	1.42
1	A	680	THR	C-O	-5.72	1.12	1.23
1	A	1195	LEU	CG-CD2	-5.72	1.30	1.51
2	B	852	ARG	N-CA	-5.72	1.34	1.46
2	B	187	SER	CB-OG	-5.72	1.34	1.42
2	B	1224	PHE	CA-C	5.72	1.67	1.52
4	E	39	LEU	CG-CD2	5.72	1.73	1.51
1	A	388	LEU	CB-CG	-5.72	1.35	1.52
1	A	561	PRO	CA-CB	5.72	1.65	1.53
1	A	696	GLU	N-CA	-5.72	1.34	1.46
3	C	149	LYS	CB-CG	5.72	1.68	1.52
8	J	26	GLN	CD-NE2	5.72	1.47	1.32
1	A	626	ASN	CB-CG	5.71	1.64	1.51
1	A	639	PRO	CG-CD	-5.71	1.31	1.50
2	B	698	GLU	N-CA	-5.71	1.34	1.46
1	A	709	THR	CB-CG2	-5.71	1.33	1.52
3	C	55	THR	CA-C	5.71	1.67	1.52
3	C	220	ASP	CG-OD1	5.71	1.38	1.25
1	A	407	ARG	CB-CG	5.71	1.68	1.52
1	A	807	GLY	C-N	-5.71	1.21	1.34
1	A	866	PHE	C-O	-5.71	1.12	1.23
1	A	923	LEU	CA-CB	5.71	1.66	1.53
2	B	531	GLN	C-N	5.71	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	445	ASN	CG-OD1	5.71	1.36	1.24
1	A	556	TRP	CD2-CE3	-5.71	1.31	1.40
1	A	1329	THR	C-O	5.70	1.34	1.23
2	B	183	GLU	CB-CG	5.70	1.62	1.52
2	B	257	LYS	N-CA	-5.70	1.34	1.46
3	C	181	ASP	C-N	-5.70	1.23	1.34
1	A	730	GLY	N-CA	-5.70	1.37	1.46
2	B	171	PRO	C-O	-5.70	1.11	1.23
2	B	401	PHE	CD1-CE1	-5.70	1.27	1.39
2	B	667	GLN	N-CA	5.70	1.57	1.46
2	B	1133	MET	CB-CG	-5.70	1.33	1.51
1	A	6	TYR	CD2-CE2	5.70	1.47	1.39
1	A	994	GLN	C-O	-5.70	1.12	1.23
3	C	99	LEU	C-N	5.70	1.47	1.34
3	C	267	GLN	CB-CG	5.70	1.68	1.52
1	A	185	TRP	CG-CD2	-5.70	1.33	1.43
1	A	391	LEU	CG-CD1	-5.70	1.30	1.51
1	A	801	GLU	CG-CD	5.70	1.60	1.51
1	A	1450	LEU	CG-CD1	5.70	1.73	1.51
2	B	999	MET	CG-SD	5.70	1.96	1.81
3	C	134	ILE	CB-CG2	-5.70	1.35	1.52
4	E	185	ALA	N-CA	-5.70	1.34	1.46
1	A	232	GLU	CG-CD	5.69	1.60	1.51
10	L	31	CYS	N-CA	5.69	1.57	1.46
1	A	494	SER	C-O	5.69	1.34	1.23
2	B	459	TYR	C-O	-5.69	1.12	1.23
2	B	1129	ARG	N-CA	-5.69	1.34	1.46
3	C	175	ALA	C-O	5.69	1.34	1.23
3	C	255	VAL	CB-CG2	-5.69	1.40	1.52
1	A	906	HIS	C-O	-5.69	1.12	1.23
2	B	664	THR	C-O	-5.69	1.12	1.23
4	E	68	SER	CA-C	-5.69	1.38	1.52
8	J	18	TRP	CZ3-CH2	5.69	1.49	1.40
8	J	35	ALA	CA-CB	5.69	1.64	1.52
8	J	37	SER	CB-OG	-5.69	1.34	1.42
6	H	25	ARG	N-CA	5.69	1.57	1.46
1	A	156	ASP	N-CA	5.69	1.57	1.46
1	A	804	TYR	CG-CD2	-5.69	1.31	1.39
1	A	958	VAL	CB-CG1	-5.69	1.41	1.52
3	C	149	LYS	C-O	5.69	1.34	1.23
9	K	43	GLY	CA-C	5.69	1.60	1.51
1	A	506	ALA	CA-C	-5.69	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	536	LEU	CA-C	5.69	1.67	1.52
4	E	42	PHE	CE2-CZ	5.69	1.48	1.37
7	I	82	GLU	CD-OE2	5.69	1.31	1.25
1	A	305	ASP	CA-C	5.68	1.67	1.52
2	B	436	VAL	CB-CG2	5.68	1.64	1.52
2	B	820	GLY	C-O	-5.68	1.14	1.23
7	I	36	GLU	C-N	-5.68	1.21	1.34
1	A	273	ASN	C-O	5.68	1.34	1.23
1	A	910	PRO	CB-CG	5.68	1.78	1.50
2	B	305	VAL	CB-CG2	5.68	1.64	1.52
1	A	616	VAL	CB-CG1	-5.68	1.41	1.52
2	B	177	LYS	CG-CD	5.68	1.71	1.52
2	B	1210	MET	CA-C	-5.68	1.38	1.52
9	K	28	PRO	C-O	-5.68	1.11	1.23
2	B	51	PHE	CA-CB	5.68	1.66	1.53
2	B	694	ASP	N-CA	5.68	1.57	1.46
2	B	1181	GLU	CB-CG	5.68	1.62	1.52
4	E	204	THR	CA-CB	-5.68	1.38	1.53
2	B	1072	MET	C-O	5.68	1.34	1.23
2	B	1094	ARG	CA-C	-5.68	1.38	1.52
4	E	167	ARG	N-CA	-5.68	1.34	1.46
7	I	101	PHE	CA-CB	-5.68	1.41	1.53
2	B	405	ARG	C-O	-5.67	1.12	1.23
2	B	529	GLU	CB-CG	5.67	1.62	1.52
1	A	518	LYS	C-O	-5.67	1.12	1.23
1	A	1225	PHE	CG-CD1	5.67	1.47	1.38
2	B	912	ILE	C-N	5.67	1.43	1.33
1	A	775	ILE	C-N	-5.67	1.21	1.34
1	A	1374	VAL	CA-CB	-5.67	1.42	1.54
4	E	205	SER	CA-C	-5.67	1.38	1.52
5	F	142	SER	CB-OG	-5.67	1.34	1.42
1	A	716	ASP	CB-CG	-5.67	1.39	1.51
2	B	1188	LYS	C-O	5.67	1.34	1.23
7	I	58	VAL	CA-C	-5.67	1.38	1.52
9	K	66	PRO	C-O	-5.67	1.11	1.23
1	A	787	PHE	CG-CD2	-5.67	1.30	1.38
2	B	1189	ILE	CA-CB	5.67	1.67	1.54
3	C	84	ARG	CB-CG	5.67	1.67	1.52
1	A	452	LYS	CB-CG	5.67	1.67	1.52
2	B	303	TYR	CB-CG	5.67	1.60	1.51
3	C	188	HIS	CA-C	5.67	1.67	1.52
1	A	1260	LEU	C-N	-5.66	1.21	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1379	GLY	N-CA	-5.66	1.37	1.46
3	C	142	VAL	CB-CG2	5.66	1.64	1.52
6	H	80	ARG	C-O	-5.66	1.12	1.23
9	K	97	LYS	CA-C	-5.66	1.38	1.52
1	A	486	GLU	CB-CG	5.66	1.62	1.52
1	A	795	GLU	CD-OE2	5.66	1.31	1.25
2	B	242	SER	C-O	-5.66	1.12	1.23
5	F	97	ARG	CZ-NH2	-5.66	1.25	1.33
5	F	154	ASP	CB-CG	5.66	1.63	1.51
1	A	970	THR	CB-CG2	-5.66	1.33	1.52
2	B	1096	ARG	CA-CB	5.66	1.66	1.53
1	A	26	GLU	CB-CG	5.66	1.62	1.52
1	A	945	GLU	CD-OE1	5.66	1.31	1.25
2	B	1220	ARG	CG-CD	5.66	1.66	1.51
4	E	21	GLU	CA-C	-5.66	1.38	1.52
2	B	39	ARG	CG-CD	-5.66	1.37	1.51
2	B	115	GLN	CA-C	5.66	1.67	1.52
1	A	1428	VAL	CB-CG1	-5.66	1.41	1.52
1	A	711	ARG	C-N	-5.65	1.21	1.34
1	A	224	PHE	CB-CG	5.65	1.60	1.51
1	A	726	ARG	CG-CD	5.65	1.66	1.51
1	A	1108	ALA	C-O	5.65	1.34	1.23
2	B	104	GLU	CG-CD	5.65	1.60	1.51
2	B	287	ARG	NE-CZ	-5.65	1.25	1.33
3	C	141	GLY	C-O	5.65	1.32	1.23
1	A	465	TYR	CA-CB	5.65	1.66	1.53
1	A	961	ARG	CZ-NH1	5.65	1.40	1.33
1	A	1262	LYS	CB-CG	5.65	1.67	1.52
2	B	980	PHE	CE2-CZ	-5.65	1.26	1.37
6	H	110	ASP	CB-CG	5.65	1.63	1.51
6	H	132	LEU	C-O	5.65	1.34	1.23
1	A	952	ALA	N-CA	-5.65	1.35	1.46
2	B	323	VAL	CA-CB	-5.65	1.42	1.54
2	B	1097	HIS	CE1-NE2	5.65	1.45	1.32
3	C	34	ARG	CG-CD	5.65	1.66	1.51
9	K	103	THR	C-O	5.65	1.34	1.23
1	A	85	ASP	C-O	5.65	1.34	1.23
1	A	819	GLY	N-CA	-5.65	1.37	1.46
2	B	484	ASN	CB-CG	-5.65	1.38	1.51
2	B	494	HIS	CA-C	-5.65	1.38	1.52
2	B	524	PRO	CA-CB	-5.65	1.42	1.53
6	H	87	ARG	CB-CG	5.65	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	446	ARG	CA-CB	-5.64	1.41	1.53
1	A	511	ILE	CA-CB	-5.64	1.41	1.54
1	A	1299	VAL	C-O	5.64	1.34	1.23
2	B	20	ASP	C-O	-5.64	1.12	1.23
1	A	535	THR	N-CA	5.64	1.57	1.46
1	A	1287	TYR	CB-CG	-5.64	1.43	1.51
4	E	157	SER	CA-C	-5.64	1.38	1.52
7	I	103	CYS	CA-C	-5.64	1.38	1.52
1	A	139	TRP	CE2-CZ2	-5.64	1.30	1.39
1	A	1093	LYS	CD-CE	5.64	1.65	1.51
2	B	465	ASN	CG-OD1	5.64	1.36	1.24
6	H	111	LEU	CA-C	5.64	1.67	1.52
1	A	769	SER	N-CA	-5.64	1.35	1.46
1	A	918	GLU	N-CA	-5.64	1.35	1.46
2	B	210	LYS	CD-CE	5.64	1.65	1.51
1	A	200	ARG	N-CA	-5.63	1.35	1.46
2	B	580	VAL	CB-CG2	-5.63	1.41	1.52
2	B	639	ILE	N-CA	-5.63	1.35	1.46
6	H	109	LYS	CA-C	5.63	1.67	1.52
2	B	57	TYR	CZ-OH	-5.63	1.28	1.37
2	B	118	ARG	CA-C	5.63	1.67	1.52
1	A	972	HIS	CA-CB	5.63	1.66	1.53
1	A	1033	GLN	N-CA	-5.63	1.35	1.46
2	B	40	GLU	CD-OE1	5.63	1.31	1.25
2	B	190	TYR	CA-CB	-5.63	1.41	1.53
2	B	194	GLU	CB-CG	5.63	1.62	1.52
2	B	482	VAL	CB-CG1	5.63	1.64	1.52
3	C	96	SER	C-O	5.63	1.34	1.23
4	E	23	VAL	CA-CB	-5.63	1.43	1.54
4	E	29	PHE	CG-CD2	-5.63	1.30	1.38
9	K	38	GLU	CD-OE2	-5.63	1.19	1.25
1	A	25	GLU	CA-CB	-5.63	1.41	1.53
1	A	373	THR	N-CA	-5.63	1.35	1.46
2	B	116	GLU	N-CA	-5.63	1.35	1.46
8	J	18	TRP	CD2-CE2	5.63	1.48	1.41
1	A	116	ASP	N-CA	-5.63	1.35	1.46
1	A	837	ILE	C-O	-5.63	1.12	1.23
1	A	976	THR	CB-CG2	5.63	1.71	1.52
1	A	1283	VAL	CB-CG1	5.62	1.64	1.52
2	B	391	ASP	CB-CG	5.62	1.63	1.51
3	C	123	ASN	CG-OD1	5.62	1.36	1.24
3	C	191	TYR	N-CA	-5.62	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	130	ARG	CD-NE	-5.62	1.36	1.46
1	A	350	ARG	CZ-NH2	-5.62	1.25	1.33
1	A	1123	GLY	N-CA	5.62	1.54	1.46
2	B	266	ALA	CA-C	5.62	1.67	1.52
2	B	678	GLU	N-CA	5.62	1.57	1.46
4	E	132	ILE	N-CA	-5.62	1.35	1.46
10	L	47	ARG	CZ-NH2	5.62	1.40	1.33
2	B	554	ILE	C-O	5.62	1.34	1.23
2	B	1025	HIS	CA-CB	5.62	1.66	1.53
3	C	86	CYS	N-CA	5.62	1.57	1.46
4	E	74	ASP	CG-OD1	-5.62	1.12	1.25
1	A	356	ASP	CA-CB	5.62	1.66	1.53
1	A	448	PRO	CB-CG	5.62	1.78	1.50
1	A	540	PHE	C-O	5.62	1.34	1.23
1	A	41	MET	CA-C	5.62	1.67	1.52
1	A	1144	LYS	CG-CD	5.62	1.71	1.52
2	B	240	ILE	CB-CG2	-5.62	1.35	1.52
4	E	205	SER	N-CA	5.62	1.57	1.46
2	B	623	GLU	CG-CD	-5.62	1.43	1.51
4	E	74	ASP	CA-C	5.62	1.67	1.52
1	A	128	ILE	CA-CB	5.62	1.67	1.54
1	A	560	ILE	CA-C	-5.62	1.38	1.52
1	A	1040	GLN	C-O	-5.62	1.12	1.23
2	B	903	VAL	CB-CG1	-5.62	1.41	1.52
1	A	112	LYS	CG-CD	5.61	1.71	1.52
1	A	840	ARG	N-CA	-5.61	1.35	1.46
2	B	267	ARG	CA-C	5.61	1.67	1.52
2	B	318	VAL	N-CA	-5.61	1.35	1.46
6	H	146	ARG	CA-CB	5.61	1.66	1.53
1	A	880	LYS	N-CA	-5.61	1.35	1.46
2	B	249	ARG	C-O	5.61	1.34	1.23
3	C	221	TYR	CD2-CE2	5.61	1.47	1.39
10	L	51	CYS	N-CA	5.61	1.57	1.46
8	J	53	HIS	N-CA	5.61	1.57	1.46
1	A	744	LYS	C-O	-5.61	1.12	1.23
2	B	516	ASN	CG-ND2	-5.61	1.18	1.32
2	B	1171	VAL	CA-C	5.61	1.67	1.52
7	I	62	ILE	CB-CG2	-5.61	1.35	1.52
1	A	521	MET	CA-CB	-5.61	1.41	1.53
1	A	973	ILE	CB-CG2	5.61	1.70	1.52
5	F	93	ILE	CA-CB	-5.61	1.42	1.54
1	A	635	ARG	CZ-NH1	5.60	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	814	PHE	CD1-CE1	5.60	1.50	1.39
4	E	112	TYR	C-O	-5.60	1.12	1.23
8	J	1	MET	CA-CB	-5.60	1.41	1.53
1	A	1001	ARG	CB-CG	5.60	1.67	1.52
1	A	1009	ASN	C-O	-5.60	1.12	1.23
1	A	605	MET	C-O	5.60	1.33	1.23
1	A	1129	GLU	CB-CG	5.60	1.62	1.52
2	B	1135	ARG	CD-NE	-5.60	1.36	1.46
1	A	22	PHE	CE2-CZ	5.60	1.48	1.37
1	A	30	ILE	CB-CG2	5.60	1.70	1.52
1	A	72	GLU	CA-C	5.60	1.67	1.52
1	A	272	ALA	CA-CB	5.60	1.64	1.52
5	F	100	GLN	N-CA	-5.60	1.35	1.46
1	A	379	VAL	CB-CG1	-5.59	1.41	1.52
1	A	795	GLU	CA-C	-5.59	1.38	1.52
1	A	963	ILE	C-N	-5.59	1.21	1.34
1	A	1161	THR	CA-CB	5.59	1.67	1.53
5	F	133	VAL	CA-CB	-5.59	1.43	1.54
6	H	145	ARG	CZ-NH1	5.59	1.40	1.33
6	H	81	PRO	CA-CB	5.59	1.64	1.53
9	K	109	TRP	C-O	5.59	1.33	1.23
2	B	761	HIS	CA-C	-5.59	1.38	1.52
2	B	933	SER	CA-CB	5.59	1.61	1.52
1	A	430	TRP	N-CA	5.59	1.57	1.46
1	A	1053	PHE	CA-C	-5.59	1.38	1.52
2	B	1023	VAL	CB-CG2	-5.59	1.41	1.52
8	J	37	SER	N-CA	5.59	1.57	1.46
1	A	1424	VAL	CA-CB	-5.59	1.43	1.54
3	C	254	LYS	CA-C	-5.59	1.38	1.52
8	J	16	ASP	CB-CG	5.59	1.63	1.51
1	A	1122	PRO	CB-CG	5.58	1.77	1.50
1	A	1417	GLU	C-O	5.58	1.33	1.23
2	B	37	PHE	CD1-CE1	-5.58	1.28	1.39
2	B	500	THR	C-N	-5.58	1.23	1.34
9	K	114	LEU	CA-CB	5.58	1.66	1.53
1	A	238	CYS	CB-SG	5.58	1.91	1.82
1	A	446	ARG	CZ-NH1	5.58	1.40	1.33
2	B	237	VAL	CB-CG1	-5.58	1.41	1.52
2	B	410	GLY	CA-C	5.58	1.60	1.51
2	B	681	TRP	CD2-CE2	-5.58	1.34	1.41
2	B	862	GLN	N-CA	5.58	1.57	1.46
8	J	12	LYS	CA-CB	-5.58	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	622	LYS	C-O	-5.58	1.12	1.23
2	B	880	THR	C-O	5.58	1.33	1.23
4	E	109	ILE	CA-C	-5.58	1.38	1.52
2	B	109	THR	CB-OG1	5.58	1.54	1.43
3	C	174	ALA	CA-C	-5.58	1.38	1.52
5	F	112	GLU	C-O	5.58	1.33	1.23
7	I	82	GLU	CA-C	5.58	1.67	1.52
1	A	372	LYS	CB-CG	5.58	1.67	1.52
4	E	60	PHE	CE1-CZ	5.58	1.48	1.37
1	A	994	GLN	CA-C	-5.58	1.38	1.52
1	A	1299	VAL	CA-CB	-5.58	1.43	1.54
2	B	902	GLY	CA-C	-5.58	1.43	1.51
2	B	1203	LEU	C-O	5.58	1.33	1.23
2	B	887	HIS	CA-CB	5.57	1.66	1.53
10	L	27	LEU	CG-CD1	5.57	1.72	1.51
7	I	105	SER	C-O	-5.57	1.12	1.23
1	A	1260	LEU	CG-CD2	-5.57	1.31	1.51
1	A	361	LEU	CG-CD1	5.57	1.72	1.51
2	B	393	LYS	CG-CD	5.57	1.71	1.52
2	B	426	LYS	CA-C	-5.57	1.38	1.52
1	A	630	ILE	C-O	5.57	1.33	1.23
1	A	981	LEU	C-O	-5.57	1.12	1.23
2	B	681	TRP	C-N	-5.57	1.21	1.34
5	F	114	GLU	CD-OE2	5.57	1.31	1.25
2	B	869	SER	CA-CB	5.57	1.61	1.52
3	C	127	ARG	CZ-NH1	5.57	1.40	1.33
5	F	150	GLU	CB-CG	-5.57	1.41	1.52
1	A	1040	GLN	CG-CD	5.56	1.63	1.51
2	B	401	PHE	CD2-CE2	-5.56	1.28	1.39
1	A	177	ASP	C-O	5.56	1.33	1.23
3	C	137	LYS	CG-CD	5.56	1.71	1.52
1	A	80	HIS	CG-CD2	5.56	1.45	1.35
1	A	1288	ASP	CG-OD1	5.56	1.38	1.25
1	A	1441	PHE	CG-CD1	-5.56	1.30	1.38
2	B	176	SER	C-O	-5.56	1.12	1.23
2	B	257	LYS	C-O	-5.56	1.12	1.23
2	B	331	LEU	CA-C	-5.56	1.38	1.52
2	B	745	PRO	N-CD	-5.56	1.40	1.47
2	B	855	PHE	C-O	-5.56	1.12	1.23
2	B	1020	ARG	N-CA	-5.56	1.35	1.46
3	C	162	GLY	C-O	5.56	1.32	1.23
1	A	996	ASN	CG-ND2	5.56	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	732	SER	CA-C	5.56	1.67	1.52
2	B	748	ILE	C-O	5.56	1.33	1.23
1	A	1362	TYR	N-CA	5.56	1.57	1.46
2	B	763	GLN	CA-C	-5.56	1.38	1.52
1	A	1418	LEU	CG-CD1	5.55	1.72	1.51
2	B	351	TYR	C-O	5.55	1.33	1.23
2	B	711	GLU	CA-C	5.55	1.67	1.52
7	I	6	PHE	C-O	-5.55	1.12	1.23
2	B	275	TYR	CE1-CZ	-5.55	1.31	1.38
1	A	689	LYS	C-O	-5.55	1.12	1.23
1	A	795	GLU	C-N	-5.55	1.21	1.34
2	B	209	GLU	CD-OE2	-5.55	1.19	1.25
1	A	24	PRO	C-O	5.55	1.34	1.23
1	A	1050	GLU	CB-CG	5.55	1.62	1.52
2	B	743	ILE	C-O	5.55	1.33	1.23
2	B	1109	GLY	N-CA	5.55	1.54	1.46
1	A	565	ILE	CB-CG2	-5.55	1.35	1.52
1	A	672	ASP	CB-CG	-5.55	1.40	1.51
1	A	122	MET	SD-CE	5.55	2.08	1.77
7	I	58	VAL	CB-CG2	-5.55	1.41	1.52
9	K	88	LYS	CD-CE	5.54	1.65	1.51
1	A	503	GLN	CD-NE2	5.54	1.46	1.32
1	A	997	LEU	C-O	-5.54	1.12	1.23
3	C	179	GLU	CA-C	-5.54	1.38	1.52
5	F	140	ASP	CG-OD2	5.54	1.38	1.25
9	K	20	LYS	C-O	5.54	1.33	1.23
1	A	818	MET	C-N	-5.54	1.23	1.33
1	A	1080	THR	CB-CG2	5.54	1.70	1.52
1	A	1366	ARG	CD-NE	-5.54	1.37	1.46
3	C	189	THR	C-O	5.54	1.33	1.23
2	B	558	LEU	C-O	5.54	1.33	1.23
9	K	71	PHE	N-CA	5.54	1.57	1.46
2	B	358	LYS	CB-CG	5.54	1.67	1.52
2	B	843	GLN	CD-OE1	-5.54	1.11	1.24
4	E	192	ARG	CB-CG	5.54	1.67	1.52
2	B	193	LYS	CD-CE	5.54	1.65	1.51
7	I	61	ASP	CA-CB	-5.54	1.41	1.53
1	A	369	SER	CA-CB	-5.53	1.44	1.52
1	A	1079	MET	CA-C	5.53	1.67	1.52
5	F	153	VAL	CA-C	-5.53	1.38	1.52
1	A	416	ARG	CA-CB	5.53	1.66	1.53
2	B	565	PRO	CA-CB	-5.53	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	733	HIS	CB-CG	5.53	1.60	1.50
9	K	73	LEU	CB-CG	-5.53	1.36	1.52
1	A	1360	GLY	CA-C	5.53	1.60	1.51
2	B	1034	VAL	CB-CG2	5.53	1.64	1.52
2	B	1097	HIS	CG-ND1	5.53	1.50	1.38
3	C	218	PRO	CB-CG	5.53	1.77	1.50
6	H	57	VAL	C-O	-5.53	1.12	1.23
10	L	55	ILE	CA-CB	-5.53	1.42	1.54
1	A	721	PHE	CE1-CZ	-5.53	1.26	1.37
1	A	686	ALA	C-O	-5.53	1.12	1.23
2	B	526	GLU	N-CA	5.53	1.57	1.46
8	J	53	HIS	CB-CG	-5.53	1.40	1.50
1	A	281	HIS	C-O	5.53	1.33	1.23
1	A	400	PRO	CB-CG	-5.53	1.22	1.50
2	B	396	ASP	C-N	5.53	1.46	1.34
1	A	650	GLN	CD-NE2	-5.52	1.19	1.32
6	H	21	ASN	C-N	-5.52	1.21	1.34
1	A	200	ARG	NE-CZ	-5.52	1.25	1.33
1	A	497	THR	N-CA	-5.52	1.35	1.46
1	A	516	SER	CA-CB	-5.52	1.44	1.52
2	B	432	MET	CB-CG	5.52	1.69	1.51
1	A	1230	GLU	N-CA	5.52	1.57	1.46
1	A	1262	LYS	CA-C	5.52	1.67	1.52
2	B	856	PHE	CG-CD2	-5.52	1.30	1.38
2	B	908	GLU	CA-CB	5.52	1.66	1.53
2	B	1179	GLN	CA-CB	5.52	1.66	1.53
3	C	34	ARG	CA-C	-5.52	1.38	1.52
4	E	147	HIS	C-O	-5.52	1.12	1.23
1	A	464	PRO	N-CD	-5.52	1.40	1.47
2	B	495	LEU	CA-CB	-5.52	1.41	1.53
2	B	569	TYR	CA-CB	5.52	1.66	1.53
4	E	94	LYS	CG-CD	5.52	1.71	1.52
5	F	104	ASN	C-O	-5.52	1.12	1.23
2	B	492	LEU	CG-CD1	-5.52	1.31	1.51
3	C	183	TRP	CA-CB	5.52	1.66	1.53
1	A	1060	PRO	N-CD	-5.51	1.40	1.47
2	B	336	ARG	C-O	5.51	1.33	1.23
3	C	121	VAL	CA-C	-5.51	1.38	1.52
4	E	103	LYS	N-CA	5.51	1.57	1.46
1	A	1239	ARG	N-CA	-5.51	1.35	1.46
1	A	1323	ASP	CA-C	5.51	1.67	1.52
2	B	734	HIS	CB-CG	5.51	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1173	ALA	C-O	5.51	1.33	1.23
2	B	1210	MET	SD-CE	5.51	2.08	1.77
3	C	241	ASP	CA-CB	5.51	1.66	1.53
2	B	724	ASP	CB-CG	5.51	1.63	1.51
1	A	300	VAL	CA-CB	-5.51	1.43	1.54
2	B	561	TRP	CB-CG	-5.51	1.40	1.50
3	C	31	ASN	C-O	5.51	1.33	1.23
1	A	451	HIS	N-CA	-5.51	1.35	1.46
2	B	113	TYR	N-CA	5.51	1.57	1.46
2	B	375	ALA	N-CA	-5.51	1.35	1.46
2	B	601	ARG	CD-NE	5.51	1.55	1.46
2	B	1181	GLU	N-CA	5.51	1.57	1.46
2	B	1181	GLU	CD-OE2	-5.50	1.19	1.25
7	I	71	SER	CA-CB	5.50	1.61	1.52
1	A	225	ASN	C-N	5.50	1.46	1.34
1	A	268	ASP	CA-C	5.50	1.67	1.52
1	A	1211	GLN	C-O	-5.50	1.12	1.23
1	A	1373	ASP	CA-CB	-5.50	1.41	1.53
2	B	320	ASP	CB-CG	5.50	1.63	1.51
7	I	51	ASN	C-O	-5.50	1.12	1.23
1	A	30	ILE	C-O	5.50	1.33	1.23
1	A	375	THR	C-O	-5.50	1.12	1.23
1	A	1281	ARG	CZ-NH2	5.50	1.40	1.33
2	B	482	VAL	CA-CB	-5.50	1.43	1.54
4	E	168	TYR	CE2-CZ	-5.50	1.31	1.38
1	A	39	GLU	CA-C	5.50	1.67	1.52
1	A	1264	GLU	C-N	-5.50	1.21	1.34
2	B	67	SER	CA-CB	5.50	1.61	1.52
8	J	1	MET	CG-SD	-5.50	1.66	1.81
1	A	238	CYS	CA-CB	5.50	1.66	1.53
1	A	268	ASP	CA-CB	5.50	1.66	1.53
1	A	1349	TYR	CE2-CZ	-5.50	1.31	1.38
3	C	46	ILE	CB-CG2	-5.50	1.35	1.52
9	K	32	VAL	N-CA	-5.50	1.35	1.46
2	B	1205	GLN	N-CA	5.50	1.57	1.46
1	A	61	ILE	CB-CG1	5.49	1.69	1.54
1	A	669	THR	CA-CB	5.49	1.67	1.53
1	A	1407	GLU	CB-CG	5.49	1.62	1.52
2	B	406	LEU	CB-CG	-5.49	1.36	1.52
2	B	864	LYS	CD-CE	5.49	1.65	1.51
8	J	48	ARG	CZ-NH2	-5.49	1.25	1.33
9	K	4	PRO	C-O	-5.49	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	63	ARG	CA-CB	5.49	1.66	1.53
1	A	455	MET	SD-CE	-5.49	1.47	1.77
2	B	579	ARG	N-CA	5.49	1.57	1.46
2	B	1147	LEU	CA-CB	-5.49	1.41	1.53
6	H	20	TYR	CZ-OH	-5.49	1.28	1.37
8	J	21	TYR	CA-CB	5.49	1.66	1.53
1	A	170	THR	C-N	5.49	1.46	1.34
1	A	286	HIS	CA-CB	5.49	1.66	1.53
1	A	704	ALA	C-O	5.49	1.33	1.23
2	B	32	ALA	CA-C	-5.49	1.38	1.52
3	C	106	GLU	CG-CD	5.49	1.60	1.51
3	C	167	HIS	C-N	-5.49	1.21	1.34
3	C	34	ARG	C-N	-5.49	1.21	1.34
8	J	33	GLY	N-CA	5.49	1.54	1.46
9	K	67	PHE	CB-CG	-5.49	1.42	1.51
7	I	70	ARG	CZ-NH1	5.49	1.40	1.33
9	K	46	ILE	CA-CB	-5.49	1.42	1.54
2	B	457	LEU	N-CA	-5.49	1.35	1.46
2	B	785	TYR	CG-CD1	-5.49	1.32	1.39
2	B	1148	LYS	N-CA	-5.49	1.35	1.46
3	C	167	HIS	CB-CG	-5.49	1.40	1.50
9	K	109	TRP	CZ3-CH2	-5.49	1.31	1.40
1	A	1377	THR	CB-OG1	-5.48	1.32	1.43
1	A	234	MET	CG-SD	-5.48	1.66	1.81
2	B	681	TRP	NE1-CE2	-5.48	1.30	1.37
2	B	1110	PRO	N-CA	5.48	1.56	1.47
4	E	166	LYS	C-O	5.48	1.33	1.23
7	I	51	ASN	CG-OD1	5.48	1.36	1.24
10	L	28	LYS	CG-CD	5.48	1.71	1.52
1	A	398	GLU	CG-CD	5.48	1.60	1.51
2	B	859	TYR	CE1-CZ	5.48	1.45	1.38
6	H	41	ASP	CG-OD1	5.48	1.38	1.25
1	A	1325	THR	CB-CG2	-5.48	1.34	1.52
1	A	206	GLU	CA-C	-5.48	1.38	1.52
1	A	445	ASN	CB-CG	-5.48	1.38	1.51
2	B	879	ARG	CG-CD	5.48	1.65	1.51
4	E	201	LYS	CA-CB	-5.48	1.41	1.53
2	B	640	VAL	CB-CG2	5.48	1.64	1.52
2	B	743	ILE	CA-C	-5.48	1.38	1.52
8	J	53	HIS	CG-CD2	-5.48	1.26	1.35
1	A	98	LYS	C-O	5.47	1.33	1.23
10	L	56	LEU	CA-C	-5.47	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	PHE	CD1-CE1	-5.47	1.28	1.39
2	B	894	ASP	CG-OD2	5.47	1.38	1.25
5	F	72	LYS	CB-CG	5.47	1.67	1.52
5	F	108	PHE	N-CA	-5.47	1.35	1.46
2	B	415	GLN	CD-NE2	5.47	1.46	1.32
2	B	1216	LEU	CG-CD2	-5.47	1.31	1.51
1	A	548	ASN	CA-C	5.47	1.67	1.52
1	A	607	ILE	CB-CG2	-5.47	1.35	1.52
2	B	446	LEU	C-O	5.47	1.33	1.23
4	E	42	PHE	CD2-CE2	5.47	1.50	1.39
1	A	463	ILE	C-O	5.47	1.33	1.23
2	B	647	GLY	C-O	-5.47	1.15	1.23
2	B	889	THR	N-CA	5.47	1.57	1.46
5	F	148	VAL	N-CA	-5.47	1.35	1.46
1	A	768	GLN	CG-CD	5.46	1.63	1.51
1	A	921	GLY	CA-C	5.46	1.60	1.51
10	L	42	ARG	N-CA	5.46	1.57	1.46
2	B	1057	LYS	N-CA	-5.46	1.35	1.46
1	A	485	ASP	N-CA	5.46	1.57	1.46
2	B	899	ILE	CA-C	-5.46	1.38	1.52
1	A	859	SER	CB-OG	-5.46	1.35	1.42
1	A	507	VAL	CB-CG2	-5.46	1.41	1.52
1	A	814	PHE	C-O	-5.46	1.12	1.23
2	B	223	VAL	CB-CG2	-5.46	1.41	1.52
5	F	103	MET	CB-CG	-5.46	1.33	1.51
1	A	883	LEU	CG-CD1	-5.46	1.31	1.51
4	E	84	ASP	CA-CB	5.46	1.66	1.53
1	A	1231	ASP	CB-CG	5.46	1.63	1.51
2	B	872	GLU	CG-CD	5.46	1.60	1.51
1	A	912	LEU	C-N	-5.45	1.21	1.34
2	B	35	SER	CA-CB	-5.45	1.44	1.52
2	B	200	GLY	CA-C	-5.45	1.43	1.51
2	B	709	ASP	CB-CG	5.45	1.63	1.51
2	B	1102	LYS	C-O	5.45	1.33	1.23
9	K	96	ASN	N-CA	5.45	1.57	1.46
1	A	767	GLN	CG-CD	-5.45	1.38	1.51
1	A	1066	VAL	CA-CB	-5.45	1.43	1.54
1	A	1433	MET	SD-CE	-5.45	1.47	1.77
2	B	269	ILE	C-O	-5.45	1.12	1.23
6	H	20	TYR	C-O	5.45	1.33	1.23
9	K	38	GLU	CD-OE1	5.45	1.31	1.25
1	A	1130	GLN	C-O	-5.45	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	30	ILE	CA-C	-5.45	1.38	1.52
1	A	561	PRO	CG-CD	5.45	1.68	1.50
1	A	1422	ARG	CG-CD	-5.45	1.38	1.51
2	B	995	ARG	NE-CZ	-5.45	1.25	1.33
2	B	1209	ALA	C-O	5.45	1.33	1.23
10	L	70	ARG	NE-CZ	5.45	1.40	1.33
1	A	496	GLU	CA-CB	5.44	1.66	1.53
2	B	25	ILE	CA-C	-5.44	1.38	1.52
2	B	127	GLY	CA-C	-5.44	1.43	1.51
1	A	805	LEU	CA-CB	-5.44	1.41	1.53
2	B	847	ASP	C-N	-5.44	1.21	1.34
5	F	146	TRP	CD2-CE3	-5.44	1.32	1.40
9	K	54	ARG	CA-C	5.44	1.67	1.52
1	A	557	ASP	N-CA	5.44	1.57	1.46
2	B	430	ARG	NE-CZ	5.44	1.40	1.33
2	B	766	ARG	CA-CB	-5.44	1.42	1.53
9	K	62	LYS	CG-CD	5.44	1.71	1.52
1	A	159	THR	CB-CG2	5.44	1.70	1.52
1	A	237	THR	C-N	5.44	1.46	1.34
1	A	1441	PHE	CD1-CE1	-5.44	1.28	1.39
2	B	376	PHE	CG-CD1	-5.44	1.30	1.38
1	A	1442	ASP	CA-C	-5.44	1.38	1.52
4	E	212	ARG	CD-NE	-5.44	1.37	1.46
1	A	1211	GLN	CD-OE1	5.43	1.35	1.24
1	A	1316	VAL	C-O	5.43	1.33	1.23
2	B	435	THR	CA-CB	5.43	1.67	1.53
2	B	756	ILE	CB-CG2	-5.43	1.36	1.52
1	A	1018	PHE	CG-CD2	-5.43	1.30	1.38
2	B	204	ILE	N-CA	5.43	1.57	1.46
3	C	179	GLU	CG-CD	-5.43	1.43	1.51
1	A	612	ILE	CA-C	-5.43	1.38	1.52
4	E	202	SER	N-CA	5.43	1.57	1.46
8	J	19	GLU	C-O	5.43	1.33	1.23
1	A	105	CYS	C-N	-5.43	1.21	1.34
5	F	88	TYR	N-CA	-5.43	1.35	1.46
1	A	893	PHE	CD2-CE2	5.43	1.50	1.39
1	A	1233	ASP	CG-OD2	5.43	1.37	1.25
2	B	124	TYR	C-N	5.43	1.46	1.34
3	C	57	VAL	N-CA	5.43	1.57	1.46
4	E	41	ASP	CG-OD2	5.43	1.37	1.25
5	F	141	GLY	N-CA	5.43	1.54	1.46
10	L	40	LEU	CG-CD1	5.43	1.72	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	PHE	CE1-CZ	-5.42	1.27	1.37
2	B	983	ARG	N-CA	-5.42	1.35	1.46
3	C	9	LYS	CA-CB	-5.42	1.42	1.53
1	A	491	VAL	CB-CG1	-5.42	1.41	1.52
1	A	977	LYS	CB-CG	5.42	1.67	1.52
1	A	1039	LYS	CG-CD	-5.42	1.34	1.52
2	B	486	TYR	CD2-CE2	5.42	1.47	1.39
6	H	102	TYR	CG-CD2	-5.42	1.32	1.39
1	A	1023	ARG	CA-CB	-5.42	1.42	1.53
2	B	44	VAL	CA-CB	-5.42	1.43	1.54
2	B	117	ALA	C-O	-5.42	1.13	1.23
4	E	173	SER	C-O	-5.42	1.13	1.23
8	J	43	ARG	CA-CB	-5.42	1.42	1.53
1	A	164	ARG	CA-CB	-5.42	1.42	1.53
1	A	430	TRP	CA-C	-5.42	1.38	1.52
2	B	169	ARG	CD-NE	5.42	1.55	1.46
2	B	455	SER	CB-OG	5.42	1.49	1.42
1	A	130	ASP	CG-OD1	5.41	1.37	1.25
1	A	562	THR	CA-CB	5.41	1.67	1.53
2	B	1139	ILE	CA-CB	-5.41	1.42	1.54
9	K	66	PRO	N-CD	-5.41	1.40	1.47
1	A	68	GLN	C-O	5.41	1.33	1.23
1	A	697	ALA	CA-C	-5.41	1.38	1.52
1	A	779	PHE	CE1-CZ	-5.41	1.27	1.37
6	H	22	LYS	N-CA	-5.41	1.35	1.46
7	I	115	LYS	CB-CG	-5.41	1.38	1.52
1	A	646	PHE	CD2-CE2	-5.41	1.28	1.39
1	A	684	ALA	CA-C	5.41	1.67	1.52
2	B	561	TRP	CE3-CZ3	5.41	1.47	1.38
2	B	567	GLU	CA-CB	5.41	1.65	1.53
2	B	585	VAL	CB-CG2	-5.41	1.41	1.52
4	E	145	THR	C-O	-5.41	1.13	1.23
6	H	109	LYS	CD-CE	5.41	1.64	1.51
1	A	690	VAL	CB-CG1	5.41	1.64	1.52
3	C	50	GLU	N-CA	5.41	1.57	1.46
4	E	170	LEU	N-CA	5.41	1.57	1.46
1	A	11	LEU	C-O	-5.41	1.13	1.23
1	A	221	SER	C-O	5.41	1.33	1.23
1	A	239	LEU	CA-CB	-5.41	1.41	1.53
1	A	1034	GLU	CA-CB	-5.41	1.42	1.53
2	B	41	LYS	N-CA	-5.41	1.35	1.46
2	B	879	ARG	CD-NE	5.41	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1054	GLY	C-O	5.41	1.32	1.23
2	B	1181	GLU	CA-CB	5.41	1.65	1.53
3	C	10	ILE	CA-CB	-5.40	1.42	1.54
3	C	70	ILE	CB-CG1	5.40	1.69	1.54
9	K	47	ARG	CG-CD	5.40	1.65	1.51
1	A	112	LYS	C-O	-5.40	1.13	1.23
1	A	226	GLU	CG-CD	5.40	1.60	1.51
1	A	553	VAL	C-N	-5.40	1.24	1.34
1	A	1414	ALA	CA-C	-5.40	1.39	1.52
2	B	661	LEU	CG-CD2	5.40	1.71	1.51
3	C	90	ASP	CG-OD2	5.40	1.37	1.25
3	C	191	TYR	CA-CB	5.40	1.65	1.53
10	L	36	SER	CA-CB	5.40	1.61	1.52
5	F	147	SER	C-O	5.40	1.33	1.23
2	B	228	LYS	C-O	5.40	1.33	1.23
2	B	694	ASP	CG-OD2	5.40	1.37	1.25
3	C	77	ILE	C-O	5.40	1.33	1.23
6	H	115	TYR	N-CA	5.40	1.57	1.46
1	A	1214	GLU	CA-CB	5.40	1.65	1.53
2	B	699	GLU	CB-CG	5.40	1.62	1.52
1	A	1024	SER	N-CA	-5.39	1.35	1.46
1	A	1270	ASN	CG-ND2	5.39	1.46	1.32
2	B	256	VAL	C-O	-5.39	1.13	1.23
1	A	556	TRP	CD2-CE2	5.39	1.47	1.41
1	A	1378	GLN	CG-CD	5.39	1.63	1.51
1	A	1447	GLU	CD-OE1	5.39	1.31	1.25
2	B	627	PHE	CB-CG	5.39	1.60	1.51
3	C	131	HIS	CA-CB	5.39	1.65	1.53
1	A	637	LYS	C-O	-5.39	1.13	1.23
2	B	233	PRO	CB-CG	5.39	1.76	1.50
1	A	22	PHE	C-O	5.39	1.33	1.23
1	A	499	ALA	C-O	-5.39	1.13	1.23
1	A	512	VAL	CA-CB	-5.39	1.43	1.54
1	A	606	LEU	CA-C	-5.39	1.39	1.52
1	A	768	GLN	CB-CG	-5.39	1.38	1.52
2	B	880	THR	CA-C	5.39	1.67	1.52
1	A	1220	PHE	CD2-CE2	5.39	1.50	1.39
2	B	1053	GLU	CA-C	-5.39	1.39	1.52
8	J	29	GLU	CA-CB	5.39	1.65	1.53
3	C	197	SER	CB-OG	5.38	1.49	1.42
1	A	385	ILE	CA-C	-5.38	1.39	1.52
1	A	1166	ASP	CG-OD1	5.38	1.37	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	209	ALA	CA-C	-5.38	1.39	1.52
1	A	536	LEU	C-O	5.38	1.33	1.23
2	B	589	VAL	CA-CB	-5.38	1.43	1.54
2	B	792	MET	CG-SD	5.38	1.95	1.81
9	K	48	ALA	CA-CB	-5.38	1.41	1.52
1	A	28	ARG	CZ-NH2	5.38	1.40	1.33
1	A	848	ILE	CA-CB	-5.38	1.42	1.54
1	A	916	GLY	CA-C	5.38	1.60	1.51
2	B	354	ASP	CB-CG	5.38	1.63	1.51
2	B	868	MET	SD-CE	5.38	2.08	1.77
2	B	1174	LYS	CB-CG	5.38	1.67	1.52
5	F	153	VAL	CB-CG2	-5.38	1.41	1.52
9	K	68	PHE	CE1-CZ	-5.38	1.27	1.37
1	A	207	ILE	CB-CG2	5.38	1.69	1.52
1	A	584	ASN	CB-CG	5.38	1.63	1.51
2	B	199	MET	SD-CE	5.38	2.08	1.77
3	C	209	TYR	N-CA	-5.38	1.35	1.46
2	B	357	GLN	CB-CG	-5.37	1.38	1.52
2	B	882	THR	CA-CB	5.37	1.67	1.53
2	B	989	THR	CB-CG2	-5.37	1.34	1.52
2	B	1081	LEU	CG-CD1	-5.37	1.31	1.51
8	J	54	VAL	C-N	5.37	1.46	1.34
1	A	164	ARG	NE-CZ	5.37	1.40	1.33
1	A	180	LYS	CD-CE	5.37	1.64	1.51
1	A	298	PHE	CE2-CZ	5.37	1.47	1.37
1	A	375	THR	CB-CG2	-5.37	1.34	1.52
2	B	287	ARG	CZ-NH1	5.37	1.40	1.33
3	C	204	SER	N-CA	-5.37	1.35	1.46
1	A	324	SER	CA-C	5.37	1.67	1.52
2	B	1104	HIS	CA-CB	5.37	1.65	1.53
3	C	177	GLU	CD-OE1	5.37	1.31	1.25
4	E	42	PHE	CG-CD2	-5.37	1.30	1.38
1	A	62	ASP	CA-CB	5.37	1.65	1.53
7	I	86	PHE	CG-CD2	-5.37	1.30	1.38
1	A	657	LEU	CB-CG	-5.37	1.36	1.52
1	A	1194	ARG	N-CA	-5.37	1.35	1.46
2	B	137	TYR	CA-C	5.37	1.66	1.52
2	B	546	SER	C-O	-5.37	1.13	1.23
2	B	871	THR	N-CA	5.37	1.57	1.46
3	C	112	ASN	CG-ND2	5.37	1.46	1.32
3	C	125	MET	CG-SD	5.37	1.95	1.81
3	C	201	TRP	CD2-CE2	-5.37	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	109	HIS	CG-ND1	5.36	1.50	1.38
1	A	591	PHE	CA-C	-5.36	1.39	1.52
2	B	246	LYS	C-O	5.36	1.33	1.23
1	A	706	HIS	C-O	5.36	1.33	1.23
1	A	731	ARG	C-O	-5.36	1.13	1.23
6	H	88	SER	N-CA	5.36	1.57	1.46
2	B	385	LEU	C-O	-5.36	1.13	1.23
2	B	542	MET	CA-C	-5.36	1.39	1.52
2	B	1001	PHE	CD1-CE1	5.36	1.50	1.39
3	C	85	ASP	N-CA	-5.36	1.35	1.46
1	A	44	THR	CA-C	5.36	1.66	1.52
1	A	468	PHE	C-O	-5.36	1.13	1.23
1	A	726	ARG	CA-CB	-5.36	1.42	1.53
1	A	1102	LYS	C-O	5.36	1.33	1.23
1	A	265	LYS	CD-CE	5.36	1.64	1.51
1	A	432	VAL	CB-CG2	5.36	1.64	1.52
1	A	445	ASN	C-O	5.36	1.33	1.23
3	C	184	ASN	N-CA	5.36	1.57	1.46
1	A	174	ILE	C-O	-5.35	1.13	1.23
4	E	177	ARG	NE-CZ	-5.35	1.26	1.33
6	H	3	ASN	CA-CB	5.35	1.67	1.53
1	A	1201	ALA	CA-C	5.35	1.66	1.52
2	B	699	GLU	CA-CB	-5.35	1.42	1.53
3	C	154	LYS	N-CA	5.35	1.57	1.46
4	E	13	TRP	CD2-CE3	5.35	1.48	1.40
4	E	27	GLY	C-O	5.35	1.32	1.23
1	A	18	GLN	CB-CG	-5.35	1.38	1.52
10	L	62	LYS	CG-CD	5.35	1.70	1.52
1	A	826	ASP	C-O	-5.35	1.13	1.23
4	E	160	GLU	CD-OE1	-5.35	1.19	1.25
1	A	726	ARG	CD-NE	-5.35	1.37	1.46
2	B	423	LYS	CG-CD	5.35	1.70	1.52
2	B	525	ALA	CA-C	-5.35	1.39	1.52
2	B	879	ARG	NE-CZ	5.35	1.40	1.33
2	B	768	THR	CB-CG2	-5.35	1.34	1.52
2	B	497	ARG	N-CA	-5.34	1.35	1.46
2	B	848	ARG	CD-NE	-5.34	1.37	1.46
2	B	982	SER	CA-C	-5.34	1.39	1.52
3	C	148	ARG	CB-CG	-5.34	1.38	1.52
1	A	629	LEU	CG-CD1	-5.34	1.32	1.51
2	B	348	ARG	CZ-NH1	-5.34	1.26	1.33
8	J	57	ILE	C-O	-5.34	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	114	LEU	CG-CD2	5.34	1.71	1.51
2	B	600	LEU	CG-CD2	-5.34	1.32	1.51
2	B	1076	HIS	C-N	-5.34	1.21	1.34
3	C	240	VAL	CA-C	-5.34	1.39	1.52
6	H	103	LYS	CA-CB	5.34	1.65	1.53
9	K	25	THR	CA-C	-5.34	1.39	1.52
1	A	609	ASP	CA-CB	-5.34	1.42	1.53
1	A	668	ASP	N-CA	-5.34	1.35	1.46
1	A	724	GLU	CB-CG	5.34	1.62	1.52
3	C	99	LEU	CG-CD1	-5.34	1.32	1.51
2	B	30	SER	CA-CB	-5.34	1.45	1.52
2	B	1034	VAL	C-N	-5.34	1.21	1.34
1	A	787	PHE	N-CA	-5.34	1.35	1.46
1	A	844	ALA	C-N	-5.34	1.21	1.34
2	B	565	PRO	CA-C	-5.34	1.42	1.52
7	I	78	CYS	C-O	-5.34	1.13	1.23
1	A	1155	ASP	CB-CG	-5.33	1.40	1.51
7	I	11	ASN	C-O	-5.33	1.13	1.23
1	A	868	TYR	N-CA	-5.33	1.35	1.46
2	B	784	ASN	CB-CG	-5.33	1.38	1.51
9	K	44	ASN	C-O	-5.33	1.13	1.23
2	B	403	LYS	CE-NZ	5.33	1.62	1.49
2	B	834	ASN	CG-ND2	5.33	1.46	1.32
2	B	870	ILE	CA-C	5.33	1.66	1.52
2	B	1071	VAL	CB-CG2	-5.33	1.41	1.52
2	B	1193	GLN	CD-NE2	5.33	1.46	1.32
2	B	1198	TYR	CZ-OH	5.33	1.47	1.37
4	E	14	ARG	CG-CD	5.33	1.65	1.51
1	A	913	LEU	CA-C	5.33	1.66	1.52
1	A	997	LEU	CG-CD2	-5.33	1.32	1.51
2	B	518	HIS	CA-C	5.33	1.66	1.52
4	E	7	ARG	CB-CG	5.33	1.67	1.52
5	F	144	GLU	C-O	-5.33	1.13	1.23
2	B	512	ARG	C-O	5.32	1.33	1.23
2	B	970	THR	C-O	-5.32	1.13	1.23
5	F	82	THR	C-O	-5.32	1.13	1.23
8	J	22	LEU	CG-CD1	-5.32	1.32	1.51
1	A	56	PRO	C-O	5.32	1.33	1.23
2	B	1058	LEU	CG-CD1	5.32	1.71	1.51
2	B	704	ALA	C-O	-5.32	1.13	1.23
2	B	889	THR	C-O	5.32	1.33	1.23
1	A	956	LEU	CG-CD2	-5.32	1.32	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	491	THR	C-O	5.32	1.33	1.23
2	B	1087	PHE	CG-CD2	-5.32	1.30	1.38
3	C	131	HIS	C-O	-5.32	1.13	1.23
1	A	599	SER	CB-OG	5.32	1.49	1.42
2	B	666	TYR	CG-CD1	5.32	1.46	1.39
2	B	419	THR	CA-CB	-5.32	1.39	1.53
2	B	799	PRO	CA-CB	-5.32	1.43	1.53
2	B	1047	PHE	CG-CD2	-5.32	1.30	1.38
2	B	1180	PHE	CG-CD2	5.31	1.46	1.38
1	A	230	ARG	CZ-NH2	5.31	1.40	1.33
2	B	244	LEU	N-CA	5.31	1.56	1.46
2	B	332	ASP	C-O	-5.31	1.13	1.23
3	C	29	MET	CB-CG	5.31	1.68	1.51
4	E	62	ALA	CA-C	-5.31	1.39	1.52
1	A	438	ASP	CB-CG	-5.31	1.40	1.51
1	A	620	LYS	CG-CD	5.31	1.70	1.52
3	C	71	PRO	N-CA	-5.31	1.38	1.47
1	A	420	ARG	NE-CZ	-5.31	1.26	1.33
1	A	866	PHE	C-N	-5.31	1.21	1.34
2	B	725	PRO	CG-CD	-5.31	1.33	1.50
1	A	36	ARG	C-O	-5.31	1.13	1.23
2	B	325	GLN	CD-OE1	5.31	1.35	1.24
10	L	67	PHE	CA-C	-5.31	1.39	1.52
1	A	356	ASP	CA-C	-5.31	1.39	1.52
1	A	836	TYR	CD1-CE1	-5.31	1.31	1.39
1	A	1152	ILE	C-O	-5.30	1.13	1.23
2	B	120	ARG	C-O	5.30	1.33	1.23
4	E	79	TRP	CG-CD2	5.30	1.52	1.43
9	K	53	ASP	CG-OD2	5.30	1.37	1.25
2	B	811	TYR	CE1-CZ	-5.30	1.31	1.38
3	C	187	LYS	CB-CG	5.30	1.66	1.52
4	E	123	LEU	CG-CD2	5.30	1.71	1.51
1	A	219	PHE	CB-CG	5.30	1.60	1.51
1	A	1117	THR	CA-CB	-5.30	1.39	1.53
1	A	1199	ARG	CZ-NH2	5.30	1.40	1.33
2	B	412	LEU	C-O	-5.30	1.13	1.23
2	B	608	ASP	C-O	-5.30	1.13	1.23
2	B	996	ARG	CA-CB	-5.30	1.42	1.53
3	C	232	VAL	CB-CG2	-5.30	1.41	1.52
4	E	66	GLU	CD-OE1	5.30	1.31	1.25
4	E	137	GLU	N-CA	-5.30	1.35	1.46
2	B	595	ARG	CD-NE	5.30	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	686	ASN	CG-OD1	5.30	1.35	1.24
1	A	694	THR	C-N	-5.30	1.21	1.34
2	B	710	LEU	CA-CB	-5.30	1.41	1.53
2	B	55	VAL	CB-CG1	-5.29	1.41	1.52
2	B	641	GLU	CD-OE1	5.29	1.31	1.25
4	E	11	ARG	NE-CZ	-5.29	1.26	1.33
1	A	1241	ARG	CG-CD	5.29	1.65	1.51
2	B	106	ASP	CG-OD2	5.29	1.37	1.25
3	C	183	TRP	CE2-CZ2	-5.29	1.30	1.39
1	A	201	VAL	CB-CG2	-5.29	1.41	1.52
1	A	636	GLU	C-O	-5.29	1.13	1.23
1	A	983	ILE	CB-CG1	5.29	1.68	1.54
2	B	577	ALA	C-O	-5.29	1.13	1.23
1	A	109	HIS	C-O	-5.29	1.13	1.23
1	A	861	GLY	CA-C	-5.29	1.43	1.51
2	B	1146	PHE	CA-CB	-5.29	1.42	1.53
1	A	233	TRP	CB-CG	-5.29	1.40	1.50
2	B	433	GLN	N-CA	5.29	1.56	1.46
1	A	1328	TYR	C-O	-5.29	1.13	1.23
2	B	353	LYS	CA-CB	-5.29	1.42	1.53
3	C	44	LEU	C-N	5.29	1.46	1.34
5	F	128	LYS	CG-CD	5.29	1.70	1.52
1	A	106	VAL	CB-CG2	-5.29	1.41	1.52
1	A	1036	ARG	CZ-NH1	5.29	1.40	1.33
2	B	834	ASN	C-O	5.29	1.33	1.23
9	K	107	THR	CA-C	-5.29	1.39	1.52
2	B	629	ASP	CA-C	-5.28	1.39	1.52
2	B	634	TYR	CG-CD2	-5.28	1.32	1.39
3	C	229	TYR	CD1-CE1	-5.28	1.31	1.39
2	B	1094	ARG	NE-CZ	-5.28	1.26	1.33
4	E	36	GLU	CG-CD	5.28	1.59	1.51
1	A	80	HIS	CB-CG	5.28	1.59	1.50
1	A	1284	MET	CB-CG	-5.28	1.34	1.51
2	B	573	GLN	CB-CG	5.28	1.66	1.52
2	B	744	HIS	N-CA	5.28	1.56	1.46
10	L	30	ILE	CB-CG1	-5.28	1.39	1.54
5	F	88	TYR	CE1-CZ	5.28	1.45	1.38
1	A	998	LEU	N-CA	-5.28	1.35	1.46
7	I	105	SER	CB-OG	5.28	1.49	1.42
2	B	397	ASP	CG-OD2	5.28	1.37	1.25
6	H	146	ARG	CA-C	5.28	1.66	1.52
2	B	251	ILE	CA-CB	5.27	1.67	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1038	THR	C-O	-5.27	1.13	1.23
1	A	1256	GLU	CA-CB	5.27	1.65	1.53
2	B	387	LEU	N-CA	-5.27	1.35	1.46
9	K	74	ARG	CD-NE	-5.27	1.37	1.46
2	B	346	GLU	CB-CG	5.27	1.62	1.52
2	B	465	ASN	CA-C	5.27	1.66	1.52
10	L	69	ALA	CA-CB	-5.27	1.41	1.52
1	A	93	VAL	CA-CB	5.27	1.65	1.54
1	A	1113	THR	C-N	-5.27	1.24	1.34
2	B	250	PHE	N-CA	5.27	1.56	1.46
4	E	42	PHE	CE1-CZ	-5.27	1.27	1.37
6	H	86	ASP	CA-CB	5.27	1.65	1.53
8	J	2	ILE	CA-C	-5.27	1.39	1.52
1	A	604	GLY	C-O	5.27	1.32	1.23
2	B	35	SER	C-O	-5.27	1.13	1.23
4	E	148	GLU	N-CA	5.26	1.56	1.46
5	F	75	PRO	C-O	-5.26	1.12	1.23
1	A	1435	PRO	N-CD	-5.26	1.40	1.47
2	B	261	ARG	C-O	5.26	1.33	1.23
2	B	803	LEU	N-CA	-5.26	1.35	1.46
6	H	37	LYS	CD-CE	5.26	1.64	1.51
9	K	71	PHE	CA-C	-5.26	1.39	1.52
1	A	393	ARG	CA-CB	-5.26	1.42	1.53
1	A	692	ASP	CB-CG	5.26	1.62	1.51
1	A	802	ASN	C-O	-5.26	1.13	1.23
1	A	719	VAL	CB-CG1	-5.26	1.41	1.52
1	A	1107	VAL	CA-CB	5.26	1.65	1.54
1	A	487	MET	C-O	-5.26	1.13	1.23
1	A	778	GLY	CA-C	-5.26	1.43	1.51
1	A	1100	ARG	CB-CG	5.26	1.66	1.52
1	A	1315	GLU	CD-OE1	5.26	1.31	1.25
2	B	887	HIS	C-N	5.26	1.42	1.33
2	B	1192	TYR	CD1-CE1	5.26	1.47	1.39
9	K	107	THR	CB-OG1	5.26	1.53	1.43
2	B	389	ALA	CA-C	-5.25	1.39	1.52
2	B	1223	ASP	CA-C	5.25	1.66	1.52
1	A	526	ASP	CG-OD1	5.25	1.37	1.25
1	A	912	LEU	CA-CB	-5.25	1.41	1.53
4	E	128	PRO	C-O	5.25	1.33	1.23
1	A	69	THR	C-N	5.25	1.46	1.34
1	A	184	SER	N-CA	5.25	1.56	1.46
1	A	505	CYS	C-N	-5.25	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1016	THR	N-CA	-5.25	1.35	1.46
2	B	710	LEU	CG-CD2	-5.25	1.32	1.51
4	E	24	LYS	CA-CB	5.25	1.65	1.53
5	F	101	ILE	CA-C	5.25	1.66	1.52
1	A	552	TRP	CD2-CE3	-5.25	1.32	1.40
1	A	637	LYS	CA-C	-5.25	1.39	1.52
1	A	956	LEU	C-O	-5.25	1.13	1.23
1	A	387	ARG	NE-CZ	5.25	1.39	1.33
2	B	357	GLN	CA-C	-5.25	1.39	1.52
2	B	835	GLN	N-CA	5.25	1.56	1.46
4	E	6	GLU	C-O	-5.25	1.13	1.23
4	E	34	GLU	CA-CB	5.25	1.65	1.53
6	H	45	GLU	CG-CD	5.25	1.59	1.51
2	B	377	PHE	CD2-CE2	5.25	1.49	1.39
3	C	127	ARG	CA-CB	-5.25	1.42	1.53
3	C	192	TRP	NE1-CE2	-5.25	1.30	1.37
3	C	63	ILE	C-N	5.25	1.46	1.34
1	A	860	LEU	N-CA	5.24	1.56	1.46
1	A	951	GLU	CA-C	-5.24	1.39	1.52
2	B	273	LEU	CG-CD2	-5.24	1.32	1.51
2	B	811	TYR	CA-C	5.24	1.66	1.52
1	A	1265	ASN	CG-OD1	5.24	1.35	1.24
2	B	850	LEU	CG-CD1	-5.24	1.32	1.51
6	H	46	LEU	CA-CB	-5.24	1.41	1.53
10	L	45	ALA	C-O	5.24	1.33	1.23
1	A	922	ASP	CA-CB	5.24	1.65	1.53
1	A	1283	VAL	CA-C	5.24	1.66	1.52
2	B	91	SER	CA-CB	5.24	1.60	1.52
2	B	1069	PHE	CB-CG	-5.24	1.42	1.51
6	H	93	TYR	CZ-OH	-5.24	1.28	1.37
1	A	22	PHE	N-CA	-5.24	1.35	1.46
1	A	575	LYS	CE-NZ	-5.24	1.35	1.49
1	A	1058	VAL	N-CA	-5.24	1.35	1.46
2	B	45	SER	CA-C	-5.24	1.39	1.52
2	B	188	ASP	N-CA	-5.24	1.35	1.46
1	A	219	PHE	C-O	-5.23	1.13	1.23
2	B	39	ARG	CB-CG	5.23	1.66	1.52
7	I	100	PHE	CA-C	-5.23	1.39	1.52
1	A	557	ASP	CG-OD2	-5.23	1.13	1.25
1	A	704	ALA	N-CA	5.23	1.56	1.46
2	B	681	TRP	CE2-CZ2	-5.23	1.30	1.39
3	C	170	TRP	CE2-CZ2	-5.23	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	186	LEU	CA-C	-5.23	1.39	1.52
7	I	75	CYS	CA-C	-5.23	1.39	1.52
1	A	76	GLU	CD-OE2	5.23	1.31	1.25
1	A	127	ALA	CA-CB	5.23	1.63	1.52
1	A	768	GLN	N-CA	-5.23	1.35	1.46
2	B	1189	ILE	N-CA	5.23	1.56	1.46
3	C	9	LYS	CG-CD	5.23	1.70	1.52
4	E	110	PHE	CA-C	-5.23	1.39	1.52
4	E	6	GLU	CG-CD	5.23	1.59	1.51
1	A	1193	LEU	C-N	-5.23	1.22	1.34
2	B	1103	ILE	CB-CG1	-5.23	1.39	1.54
4	E	77	SER	N-CA	-5.23	1.35	1.46
1	A	5	GLN	CA-C	-5.22	1.39	1.52
1	A	622	VAL	CA-CB	-5.22	1.43	1.54
1	A	684	ALA	N-CA	-5.22	1.35	1.46
1	A	1426	GLU	N-CA	-5.22	1.35	1.46
2	B	572	HIS	CA-CB	5.22	1.65	1.53
2	B	790	ASP	CG-OD1	5.22	1.37	1.25
10	L	27	LEU	C-O	5.22	1.33	1.23
1	A	935	GLN	CD-OE1	-5.22	1.12	1.24
2	B	661	LEU	CA-C	-5.22	1.39	1.52
2	B	986	GLN	CA-CB	5.22	1.65	1.53
2	B	1146	PHE	CD1-CE1	-5.22	1.28	1.39
7	I	21	GLU	C-N	-5.22	1.22	1.34
7	I	29	CYS	CA-CB	-5.22	1.42	1.53
1	A	412	ARG	C-O	-5.22	1.13	1.23
1	A	1208	THR	CB-CG2	5.22	1.69	1.52
3	C	24	ASN	CG-ND2	5.22	1.46	1.32
8	J	60	PHE	CG-CD1	5.22	1.46	1.38
1	A	72	GLU	CD-OE1	5.22	1.31	1.25
1	A	77	CYS	N-CA	5.22	1.56	1.46
1	A	514	PRO	N-CD	5.22	1.55	1.47
1	A	660	ASN	CG-ND2	-5.22	1.19	1.32
3	C	52	GLU	N-CA	-5.22	1.35	1.46
6	H	36	CYS	N-CA	5.22	1.56	1.46
7	I	25	LEU	CG-CD2	-5.22	1.32	1.51
2	B	622	LYS	CD-CE	5.22	1.64	1.51
1	A	460	VAL	CA-C	-5.22	1.39	1.52
1	A	1326	ARG	C-O	-5.22	1.13	1.23
7	I	52	ILE	C-N	-5.22	1.23	1.33
2	B	588	GLY	CA-C	-5.21	1.43	1.51
1	A	662	PHE	CG-CD1	5.21	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	958	GLN	CD-OE1	5.21	1.35	1.24
1	A	224	PHE	CE1-CZ	-5.21	1.27	1.37
1	A	545	GLN	C-O	-5.21	1.13	1.23
1	A	698	GLN	CA-CB	-5.21	1.42	1.53
2	B	261	ARG	CA-C	5.21	1.66	1.52
2	B	466	TRP	CZ3-CH2	-5.21	1.31	1.40
1	A	171	GLN	CA-CB	-5.21	1.42	1.53
1	A	209	ASN	CA-CB	5.21	1.66	1.53
1	A	580	VAL	CB-CG1	-5.21	1.42	1.52
1	A	590	ARG	NE-CZ	-5.21	1.26	1.33
2	B	388	CYS	CA-CB	-5.21	1.42	1.53
2	B	737	THR	C-O	5.21	1.33	1.23
4	E	61	GLN	CG-CD	5.21	1.63	1.51
1	A	761	MET	N-CA	-5.21	1.35	1.46
1	A	6	TYR	CG-CD2	5.20	1.46	1.39
1	A	1314	SER	CB-OG	5.20	1.49	1.42
1	A	1080	THR	C-O	5.20	1.33	1.23
1	A	1365	TYR	CE2-CZ	-5.20	1.31	1.38
2	B	200	GLY	N-CA	-5.20	1.38	1.46
3	C	183	TRP	NE1-CE2	-5.20	1.30	1.37
1	A	12	ARG	CZ-NH2	5.20	1.39	1.33
1	A	408	ASP	C-O	5.20	1.33	1.23
3	C	239	PRO	C-N	-5.20	1.22	1.34
9	K	46	ILE	N-CA	-5.20	1.35	1.46
10	L	40	LEU	C-N	5.20	1.46	1.34
7	I	66	PRO	C-O	5.20	1.33	1.23
1	A	483	ASP	CA-CB	-5.20	1.42	1.53
2	B	381	MET	CB-CG	-5.20	1.34	1.51
2	B	708	GLU	C-O	-5.20	1.13	1.23
2	B	764	SER	C-N	-5.20	1.24	1.34
4	E	14	ARG	CB-CG	5.20	1.66	1.52
5	F	83	PRO	N-CD	-5.20	1.40	1.47
7	I	79	HIS	CA-CB	5.20	1.65	1.53
10	L	68	GLU	N-CA	-5.20	1.35	1.46
2	B	325	GLN	CD-NE2	5.19	1.45	1.32
3	C	249	ASP	CG-OD1	5.19	1.37	1.25
9	K	40	HIS	CA-CB	5.19	1.65	1.53
1	A	712	GLU	CD-OE1	5.19	1.31	1.25
1	A	1113	THR	CB-OG1	-5.19	1.32	1.43
2	B	785	TYR	CG-CD2	5.19	1.46	1.39
3	C	180	TYR	CB-CG	-5.19	1.43	1.51
4	E	144	ILE	CB-CG2	-5.19	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	23	VAL	CB-CG2	-5.19	1.42	1.52
1	A	70	CYS	N-CA	5.19	1.56	1.46
2	B	37	PHE	CD2-CE2	5.19	1.49	1.39
2	B	417	PHE	CG-CD1	5.19	1.46	1.38
6	H	35	GLN	CB-CG	5.19	1.66	1.52
7	I	24	ARG	N-CA	5.19	1.56	1.46
9	K	18	LYS	C-O	-5.19	1.13	1.23
2	B	343	ILE	CA-CB	-5.19	1.43	1.54
1	A	976	THR	N-CA	5.19	1.56	1.46
2	B	89	GLU	C-N	5.19	1.46	1.34
2	B	946	ASN	C-O	-5.19	1.13	1.23
3	C	253	LYS	CA-CB	5.19	1.65	1.53
1	A	593	GLU	CG-CD	5.19	1.59	1.51
2	B	1182	CYS	C-O	5.19	1.33	1.23
4	E	38	PRO	CG-CD	5.19	1.67	1.50
9	K	81	TYR	CG-CD2	-5.19	1.32	1.39
1	A	179	LEU	CG-CD1	5.18	1.71	1.51
1	A	1322	ILE	C-O	5.18	1.33	1.23
2	B	527	THR	CA-C	-5.18	1.39	1.52
2	B	893	LEU	CG-CD1	5.18	1.71	1.51
3	C	157	CYS	CB-SG	-5.18	1.73	1.81
3	C	233	GLU	CB-CG	5.18	1.61	1.52
7	I	98	VAL	CB-CG1	-5.18	1.42	1.52
1	A	150	THR	CA-CB	5.18	1.66	1.53
6	H	83	GLN	CG-CD	5.18	1.62	1.51
1	A	1347	ALA	CA-CB	-5.18	1.41	1.52
1	A	924	LYS	CG-CD	5.18	1.70	1.52
1	A	1110	ASN	CA-CB	5.18	1.66	1.53
2	B	810	GLU	CG-CD	5.18	1.59	1.51
4	E	167	ARG	CG-CD	5.18	1.65	1.51
6	H	45	GLU	CD-OE2	5.18	1.31	1.25
1	A	1203	ASN	CB-CG	-5.18	1.39	1.51
2	B	451	LYS	CE-NZ	-5.18	1.36	1.49
2	B	116	GLU	C-O	5.18	1.33	1.23
2	B	1207	LEU	C-O	5.18	1.33	1.23
3	C	148	ARG	N-CA	-5.18	1.35	1.46
7	I	68	LEU	CA-C	-5.17	1.39	1.52
9	K	19	LEU	CB-CG	-5.17	1.37	1.52
6	H	145	ARG	CB-CG	5.17	1.66	1.52
1	A	614	PHE	N-CA	-5.17	1.36	1.46
1	A	1211	GLN	N-CA	5.17	1.56	1.46
2	B	328	GLU	C-O	-5.17	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	160	LYS	C-O	5.17	1.33	1.23
8	J	61	LEU	CG-CD1	5.17	1.71	1.51
3	C	108	GLU	CD-OE1	5.17	1.31	1.25
1	A	704	ALA	CA-C	-5.17	1.39	1.52
2	B	800	GLN	CA-CB	-5.17	1.42	1.53
1	A	109	HIS	CA-C	5.17	1.66	1.52
1	A	379	VAL	C-N	5.17	1.46	1.34
1	A	759	ALA	C-O	5.17	1.33	1.23
2	B	986	GLN	N-CA	5.17	1.56	1.46
3	C	218	PRO	CA-CB	5.17	1.63	1.53
8	J	56	LEU	CG-CD1	-5.17	1.32	1.51
1	A	66	LYS	CA-C	5.17	1.66	1.52
2	B	70	ILE	CB-CG2	5.17	1.68	1.52
2	B	899	ILE	CB-CG1	-5.17	1.39	1.54
2	B	974	PRO	N-CA	-5.16	1.38	1.47
4	E	91	LYS	CE-NZ	-5.16	1.36	1.49
1	A	749	ALA	N-CA	-5.16	1.36	1.46
1	A	880	LYS	CG-CD	5.16	1.70	1.52
9	K	65	HIS	CB-CG	-5.16	1.40	1.50
1	A	524	VAL	C-O	-5.16	1.13	1.23
1	A	1370	LEU	C-N	-5.16	1.22	1.34
2	B	97	VAL	CA-C	-5.16	1.39	1.52
2	B	560	GLU	CB-CG	5.16	1.61	1.52
7	I	11	ASN	CG-OD1	-5.16	1.12	1.24
9	K	96	ASN	CG-OD1	5.16	1.35	1.24
1	A	488	ASN	CG-OD1	-5.16	1.12	1.24
2	B	1192	TYR	CA-CB	-5.16	1.42	1.53
1	A	1146	VAL	CA-CB	-5.16	1.44	1.54
1	A	1431	GLY	CA-C	-5.16	1.43	1.51
3	C	83	SER	N-CA	-5.16	1.36	1.46
7	I	87	GLN	CA-CB	5.16	1.65	1.53
1	A	694	THR	C-O	-5.15	1.13	1.23
2	B	108	VAL	N-CA	5.15	1.56	1.46
2	B	734	HIS	CA-C	5.15	1.66	1.52
2	B	1046	PRO	C-O	5.15	1.33	1.23
2	B	1150	ARG	CG-CD	-5.15	1.39	1.51
6	H	22	LYS	CE-NZ	5.15	1.61	1.49
1	A	210	ILE	CA-C	5.15	1.66	1.52
2	B	121	ASN	CG-ND2	5.15	1.45	1.32
2	B	700	SER	CB-OG	-5.15	1.35	1.42
2	B	821	GLN	CB-CG	-5.15	1.38	1.52
2	B	1072	MET	CB-CG	-5.15	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1091	TYR	CA-CB	-5.15	1.42	1.53
2	B	1169	MET	CA-CB	-5.15	1.42	1.53
4	E	51	GLY	C-O	5.15	1.31	1.23
1	A	113	LEU	C-O	5.15	1.33	1.23
1	A	436	ILE	CB-CG2	5.15	1.68	1.52
2	B	292	ILE	CA-CB	5.15	1.66	1.54
1	A	907	THR	CB-OG1	5.15	1.53	1.43
1	A	1150	SER	CA-CB	-5.15	1.45	1.52
6	H	120	GLY	N-CA	5.15	1.53	1.46
7	I	59	VAL	C-O	-5.15	1.13	1.23
9	K	52	ASN	CG-ND2	5.15	1.45	1.32
1	A	58	LEU	N-CA	5.14	1.56	1.46
1	A	1112	LYS	CE-NZ	5.14	1.61	1.49
2	B	589	VAL	CB-CG1	-5.14	1.42	1.52
1	A	65	LEU	CG-CD2	5.14	1.70	1.51
1	A	1384	VAL	N-CA	5.14	1.56	1.46
2	B	24	PRO	CA-CB	-5.14	1.43	1.53
2	B	884	ARG	CG-CD	5.14	1.64	1.51
3	C	43	THR	N-CA	-5.14	1.36	1.46
4	E	112	TYR	CD1-CE1	5.14	1.47	1.39
7	I	72	ASP	N-CA	5.14	1.56	1.46
1	A	361	LEU	CA-C	-5.14	1.39	1.52
1	A	1285	MET	CA-C	-5.14	1.39	1.52
1	A	463	ILE	CB-CG2	-5.14	1.36	1.52
1	A	726	ARG	CA-C	-5.14	1.39	1.52
2	B	1138	MET	CG-SD	5.14	1.94	1.81
1	A	540	PHE	CD2-CE2	-5.14	1.28	1.39
1	A	897	TYR	CB-CG	5.14	1.59	1.51
1	A	771	GLU	CD-OE1	5.14	1.31	1.25
2	B	638	PHE	C-O	-5.14	1.13	1.23
2	B	968	VAL	CB-CG1	-5.14	1.42	1.52
2	B	1207	LEU	N-CA	-5.14	1.36	1.46
9	K	73	LEU	N-CA	5.14	1.56	1.46
1	A	499	ALA	CA-C	-5.13	1.39	1.52
2	B	18	PHE	CE2-CZ	5.13	1.47	1.37
2	B	315	LYS	CB-CG	-5.13	1.38	1.52
2	B	769	TYR	N-CA	-5.13	1.36	1.46
2	B	1083	ALA	C-O	5.13	1.33	1.23
5	F	112	GLU	CB-CG	5.13	1.61	1.52
1	A	29	ALA	CA-C	5.13	1.66	1.52
4	E	6	GLU	CB-CG	5.13	1.61	1.52
7	I	60	GLN	CA-CB	-5.13	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	302	THR	CA-C	5.13	1.66	1.52
1	A	807	GLY	CA-C	5.13	1.60	1.51
1	A	1078	GLN	N-CA	5.13	1.56	1.46
1	A	1299	VAL	CB-CG1	-5.13	1.42	1.52
7	I	85	PHE	CE2-CZ	-5.13	1.27	1.37
1	A	169	ASN	C-O	5.13	1.33	1.23
1	A	619	LYS	N-CA	5.13	1.56	1.46
1	A	1320	PRO	N-CA	-5.13	1.38	1.47
1	A	66	LYS	CG-CD	5.13	1.69	1.52
1	A	1173	HIS	CA-C	5.13	1.66	1.52
1	A	1406	VAL	CB-CG1	5.13	1.63	1.52
2	B	246	LYS	CB-CG	5.13	1.66	1.52
6	H	26	ILE	CB-CG2	-5.13	1.36	1.52
6	H	121	LEU	CG-CD1	-5.13	1.32	1.51
7	I	22	ASN	N-CA	-5.13	1.36	1.46
1	A	1291	VAL	CA-CB	-5.12	1.44	1.54
2	B	262	GLU	CA-CB	5.12	1.65	1.53
2	B	785	TYR	CE2-CZ	-5.12	1.31	1.38
2	B	1183	LYS	CG-CD	5.12	1.69	1.52
7	I	53	GLY	C-O	5.12	1.31	1.23
1	A	482	PHE	CG-CD2	-5.12	1.31	1.38
1	A	878	ILE	CB-CG1	-5.12	1.39	1.54
7	I	47	GLU	CD-OE1	5.12	1.31	1.25
7	I	113	ASP	CA-CB	-5.12	1.42	1.53
10	L	58	LYS	CB-CG	5.12	1.66	1.52
1	A	161	LEU	CA-C	-5.12	1.39	1.52
1	A	812	GLU	C-O	5.12	1.33	1.23
1	A	862	ASN	C-O	-5.12	1.13	1.23
1	A	1339	LEU	CA-C	-5.12	1.39	1.52
5	F	138	LEU	CG-CD2	-5.12	1.32	1.51
7	I	29	CYS	CB-SG	5.12	1.91	1.82
7	I	35	VAL	C-O	-5.12	1.13	1.23
7	I	23	ASN	C-O	5.12	1.33	1.23
1	A	143	LYS	CG-CD	5.12	1.69	1.52
1	A	1000	LEU	N-CA	-5.12	1.36	1.46
2	B	617	ARG	CB-CG	-5.12	1.38	1.52
2	B	874	PHE	CA-CB	5.12	1.65	1.53
9	K	13	GLY	C-O	5.12	1.31	1.23
2	B	581	PHE	CD1-CE1	-5.12	1.29	1.39
2	B	1073	TYR	CZ-OH	5.12	1.46	1.37
1	A	447	GLN	CB-CG	5.12	1.66	1.52
1	A	1098	VAL	CA-C	-5.12	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	41	LEU	CA-C	-5.12	1.39	1.52
2	B	268	THR	C-N	-5.11	1.22	1.34
2	B	1055	ILE	C-O	-5.11	1.13	1.23
2	B	128	LEU	C-O	-5.11	1.13	1.23
1	A	280	GLU	CA-C	5.11	1.66	1.52
1	A	408	ASP	CA-C	5.11	1.66	1.52
1	A	672	ASP	CG-OD1	5.11	1.37	1.25
2	B	166	PHE	CG-CD1	5.11	1.46	1.38
2	B	539	LEU	CG-CD2	-5.11	1.32	1.51
1	A	920	LEU	C-N	-5.11	1.23	1.33
1	A	1029	ARG	CZ-NH2	-5.11	1.26	1.33
2	B	31	TRP	CZ2-CH2	5.11	1.47	1.37
2	B	1189	ILE	CB-CG1	5.11	1.68	1.54
9	K	13	GLY	N-CA	5.11	1.53	1.46
1	A	865	GLN	CD-NE2	-5.11	1.20	1.32
1	A	1300	LYS	CE-NZ	-5.11	1.36	1.49
2	B	561	TRP	CZ3-CH2	5.11	1.48	1.40
2	B	1068	GLY	N-CA	5.11	1.53	1.46
3	C	222	LYS	N-CA	-5.11	1.36	1.46
6	H	37	LYS	C-O	5.11	1.33	1.23
9	K	80	GLY	C-O	5.11	1.31	1.23
1	A	940	ARG	CZ-NH1	-5.10	1.26	1.33
3	C	159	ALA	CA-C	-5.10	1.39	1.52
1	A	989	GLY	C-O	5.10	1.31	1.23
2	B	616	ILE	CA-CB	5.10	1.66	1.54
4	E	188	LEU	C-O	5.10	1.33	1.23
2	B	274	PRO	CG-CD	5.10	1.67	1.50
2	B	595	ARG	C-N	-5.10	1.22	1.34
2	B	751	VAL	C-N	-5.10	1.22	1.34
6	H	14	GLU	CD-OE1	5.10	1.31	1.25
1	A	1121	GLU	CD-OE2	-5.10	1.20	1.25
2	B	535	LEU	N-CA	5.10	1.56	1.46
3	C	228	PHE	CA-C	-5.10	1.39	1.52
2	B	789	MET	C-O	5.10	1.33	1.23
4	E	201	LYS	CE-NZ	5.10	1.61	1.49
8	J	31	ASP	C-N	5.10	1.45	1.34
1	A	1147	THR	N-CA	5.10	1.56	1.46
2	B	686	ASN	C-O	5.10	1.33	1.23
3	C	6	PRO	N-CD	5.09	1.54	1.47
10	L	56	LEU	CG-CD1	-5.09	1.33	1.51
1	A	356	ASP	C-N	-5.09	1.24	1.34
2	B	272	THR	CA-CB	-5.09	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	747	MET	N-CA	5.09	1.56	1.46
1	A	921	GLY	C-O	5.09	1.31	1.23
2	B	31	TRP	CG-CD2	-5.09	1.34	1.43
2	B	946	ASN	CB-CG	5.09	1.62	1.51
1	A	492	PRO	C-O	-5.09	1.13	1.23
1	A	549	MET	CG-SD	-5.09	1.68	1.81
2	B	351	TYR	CA-C	5.09	1.66	1.52
2	B	596	LEU	C-O	-5.09	1.13	1.23
3	C	182	PRO	CG-CD	5.09	1.67	1.50
7	I	101	PHE	CG-CD1	-5.09	1.31	1.38
9	K	58	PHE	CG-CD2	5.09	1.46	1.38
4	E	81	GLU	CD-OE1	5.09	1.31	1.25
9	K	72	LYS	CB-CG	-5.09	1.38	1.52
1	A	1422	ARG	N-CA	5.09	1.56	1.46
3	C	101	LEU	CG-CD1	5.09	1.70	1.51
4	E	172	GLU	CA-C	-5.09	1.39	1.52
6	H	11	GLN	CA-C	-5.09	1.39	1.52
8	J	43	ARG	CZ-NH1	-5.09	1.26	1.33
1	A	921	GLY	C-N	-5.08	1.22	1.34
2	B	344	LYS	CG-CD	5.08	1.69	1.52
2	B	515	HIS	CA-C	-5.08	1.39	1.52
1	A	1165	GLU	CA-CB	-5.08	1.42	1.53
2	B	19	GLU	CD-OE1	5.08	1.31	1.25
3	C	192	TRP	N-CA	-5.08	1.36	1.46
9	K	14	GLU	C-O	5.08	1.33	1.23
1	A	583	PRO	CA-CB	-5.08	1.43	1.53
1	A	931	GLU	C-O	-5.08	1.13	1.23
3	C	174	ALA	C-O	-5.08	1.13	1.23
6	H	137	GLN	CB-CG	5.08	1.66	1.52
2	B	123	THR	CB-OG1	-5.08	1.33	1.43
2	B	210	LYS	CA-CB	5.08	1.65	1.53
2	B	564	GLU	C-O	-5.08	1.13	1.23
1	A	593	GLU	CA-CB	5.08	1.65	1.53
1	A	635	ARG	C-O	-5.08	1.13	1.23
2	B	322	PHE	CB-CG	5.08	1.59	1.51
3	C	62	PHE	CG-CD1	-5.08	1.31	1.38
4	E	66	GLU	N-CA	5.08	1.56	1.46
1	A	346	ASP	CG-OD2	5.08	1.37	1.25
1	A	452	LYS	C-O	-5.08	1.13	1.23
1	A	1157	ASP	C-O	5.08	1.32	1.23
1	A	1300	LYS	C-O	5.08	1.32	1.23
2	B	1135	ARG	N-CA	-5.08	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	76	GLN	CG-CD	5.08	1.62	1.51
2	B	994	TYR	CB-CG	5.07	1.59	1.51
2	B	1081	LEU	CA-CB	5.07	1.65	1.53
3	C	168	ALA	CA-C	5.07	1.66	1.52
9	K	74	ARG	CZ-NH1	-5.07	1.26	1.33
1	A	679	ILE	CB-CG2	-5.07	1.37	1.52
6	H	20	TYR	CB-CG	-5.07	1.44	1.51
6	H	97	MET	CA-CB	-5.07	1.42	1.53
1	A	236	LEU	CG-CD2	-5.07	1.33	1.51
2	B	975	GLN	CA-C	-5.07	1.39	1.52
7	I	87	GLN	CD-OE1	5.07	1.35	1.24
4	E	73	PRO	CB-CG	5.07	1.75	1.50
1	A	102	VAL	CB-CG1	5.07	1.63	1.52
1	A	368	LYS	C-O	-5.07	1.13	1.23
2	B	211	VAL	CA-C	-5.07	1.39	1.52
2	B	887	HIS	CA-C	5.07	1.66	1.52
3	C	95	CYS	CB-SG	-5.07	1.73	1.81
7	I	60	GLN	CD-OE1	5.07	1.35	1.24
9	K	68	PHE	CA-CB	-5.07	1.42	1.53
1	A	279	LEU	CA-C	-5.06	1.39	1.52
2	B	264	SER	CA-CB	-5.06	1.45	1.52
4	E	1	MET	SD-CE	5.06	2.06	1.77
4	E	96	PHE	CE1-CZ	-5.06	1.27	1.37
8	J	10	CYS	CA-CB	5.06	1.65	1.53
1	A	135	PHE	CE2-CZ	-5.06	1.27	1.37
1	A	264	PHE	CA-C	5.06	1.66	1.52
1	A	1293	SER	N-CA	-5.06	1.36	1.46
2	B	383	ASN	CG-ND2	5.06	1.45	1.32
1	A	100	LYS	CE-NZ	-5.06	1.36	1.49
1	A	681	GLU	CA-CB	5.06	1.65	1.53
1	A	134	ARG	NE-CZ	5.06	1.39	1.33
1	A	358	ASN	C-O	-5.06	1.13	1.23
2	B	114	PRO	CG-CD	-5.06	1.33	1.50
2	B	791	THR	C-O	-5.06	1.13	1.23
2	B	875	GLU	C-O	-5.06	1.13	1.23
1	A	1196	GLU	C-O	-5.06	1.13	1.23
1	A	1342	GLU	CB-CG	-5.06	1.42	1.52
2	B	617	ARG	CA-CB	-5.06	1.42	1.53
1	A	484	GLY	CA-C	-5.05	1.43	1.51
1	A	728	LYS	CB-CG	-5.05	1.39	1.52
1	A	947	PHE	CB-CG	5.05	1.59	1.51
2	B	750	GLY	CA-C	-5.05	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	138	GLU	C-O	5.05	1.32	1.23
1	A	57	ARG	CZ-NH2	5.05	1.39	1.33
1	A	406	ILE	CA-CB	-5.05	1.43	1.54
1	A	1427	ASN	CB-CG	5.05	1.62	1.51
2	B	1055	ILE	C-N	-5.05	1.22	1.34
1	A	298	PHE	CE1-CZ	5.05	1.47	1.37
4	E	95	THR	CA-CB	5.05	1.66	1.53
7	I	73	ARG	CB-CG	-5.05	1.39	1.52
2	B	1162	ILE	CB-CG1	-5.05	1.40	1.54
3	C	252	GLN	CA-C	-5.05	1.39	1.52
1	A	818	MET	C-O	-5.05	1.13	1.23
2	B	358	LYS	C-O	-5.05	1.13	1.23
2	B	464	GLY	C-O	5.05	1.31	1.23
2	B	892	LYS	CG-CD	5.05	1.69	1.52
9	K	75	ILE	CB-CG2	-5.05	1.37	1.52
9	K	109	TRP	CZ2-CH2	5.05	1.47	1.37
6	H	99	GLY	C-O	5.04	1.31	1.23
7	I	101	PHE	C-O	-5.04	1.13	1.23
1	A	224	PHE	CE2-CZ	-5.04	1.27	1.37
1	A	902	LEU	N-CA	-5.04	1.36	1.46
1	A	946	VAL	C-O	-5.04	1.13	1.23
1	A	960	ILE	CB-CG1	-5.04	1.40	1.54
2	B	553	PRO	C-N	5.04	1.45	1.34
2	B	1219	ASP	CG-OD2	5.04	1.36	1.25
9	K	91	CYS	N-CA	-5.04	1.36	1.46
2	B	697	GLU	CG-CD	5.04	1.59	1.51
3	C	264	GLN	CB-CG	5.04	1.66	1.52
1	A	943	LEU	N-CA	-5.04	1.36	1.46
2	B	89	GLU	CA-C	5.04	1.66	1.52
1	A	53	LEU	N-CA	5.04	1.56	1.46
2	B	1085	ILE	C-O	-5.04	1.13	1.23
1	A	288	ALA	N-CA	5.04	1.56	1.46
1	A	305	ASP	N-CA	5.04	1.56	1.46
1	A	687	LYS	CE-NZ	5.04	1.61	1.49
1	A	704	ALA	CA-CB	-5.04	1.41	1.52
1	A	184	SER	CB-OG	-5.04	1.35	1.42
2	B	1031	LEU	C-O	-5.04	1.13	1.23
5	F	149	GLU	N-CA	5.04	1.56	1.46
9	K	58	PHE	CD1-CE1	-5.04	1.29	1.39
9	K	75	ILE	CB-CG1	5.04	1.68	1.54
1	A	525	GLN	C-O	-5.03	1.13	1.23
1	A	572	TRP	CA-C	5.03	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	893	PHE	CG-CD2	-5.03	1.31	1.38
2	B	181	LEU	N-CA	-5.03	1.36	1.46
2	B	607	GLY	CA-C	5.03	1.59	1.51
7	I	15	TYR	N-CA	-5.03	1.36	1.46
1	A	807	GLY	N-CA	5.03	1.53	1.46
1	A	1368	MET	CA-C	-5.03	1.39	1.52
2	B	635	ARG	CG-CD	5.03	1.64	1.51
2	B	1101	ASP	CA-CB	5.03	1.65	1.53
4	E	24	LYS	CG-CD	-5.03	1.35	1.52
1	A	573	SER	CB-OG	5.03	1.48	1.42
2	B	1098	MET	SD-CE	5.03	2.06	1.77
2	B	96	TYR	C-O	5.03	1.32	1.23
2	B	360	PHE	CD2-CE2	-5.03	1.29	1.39
2	B	595	ARG	N-CA	5.03	1.56	1.46
2	B	1100	ASP	CA-CB	5.03	1.65	1.53
3	C	267	GLN	CD-OE1	5.03	1.35	1.24
1	A	1037	LEU	CB-CG	5.03	1.67	1.52
1	A	1323	ASP	C-N	-5.03	1.24	1.34
2	B	416	LEU	CA-C	-5.03	1.39	1.52
2	B	421	PHE	CE1-CZ	-5.03	1.27	1.37
2	B	431	TYR	CE2-CZ	5.03	1.45	1.38
1	A	17	VAL	CB-CG1	-5.02	1.42	1.52
1	A	852	TYR	CZ-OH	-5.02	1.29	1.37
2	B	406	LEU	C-O	5.02	1.32	1.23
2	B	422	LYS	CD-CE	5.02	1.63	1.51
2	B	711	GLU	CD-OE2	5.02	1.31	1.25
4	E	112	TYR	CD2-CE2	5.02	1.46	1.39
5	F	74	ILE	CB-CG2	5.02	1.68	1.52
2	B	972	LYS	CE-NZ	5.02	1.61	1.49
6	H	141	TYR	CG-CD2	5.02	1.45	1.39
1	A	72	GLU	CA-CB	5.02	1.65	1.53
1	A	721	PHE	CG-CD2	-5.02	1.31	1.38
1	A	1265	ASN	C-O	-5.02	1.13	1.23
2	B	389	ALA	C-O	-5.02	1.13	1.23
4	E	115	ASN	CG-OD1	5.02	1.34	1.24
7	I	79	HIS	CA-C	5.02	1.66	1.52
1	A	303	TYR	C-N	-5.02	1.22	1.34
2	B	485	ARG	C-N	-5.02	1.22	1.34
2	B	773	MET	CA-CB	-5.02	1.43	1.53
2	B	1061	GLU	CA-CB	5.02	1.65	1.53
2	B	1061	GLU	C-O	5.02	1.32	1.23
3	C	161	LYS	CD-CE	-5.02	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1332	PHE	CD1-CE1	-5.02	1.29	1.39
5	F	136	ARG	C-O	-5.02	1.13	1.23
1	A	792	TYR	CD1-CE1	-5.01	1.31	1.39
1	A	1304	TRP	CD2-CE2	-5.01	1.35	1.41
2	B	239	GLU	CD-OE1	5.01	1.31	1.25
2	B	603	LEU	CG-CD2	-5.01	1.33	1.51
1	A	47	ARG	CG-CD	5.01	1.64	1.51
1	A	63	ARG	CG-CD	5.01	1.64	1.51
1	A	415	LEU	C-O	5.01	1.32	1.23
1	A	944	ARG	CZ-NH1	-5.01	1.26	1.33
2	B	485	ARG	C-O	5.01	1.32	1.23
2	B	1035	ALA	N-CA	-5.01	1.36	1.46
1	A	511	ILE	C-N	-5.01	1.22	1.34
1	A	1222	ASN	C-O	5.01	1.32	1.23
2	B	131	ASP	CA-CB	5.01	1.65	1.53
3	C	25	VAL	CB-CG1	5.01	1.63	1.52
3	C	67	LEU	CG-CD1	-5.01	1.33	1.51
4	E	5	ASN	CA-C	-5.01	1.40	1.52
7	I	120	GLN	C-O	5.01	1.32	1.23
3	C	21	ILE	CA-CB	-5.01	1.43	1.54
3	C	215	GLU	N-CA	5.01	1.56	1.46
6	H	99	GLY	N-CA	-5.01	1.38	1.46
6	H	141	TYR	CZ-OH	-5.01	1.29	1.37
9	K	26	LYS	C-O	-5.00	1.13	1.23
1	A	1242	VAL	N-CA	-5.00	1.36	1.46
2	B	215	GLN	CA-CB	5.00	1.65	1.53
2	B	1000	PRO	CG-CD	5.00	1.67	1.50
3	C	26	ASP	CA-C	5.00	1.66	1.52
3	C	205	LYS	N-CA	5.00	1.56	1.46
6	H	7	ASP	CG-OD2	5.00	1.36	1.25
1	A	476	SER	C-O	-5.00	1.13	1.23
1	A	867	ILE	CB-CG1	-5.00	1.40	1.54
2	B	376	PHE	CE1-CZ	-5.00	1.27	1.37
2	B	678	GLU	CD-OE2	5.00	1.31	1.25
3	C	204	SER	CB-OG	5.00	1.48	1.42
5	F	88	TYR	CG-CD1	-5.00	1.32	1.39

All (3318) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	774	ARG	NE-CZ-NH1	45.06	142.83	120.30
2	B	995	ARG	NE-CZ-NH2	-36.16	102.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	91	ARG	NE-CZ-NH1	32.74	136.67	120.30
2	B	995	ARG	NE-CZ-NH1	32.13	136.37	120.30
1	A	469	ARG	NE-CZ-NH1	31.48	136.04	120.30
3	C	66	ARG	NE-CZ-NH1	-30.55	105.03	120.30
1	A	1289	ARG	NE-CZ-NH1	-29.63	105.48	120.30
1	A	774	ARG	NE-CZ-NH2	-29.52	105.54	120.30
1	A	821	ARG	NE-CZ-NH2	-29.06	105.77	120.30
1	A	1366	ARG	NE-CZ-NH2	-28.67	105.96	120.30
3	C	35	ARG	NE-CZ-NH1	28.29	134.44	120.30
2	B	496	ARG	NE-CZ-NH1	27.94	134.27	120.30
6	H	77	ARG	NE-CZ-NH1	26.68	133.64	120.30
2	B	591	ARG	NE-CZ-NH1	26.48	133.54	120.30
2	B	496	ARG	NE-CZ-NH2	-26.00	107.30	120.30
3	C	66	ARG	NE-CZ-NH2	24.94	132.77	120.30
9	K	47	ARG	NE-CZ-NH2	-24.91	107.84	120.30
2	B	807	ARG	NE-CZ-NH2	-24.42	108.09	120.30
2	B	983	ARG	NE-CZ-NH2	-24.37	108.12	120.30
7	I	91	ARG	NE-CZ-NH2	-24.31	108.15	120.30
1	A	416	ARG	NE-CZ-NH1	23.85	132.23	120.30
2	B	604	ARG	NE-CZ-NH1	23.73	132.16	120.30
2	B	1135	ARG	NE-CZ-NH2	-23.53	108.53	120.30
2	B	983	ARG	NE-CZ-NH1	23.41	132.00	120.30
1	A	434	ARG	NE-CZ-NH2	-23.39	108.60	120.30
2	B	620	ARG	NE-CZ-NH1	-23.31	108.64	120.30
1	A	434	ARG	NE-CZ-NH1	23.03	131.81	120.30
2	B	604	ARG	NE-CZ-NH2	-22.97	108.81	120.30
1	A	1422	ARG	NE-CZ-NH1	22.94	131.77	120.30
1	A	985	ASP	CB-CG-OD1	-22.54	98.02	118.30
2	B	591	ARG	NE-CZ-NH2	-22.46	109.07	120.30
3	C	35	ARG	NE-CZ-NH2	-22.40	109.10	120.30
1	A	446	ARG	NE-CZ-NH2	-22.26	109.17	120.30
1	A	459	ARG	NE-CZ-NH2	-20.99	109.80	120.30
5	F	97	ARG	NE-CZ-NH1	20.80	130.70	120.30
2	B	106	ASP	CB-CG-OD2	20.75	136.97	118.30
4	E	192	ARG	NE-CZ-NH2	20.60	130.60	120.30
1	A	407	ARG	NE-CZ-NH2	-20.48	110.06	120.30
1	A	386	ASP	CB-CG-OD1	20.46	136.71	118.30
1	A	469	ARG	NE-CZ-NH2	-20.28	110.16	120.30
1	A	806	ARG	NE-CZ-NH1	-20.01	110.30	120.30
1	A	1241	ARG	NE-CZ-NH2	-19.85	110.37	120.30
1	A	884	ASP	CB-CG-OD2	19.84	136.15	118.30
1	A	940	ARG	NE-CZ-NH2	-19.74	110.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1100	ARG	NE-CZ-NH1	19.54	130.07	120.30
2	B	1129	ARG	NE-CZ-NH2	-19.33	110.64	120.30
1	A	731	ARG	NE-CZ-NH1	-19.16	110.72	120.30
2	B	1129	ARG	NE-CZ-NH1	19.14	129.87	120.30
1	A	940	ARG	NE-CZ-NH1	18.91	129.75	120.30
3	C	26	ASP	CB-CG-OD2	-18.79	101.39	118.30
1	A	1366	ARG	NE-CZ-NH1	18.59	129.60	120.30
2	B	348	ARG	NE-CZ-NH1	18.38	129.49	120.30
2	B	839	MET	CG-SD-CE	-18.25	70.99	100.20
8	J	49	MET	CG-SD-CE	-18.01	71.38	100.20
1	A	962	ARG	NE-CZ-NH2	-17.98	111.31	120.30
4	E	207	ARG	NE-CZ-NH1	17.88	129.24	120.30
2	B	564	GLU	OE1-CD-OE2	17.76	144.61	123.30
1	A	1442	ASP	CB-CG-OD2	17.70	134.22	118.30
2	B	392	ARG	NE-CZ-NH2	-17.59	111.51	120.30
1	A	884	ASP	CB-CG-OD1	-17.38	102.66	118.30
1	A	1202	MET	CG-SD-CE	17.32	127.91	100.20
1	A	1121	GLU	OE1-CD-OE2	-17.27	102.57	123.30
4	E	180	ARG	NE-CZ-NH1	-17.19	111.70	120.30
8	J	43	ARG	NE-CZ-NH1	-17.03	111.78	120.30
1	A	1442	ASP	CB-CG-OD1	-16.98	103.01	118.30
4	E	14	ARG	NE-CZ-NH2	-16.81	111.90	120.30
2	B	320	ASP	CB-CG-OD1	16.74	133.37	118.30
2	B	1019	SER	CB-CA-C	-16.70	78.37	110.10
1	A	459	ARG	NE-CZ-NH1	16.59	128.60	120.30
1	A	532	ARG	NE-CZ-NH1	16.56	128.58	120.30
10	L	68	GLU	OE1-CD-OE2	-16.51	103.49	123.30
2	B	188	ASP	CB-CG-OD1	-16.50	103.45	118.30
10	L	70	ARG	NE-CZ-NH1	16.41	128.51	120.30
1	A	896	ARG	NE-CZ-NH2	-16.34	112.13	120.30
8	J	2	ILE	CG1-CB-CG2	-16.30	75.55	111.40
1	A	590	ARG	NE-CZ-NH2	-16.25	112.18	120.30
2	B	760	ASP	CB-CG-OD2	16.06	132.75	118.30
2	B	316	PRO	N-CD-CG	-16.05	79.13	103.20
1	A	350	ARG	NE-CZ-NH1	15.98	128.29	120.30
1	A	393	ARG	NE-CZ-NH1	-15.94	112.33	120.30
2	B	294	ASP	CB-CG-OD2	15.75	132.48	118.30
9	K	114	LEU	CB-CG-CD2	15.67	137.64	111.00
7	I	34	TYR	CB-CG-CD1	15.64	130.39	121.00
2	B	327	ARG	NE-CZ-NH1	-15.60	112.50	120.30
1	A	605	MET	CG-SD-CE	-15.51	75.39	100.20
1	A	532	ARG	NE-CZ-NH2	-15.49	112.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	722	ASP	CB-CG-OD1	15.42	132.18	118.30
2	B	790	ASP	CB-CG-OD2	-15.34	104.49	118.30
1	A	1023	ARG	NE-CZ-NH2	15.34	127.97	120.30
1	A	188	ASP	CB-CG-OD2	15.32	132.09	118.30
2	B	326	ASP	CB-CG-OD2	15.31	132.08	118.30
1	A	305	ASP	CB-CG-OD2	15.28	132.05	118.30
1	A	949	ASP	CB-CG-OD2	15.24	132.02	118.30
1	A	1336	MET	CG-SD-CE	15.22	124.56	100.20
1	A	359	LEU	CB-CG-CD2	-15.20	85.17	111.00
2	B	612	GLU	OE1-CD-OE2	15.12	141.45	123.30
1	A	42	ASP	CB-CG-OD2	15.05	131.84	118.30
9	K	5	ASP	CB-CG-OD1	-15.02	104.78	118.30
1	A	1100	ARG	NE-CZ-NH2	-15.02	112.79	120.30
2	B	935	ARG	NE-CZ-NH1	14.88	127.74	120.30
2	B	408	LEU	CB-CG-CD2	-14.87	85.73	111.00
1	A	12	ARG	NE-CZ-NH2	-14.86	112.87	120.30
6	H	146	ARG	NE-CZ-NH1	14.76	127.68	120.30
2	B	1043	ASP	CB-CG-OD2	14.74	131.57	118.30
1	A	1326	ARG	NE-CZ-NH1	14.71	127.65	120.30
1	A	412	ARG	NE-CZ-NH2	-14.62	112.99	120.30
8	J	43	ARG	NE-CZ-NH2	14.60	127.60	120.30
2	B	552	MET	CG-SD-CE	14.59	123.53	100.20
1	A	1241	ARG	NE-CZ-NH1	14.45	127.53	120.30
1	A	728	LYS	CD-CE-NZ	14.45	144.92	111.70
1	A	74	MET	CG-SD-CE	14.35	123.16	100.20
4	E	48	ASP	CB-CG-OD2	14.30	131.18	118.30
1	A	1198	ASP	CB-CG-OD1	14.29	131.16	118.30
1	A	1267	MET	CG-SD-CE	-14.26	77.38	100.20
2	B	1028	GLU	OE1-CD-OE2	-14.25	106.20	123.30
6	H	41	ASP	CB-CG-OD1	14.22	131.10	118.30
2	B	1150	ARG	NE-CZ-NH2	-14.21	113.19	120.30
2	B	883	LEU	CA-CB-CG	14.20	147.96	115.30
2	B	348	ARG	NE-CZ-NH2	-14.18	113.21	120.30
4	E	11	ARG	NE-CZ-NH1	-14.13	113.24	120.30
5	F	154	ASP	CB-CG-OD1	14.10	130.99	118.30
2	B	49	ASP	CB-CG-OD2	14.04	130.94	118.30
2	B	267	ARG	NE-CZ-NH2	-14.01	113.30	120.30
1	A	1204	ASP	CB-CG-OD2	14.00	130.90	118.30
7	I	92	ARG	NE-CZ-NH1	-13.97	113.31	120.30
1	A	1043	ASP	CB-CG-OD2	13.85	130.76	118.30
1	A	420	ARG	NE-CZ-NH1	13.80	127.20	120.30
4	E	192	ARG	NE-CZ-NH1	-13.73	113.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	7	ASP	CB-CG-OD2	13.62	130.56	118.30
3	C	246	ARG	NE-CZ-NH2	13.62	127.11	120.30
1	A	130	ASP	CB-CG-OD1	13.61	130.55	118.30
2	B	837	ASP	CB-CG-OD2	13.61	130.55	118.30
2	B	209	GLU	N-CA-CB	-13.57	86.17	110.60
1	A	812	GLU	OE1-CD-OE2	-13.57	107.02	123.30
4	E	180	ARG	NE-CZ-NH2	13.54	127.07	120.30
3	C	143	LEU	CB-CG-CD2	-13.53	87.99	111.00
1	A	1006	ILE	CG1-CB-CG2	-13.48	81.74	111.40
2	B	1096	ARG	NE-CZ-NH2	-13.44	113.58	120.30
1	A	352	VAL	CG1-CB-CG2	-13.41	89.44	110.90
1	A	652	VAL	CG1-CB-CG2	-13.38	89.49	110.90
2	B	601	ARG	NE-CZ-NH1	-13.35	113.63	120.30
1	A	1231	ASP	CB-CG-OD1	-13.33	106.31	118.30
7	I	7	CYS	CA-CB-SG	13.30	137.94	114.00
7	I	106	CYS	CA-CB-SG	13.30	137.94	114.00
7	I	54	GLU	OE1-CD-OE2	13.26	139.21	123.30
4	E	149	LEU	CB-CG-CD1	13.25	133.52	111.00
10	L	47	ARG	NE-CZ-NH2	13.24	126.92	120.30
3	C	136	ASP	CB-CG-OD2	13.16	130.15	118.30
1	A	590	ARG	NE-CZ-NH1	13.16	126.88	120.30
1	A	170	THR	OG1-CB-CG2	-13.16	79.73	110.00
1	A	557	ASP	CB-CG-OD1	13.15	130.14	118.30
1	A	1129	GLU	OE1-CD-OE2	-13.15	107.52	123.30
7	I	61	ASP	CB-CG-OD2	13.14	130.12	118.30
4	E	212	ARG	CD-NE-CZ	13.13	141.98	123.60
1	A	1155	ASP	CB-CG-OD1	13.11	130.10	118.30
1	A	544	ASP	CB-CG-OD1	13.10	130.09	118.30
4	E	84	ASP	CB-CG-OD1	13.08	130.07	118.30
7	I	113	ASP	CB-CG-OD2	13.07	130.06	118.30
2	B	287	ARG	NE-CZ-NH2	-13.06	113.77	120.30
3	C	155	LEU	CB-CA-C	-13.05	85.41	110.20
9	K	6	ARG	NE-CZ-NH1	13.04	126.82	120.30
2	B	385	LEU	CB-CG-CD1	-12.96	88.96	111.00
3	C	160	LYS	CD-CE-NZ	12.95	141.49	111.70
8	J	6	ARG	NE-CZ-NH1	-12.95	113.83	120.30
3	C	34	ARG	NE-CZ-NH2	-12.87	113.87	120.30
1	A	1032	LEU	CB-CG-CD2	12.84	132.83	111.00
5	F	97	ARG	NE-CZ-NH2	-12.84	113.88	120.30
2	B	1185	CYS	CA-CB-SG	12.82	137.08	114.00
1	A	1176	LEU	N-CA-C	-12.82	76.39	111.00
2	B	284	ILE	CG1-CB-CG2	-12.80	83.24	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	748	MET	CG-SD-CE	12.78	120.64	100.20
1	A	801	GLU	OE1-CD-OE2	12.72	138.57	123.30
2	B	1041	GLU	OE1-CD-OE2	12.71	138.55	123.30
2	B	407	ASP	CB-CG-OD1	12.64	129.68	118.30
2	B	394	ASP	CB-CG-OD1	-12.61	106.95	118.30
2	B	131	ASP	CB-CG-OD2	12.59	129.63	118.30
3	C	163	ILE	CA-CB-CG2	12.54	135.97	110.90
1	A	944	ARG	NE-CZ-NH1	12.51	126.56	120.30
2	B	100	PRO	N-CD-CG	-12.51	84.44	103.20
6	H	135	LEU	CB-CG-CD2	12.50	132.25	111.00
10	L	70	ARG	NE-CZ-NH2	-12.50	114.05	120.30
4	E	50	MET	CG-SD-CE	12.48	120.17	100.20
2	B	568	ASP	CB-CG-OD2	12.48	129.53	118.30
3	C	125	MET	CG-SD-CE	12.45	120.12	100.20
1	A	821	ARG	CG-CD-NE	-12.44	85.69	111.80
2	B	384	ARG	NE-CZ-NH2	-12.42	114.09	120.30
1	A	1418	LEU	CB-CG-CD1	12.41	132.10	111.00
2	B	654	ARG	NE-CZ-NH1	-12.41	114.09	120.30
2	B	747	MET	CG-SD-CE	-12.41	80.34	100.20
3	C	26	ASP	CB-CG-OD1	12.41	129.47	118.30
1	A	32	VAL	CG1-CB-CG2	-12.38	91.10	110.90
9	K	1	MET	CG-SD-CE	12.37	119.99	100.20
2	B	391	ASP	CB-CG-OD2	12.35	129.41	118.30
1	A	416	ARG	NE-CZ-NH2	-12.35	114.13	120.30
4	E	24	LYS	CD-CE-NZ	-12.35	83.30	111.70
6	H	77	ARG	NH1-CZ-NH2	-12.35	105.82	119.40
1	A	174	ILE	CG1-CB-CG2	-12.35	84.24	111.40
1	A	163	SER	N-CA-CB	12.32	128.99	110.50
1	A	866	PHE	CB-CG-CD2	12.29	129.40	120.80
2	B	629	ASP	CB-CG-OD2	12.29	129.36	118.30
1	A	1133	LEU	CB-CG-CD2	-12.28	90.13	111.00
1	A	1055	ARG	CG-CD-NE	-12.23	86.11	111.80
1	A	962	ARG	NE-CZ-NH1	12.22	126.41	120.30
2	B	967	ARG	NE-CZ-NH1	-12.19	114.20	120.30
2	B	641	GLU	OE1-CD-OE2	-12.17	108.70	123.30
2	B	227	LYS	CD-CE-NZ	12.17	139.69	111.70
1	A	541	ILE	CG1-CB-CG2	-12.16	84.65	111.40
1	A	752	LYS	CD-CE-NZ	12.15	139.64	111.70
2	B	312	GLU	OE1-CD-OE2	12.13	137.86	123.30
1	A	70	CYS	CA-CB-SG	12.12	135.82	114.00
5	F	135	ARG	NE-CZ-NH2	12.10	126.35	120.30
1	A	636	GLU	OE1-CD-OE2	-12.10	108.78	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	949	ASP	N-CA-CB	-12.09	88.84	110.60
2	B	884	ARG	NE-CZ-NH1	12.08	126.34	120.30
1	A	424	ILE	CG1-CB-CG2	-12.07	84.84	111.40
2	B	188	ASP	CB-CG-OD2	12.06	129.15	118.30
7	I	75	CYS	CA-CB-SG	12.05	135.69	114.00
2	B	598	GLU	OE1-CD-OE2	-12.04	108.85	123.30
2	B	1166	CYS	CA-CB-SG	12.04	135.68	114.00
1	A	164	ARG	NE-CZ-NH2	-11.97	114.31	120.30
4	E	46	TYR	CB-CG-CD2	11.97	128.18	121.00
1	A	504	LEU	CA-CB-CG	11.96	142.82	115.30
1	A	1231	ASP	CB-CG-OD2	11.95	129.06	118.30
7	I	34	TYR	CD1-CG-CD2	-11.95	104.75	117.90
2	B	851	PHE	CB-CG-CD2	11.92	129.14	120.80
1	A	922	ASP	CB-CG-OD1	11.91	129.02	118.30
2	B	181	LEU	CB-CG-CD2	-11.89	90.79	111.00
2	B	994	TYR	CZ-CE2-CD2	11.88	130.49	119.80
1	A	985	ASP	CB-CG-OD2	11.86	128.97	118.30
1	A	761	MET	CG-SD-CE	11.85	119.16	100.20
7	I	72	ASP	CB-CG-OD1	11.84	128.96	118.30
1	A	1062	GLU	OE1-CD-OE2	11.84	137.51	123.30
1	A	1257	ASP	CB-CG-OD1	-11.84	107.64	118.30
1	A	1284	MET	CA-CB-CG	-11.82	93.21	113.30
2	B	618	ASP	CB-CG-OD2	-11.82	107.67	118.30
6	H	46	LEU	CB-CG-CD1	-11.81	90.92	111.00
10	L	27	LEU	CA-CB-CG	11.81	142.46	115.30
2	B	198	ASP	CB-CG-OD1	11.77	128.89	118.30
2	B	497	ARG	NE-CZ-NH1	11.74	126.17	120.30
1	A	1025	ARG	NE-CZ-NH2	11.73	126.17	120.30
2	B	642	ASP	N-CA-C	-11.72	79.35	111.00
2	B	1020	ARG	NE-CZ-NH2	-11.72	114.44	120.30
9	K	53	ASP	CB-CG-OD2	11.71	128.84	118.30
6	H	92	ASP	CB-CG-OD2	11.71	128.84	118.30
2	B	396	ASP	CB-CG-OD1	11.71	128.84	118.30
9	K	61	TYR	CB-CG-CD2	11.70	128.02	121.00
1	A	193	ASP	CB-CG-OD1	11.70	128.83	118.30
1	A	720	ARG	NE-CZ-NH2	11.70	126.15	120.30
2	B	833	TYR	CB-CG-CD2	-11.69	113.99	121.00
1	A	899	VAL	CG1-CB-CG2	-11.69	92.20	110.90
2	B	942	ARG	NE-CZ-NH1	-11.68	114.46	120.30
2	B	646	LEU	CB-CG-CD2	11.67	130.85	111.00
1	A	826	ASP	CB-CG-OD2	11.67	128.80	118.30
1	A	1349	TYR	CB-CG-CD1	11.66	128.00	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	38	ARG	NE-CZ-NH1	11.65	126.13	120.30
2	B	620	ARG	NH1-CZ-NH2	11.65	132.21	119.40
1	A	107	CYS	CA-CB-SG	11.64	134.96	114.00
1	A	538	ASP	CB-CA-C	-11.62	87.16	110.40
1	A	992	ASP	CB-CG-OD2	11.62	128.75	118.30
9	K	24	ASP	CB-CG-OD1	-11.62	107.84	118.30
2	B	833	TYR	CB-CG-CD1	11.60	127.96	121.00
9	K	85	ASP	CB-CG-OD1	11.58	128.72	118.30
2	B	579	ARG	NE-CZ-NH2	-11.54	114.53	120.30
2	B	170	LEU	CB-CG-CD1	-11.54	91.39	111.00
2	B	270	LYS	CD-CE-NZ	-11.52	85.20	111.70
3	C	90	ASP	CB-CG-OD2	-11.51	107.94	118.30
1	A	645	LEU	CB-CG-CD2	11.49	130.53	111.00
5	F	81	THR	N-CA-CB	-11.47	88.50	110.30
1	A	781	ASP	CB-CG-OD1	11.47	128.62	118.30
2	B	936	ASP	CB-CG-OD2	11.47	128.62	118.30
8	J	3	VAL	CB-CA-C	-11.45	89.65	111.40
4	E	52	ARG	NE-CZ-NH2	-11.43	114.59	120.30
1	A	974	ASP	N-CA-CB	11.43	131.17	110.60
7	I	19	ASP	CB-CG-OD2	11.42	128.57	118.30
9	K	68	PHE	CB-CG-CD1	-11.39	112.83	120.80
1	A	1345	ARG	NE-CZ-NH1	-11.38	114.61	120.30
1	A	547	LEU	CB-CG-CD2	-11.38	91.66	111.00
3	C	11	ARG	NE-CZ-NH1	11.36	125.98	120.30
1	A	804	TYR	CB-CG-CD1	11.33	127.80	121.00
2	B	392	ARG	NE-CZ-NH1	11.33	125.96	120.30
9	K	68	PHE	CB-CG-CD2	11.30	128.71	120.80
5	F	125	LEU	CB-CG-CD1	-11.21	91.95	111.00
1	A	656	TRP	CD1-NE1-CE2	-11.20	98.92	109.00
2	B	709	ASP	CB-CG-OD2	11.20	128.38	118.30
7	I	5	ARG	NE-CZ-NH2	11.20	125.90	120.30
8	J	62	ARG	NE-CZ-NH2	-11.19	114.70	120.30
1	A	618	GLU	OE1-CD-OE2	11.19	136.72	123.30
1	A	268	ASP	CB-CG-OD2	11.18	128.36	118.30
1	A	1357	ALA	CB-CA-C	-11.13	93.41	110.10
7	I	81	ARG	NE-CZ-NH1	11.07	125.84	120.30
1	A	982	THR	CA-CB-CG2	11.07	127.89	112.40
2	B	1219	ASP	CB-CG-OD2	11.06	128.25	118.30
2	B	967	ARG	NE-CZ-NH2	11.05	125.83	120.30
1	A	782	ARG	NE-CZ-NH2	-11.05	114.77	120.30
1	A	1366	ARG	CD-NE-CZ	11.05	139.07	123.60
1	A	1271	ILE	CG1-CB-CG2	-11.02	87.16	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1407	GLU	OE1-CD-OE2	-11.02	110.08	123.30
7	I	4	PHE	CB-CG-CD1	-11.02	113.09	120.80
3	C	18	VAL	CB-CA-C	-11.01	90.47	111.40
1	A	96	ILE	CG1-CB-CG2	-11.01	87.19	111.40
1	A	218	ASP	CB-CG-OD2	-11.00	108.40	118.30
9	K	24	ASP	CB-CG-OD2	10.98	128.19	118.30
2	B	807	ARG	NE-CZ-NH1	10.93	125.77	120.30
1	A	709	THR	N-CA-CB	-10.92	89.55	110.30
6	H	8	ASP	CB-CG-OD2	10.92	128.13	118.30
1	A	635	ARG	NE-CZ-NH2	-10.91	114.84	120.30
2	B	995	ARG	CD-NE-CZ	10.89	138.85	123.60
1	A	1036	ARG	NE-CZ-NH2	-10.88	114.86	120.30
2	B	766	ARG	NE-CZ-NH1	10.88	125.74	120.30
2	B	1010	LEU	CB-CG-CD1	-10.88	92.51	111.00
9	K	5	ASP	CB-CG-OD2	10.87	128.08	118.30
4	E	2	ASP	CB-CG-OD1	10.86	128.07	118.30
1	A	821	ARG	NE-CZ-NH1	10.86	125.73	120.30
3	C	19	ASP	CB-CG-OD1	-10.85	108.54	118.30
2	B	1160	VAL	CB-CA-C	-10.82	90.83	111.40
8	J	7	CYS	CA-CB-SG	10.81	133.47	114.00
2	B	329	THR	OG1-CB-CG2	-10.81	85.15	110.00
4	E	163	GLU	OE1-CD-OE2	-10.80	110.33	123.30
2	B	653	VAL	CB-CA-C	-10.78	90.92	111.40
4	E	167	ARG	NE-CZ-NH1	-10.78	114.91	120.30
7	I	118	ARG	NE-CZ-NH2	10.77	125.68	120.30
9	K	114	LEU	CA-CB-CG	10.74	140.00	115.30
9	K	70	ARG	NE-CZ-NH2	10.72	125.66	120.30
2	B	852	ARG	N-CA-CB	-10.70	91.34	110.60
1	A	386	ASP	CB-CG-OD2	-10.70	108.67	118.30
2	B	633	VAL	CG1-CB-CG2	-10.69	93.79	110.90
1	A	1301	GLU	OE1-CD-OE2	10.68	136.12	123.30
2	B	1182	CYS	CA-CB-SG	10.68	133.23	114.00
9	K	49	GLU	OE1-CD-OE2	10.68	136.12	123.30
2	B	710	LEU	CB-CG-CD2	10.68	129.15	111.00
2	B	966	VAL	CG1-CB-CG2	-10.67	93.83	110.90
2	B	552	MET	CA-CB-CG	10.66	131.42	113.30
2	B	1099	VAL	CB-CA-C	-10.65	91.16	111.40
1	A	85	ASP	CB-CG-OD1	-10.64	108.73	118.30
2	B	1159	ARG	NE-CZ-NH2	-10.64	114.98	120.30
1	A	731	ARG	NH1-CZ-NH2	10.63	131.09	119.40
2	B	138	GLU	OE1-CD-OE2	-10.63	110.54	123.30
4	E	168	TYR	CB-CG-CD2	10.63	127.38	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1058	LEU	CB-CG-CD2	-10.63	92.94	111.00
7	I	30	ARG	CG-CD-NE	-10.63	89.48	111.80
1	A	514	PRO	N-CA-CB	-10.60	90.59	103.30
2	B	497	ARG	NE-CZ-NH2	-10.59	115.01	120.30
1	A	486	GLU	OE1-CD-OE2	-10.58	110.60	123.30
1	A	1107	VAL	CG1-CB-CG2	-10.58	93.97	110.90
4	E	182	ASP	CB-CG-OD1	10.57	127.81	118.30
2	B	336	ARG	NE-CZ-NH1	-10.57	115.02	120.30
2	B	387	LEU	CB-CG-CD1	-10.57	93.03	111.00
2	B	137	TYR	CA-CB-CG	10.56	133.47	113.40
2	B	791	THR	OG1-CB-CG2	-10.56	85.71	110.00
2	B	391	ASP	OD1-CG-OD2	-10.55	103.26	123.30
1	A	1284	MET	CG-SD-CE	-10.53	83.34	100.20
2	B	353	LYS	CD-CE-NZ	10.53	135.93	111.70
4	E	25	ASP	CB-CG-OD1	10.53	127.77	118.30
1	A	346	ASP	CB-CG-OD1	10.52	127.77	118.30
1	A	549	MET	CG-SD-CE	10.52	117.03	100.20
2	B	249	ARG	NE-CZ-NH1	10.51	125.56	120.30
7	I	70	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	A	1329	THR	OG1-CB-CG2	-10.49	85.87	110.00
1	A	1417	GLU	OE1-CD-OE2	-10.49	110.71	123.30
3	C	116	LYS	CD-CE-NZ	-10.49	87.57	111.70
2	B	785	TYR	CB-CG-CD1	-10.47	114.72	121.00
1	A	200	ARG	NE-CZ-NH2	-10.46	115.07	120.30
4	E	14	ARG	NE-CZ-NH1	10.45	125.53	120.30
3	C	204	SER	N-CA-CB	-10.44	94.84	110.50
7	I	34	TYR	CD1-CE1-CZ	10.44	129.19	119.80
2	B	398	ARG	NE-CZ-NH1	-10.43	115.08	120.30
1	A	53	LEU	CA-CB-CG	10.43	139.28	115.30
1	A	290	GLU	OE1-CD-OE2	10.40	135.78	123.30
9	K	70	ARG	NE-CZ-NH1	-10.40	115.10	120.30
6	H	118	PHE	CB-CG-CD2	10.40	128.08	120.80
2	B	405	ARG	NE-CZ-NH1	10.40	125.50	120.30
1	A	1176	LEU	CA-CB-CG	10.38	139.18	115.30
1	A	1372	VAL	CG1-CB-CG2	-10.38	94.29	110.90
2	B	57	TYR	CB-CG-CD2	10.37	127.22	121.00
1	A	93	VAL	CB-CA-C	-10.36	91.71	111.40
1	A	511	ILE	CG1-CB-CG2	-10.36	88.60	111.40
1	A	483	ASP	CB-CG-OD2	10.35	127.62	118.30
2	B	680	THR	OG1-CB-CG2	-10.35	86.19	110.00
2	B	304	ASP	CB-CG-OD1	10.34	127.61	118.30
2	B	1072	MET	CG-SD-CE	10.34	116.74	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1328	TYR	CD1-CE1-CZ	10.32	129.09	119.80
1	A	65	LEU	CB-CG-CD2	10.32	128.54	111.00
3	C	84	ARG	NE-CZ-NH2	10.31	125.46	120.30
4	E	204	THR	CA-CB-CG2	10.31	126.83	112.40
2	B	684	LEU	CB-CG-CD1	-10.30	93.48	111.00
1	A	1012	ARG	CG-CD-NE	-10.29	90.18	111.80
2	B	1019	SER	CA-C-N	10.29	139.84	117.20
1	A	291	GLU	OE1-CD-OE2	-10.28	110.96	123.30
1	A	1362	TYR	CB-CG-CD2	-10.28	114.83	121.00
1	A	806	ARG	NH1-CZ-NH2	10.26	130.69	119.40
9	K	6	ARG	NE-CZ-NH2	-10.24	115.18	120.30
1	A	1259	MET	CG-SD-CE	10.24	116.58	100.20
2	B	935	ARG	NE-CZ-NH2	-10.24	115.18	120.30
1	A	596	THR	CA-CB-CG2	-10.23	98.08	112.40
7	I	31	THR	N-CA-CB	-10.21	90.90	110.30
4	E	66	GLU	N-CA-CB	10.20	128.97	110.60
1	A	356	ASP	CB-CG-OD1	-10.20	109.12	118.30
1	A	782	ARG	NE-CZ-NH1	10.18	125.39	120.30
1	A	1356	ILE	CG1-CB-CG2	-10.18	89.00	111.40
1	A	1289	ARG	NE-CZ-NH2	10.17	125.39	120.30
1	A	86	LEU	CB-CG-CD2	10.17	128.29	111.00
1	A	1376	THR	N-CA-CB	-10.15	91.01	110.30
2	B	287	ARG	NE-CZ-NH1	10.14	125.37	120.30
2	B	1097	HIS	CB-CG-ND1	-10.14	97.84	123.20
1	A	1176	LEU	CB-CG-CD1	10.13	128.23	111.00
1	A	512	VAL	CA-CB-CG2	-10.13	95.70	110.90
1	A	912	LEU	CB-CG-CD2	10.12	128.21	111.00
1	A	498	ARG	CD-NE-CZ	-10.10	109.46	123.60
1	A	1298	TYR	CG-CD2-CE2	10.08	129.37	121.30
2	B	24	PRO	N-CD-CG	-10.07	88.09	103.20
1	A	789	LYS	CD-CE-NZ	-10.05	88.58	111.70
2	B	598	GLU	N-CA-CB	10.05	128.68	110.60
3	C	76	ASP	CB-CG-OD1	10.04	127.33	118.30
2	B	241	ARG	NE-CZ-NH1	10.03	125.32	120.30
6	H	5	LEU	CB-CG-CD1	-10.02	93.96	111.00
1	A	696	GLU	OE1-CD-OE2	-10.02	111.28	123.30
9	K	51	LEU	CB-CG-CD1	-10.01	93.99	111.00
4	E	207	ARG	NH1-CZ-NH2	-10.00	108.39	119.40
1	A	1422	ARG	NH1-CZ-NH2	-10.00	108.40	119.40
1	A	982	THR	N-CA-CB	-10.00	91.31	110.30
2	B	1220	ARG	NE-CZ-NH2	10.00	125.30	120.30
1	A	646	PHE	CZ-CE2-CD2	-9.98	108.13	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	567	LYS	CD-CE-NZ	9.97	134.62	111.70
1	A	466	SER	CB-CA-C	-9.95	91.20	110.10
1	A	164	ARG	NE-CZ-NH1	9.94	125.27	120.30
2	B	1043	ASP	CB-CG-OD1	-9.94	109.36	118.30
1	A	1192	LEU	CB-CG-CD1	-9.92	94.13	111.00
1	A	483	ASP	CB-CG-OD1	-9.92	109.37	118.30
1	A	464	PRO	O-C-N	-9.92	106.83	122.70
4	E	25	ASP	CB-CG-OD2	9.92	127.22	118.30
2	B	303	TYR	CZ-CE2-CD2	9.90	128.71	119.80
8	J	3	VAL	CA-CB-CG2	-9.90	96.05	110.90
1	A	646	PHE	CB-CG-CD2	-9.88	113.88	120.80
1	A	1032	LEU	CB-CG-CD1	-9.87	94.22	111.00
4	E	80	VAL	CB-CA-C	-9.85	92.69	111.40
8	J	51	LEU	CB-CG-CD1	9.84	127.72	111.00
2	B	165	VAL	CB-CA-C	-9.83	92.72	111.40
1	A	446	ARG	NH1-CZ-NH2	9.82	130.20	119.40
1	A	305	ASP	OD1-CG-OD2	-9.81	104.66	123.30
1	A	653	VAL	CG1-CB-CG2	-9.81	95.21	110.90
3	C	165	LYS	CD-CE-NZ	9.80	134.25	111.70
2	B	327	ARG	NH1-CZ-NH2	9.79	130.17	119.40
2	B	705	MET	CG-SD-CE	-9.79	84.53	100.20
1	A	472	LEU	CA-CB-CG	-9.77	92.82	115.30
2	B	879	ARG	NE-CZ-NH2	-9.77	115.41	120.30
1	A	477	PRO	N-CD-CG	9.77	117.86	103.20
7	I	18	GLU	OE1-CD-OE2	9.76	135.01	123.30
4	E	46	TYR	CD1-CE1-CZ	9.76	128.58	119.80
2	B	46	GLN	CA-CB-CG	-9.75	91.95	113.40
1	A	1196	GLU	OE1-CD-OE2	9.73	134.97	123.30
1	A	1042	PHE	CB-CG-CD2	-9.72	113.99	120.80
5	F	122	MET	CG-SD-CE	9.72	115.75	100.20
1	A	913	LEU	CB-CG-CD1	-9.71	94.49	111.00
3	C	72	LEU	CB-CG-CD1	-9.70	94.51	111.00
2	B	879	ARG	NE-CZ-NH1	9.69	125.15	120.30
3	C	34	ARG	NE-CZ-NH1	9.69	125.14	120.30
2	B	498	THR	N-CA-CB	-9.68	91.91	110.30
1	A	238	CYS	CA-CB-SG	-9.68	96.58	114.00
8	J	44	TYR	CG-CD1-CE1	9.67	129.04	121.30
2	B	963	PHE	CB-CA-C	-9.67	91.06	110.40
7	I	110	PHE	CZ-CE2-CD2	9.66	131.70	120.10
4	E	159	ASP	CB-CG-OD1	9.66	127.00	118.30
2	B	1150	ARG	NH1-CZ-NH2	9.66	130.02	119.40
3	C	11	ARG	CB-CA-C	-9.65	91.09	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	48	ARG	CD-NE-CZ	9.65	137.11	123.60
4	E	25	ASP	OD1-CG-OD2	-9.65	104.97	123.30
2	B	578	THR	CA-CB-CG2	-9.64	98.90	112.40
4	E	188	LEU	CB-CG-CD1	-9.64	94.61	111.00
2	B	837	ASP	CB-CG-OD1	-9.64	109.63	118.30
6	H	132	LEU	CB-CG-CD2	9.64	127.38	111.00
7	I	81	ARG	NE-CZ-NH2	-9.63	115.48	120.30
2	B	118	ARG	NE-CZ-NH1	9.63	125.11	120.30
3	C	86	CYS	CA-CB-SG	9.62	131.32	114.00
3	C	268	ASP	CB-CG-OD2	9.62	126.96	118.30
1	A	960	ILE	CG1-CB-CG2	-9.61	90.25	111.40
2	B	1198	TYR	CD1-CE1-CZ	9.61	128.45	119.80
2	B	848	ARG	N-CA-CB	-9.61	93.30	110.60
1	A	399	HIS	C-N-CD	-9.60	99.48	120.60
7	I	84	VAL	N-CA-CB	-9.59	90.40	111.50
1	A	1220	PHE	CB-CG-CD1	9.58	127.50	120.80
2	B	916	THR	N-CA-C	9.57	136.85	111.00
1	A	157	ASP	CB-CG-OD1	9.57	126.91	118.30
2	B	668	ASP	CB-CG-OD1	9.56	126.91	118.30
1	A	588	LEU	CB-CG-CD1	-9.55	94.77	111.00
1	A	1349	TYR	CB-CG-CD2	-9.54	115.27	121.00
2	B	654	ARG	NE-CZ-NH2	9.54	125.07	120.30
8	J	58	GLU	OE1-CD-OE2	-9.54	111.85	123.30
2	B	680	THR	N-CA-CB	-9.54	92.17	110.30
2	B	169	ARG	NE-CZ-NH1	9.51	125.06	120.30
1	A	836	TYR	CZ-CE2-CD2	-9.50	111.25	119.80
1	A	879	GLU	OE1-CD-OE2	9.50	134.70	123.30
1	A	557	ASP	C-N-CA	-9.49	102.37	122.30
7	I	113	ASP	OD1-CG-OD2	-9.49	105.27	123.30
4	E	11	ARG	NH1-CZ-NH2	9.48	129.83	119.40
9	K	61	TYR	CZ-CE2-CD2	9.47	128.33	119.80
2	B	996	ARG	NE-CZ-NH1	-9.46	115.57	120.30
7	I	1	MET	CA-CB-CG	9.45	129.37	113.30
2	B	416	LEU	CB-CA-C	-9.44	92.27	110.20
4	E	81	GLU	OE1-CD-OE2	9.44	134.62	123.30
1	A	864	ILE	CG1-CB-CG2	-9.43	90.66	111.40
8	J	49	MET	CB-CG-SD	9.42	140.65	112.40
1	A	1446	ASP	CB-CG-OD2	9.41	126.77	118.30
3	C	118	LEU	CB-CG-CD2	9.41	126.99	111.00
3	C	149	LYS	CD-CE-NZ	-9.40	90.07	111.70
2	B	267	ARG	O-C-N	-9.40	107.66	122.70
1	A	1241	ARG	CG-CD-NE	-9.38	92.11	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	28	TYR	CD1-CE1-CZ	9.38	128.24	119.80
1	A	22	PHE	CB-CG-CD1	-9.36	114.25	120.80
2	B	174	LEU	CB-CG-CD2	9.36	126.91	111.00
2	B	1192	TYR	CB-CG-CD2	9.36	126.61	121.00
2	B	1037	LEU	CB-CG-CD1	9.35	126.89	111.00
4	E	113	GLN	N-CA-CB	9.34	127.42	110.60
1	A	117	GLU	OE1-CD-OE2	9.34	134.50	123.30
1	A	426	LEU	CB-CG-CD1	9.33	126.87	111.00
6	H	126	GLU	OE1-CD-OE2	-9.32	112.12	123.30
1	A	481	ASP	CB-CG-OD1	9.32	126.69	118.30
5	F	90	ARG	NE-CZ-NH1	-9.32	115.64	120.30
2	B	398	ARG	CB-CA-C	-9.31	91.78	110.40
6	H	89	LEU	CA-CB-CG	9.31	136.71	115.30
1	A	1062	GLU	CB-CA-C	-9.30	91.79	110.40
1	A	396	PRO	N-CD-CG	-9.30	89.25	103.20
1	A	793	SER	N-CA-CB	-9.30	96.55	110.50
3	C	238	ILE	CG1-CB-CG2	-9.30	90.94	111.40
1	A	908	LEU	CB-CG-CD2	-9.30	95.20	111.00
9	K	96	ASN	N-CA-CB	9.29	127.33	110.60
2	B	398	ARG	NE-CZ-NH2	9.29	124.94	120.30
3	C	47	ASP	CB-CG-OD1	-9.27	109.95	118.30
1	A	1274	ARG	NE-CZ-NH1	-9.27	115.66	120.30
6	H	110	ASP	CB-CG-OD2	9.26	126.64	118.30
1	A	30	ILE	CG1-CB-CG2	9.25	131.75	111.40
4	E	208	TYR	CZ-CE2-CD2	9.23	128.10	119.80
1	A	635	ARG	NE-CZ-NH1	-9.22	115.69	120.30
2	B	999	MET	CG-SD-CE	-9.22	85.44	100.20
2	B	268	THR	N-CA-CB	-9.22	92.78	110.30
1	A	909	ASP	CB-CG-OD2	-9.21	110.01	118.30
1	A	1242	VAL	CA-CB-CG2	-9.21	97.08	110.90
6	H	91	ASP	CB-CG-OD2	9.21	126.59	118.30
2	B	712	PRO	N-CD-CG	-9.20	89.39	103.20
1	A	50	ILE	CB-CA-C	-9.20	93.21	111.60
2	B	384	ARG	NE-CZ-NH1	9.19	124.90	120.30
1	A	61	ILE	N-CA-C	-9.17	86.24	111.00
5	F	124	GLU	OE1-CD-OE2	-9.17	112.29	123.30
2	B	618	ASP	CB-CG-OD1	9.15	126.54	118.30
2	B	853	SER	CB-CA-C	-9.15	92.72	110.10
1	A	1223	ASP	CB-CG-OD1	9.14	126.52	118.30
4	E	17	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	A	571	LEU	CB-CG-CD2	9.13	126.53	111.00
2	B	576	ASP	CB-CG-OD1	9.13	126.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	337	ARG	CG-CD-NE	-9.12	92.64	111.80
2	B	620	ARG	CG-CD-NE	-9.12	92.65	111.80
1	A	41	MET	CG-SD-CE	9.12	114.79	100.20
8	J	43	ARG	CG-CD-NE	-9.11	92.67	111.80
1	A	716	ASP	CB-CG-OD1	-9.10	110.11	118.30
2	B	595	ARG	NE-CZ-NH2	9.10	124.85	120.30
9	K	64	GLU	CG-CD-OE2	-9.09	100.12	118.30
2	B	536	VAL	CG1-CB-CG2	-9.06	96.40	110.90
2	B	816	GLU	CG-CD-OE2	-9.05	100.19	118.30
2	B	547	VAL	CG1-CB-CG2	9.05	125.38	110.90
4	E	162	ARG	CB-CG-CD	9.05	135.12	111.60
7	I	13	MET	CG-SD-CE	-9.05	85.72	100.20
1	A	1199	ARG	NE-CZ-NH1	-9.04	115.78	120.30
1	A	1119	TYR	CG-CD1-CE1	-9.04	114.07	121.30
1	A	264	PHE	CB-CA-C	9.02	128.45	110.40
10	L	28	LYS	O-C-N	-9.02	108.27	122.70
4	E	201	LYS	CD-CE-NZ	-9.02	90.95	111.70
2	B	391	ASP	CB-CG-OD1	9.02	126.42	118.30
5	F	85	MET	CG-SD-CE	-9.01	85.78	100.20
6	H	34	ASP	CB-CG-OD1	-9.01	110.19	118.30
3	C	53	THR	OG1-CB-CG2	-9.01	89.28	110.00
2	B	289	LEU	C-N-CA	-9.01	103.39	122.30
2	B	909	ASP	CB-CG-OD2	9.00	126.40	118.30
2	B	1097	HIS	CB-CA-C	8.99	128.38	110.40
3	C	55	THR	OG1-CB-CG2	-8.99	89.32	110.00
2	B	652	LYS	CD-CE-NZ	8.97	132.33	111.70
1	A	748	MET	CA-CB-CG	-8.96	98.06	113.30
2	B	807	ARG	CG-CD-NE	-8.96	92.98	111.80
1	A	1280	GLU	CA-CB-CG	8.96	133.11	113.40
3	C	118	LEU	CB-CG-CD1	-8.96	95.77	111.00
2	B	341	LEU	CB-CG-CD1	8.95	126.22	111.00
1	A	608	ILE	CA-CB-CG1	8.95	128.00	111.00
2	B	629	ASP	CB-CG-OD1	-8.95	110.25	118.30
2	B	816	GLU	CG-CD-OE1	8.91	136.13	118.30
1	A	203	SER	N-CA-CB	8.90	123.85	110.50
1	A	407	ARG	NH1-CZ-NH2	8.90	129.19	119.40
1	A	47	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	A	134	ARG	NE-CZ-NH1	8.90	124.75	120.30
2	B	650	GLU	OE1-CD-OE2	8.90	133.98	123.30
2	B	630	ALA	CB-CA-C	-8.89	96.77	110.10
1	A	635	ARG	NH1-CZ-NH2	8.87	129.16	119.40
3	C	121	VAL	CG1-CB-CG2	-8.86	96.72	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1020	ARG	N-CA-C	8.86	134.91	111.00
4	E	11	ARG	NE-CZ-NH2	-8.85	115.88	120.30
1	A	113	LEU	CB-CG-CD1	-8.85	95.96	111.00
1	A	1289	ARG	NH1-CZ-NH2	8.84	129.12	119.40
2	B	879	ARG	CB-CA-C	-8.83	92.74	110.40
1	A	1046	LEU	O-C-N	-8.83	108.58	122.70
1	A	1176	LEU	CB-CG-CD2	8.82	126.00	111.00
1	A	151	ASP	CB-CG-OD1	8.82	126.24	118.30
2	B	89	GLU	OE1-CD-OE2	-8.82	112.72	123.30
6	H	19	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	A	326	ARG	NE-CZ-NH2	8.81	124.71	120.30
6	H	77	ARG	CD-NE-CZ	8.81	135.94	123.60
2	B	297	ILE	CA-CB-CG1	8.81	127.74	111.00
1	A	1285	MET	CG-SD-CE	8.80	114.28	100.20
2	B	587	HIS	CA-C-N	8.80	133.80	116.20
2	B	231	PRO	N-CD-CG	8.79	116.39	103.20
1	A	1136	SER	N-CA-CB	-8.79	97.31	110.50
1	A	678	GLU	OE1-CD-OE2	-8.79	112.75	123.30
2	B	1148	LYS	CD-CE-NZ	-8.79	91.48	111.70
9	K	17	SER	CB-CA-C	-8.78	93.42	110.10
4	E	21	GLU	OE1-CD-OE2	-8.76	112.78	123.30
4	E	74	ASP	CB-CG-OD1	8.76	126.19	118.30
5	F	72	LYS	N-CA-C	8.76	134.66	111.00
8	J	44	TYR	CB-CG-CD2	-8.76	115.75	121.00
2	B	1108	ARG	NE-CZ-NH2	-8.76	115.92	120.30
2	B	314	LEU	CB-CG-CD2	8.76	125.88	111.00
1	A	1062	GLU	CA-CB-CG	8.75	132.65	113.40
2	B	310	MET	CG-SD-CE	8.75	114.20	100.20
1	A	940	ARG	CG-CD-NE	-8.73	93.46	111.80
6	H	14	GLU	OE1-CD-OE2	8.72	133.76	123.30
6	H	95	TYR	CB-CG-CD2	8.72	126.23	121.00
3	C	210	GLU	CG-CD-OE2	-8.71	100.88	118.30
2	B	1021	MET	N-CA-CB	-8.71	94.93	110.60
4	E	159	ASP	CB-CG-OD2	-8.70	110.47	118.30
2	B	711	GLU	CB-CA-C	-8.69	93.01	110.40
1	A	1109	LYS	CD-CE-NZ	8.69	131.68	111.70
10	L	68	GLU	CG-CD-OE1	8.69	135.67	118.30
1	A	1073	GLY	N-CA-C	8.68	134.81	113.10
2	B	915	THR	OG1-CB-CG2	-8.68	90.03	110.00
1	A	438	ASP	CB-CG-OD2	8.68	126.11	118.30
2	B	607	GLY	O-C-N	-8.68	108.81	122.70
1	A	565	ILE	CG1-CB-CG2	-8.67	92.32	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	857	ARG	NE-CZ-NH1	-8.67	115.97	120.30
1	A	1301	GLU	CG-CD-OE2	-8.67	100.97	118.30
2	B	640	VAL	CG1-CB-CG2	8.66	124.76	110.90
3	C	246	ARG	N-CA-CB	-8.66	95.00	110.60
1	A	941	LYS	CD-CE-NZ	-8.66	91.78	111.70
2	B	1073	TYR	CZ-CE2-CD2	8.65	127.59	119.80
1	A	1239	ARG	CB-CA-C	8.64	127.69	110.40
1	A	1348	LEU	CB-CG-CD1	-8.64	96.31	111.00
2	B	915	THR	CA-CB-CG2	8.64	124.49	112.40
1	A	63	ARG	NE-CZ-NH2	-8.64	115.98	120.30
6	H	93	TYR	CB-CG-CD2	-8.63	115.82	121.00
1	A	620	LYS	CD-CE-NZ	8.62	131.52	111.70
1	A	616	VAL	CG1-CB-CG2	-8.62	97.12	110.90
2	B	589	VAL	CB-CA-C	8.62	127.77	111.40
5	F	135	ARG	NE-CZ-NH1	-8.61	115.99	120.30
1	A	466	SER	N-CA-C	8.61	134.25	111.00
7	I	98	VAL	CA-CB-CG2	-8.61	97.99	110.90
1	A	1012	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	A	581	ALA	N-CA-CB	-8.59	98.07	110.10
2	B	550	ASP	CB-CG-OD1	8.58	126.02	118.30
6	H	111	LEU	CB-CG-CD1	8.57	125.58	111.00
2	B	509	ALA	CB-CA-C	8.57	122.96	110.10
2	B	1033	LYS	CD-CE-NZ	-8.57	92.00	111.70
2	B	1190	ASP	CB-CG-OD1	-8.56	110.59	118.30
9	K	12	LEU	CA-CB-CG	-8.56	95.62	115.30
8	J	22	LEU	N-CA-CB	-8.55	93.31	110.40
3	C	100	THR	OG1-CB-CG2	-8.54	90.35	110.00
3	C	183	TRP	C-N-CA	-8.54	100.34	121.70
1	A	1012	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	A	1438	THR	N-CA-CB	-8.53	94.09	110.30
10	L	58	LYS	N-CA-C	8.53	134.02	111.00
1	A	437	MET	CB-CA-C	-8.52	93.36	110.40
2	B	305	VAL	CG1-CB-CG2	8.52	124.53	110.90
9	K	64	GLU	CG-CD-OE1	8.50	135.30	118.30
1	A	887	GLY	C-N-CA	-8.49	104.47	122.30
1	A	1257	ASP	CB-CG-OD2	8.49	125.94	118.30
1	A	1309	ASP	CB-CG-OD2	-8.48	110.67	118.30
2	B	1052	VAL	CA-CB-CG2	-8.47	98.19	110.90
2	B	368	GLU	OE1-CD-OE2	-8.46	113.15	123.30
5	F	150	GLU	N-CA-CB	-8.46	95.38	110.60
1	A	391	LEU	CB-CG-CD2	-8.45	96.63	111.00
7	I	104	LEU	CB-CG-CD1	8.45	125.37	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	204	ILE	CA-CB-CG2	-8.45	94.00	110.90
4	E	164	LEU	CB-CG-CD1	8.45	125.36	111.00
1	A	389	THR	OG1-CB-CG2	-8.45	90.58	110.00
2	B	848	ARG	CG-CD-NE	-8.45	94.06	111.80
1	A	1318	THR	N-CA-CB	-8.44	94.27	110.30
2	B	331	LEU	CB-CG-CD1	8.43	125.33	111.00
1	A	472	LEU	CB-CG-CD1	8.43	125.33	111.00
1	A	486	GLU	CG-CD-OE1	8.43	135.16	118.30
2	B	778	MET	CG-SD-CE	8.43	113.69	100.20
1	A	1334	ASP	CB-CG-OD1	8.42	125.88	118.30
3	C	50	GLU	OE1-CD-OE2	-8.42	113.20	123.30
2	B	303	TYR	CB-CG-CD1	8.42	126.05	121.00
7	I	118	ARG	CD-NE-CZ	8.42	135.38	123.60
1	A	776	ALA	CB-CA-C	-8.41	97.48	110.10
2	B	964	VAL	CA-CB-CG2	-8.41	98.29	110.90
2	B	118	ARG	CD-NE-CZ	8.40	135.37	123.60
1	A	1326	ARG	NH1-CZ-NH2	-8.40	110.16	119.40
2	B	1019	SER	O-C-N	-8.40	109.27	122.70
4	E	207	ARG	CB-CG-CD	8.40	133.43	111.60
9	K	105	PHE	CZ-CE2-CD2	-8.40	110.02	120.10
1	A	1215	ARG	N-CA-CB	8.39	125.70	110.60
2	B	175	ARG	CB-CG-CD	8.38	133.40	111.60
3	C	122	SER	N-CA-CB	8.38	123.08	110.50
7	I	45	ARG	CA-CB-CG	8.38	131.84	113.40
3	C	220	ASP	CB-CG-OD1	8.38	125.84	118.30
7	I	29	CYS	CA-CB-SG	8.37	129.07	114.00
3	C	254	LYS	CD-CE-NZ	-8.37	92.46	111.70
2	B	1127	GLY	N-CA-C	8.36	134.00	113.10
2	B	1166	CYS	N-CA-CB	-8.36	95.55	110.60
1	A	1198	ASP	CB-CG-OD2	-8.36	110.78	118.30
1	A	629	LEU	CB-CG-CD2	-8.36	96.79	111.00
2	B	1077	THR	N-CA-CB	-8.36	94.42	110.30
1	A	504	LEU	N-CA-CB	-8.35	93.70	110.40
2	B	1054	GLY	CA-C-O	-8.35	105.57	120.60
9	K	14	GLU	CB-CA-C	8.35	127.10	110.40
1	A	912	LEU	N-CA-CB	8.34	127.08	110.40
1	A	115	LEU	CB-CG-CD1	8.34	125.17	111.00
1	A	176	LYS	CD-CE-NZ	8.33	130.86	111.70
2	B	898	LEU	CB-CG-CD2	8.32	125.14	111.00
1	A	1035	TYR	CD1-CE1-CZ	8.31	127.28	119.80
1	A	434	ARG	CD-NE-CZ	8.31	135.23	123.60
1	A	1311	VAL	CG1-CB-CG2	-8.30	97.62	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	895	ASP	N-CA-CB	8.29	125.52	110.60
2	B	226	PHE	CB-CG-CD1	-8.29	115.00	120.80
7	I	1	MET	CG-SD-CE	8.29	113.46	100.20
1	A	17	VAL	CG1-CB-CG2	-8.29	97.64	110.90
2	B	203	PHE	N-CA-CB	-8.29	95.68	110.60
1	A	649	ILE	CA-CB-CG1	8.29	126.74	111.00
8	J	22	LEU	CA-CB-CG	8.28	134.35	115.30
2	B	1050	ILE	CG1-CB-CG2	-8.27	93.20	111.40
1	A	12	ARG	CG-CD-NE	-8.27	94.44	111.80
1	A	117	GLU	CG-CD-OE2	-8.27	101.77	118.30
2	B	452	THR	OG1-CB-CG2	-8.27	90.99	110.00
2	B	582	VAL	CG1-CB-CG2	-8.26	97.69	110.90
6	H	86	ASP	CB-CA-C	8.26	126.91	110.40
8	J	3	VAL	CG1-CB-CG2	8.26	124.11	110.90
4	E	53	PRO	N-CD-CG	-8.24	90.83	103.20
1	A	586	ILE	O-C-N	8.24	135.88	122.70
9	K	79	GLU	CB-CA-C	8.24	126.88	110.40
1	A	518	LYS	CD-CE-NZ	-8.23	92.76	111.70
2	B	642	ASP	CB-CA-C	8.23	126.86	110.40
2	B	29	ASP	CB-CG-OD2	-8.23	110.90	118.30
2	B	406	LEU	CB-CG-CD2	-8.22	97.03	111.00
10	L	63	ARG	NE-CZ-NH1	8.21	124.41	120.30
3	C	38	ILE	CG1-CB-CG2	-8.21	93.33	111.40
1	A	455	MET	CG-SD-CE	-8.21	87.06	100.20
1	A	952	ALA	N-CA-CB	-8.21	98.61	110.10
4	E	29	PHE	CB-CG-CD2	-8.19	115.06	120.80
1	A	452	LYS	CB-CG-CD	-8.19	90.31	111.60
2	B	1224	PHE	CB-CG-CD1	-8.18	115.07	120.80
3	C	233	GLU	CA-C-O	-8.18	102.92	120.10
1	A	833	GLU	CG-CD-OE1	8.18	134.65	118.30
2	B	434	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	A	11	LEU	CB-CG-CD2	8.17	124.88	111.00
2	B	945	GLU	CG-CD-OE1	8.17	134.63	118.30
6	H	132	LEU	CA-CB-CG	8.17	134.08	115.30
2	B	738	PHE	CB-CG-CD1	-8.16	115.09	120.80
1	A	53	LEU	CB-CG-CD1	8.16	124.86	111.00
1	A	1281	ARG	NE-CZ-NH2	8.16	124.38	120.30
2	B	963	PHE	CB-CG-CD2	-8.15	115.09	120.80
2	B	798	TYR	CD1-CE1-CZ	8.15	127.13	119.80
1	A	609	ASP	CB-CG-OD2	8.15	125.63	118.30
2	B	37	PHE	CD1-CE1-CZ	8.15	129.88	120.10
1	A	59	GLY	N-CA-C	8.14	133.46	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	666	ILE	CG1-CB-CG2	8.14	129.32	111.40
2	B	1002	THR	OG1-CB-CG2	-8.14	91.28	110.00
2	B	373	ARG	NE-CZ-NH2	-8.14	116.23	120.30
3	C	62	PHE	CZ-CE2-CD2	-8.13	110.34	120.10
9	K	23	PRO	N-CD-CG	-8.13	91.00	103.20
1	A	1055	ARG	NE-CZ-NH1	8.13	124.36	120.30
2	B	511	PRO	N-CD-CG	-8.13	91.01	103.20
3	C	260	LEU	CB-CG-CD2	8.11	124.79	111.00
2	B	316	PRO	CA-CB-CG	-8.11	88.59	104.00
1	A	1384	VAL	CA-CB-CG1	-8.10	98.75	110.90
1	A	662	PHE	CZ-CE2-CD2	8.10	129.82	120.10
6	H	102	TYR	CD1-CE1-CZ	-8.10	112.51	119.80
3	C	228	PHE	N-CA-CB	-8.09	96.05	110.60
1	A	790	ASP	CB-CG-OD2	8.07	125.56	118.30
2	B	838	SER	N-CA-CB	-8.06	98.41	110.50
1	A	423	ASP	CB-CG-OD1	8.06	125.55	118.30
7	I	2	THR	CA-CB-CG2	-8.06	101.12	112.40
1	A	134	ARG	NE-CZ-NH2	8.05	124.33	120.30
1	A	1313	LEU	CB-CG-CD1	-8.04	97.32	111.00
2	B	799	PRO	N-CD-CG	-8.04	91.13	103.20
2	B	1212	ILE	CA-CB-CG1	-8.04	95.72	111.00
4	E	176	PRO	CB-CA-C	-8.04	91.89	112.00
4	E	195	VAL	CG1-CB-CG2	-8.04	98.03	110.90
2	B	768	THR	CA-CB-CG2	-8.04	101.14	112.40
3	C	76	ASP	CB-CG-OD2	-8.04	111.07	118.30
2	B	895	ASP	CB-CG-OD2	8.03	125.53	118.30
1	A	948	VAL	N-CA-CB	-8.03	93.83	111.50
1	A	218	ASP	OD1-CG-OD2	8.02	138.54	123.30
2	B	387	LEU	CA-CB-CG	8.02	133.74	115.30
2	B	396	ASP	CB-CG-OD2	-8.01	111.09	118.30
4	E	156	LEU	CB-CG-CD2	-8.01	97.39	111.00
2	B	370	PHE	CB-CA-C	8.00	126.41	110.40
10	L	40	LEU	CA-CB-CG	8.00	133.69	115.30
2	B	564	GLU	CG-CD-OE1	-8.00	102.31	118.30
2	B	97	VAL	N-CA-C	-7.99	89.42	111.00
2	B	696	GLU	CG-CD-OE2	7.99	134.29	118.30
1	A	1368	MET	CG-SD-CE	7.99	112.98	100.20
3	C	44	LEU	CA-CB-CG	-7.99	96.92	115.30
1	A	1129	GLU	CB-CA-C	7.99	126.37	110.40
1	A	722	LEU	CB-CG-CD1	7.98	124.56	111.00
2	B	617	ARG	NE-CZ-NH2	-7.98	116.31	120.30
2	B	945	GLU	CG-CD-OE2	-7.97	102.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	114	TYR	CG-CD1-CE1	-7.97	114.93	121.30
1	A	140	THR	OG1-CB-CG2	-7.96	91.69	110.00
1	A	379	VAL	CG1-CB-CG2	-7.96	98.16	110.90
1	A	157	ASP	OD1-CG-OD2	-7.96	108.18	123.30
4	E	96	PHE	CB-CG-CD2	7.96	126.37	120.80
7	I	43	VAL	N-CA-CB	-7.95	94.00	111.50
2	B	983	ARG	CD-NE-CZ	-7.95	112.47	123.60
2	B	336	ARG	CB-CA-C	-7.95	94.51	110.40
1	A	1377	THR	N-CA-CB	7.95	125.40	110.30
2	B	852	ARG	NE-CZ-NH2	7.95	124.27	120.30
7	I	92	ARG	CA-C-N	-7.95	99.72	117.20
2	B	484	ASN	CB-CA-C	-7.94	94.51	110.40
4	E	198	ILE	CG1-CB-CG2	-7.94	93.93	111.40
1	A	283	GLY	N-CA-C	-7.93	93.26	113.10
2	B	95	ILE	CG1-CB-CG2	-7.92	93.97	111.40
1	A	821	ARG	NH1-CZ-NH2	7.92	128.11	119.40
3	C	245	VAL	CA-CB-CG1	7.92	122.77	110.90
1	A	1359	ASP	CB-CG-OD2	7.91	125.42	118.30
3	C	230	MET	CG-SD-CE	7.91	112.86	100.20
1	A	372	LYS	CD-CE-NZ	-7.91	93.51	111.70
5	F	132	LEU	CB-CG-CD2	7.91	124.44	111.00
2	B	38	PHE	CB-CG-CD1	-7.91	115.27	120.80
2	B	378	LEU	CB-CG-CD2	-7.90	97.57	111.00
8	J	48	ARG	NE-CZ-NH1	7.90	124.25	120.30
2	B	434	ARG	CG-CD-NE	7.90	128.38	111.80
7	I	112	SER	N-CA-CB	-7.89	98.66	110.50
1	A	1136	SER	CB-CA-C	7.88	125.08	110.10
1	A	1385	THR	N-CA-C	7.88	132.28	111.00
1	A	929	LEU	CB-CG-CD2	-7.86	97.63	111.00
2	B	244	LEU	CB-CG-CD2	-7.86	97.63	111.00
2	B	1220	ARG	N-CA-CB	7.86	124.76	110.60
2	B	275	TYR	CZ-CE2-CD2	-7.86	112.72	119.80
10	L	64	LEU	CB-CG-CD2	-7.86	97.64	111.00
6	H	114	VAL	CG1-CB-CG2	-7.86	98.33	110.90
9	K	114	LEU	CB-CA-C	7.86	125.13	110.20
7	I	31	THR	C-N-CA	7.85	141.31	121.70
1	A	1121	GLU	CG-CD-OE1	7.84	133.99	118.30
9	K	87	LEU	CB-CG-CD2	7.84	124.33	111.00
9	K	77	THR	O-C-N	7.83	135.23	122.70
1	A	546	VAL	CG1-CB-CG2	-7.83	98.37	110.90
8	J	28	ASP	CB-CG-OD1	7.83	125.35	118.30
1	A	134	ARG	NH1-CZ-NH2	-7.83	110.79	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1083	ALA	N-CA-CB	-7.83	99.14	110.10
1	A	1066	VAL	CG1-CB-CG2	-7.83	98.38	110.90
9	K	47	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	A	1055	ARG	NE-CZ-NH2	-7.82	116.39	120.30
6	H	107	VAL	CA-CB-CG1	7.82	122.64	110.90
1	A	1035	TYR	CG-CD1-CE1	-7.82	115.05	121.30
7	I	9	ASP	CB-CG-OD1	-7.81	111.27	118.30
1	A	739	ASP	N-CA-CB	-7.81	96.54	110.60
9	K	114	LEU	CB-CG-CD1	-7.81	97.72	111.00
5	F	93	ILE	CG1-CB-CG2	-7.81	94.22	111.40
1	A	193	ASP	N-CA-CB	7.80	124.65	110.60
9	K	88	LYS	CA-CB-CG	7.80	130.56	113.40
4	E	208	TYR	CB-CG-CD1	7.80	125.68	121.00
5	F	106	PRO	N-CD-CG	7.80	114.89	103.20
1	A	885	THR	CA-CB-CG2	7.79	123.31	112.40
2	B	1067	ARG	NE-CZ-NH2	-7.79	116.40	120.30
3	C	124	LEU	N-CA-C	7.79	132.04	111.00
2	B	131	ASP	N-CA-C	-7.79	89.97	111.00
3	C	72	LEU	CA-CB-CG	-7.79	97.38	115.30
6	H	26	ILE	CB-CA-C	-7.79	96.02	111.60
2	B	399	ASP	N-CA-C	7.79	132.02	111.00
4	E	191	LYS	O-C-N	-7.79	110.24	122.70
3	C	96	SER	N-CA-CB	-7.78	98.83	110.50
2	B	615	MET	N-CA-CB	-7.77	96.61	110.60
3	C	73	GLN	CA-CB-CG	-7.77	96.31	113.40
1	A	739	ASP	CB-CG-OD2	7.76	125.29	118.30
1	A	1161	THR	OG1-CB-CG2	-7.76	92.15	110.00
2	B	273	LEU	CB-CA-C	-7.76	95.46	110.20
4	E	208	TYR	CD1-CG-CD2	-7.76	109.37	117.90
1	A	1081	LEU	CB-CG-CD2	7.75	124.18	111.00
2	B	344	LYS	N-CA-CB	-7.75	96.64	110.60
4	E	172	GLU	CG-CD-OE1	-7.75	102.80	118.30
8	J	44	TYR	CG-CD2-CE2	-7.75	115.10	121.30
1	A	603	ASN	N-CA-CB	-7.74	96.66	110.60
1	A	1044	TRP	CD1-NE1-CE2	-7.74	102.03	109.00
4	E	137	GLU	OE1-CD-OE2	7.74	132.59	123.30
3	C	81	GLU	OE1-CD-OE2	7.74	132.59	123.30
9	K	95	ILE	O-C-N	7.74	135.08	122.70
2	B	185	THR	OG1-CB-CG2	-7.74	92.20	110.00
1	A	1212	VAL	CG1-CB-CG2	-7.74	98.52	110.90
1	A	1228	TRP	CB-CA-C	-7.73	94.94	110.40
7	I	13	MET	N-CA-CB	-7.73	96.68	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	57	TYR	CD1-CG-CD2	-7.73	109.40	117.90
1	A	962	ARG	CG-CD-NE	-7.72	95.58	111.80
1	A	703	THR	CA-CB-CG2	-7.72	101.59	112.40
9	K	73	LEU	CA-CB-CG	7.72	133.05	115.30
1	A	1277	GLU	CB-CA-C	-7.71	94.97	110.40
3	C	127	ARG	NE-CZ-NH2	7.71	124.16	120.30
2	B	1135	ARG	NH1-CZ-NH2	7.71	127.88	119.40
1	A	968	GLN	CA-CB-CG	-7.70	96.47	113.40
2	B	1095	LEU	CB-CG-CD2	-7.70	97.92	111.00
3	C	266	ASP	CB-CG-OD2	7.70	125.23	118.30
1	A	901	LEU	CB-CG-CD2	7.69	124.08	111.00
6	H	46	LEU	CB-CG-CD2	7.69	124.08	111.00
3	C	211	ASP	CB-CG-OD2	7.69	125.22	118.30
1	A	705	LYS	N-CA-CB	7.69	124.44	110.60
1	A	918	GLU	CA-CB-CG	7.69	130.31	113.40
1	A	1237	ILE	CG1-CB-CG2	-7.69	94.49	111.40
7	I	99	LEU	CB-CG-CD1	7.68	124.06	111.00
1	A	468	PHE	CG-CD1-CE1	-7.68	112.35	120.80
1	A	774	ARG	NH1-CZ-NH2	-7.68	110.95	119.40
1	A	728	LYS	N-CA-CB	7.68	124.42	110.60
1	A	634	THR	CA-CB-CG2	-7.67	101.66	112.40
2	B	477	ALA	CB-CA-C	7.67	121.61	110.10
1	A	937	VAL	CA-CB-CG2	-7.67	99.40	110.90
2	B	19	GLU	OE1-CD-OE2	-7.66	114.11	123.30
1	A	1276	VAL	CG1-CB-CG2	-7.66	98.64	110.90
1	A	1323	ASP	CB-CG-OD2	7.66	125.20	118.30
1	A	1280	GLU	CA-C-N	7.66	134.05	117.20
2	B	620	ARG	N-CA-CB	-7.66	96.81	110.60
2	B	175	ARG	CD-NE-CZ	-7.66	112.88	123.60
1	A	537	ARG	NE-CZ-NH1	-7.65	116.47	120.30
8	J	41	LEU	N-CA-C	-7.65	90.34	111.00
4	E	12	LEU	CB-CG-CD1	7.65	124.01	111.00
6	H	6	PHE	CB-CG-CD2	7.65	126.15	120.80
7	I	93	LYS	CD-CE-NZ	7.65	129.29	111.70
2	B	180	TYR	CD1-CE1-CZ	-7.64	112.92	119.80
1	A	664	THR	CA-CB-CG2	-7.64	101.70	112.40
1	A	557	ASP	OD1-CG-OD2	-7.64	108.78	123.30
1	A	1373	ASP	CB-CG-OD2	7.63	125.17	118.30
2	B	1047	PHE	CB-CG-CD1	-7.63	115.46	120.80
1	A	232	GLU	CG-CD-OE1	7.63	133.55	118.30
2	B	97	VAL	CG1-CB-CG2	-7.62	98.71	110.90
2	B	393	LYS	CD-CE-NZ	-7.61	94.19	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1102	LYS	CD-CE-NZ	-7.59	94.23	111.70
1	A	112	LYS	CD-CE-NZ	-7.59	94.24	111.70
2	B	1215	ARG	NE-CZ-NH2	-7.58	116.51	120.30
7	I	38	ALA	C-N-CA	7.58	138.23	122.30
2	B	270	LYS	CB-CA-C	-7.58	95.23	110.40
4	E	23	VAL	CA-CB-CG2	-7.58	99.53	110.90
2	B	365	THR	OG1-CB-CG2	-7.58	92.56	110.00
7	I	83	ASN	CB-CA-C	-7.58	95.24	110.40
1	A	917	SER	N-CA-CB	-7.58	99.13	110.50
2	B	365	THR	N-CA-C	-7.58	90.55	111.00
1	A	239	LEU	CA-CB-CG	7.57	132.72	115.30
6	H	107	VAL	N-CA-C	-7.57	90.57	111.00
2	B	1155	SER	N-CA-CB	7.57	121.85	110.50
1	A	883	LEU	N-CA-C	-7.56	90.58	111.00
1	A	710	LEU	CB-CG-CD2	7.56	123.85	111.00
1	A	1153	TYR	CB-CG-CD2	7.56	125.54	121.00
3	C	207	CYS	CA-CB-SG	7.56	127.61	114.00
2	B	346	GLU	OE1-CD-OE2	-7.56	114.23	123.30
1	A	908	LEU	N-CA-CB	-7.55	95.31	110.40
2	B	996	ARG	NH1-CZ-NH2	7.54	127.70	119.40
4	E	17	ARG	CG-CD-NE	-7.54	95.97	111.80
1	A	928	LEU	CB-CG-CD1	-7.54	98.19	111.00
1	A	1194	ARG	CA-CB-CG	7.54	129.98	113.40
1	A	188	ASP	CB-CG-OD1	-7.53	111.52	118.30
1	A	1122	PRO	N-CD-CG	7.53	114.50	103.20
2	B	175	ARG	NE-CZ-NH2	7.53	124.07	120.30
2	B	217	ARG	NE-CZ-NH2	-7.53	116.53	120.30
8	J	62	ARG	NE-CZ-NH1	7.53	124.06	120.30
2	B	1132	GLU	CG-CD-OE1	7.53	133.35	118.30
3	C	121	VAL	CA-CB-CG1	7.52	122.19	110.90
2	B	419	THR	OG1-CB-CG2	-7.52	92.71	110.00
6	H	96	VAL	CG1-CB-CG2	7.52	122.92	110.90
2	B	806	THR	N-CA-CB	-7.51	96.02	110.30
2	B	1185	CYS	CB-CA-C	7.51	125.42	110.40
4	E	55	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	A	589	GLN	CB-CA-C	-7.50	95.39	110.40
1	A	1307	GLU	CG-CD-OE1	7.50	133.31	118.30
2	B	1019	SER	N-CA-CB	7.50	121.75	110.50
1	A	676	MET	CG-SD-CE	7.50	112.20	100.20
3	C	172	PRO	N-CD-CG	7.50	114.45	103.20
6	H	20	TYR	CB-CG-CD2	-7.50	116.50	121.00
1	A	325	ILE	CG1-CB-CG2	-7.50	94.90	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1012	ARG	CD-NE-CZ	7.50	134.10	123.60
1	A	1141	THR	OG1-CB-CG2	-7.50	92.75	110.00
1	A	1225	PHE	CB-CG-CD1	-7.50	115.55	120.80
1	A	1240	CYS	CA-CB-SG	-7.50	100.50	114.00
10	L	69	ALA	N-CA-CB	7.50	120.60	110.10
3	C	57	VAL	CG1-CB-CG2	7.50	122.89	110.90
2	B	1002	THR	N-CA-CB	-7.49	96.07	110.30
2	B	639	ILE	CA-CB-CG1	7.49	125.23	111.00
2	B	389	ALA	N-CA-CB	-7.48	99.62	110.10
1	A	1064	VAL	N-CA-CB	-7.48	95.05	111.50
1	A	468	PHE	CB-CG-CD1	-7.48	115.57	120.80
1	A	469	ARG	CG-CD-NE	-7.47	96.10	111.80
2	B	197	PHE	CB-CG-CD1	-7.47	115.57	120.80
1	A	896	ARG	NH1-CZ-NH2	7.47	127.62	119.40
2	B	1156	ASP	CB-CG-OD2	7.46	125.02	118.30
2	B	711	GLU	OE1-CD-OE2	-7.46	114.34	123.30
6	H	135	LEU	CA-CB-CG	7.46	132.46	115.30
1	A	910	PRO	CA-N-CD	7.46	122.14	111.70
7	I	29	CYS	CB-CA-C	-7.46	95.48	110.40
7	I	8	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	718	VAL	CG1-CB-CG2	-7.45	98.97	110.90
7	I	93	LYS	CA-CB-CG	7.45	129.79	113.40
1	A	1001	ARG	NE-CZ-NH2	-7.45	116.57	120.30
8	J	51	LEU	CB-CG-CD2	-7.45	98.34	111.00
6	H	32	THR	OG1-CB-CG2	-7.45	92.87	110.00
2	B	102	VAL	CB-CA-C	-7.45	97.25	111.40
2	B	1153	GLU	CB-CA-C	7.44	125.29	110.40
3	C	153	LEU	CB-CG-CD1	-7.44	98.36	111.00
4	E	179	GLN	CB-CA-C	-7.44	95.53	110.40
7	I	54	GLU	CG-CD-OE2	-7.43	103.43	118.30
7	I	52	ILE	CA-C-N	-7.43	101.34	116.20
3	C	245	VAL	CA-CB-CG2	-7.43	99.76	110.90
2	B	510	LYS	CB-CG-CD	-7.43	92.29	111.60
1	A	557	ASP	O-C-N	-7.42	110.58	123.20
5	F	149	GLU	N-CA-CB	7.42	123.97	110.60
1	A	24	PRO	N-CD-CG	7.42	114.33	103.20
2	B	998	ASP	CB-CG-OD2	7.42	124.97	118.30
1	A	793	SER	N-CA-C	7.41	131.01	111.00
4	E	111	VAL	CG1-CB-CG2	7.40	122.75	110.90
2	B	1136	ASP	CB-CG-OD2	7.40	124.96	118.30
1	A	1056	SER	N-CA-CB	-7.40	99.40	110.50
2	B	589	VAL	N-CA-CB	-7.40	95.22	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	961	ARG	CD-NE-CZ	7.40	133.96	123.60
1	A	537	ARG	CB-CG-CD	7.39	130.82	111.60
1	A	555	ASP	CB-CG-OD2	7.39	124.95	118.30
3	C	152	GLU	OE1-CD-OE2	7.39	132.17	123.30
2	B	61	ASP	CB-CG-OD2	-7.39	111.65	118.30
5	F	87	LYS	CD-CE-NZ	-7.39	94.70	111.70
2	B	980	PHE	CG-CD2-CE2	7.39	128.93	120.80
1	A	706	HIS	CA-C-N	-7.38	101.43	116.20
2	B	595	ARG	N-CA-CB	7.38	123.88	110.60
8	J	18	TRP	CD1-NE1-CE2	-7.38	102.36	109.00
1	A	712	GLU	OE1-CD-OE2	-7.38	114.45	123.30
1	A	1377	THR	CA-CB-CG2	7.37	122.72	112.40
2	B	370	PHE	CB-CG-CD2	7.37	125.96	120.80
2	B	186	GLU	OE1-CD-OE2	7.37	132.14	123.30
7	I	3	THR	O-C-N	7.37	134.49	122.70
9	K	92	ASN	CB-CA-C	7.36	125.13	110.40
10	L	42	ARG	NE-CZ-NH1	7.36	123.98	120.30
2	B	434	ARG	CA-CB-CG	7.36	129.58	113.40
4	E	133	GLU	CG-CD-OE2	-7.36	103.59	118.30
6	H	112	ILE	CG1-CB-CG2	-7.35	95.22	111.40
1	A	704	ALA	C-N-CA	-7.35	103.32	121.70
2	B	1012	ILE	CG1-CB-CG2	-7.35	95.23	111.40
5	F	152	ILE	CG1-CB-CG2	-7.35	95.23	111.40
2	B	181	LEU	CA-CB-CG	7.35	132.20	115.30
1	A	278	THR	OG1-CB-CG2	-7.35	93.10	110.00
1	A	803	SER	N-CA-CB	-7.34	99.48	110.50
8	J	34	THR	OG1-CB-CG2	-7.34	93.11	110.00
4	E	182	ASP	CB-CG-OD2	-7.34	111.69	118.30
2	B	274	PRO	N-CD-CG	7.34	114.21	103.20
1	A	928	LEU	CB-CG-CD2	-7.33	98.53	111.00
6	H	116	TYR	N-CA-C	7.33	130.80	111.00
2	B	1156	ASP	CB-CG-OD1	7.33	124.90	118.30
9	K	6	ARG	CD-NE-CZ	7.33	133.86	123.60
10	L	58	LYS	C-N-CA	-7.33	103.38	121.70
2	B	896	ASP	N-CA-CB	7.33	123.79	110.60
2	B	272	THR	N-CA-C	-7.32	91.23	111.00
1	A	1362	TYR	CD1-CE1-CZ	-7.32	113.21	119.80
1	A	1135	ARG	CD-NE-CZ	7.32	133.84	123.60
2	B	1183	LYS	CB-CA-C	7.31	125.03	110.40
2	B	56	ASP	O-C-N	-7.31	111.00	122.70
4	E	79	TRP	O-C-N	-7.31	111.01	122.70
7	I	17	ARG	NE-CZ-NH2	-7.31	116.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	597	LEU	CB-CG-CD1	7.30	123.42	111.00
1	A	124	GLN	N-CA-CB	7.30	123.74	110.60
1	A	706	HIS	N-CA-CB	7.30	123.74	110.60
7	I	106	CYS	CB-CA-C	-7.30	95.80	110.40
1	A	982	THR	CB-CA-C	-7.30	91.90	111.60
2	B	326	ASP	CB-CG-OD1	-7.29	111.73	118.30
1	A	968	GLN	CB-CA-C	-7.29	95.81	110.40
2	B	1221	SER	CB-CA-C	7.29	123.95	110.10
4	E	169	ARG	NE-CZ-NH2	-7.28	116.66	120.30
9	K	110	ASN	CB-CA-C	7.28	124.96	110.40
1	A	710	LEU	CA-CB-CG	7.28	132.03	115.30
1	A	938	LYS	CB-CA-C	-7.28	95.85	110.40
1	A	1153	TYR	CB-CG-CD1	-7.27	116.64	121.00
4	E	133	GLU	OE1-CD-OE2	7.27	132.03	123.30
1	A	503	GLN	O-C-N	-7.27	111.07	122.70
1	A	181	LEU	CB-CG-CD2	-7.26	98.65	111.00
3	C	55	THR	CA-CB-CG2	-7.26	102.23	112.40
1	A	968	GLN	N-CA-CB	7.26	123.67	110.60
2	B	983	ARG	CA-CB-CG	7.26	129.37	113.40
10	L	38	LEU	CB-CG-CD1	7.26	123.34	111.00
2	B	513	GLN	CA-CB-CG	7.25	129.36	113.40
1	A	939	ASP	CB-CG-OD2	-7.25	111.78	118.30
2	B	723	VAL	CG1-CB-CG2	7.25	122.49	110.90
4	E	195	VAL	CA-CB-CG1	7.25	121.77	110.90
2	B	399	ASP	N-CA-CB	-7.24	97.56	110.60
1	A	980	ASP	CB-CA-C	-7.24	95.92	110.40
1	A	516	SER	N-CA-CB	-7.24	99.64	110.50
3	C	16	ASP	CB-CG-OD2	7.24	124.82	118.30
5	F	94	LEU	C-N-CA	-7.24	107.10	122.30
2	B	399	ASP	CB-CG-OD1	-7.24	111.79	118.30
2	B	961	LEU	CA-CB-CG	7.24	131.94	115.30
2	B	237	VAL	CB-CA-C	-7.23	97.66	111.40
1	A	1042	PHE	CB-CG-CD1	7.23	125.86	120.80
9	K	54	ARG	CD-NE-CZ	7.23	133.72	123.60
6	H	53	ASP	CB-CG-OD2	7.23	124.81	118.30
9	K	22	ASP	CB-CG-OD1	7.23	124.80	118.30
1	A	291	GLU	CA-CB-CG	7.22	129.27	113.40
1	A	462	VAL	CG1-CB-CG2	-7.22	99.35	110.90
1	A	656	TRP	CG-CD1-NE1	7.22	117.32	110.10
2	B	790	ASP	CB-CG-OD1	7.22	124.80	118.30
1	A	277	GLU	CA-CB-CG	7.21	129.27	113.40
3	C	199	LYS	CB-CG-CD	7.21	130.35	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	79	ARG	CA-CB-CG	7.21	129.26	113.40
1	A	120	GLU	OE1-CD-OE2	7.21	131.95	123.30
1	A	472	LEU	CB-CG-CD2	-7.20	98.75	111.00
7	I	44	TYR	CB-CG-CD1	-7.20	116.68	121.00
10	L	69	ALA	CA-C-N	-7.20	101.37	117.20
6	H	139	ASN	N-CA-C	-7.20	91.57	111.00
8	J	62	ARG	CG-CD-NE	-7.20	96.69	111.80
1	A	586	ILE	N-CA-C	-7.19	91.58	111.00
2	B	226	PHE	CG-CD1-CE1	-7.19	112.89	120.80
1	A	1143	LEU	CB-CG-CD2	-7.19	98.78	111.00
9	K	47	ARG	NH1-CZ-NH2	7.18	127.30	119.40
1	A	123	ARG	CD-NE-CZ	7.18	133.66	123.60
3	C	17	ASN	CB-CA-C	-7.18	96.03	110.40
1	A	716	ASP	OD1-CG-OD2	7.18	136.94	123.30
2	B	996	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	362	ASP	CB-CG-OD1	7.17	124.76	118.30
3	C	6	PRO	CA-C-N	-7.17	101.42	117.20
1	A	846	GLU	N-CA-CB	-7.17	97.69	110.60
1	A	413	ILE	CG1-CB-CG2	-7.17	95.62	111.40
2	B	737	THR	CA-CB-CG2	-7.17	102.36	112.40
1	A	1203	ASN	CB-CA-C	7.17	124.74	110.40
6	H	120	GLY	N-CA-C	7.16	131.01	113.10
2	B	914	LYS	CD-CE-NZ	-7.16	95.23	111.70
1	A	266	LEU	CA-CB-CG	7.16	131.77	115.30
1	A	834	THR	CA-CB-CG2	-7.16	102.38	112.40
4	E	41	ASP	CB-CG-OD1	7.16	124.74	118.30
2	B	976	ILE	CG1-CB-CG2	-7.16	95.65	111.40
1	A	782	ARG	O-C-N	7.16	134.15	122.70
2	B	252	SER	N-CA-CB	7.15	121.23	110.50
2	B	381	MET	CG-SD-CE	-7.15	88.76	100.20
3	C	39	ALA	N-CA-CB	-7.15	100.09	110.10
1	A	232	GLU	CG-CD-OE2	-7.15	104.00	118.30
2	B	1041	GLU	N-CA-CB	7.15	123.47	110.60
1	A	1243	VAL	CA-CB-CG2	7.15	121.62	110.90
1	A	1415	SER	CB-CA-C	-7.15	96.52	110.10
1	A	49	LYS	CB-CG-CD	7.14	130.18	111.60
2	B	124	TYR	CD1-CG-CD2	-7.14	110.04	117.90
3	C	191	TYR	CZ-CE2-CD2	7.14	126.23	119.80
1	A	840	ARG	CG-CD-NE	-7.14	96.81	111.80
3	C	180	TYR	CD1-CE1-CZ	7.14	126.23	119.80
1	A	361	LEU	CB-CG-CD2	-7.14	98.86	111.00
1	A	1239	ARG	NE-CZ-NH1	-7.14	116.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	600	PRO	N-CD-CG	-7.14	92.50	103.20
2	B	53	GLN	CB-CG-CD	-7.13	93.05	111.60
2	B	972	LYS	CD-CE-NZ	-7.13	95.30	111.70
3	C	90	ASP	N-CA-C	7.13	130.26	111.00
1	A	1371	LEU	CB-CG-CD1	-7.13	98.88	111.00
9	K	78	THR	CB-CA-C	-7.12	92.36	111.60
1	A	278	THR	CA-CB-CG2	7.12	122.37	112.40
1	A	464	PRO	CA-C-N	7.12	132.86	117.20
1	A	856	THR	N-CA-CB	-7.12	96.78	110.30
6	H	27	GLU	OE1-CD-OE2	-7.12	114.76	123.30
6	H	34	ASP	CB-CG-OD2	7.12	124.71	118.30
2	B	899	ILE	N-CA-C	-7.12	91.79	111.00
7	I	6	PHE	CG-CD1-CE1	7.11	128.62	120.80
1	A	177	ASP	CB-CG-OD1	-7.11	111.90	118.30
1	A	857	ARG	NE-CZ-NH2	7.11	123.86	120.30
9	K	10	PHE	CB-CG-CD2	7.11	125.78	120.80
1	A	656	TRP	NE1-CE2-CZ2	-7.11	122.58	130.40
2	B	1166	CYS	O-C-N	-7.11	111.11	123.20
1	A	121	LEU	CB-CG-CD1	7.09	123.06	111.00
2	B	1150	ARG	NE-CZ-NH1	-7.09	116.75	120.30
3	C	20	PHE	CB-CG-CD1	-7.09	115.83	120.80
3	C	119	VAL	CA-CB-CG1	-7.09	100.26	110.90
2	B	745	PRO	CA-C-O	-7.09	103.18	120.20
7	I	17	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	A	1193	LEU	CB-CG-CD2	-7.09	98.95	111.00
1	A	994	GLN	CA-CB-CG	-7.09	97.81	113.40
2	B	1109	GLY	N-CA-C	7.09	130.82	113.10
2	B	1006	ILE	CG1-CB-CG2	-7.08	95.81	111.40
1	A	384	ASN	N-CA-CB	-7.08	97.85	110.60
4	E	26	ARG	NE-CZ-NH1	-7.08	116.76	120.30
3	C	25	VAL	CB-CA-C	-7.08	97.95	111.40
8	J	2	ILE	CB-CA-C	-7.08	97.44	111.60
1	A	822	GLU	C-N-CA	-7.08	107.44	122.30
5	F	72	LYS	CD-CE-NZ	7.07	127.97	111.70
1	A	709	THR	N-CA-C	7.07	130.09	111.00
7	I	20	LYS	CD-CE-NZ	7.07	127.97	111.70
1	A	1164	PRO	N-CD-CG	7.06	113.79	103.20
3	C	113	VAL	O-C-N	-7.06	111.40	122.70
1	A	1129	GLU	CG-CD-OE1	7.06	132.42	118.30
3	C	9	LYS	CD-CE-NZ	7.06	127.94	111.70
8	J	38	ARG	NH1-CZ-NH2	-7.06	111.64	119.40
1	A	297	GLN	CA-CB-CG	7.06	128.92	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1149	GLU	CG-CD-OE2	7.05	132.41	118.30
2	B	1224	PHE	CB-CG-CD2	7.05	125.74	120.80
2	B	1085	ILE	N-CA-CB	-7.05	94.59	110.80
1	A	705	LYS	CA-CB-CG	7.04	128.89	113.40
8	J	42	LYS	CD-CE-NZ	7.04	127.90	111.70
1	A	645	LEU	O-C-N	-7.04	111.43	122.70
2	B	679	TYR	CD1-CE1-CZ	-7.04	113.47	119.80
2	B	1028	GLU	CG-CD-OE2	7.04	132.38	118.30
1	A	657	LEU	CB-CG-CD1	-7.04	99.04	111.00
7	I	113	ASP	CB-CG-OD1	7.04	124.63	118.30
10	L	58	LYS	O-C-N	-7.04	111.44	122.70
2	B	113	TYR	CB-CG-CD2	-7.03	116.78	121.00
1	A	571	LEU	CB-CG-CD1	-7.03	99.06	111.00
2	B	482	VAL	CB-CA-C	-7.02	98.05	111.40
4	E	63	ASN	N-CA-C	7.02	129.95	111.00
7	I	44	TYR	CB-CG-CD2	7.02	125.21	121.00
1	A	790	ASP	OD1-CG-OD2	-7.01	109.97	123.30
2	B	481	GLN	N-CA-CB	-7.01	97.97	110.60
1	A	1080	THR	CA-CB-CG2	7.01	122.21	112.40
2	B	249	ARG	CA-CB-CG	7.01	128.82	113.40
7	I	45	ARG	NE-CZ-NH1	-7.00	116.80	120.30
3	C	265	MET	CG-SD-CE	-7.00	89.00	100.20
7	I	53	GLY	N-CA-C	7.00	130.60	113.10
1	A	226	GLU	N-CA-CB	7.00	123.20	110.60
1	A	699	ALA	N-CA-CB	-7.00	100.30	110.10
1	A	12	ARG	NE-CZ-NH1	7.00	123.80	120.30
3	C	20	PHE	CB-CG-CD2	-7.00	115.90	120.80
3	C	95	CYS	N-CA-CB	-6.99	98.01	110.60
1	A	984	LYS	CA-CB-CG	6.99	128.78	113.40
5	F	153	VAL	O-C-N	6.99	133.89	122.70
1	A	360	GLU	OE1-CD-OE2	-6.99	114.91	123.30
3	C	33	LEU	CB-CG-CD1	-6.99	99.11	111.00
1	A	801	GLU	CG-CD-OE2	-6.99	104.32	118.30
6	H	11	GLN	CB-CA-C	-6.99	96.43	110.40
2	B	1136	ASP	CB-CG-OD1	6.98	124.58	118.30
1	A	613	ILE	CG1-CB-CG2	-6.98	96.05	111.40
5	F	120	ILE	CG1-CB-CG2	-6.98	96.05	111.40
3	C	142	VAL	CB-CA-C	-6.98	98.15	111.40
1	A	243	PRO	N-CD-CG	-6.97	92.74	103.20
1	A	993	LEU	CB-CG-CD1	-6.97	99.14	111.00
1	A	1307	GLU	CG-CD-OE2	-6.97	104.35	118.30
8	J	21	TYR	N-CA-C	-6.97	92.17	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	339	THR	OG1-CB-CG2	-6.97	93.97	110.00
1	A	268	ASP	OD1-CG-OD2	-6.97	110.06	123.30
5	F	76	LYS	CD-CE-NZ	6.97	127.73	111.70
2	B	622	LYS	CA-CB-CG	6.97	128.72	113.40
6	H	40	LEU	CB-CG-CD1	-6.97	99.16	111.00
2	B	1156	ASP	OD1-CG-OD2	-6.96	110.08	123.30
3	C	154	LYS	CD-CE-NZ	6.96	127.70	111.70
2	B	1086	PHE	CD1-CE1-CZ	6.95	128.44	120.10
1	A	739	ASP	OD1-CG-OD2	-6.95	110.09	123.30
1	A	1269	GLU	OE1-CD-OE2	6.95	131.64	123.30
2	B	131	ASP	CA-C-N	-6.95	101.91	117.20
8	J	45	CYS	CA-CB-SG	6.95	126.51	114.00
1	A	72	GLU	OE1-CD-OE2	-6.95	114.96	123.30
4	E	208	TYR	CG-CD1-CE1	6.95	126.86	121.30
2	B	259	TYR	CB-CG-CD2	6.95	125.17	121.00
1	A	1118	VAL	CA-CB-CG1	6.94	121.32	110.90
1	A	1269	GLU	CB-CA-C	-6.94	96.51	110.40
3	C	243	VAL	CA-CB-CG1	6.94	121.31	110.90
1	A	199	LEU	CA-CB-CG	6.93	131.24	115.30
1	A	576	GLN	CB-CA-C	-6.93	96.54	110.40
1	A	1002	GLY	N-CA-C	6.93	130.42	113.10
1	A	598	LEU	CA-CB-CG	6.93	131.24	115.30
2	B	1136	ASP	OD1-CG-OD2	-6.93	110.14	123.30
2	B	519	TRP	CG-CD1-NE1	-6.93	103.17	110.10
1	A	1163	ILE	CG1-CB-CG2	-6.92	96.16	111.40
2	B	538	ASN	N-CA-CB	-6.92	98.14	110.60
3	C	193	TYR	CZ-CE2-CD2	-6.92	113.57	119.80
1	A	1107	VAL	CB-CA-C	6.92	124.55	111.40
6	H	118	PHE	CG-CD1-CE1	6.92	128.41	120.80
3	C	119	VAL	CA-CB-CG2	6.92	121.28	110.90
1	A	1265	ASN	O-C-N	-6.92	111.63	122.70
2	B	803	LEU	CB-CG-CD2	6.92	122.76	111.00
8	J	29	GLU	OE1-CD-OE2	6.92	131.60	123.30
2	B	44	VAL	CG1-CB-CG2	-6.92	99.84	110.90
1	A	150	THR	OG1-CB-CG2	-6.91	94.10	110.00
4	E	210	SER	CB-CA-C	-6.91	96.97	110.10
2	B	186	GLU	CG-CD-OE1	-6.91	104.48	118.30
2	B	981	ALA	CB-CA-C	-6.91	99.74	110.10
1	A	516	SER	O-C-N	-6.90	111.66	122.70
2	B	978	ASP	CB-CG-OD2	6.90	124.51	118.30
1	A	941	LYS	N-CA-CB	6.90	123.02	110.60
3	C	20	PHE	N-CA-C	6.90	129.63	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	59	VAL	O-C-N	-6.90	111.67	122.70
2	B	982	SER	O-C-N	6.89	133.73	122.70
1	A	911	SER	O-C-N	6.89	133.72	122.70
2	B	58	THR	OG1-CB-CG2	-6.89	94.15	110.00
2	B	899	ILE	CG1-CB-CG2	-6.89	96.24	111.40
2	B	454	THR	CA-CB-CG2	-6.89	102.76	112.40
2	B	1017	ILE	CA-CB-CG1	-6.89	97.92	111.00
3	C	94	LYS	CA-CB-CG	6.88	128.55	113.40
1	A	895	LYS	CD-CE-NZ	-6.88	95.87	111.70
1	A	727	ASP	CB-CG-OD1	6.88	124.49	118.30
1	A	995	GLU	OE1-CD-OE2	6.88	131.55	123.30
6	H	96	VAL	N-CA-CB	-6.88	96.37	111.50
7	I	97	MET	CG-SD-CE	-6.88	89.20	100.20
4	E	85	GLU	CG-CD-OE1	-6.88	104.55	118.30
1	A	1005	GLU	CG-CD-OE1	6.87	132.04	118.30
2	B	373	ARG	CB-CG-CD	6.87	129.47	111.60
2	B	889	THR	CB-CA-C	-6.87	93.05	111.60
10	L	58	LYS	CA-C-N	6.87	132.32	117.20
1	A	874	ASP	CB-CG-OD1	-6.87	112.12	118.30
8	J	63	TYR	CB-CG-CD1	6.87	125.12	121.00
6	H	57	VAL	N-CA-C	6.87	129.55	111.00
4	E	109	ILE	CG1-CB-CG2	-6.86	96.30	111.40
9	K	34	THR	N-CA-CB	-6.86	97.27	110.30
5	F	129	LYS	CD-CE-NZ	6.85	127.46	111.70
1	A	157	ASP	CB-CG-OD2	6.85	124.47	118.30
1	A	65	LEU	CA-CB-CG	6.85	131.05	115.30
1	A	138	ILE	CA-CB-CG2	6.84	124.58	110.90
2	B	479	VAL	CG1-CB-CG2	-6.84	99.95	110.90
3	C	97	VAL	CA-CB-CG1	-6.84	100.64	110.90
2	B	567	GLU	OE1-CD-OE2	-6.84	115.10	123.30
1	A	123	ARG	NE-CZ-NH2	6.83	123.72	120.30
1	A	836	TYR	CD1-CE1-CZ	6.83	125.94	119.80
1	A	1405	THR	OG1-CB-CG2	-6.82	94.31	110.00
4	E	20	LYS	CA-CB-CG	6.82	128.40	113.40
1	A	35	ILE	CG1-CB-CG2	-6.82	96.40	111.40
2	B	106	ASP	CB-CG-OD1	-6.82	112.17	118.30
2	B	1149	GLU	CA-CB-CG	6.82	128.39	113.40
3	C	70	ILE	CB-CA-C	-6.81	97.97	111.60
9	K	94	ILE	O-C-N	6.81	133.60	122.70
1	A	54	ASN	CA-C-N	6.81	132.19	117.20
1	A	90	VAL	N-CA-CB	-6.81	96.51	111.50
1	A	580	VAL	CG1-CB-CG2	-6.81	100.00	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1097	HIS	CA-CB-CG	-6.81	102.02	113.60
1	A	107	CYS	N-CA-C	-6.81	92.62	111.00
3	C	94	LYS	N-CA-CB	6.81	122.85	110.60
1	A	1176	LEU	CB-CA-C	6.80	123.13	110.20
2	B	601	ARG	NH1-CZ-NH2	6.80	126.88	119.40
7	I	93	LYS	N-CA-C	-6.80	92.63	111.00
2	B	101	MET	CG-SD-CE	6.80	111.08	100.20
1	A	1259	MET	CA-CB-CG	6.80	124.86	113.30
2	B	979	LYS	CD-CE-NZ	-6.80	96.06	111.70
3	C	84	ARG	NH1-CZ-NH2	-6.80	111.92	119.40
7	I	19	ASP	OD1-CG-OD2	-6.80	110.38	123.30
1	A	1242	VAL	N-CA-CB	-6.80	96.54	111.50
1	A	678	GLU	CG-CD-OE2	6.80	131.89	118.30
2	B	499	ASN	CB-CA-C	-6.80	96.81	110.40
2	B	722	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	A	1119	TYR	CG-CD2-CE2	6.79	126.73	121.30
4	E	14	ARG	C-N-CA	-6.79	104.72	121.70
1	A	95	PHE	N-CA-CB	-6.79	98.38	110.60
1	A	842	VAL	O-C-N	-6.79	111.84	122.70
2	B	322	PHE	CZ-CE2-CD2	-6.79	111.95	120.10
2	B	553	PRO	N-CD-CG	-6.79	93.02	103.20
1	A	933	TYR	CB-CG-CD1	-6.79	116.93	121.00
9	K	49	GLU	N-CA-CB	6.78	122.81	110.60
3	C	87	PHE	CD1-CE1-CZ	6.78	128.24	120.10
2	B	696	GLU	CG-CD-OE1	-6.78	104.74	118.30
2	B	844	SER	N-CA-CB	-6.78	100.33	110.50
3	C	175	ALA	N-CA-CB	-6.78	100.61	110.10
9	K	78	THR	N-CA-CB	6.78	123.17	110.30
10	L	55	ILE	CB-CA-C	-6.78	98.05	111.60
1	A	350	ARG	NH1-CZ-NH2	-6.77	111.95	119.40
10	L	40	LEU	CB-CG-CD2	6.77	122.51	111.00
1	A	916	GLY	N-CA-C	6.77	130.03	113.10
2	B	35	SER	CB-CA-C	-6.76	97.25	110.10
4	E	138	ALA	N-CA-CB	-6.76	100.63	110.10
9	K	109	TRP	N-CA-CB	-6.76	98.42	110.60
2	B	1183	LYS	N-CA-C	-6.76	92.74	111.00
1	A	585	GLY	O-C-N	6.76	133.52	122.70
2	B	856	PHE	CD1-CE1-CZ	-6.76	111.99	120.10
1	A	351	THR	N-CA-CB	6.76	123.14	110.30
2	B	959	ASP	CB-CG-OD1	6.76	124.38	118.30
5	F	133	VAL	CG1-CB-CG2	-6.75	100.09	110.90
9	K	73	LEU	CB-CG-CD1	-6.75	99.52	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	890	ASP	CB-CG-OD1	6.75	124.38	118.30
1	A	987	VAL	CB-CA-C	-6.74	98.59	111.40
2	B	327	ARG	NE-CZ-NH2	-6.74	116.93	120.30
2	B	372	SER	CA-C-O	6.74	134.25	120.10
2	B	1061	GLU	CG-CD-OE2	-6.74	104.82	118.30
5	F	112	GLU	CG-CD-OE2	6.74	131.78	118.30
1	A	1299	VAL	CA-CB-CG2	-6.74	100.80	110.90
1	A	1372	VAL	CA-CB-CG2	6.74	121.00	110.90
6	H	106	GLU	CB-CA-C	6.73	123.87	110.40
1	A	1274	ARG	CB-CA-C	-6.73	96.94	110.40
2	B	746	SER	N-CA-CB	6.73	120.60	110.50
2	B	1183	LYS	CD-CE-NZ	6.73	127.18	111.70
1	A	1332	PHE	CG-CD2-CE2	-6.72	113.40	120.80
6	H	49	VAL	CB-CA-C	-6.72	98.62	111.40
1	A	918	GLU	OE1-CD-OE2	-6.72	115.23	123.30
1	A	1301	GLU	N-CA-CB	6.72	122.70	110.60
3	C	263	THR	N-CA-CB	-6.72	97.53	110.30
1	A	864	ILE	CA-CB-CG1	6.72	123.76	111.00
2	B	136	THR	N-CA-CB	6.71	123.06	110.30
2	B	710	LEU	CD1-CG-CD2	-6.71	90.36	110.50
3	C	124	LEU	CB-CA-C	-6.71	97.44	110.20
1	A	1155	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	A	1023	ARG	NH1-CZ-NH2	-6.71	112.02	119.40
4	E	206	GLY	CA-C-O	-6.71	108.52	120.60
1	A	495	GLU	N-CA-CB	-6.71	98.53	110.60
2	B	398	ARG	N-CA-C	6.71	129.11	111.00
1	A	438	ASP	OD1-CG-OD2	-6.71	110.56	123.30
2	B	194	GLU	CB-CA-C	6.71	123.81	110.40
2	B	856	PHE	CB-CG-CD2	6.71	125.50	120.80
2	B	209	GLU	O-C-N	-6.70	111.98	122.70
3	C	71	PRO	CA-CB-CG	6.70	117.54	104.80
7	I	30	ARG	N-CA-C	6.70	129.10	111.00
4	E	74	ASP	OD1-CG-OD2	-6.70	110.57	123.30
5	F	139	PRO	N-CD-CG	6.70	113.25	103.20
1	A	739	ASP	N-CA-C	6.70	129.08	111.00
2	B	422	LYS	CD-CE-NZ	-6.70	96.29	111.70
2	B	957	ASN	N-CA-CB	-6.70	98.54	110.60
4	E	19	VAL	CA-CB-CG1	-6.70	100.85	110.90
1	A	506	ALA	CB-CA-C	-6.70	100.06	110.10
2	B	817	LEU	CB-CG-CD2	-6.70	99.62	111.00
2	B	1198	TYR	CB-CA-C	6.69	123.79	110.40
1	A	81	PHE	CD1-CG-CD2	-6.69	109.60	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	1	MET	CB-CG-SD	-6.69	92.32	112.40
2	B	360	PHE	CB-CG-CD2	6.69	125.48	120.80
6	H	62	SER	N-CA-CB	6.69	120.54	110.50
3	C	95	CYS	CA-CB-SG	6.69	126.04	114.00
3	C	240	VAL	CB-CA-C	-6.69	98.69	111.40
3	C	20	PHE	CB-CA-C	-6.69	97.03	110.40
1	A	196	GLU	CA-CB-CG	6.68	128.11	113.40
1	A	1191	TRP	CD1-NE1-CE2	-6.68	102.98	109.00
1	A	645	LEU	CB-CG-CD1	-6.68	99.64	111.00
9	K	79	GLU	OE1-CD-OE2	-6.68	115.28	123.30
2	B	541	LEU	CA-CB-CG	6.68	130.67	115.30
1	A	372	LYS	N-CA-C	6.68	129.03	111.00
2	B	394	ASP	CB-CG-OD2	6.68	124.31	118.30
2	B	1162	ILE	CA-CB-CG2	6.68	124.26	110.90
2	B	106	ASP	OD1-CG-OD2	-6.68	110.62	123.30
6	H	126	GLU	CA-CB-CG	6.67	128.08	113.40
3	C	226	ASP	CB-CG-OD2	6.67	124.30	118.30
4	E	103	LYS	N-CA-CB	6.67	122.60	110.60
1	A	1287	TYR	CD1-CE1-CZ	-6.67	113.80	119.80
3	C	233	GLU	O-C-N	6.67	133.37	122.70
4	E	178	ILE	CG1-CB-CG2	-6.67	96.73	111.40
2	B	547	VAL	N-CA-CB	-6.67	96.84	111.50
1	A	656	TRP	CZ3-CH2-CZ2	-6.66	113.61	121.60
2	B	739	THR	CA-CB-CG2	-6.65	103.09	112.40
1	A	498	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	A	1129	GLU	CA-CB-CG	6.64	128.02	113.40
2	B	124	TYR	CB-CG-CD2	6.64	124.99	121.00
2	B	223	VAL	CB-CA-C	-6.64	98.78	111.40
2	B	621	GLU	CG-CD-OE1	-6.64	105.02	118.30
3	C	5	GLY	N-CA-C	6.64	129.70	113.10
4	E	187	TYR	CD1-CE1-CZ	6.64	125.78	119.80
9	K	49	GLU	CA-C-O	-6.64	106.16	120.10
2	B	102	VAL	CG1-CB-CG2	6.64	121.52	110.90
2	B	1185	CYS	N-CA-C	-6.64	93.08	111.00
3	C	172	PRO	O-C-N	6.64	133.32	122.70
2	B	324	ILE	CG1-CB-CG2	-6.63	96.80	111.40
2	B	851	PHE	CB-CG-CD1	-6.63	116.16	120.80
1	A	514	PRO	CA-CB-CG	6.63	117.40	104.80
10	L	40	LEU	CB-CA-C	6.63	122.80	110.20
8	J	6	ARG	CB-CA-C	-6.63	97.14	110.40
1	A	1135	ARG	CA-CB-CG	6.62	127.97	113.40
1	A	522	GLY	CA-C-O	-6.62	108.68	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1046	LEU	CB-CA-C	-6.62	97.62	110.20
1	A	1199	ARG	NE-CZ-NH2	6.62	123.61	120.30
2	B	180	TYR	CG-CD2-CE2	-6.62	116.00	121.30
1	A	4	GLN	CB-CA-C	6.62	123.64	110.40
3	C	253	LYS	CB-CA-C	-6.62	97.16	110.40
4	E	136	ASN	CB-CA-C	-6.62	97.16	110.40
4	E	47	CYS	CA-CB-SG	-6.62	102.09	114.00
1	A	1043	ASP	OD1-CG-OD2	-6.61	110.73	123.30
9	K	107	THR	O-C-N	6.61	133.28	122.70
1	A	948	VAL	C-N-CA	6.61	138.22	121.70
3	C	14	SER	N-CA-C	-6.61	93.16	111.00
5	F	112	GLU	OE1-CD-OE2	-6.60	115.38	123.30
1	A	79	GLY	N-CA-C	-6.60	96.59	113.10
2	B	1151	LEU	CB-CG-CD1	-6.60	99.78	111.00
1	A	1230	GLU	OE1-CD-OE2	6.60	131.22	123.30
2	B	90	ILE	CB-CA-C	-6.60	98.40	111.60
3	C	200	GLU	OE1-CD-OE2	-6.60	115.38	123.30
3	C	233	GLU	CG-CD-OE2	-6.60	105.10	118.30
4	E	81	GLU	CG-CD-OE2	-6.60	105.10	118.30
9	K	73	LEU	CB-CA-C	-6.60	97.66	110.20
1	A	261	ASP	N-CA-C	6.60	128.82	111.00
1	A	1051	ALA	N-CA-CB	-6.60	100.86	110.10
2	B	272	THR	OG1-CB-CG2	-6.60	94.83	110.00
1	A	1038	THR	CA-CB-CG2	-6.59	103.17	112.40
2	B	501	PRO	CA-C-O	-6.59	104.38	120.20
1	A	1058	VAL	CB-CA-C	6.59	123.92	111.40
1	A	1192	LEU	CA-CB-CG	6.59	130.45	115.30
2	B	18	PHE	N-CA-C	-6.59	93.21	111.00
4	E	208	TYR	CB-CG-CD2	6.59	124.95	121.00
2	B	501	PRO	O-C-N	6.59	133.24	122.70
10	L	57	LEU	N-CA-C	6.58	128.78	111.00
1	A	826	ASP	CB-CG-OD1	-6.58	112.38	118.30
2	B	681	TRP	CE3-CZ3-CH2	-6.58	113.96	121.20
1	A	988	LEU	CB-CG-CD2	6.58	122.18	111.00
2	B	905	VAL	CG1-CB-CG2	-6.58	100.38	110.90
1	A	162	VAL	CG1-CB-CG2	6.57	121.42	110.90
1	A	807	GLY	O-C-N	-6.57	112.18	122.70
1	A	1242	VAL	N-CA-C	6.57	128.74	111.00
2	B	488	TYR	CB-CG-CD2	-6.57	117.06	121.00
2	B	134	LYS	CD-CE-NZ	6.57	126.81	111.70
3	C	75	MET	N-CA-CB	-6.57	98.78	110.60
1	A	790	ASP	CB-CG-OD1	6.56	124.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	24	ARG	CG-CD-NE	-6.56	98.02	111.80
1	A	56	PRO	O-C-N	6.56	133.20	122.70
1	A	326	ARG	NH1-CZ-NH2	-6.56	112.19	119.40
1	A	861	GLY	C-N-CA	-6.56	105.30	121.70
2	B	106	ASP	N-CA-CB	-6.56	98.80	110.60
2	B	1067	ARG	NE-CZ-NH1	6.56	123.58	120.30
2	B	418	LYS	CA-C-O	-6.55	106.34	120.10
3	C	20	PHE	CG-CD2-CE2	-6.55	113.59	120.80
2	B	57	TYR	CG-CD1-CE1	6.55	126.54	121.30
1	A	602	ASP	CB-CG-OD2	6.55	124.19	118.30
1	A	1367	HIS	O-C-N	-6.55	112.22	122.70
2	B	312	GLU	CB-CA-C	6.55	123.50	110.40
7	I	15	TYR	CZ-CE2-CD2	6.55	125.69	119.80
2	B	102	VAL	N-CA-C	6.55	128.68	111.00
2	B	942	ARG	CB-CA-C	-6.54	97.31	110.40
1	A	1003	LYS	CA-CB-CG	-6.54	99.00	113.40
2	B	602	THR	CA-CB-CG2	-6.54	103.24	112.40
2	B	1135	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	482	PHE	CB-CG-CD1	6.54	125.38	120.80
2	B	966	VAL	CA-CB-CG1	6.54	120.70	110.90
2	B	34	ILE	CG1-CB-CG2	-6.53	97.03	111.40
1	A	684	ALA	CB-CA-C	6.53	119.90	110.10
1	A	566	ILE	O-C-N	6.53	133.15	122.70
6	H	93	TYR	CB-CG-CD1	6.53	124.92	121.00
9	K	76	GLN	CB-CA-C	-6.53	97.34	110.40
2	B	595	ARG	CB-CA-C	-6.53	97.35	110.40
2	B	739	THR	CB-CA-C	-6.53	93.98	111.60
2	B	785	TYR	O-C-N	6.53	133.14	122.70
6	H	125	LEU	CB-CG-CD1	6.52	122.09	111.00
1	A	1211	GLN	N-CA-CB	6.52	122.34	110.60
1	A	415	LEU	C-N-CA	-6.52	105.40	121.70
2	B	1023	VAL	CA-CB-CG2	-6.52	101.12	110.90
2	B	773	MET	O-C-N	-6.51	112.12	123.20
1	A	237	THR	O-C-N	6.51	133.12	122.70
3	C	87	PHE	CE1-CZ-CE2	-6.51	108.28	120.00
2	B	1103	ILE	CB-CA-C	-6.51	98.58	111.60
7	I	55	THR	N-CA-CB	-6.51	97.93	110.30
2	B	124	TYR	CD1-CE1-CZ	6.50	125.65	119.80
2	B	1036	ALA	CB-CA-C	-6.50	100.35	110.10
9	K	7	PHE	CB-CG-CD1	-6.50	116.25	120.80
1	A	42	ASP	CB-CG-OD1	-6.50	112.45	118.30
2	B	57	TYR	N-CA-CB	6.50	122.29	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	8	GLU	OE1-CD-OE2	-6.50	115.51	123.30
2	B	312	GLU	N-CA-CB	-6.49	98.91	110.60
2	B	595	ARG	NH1-CZ-NH2	-6.49	112.26	119.40
7	I	100	PHE	N-CA-CB	6.49	122.29	110.60
1	A	25	GLU	CG-CD-OE2	-6.49	105.33	118.30
1	A	830	LYS	N-CA-CB	6.48	122.27	110.60
1	A	946	VAL	CB-CA-C	-6.48	99.08	111.40
1	A	1034	GLU	OE1-CD-OE2	-6.48	115.52	123.30
2	B	48	LEU	CB-CA-C	-6.48	97.88	110.20
2	B	581	PHE	CG-CD2-CE2	6.48	127.93	120.80
2	B	223	VAL	CA-CB-CG1	-6.48	101.18	110.90
2	B	1046	PRO	CA-CB-CG	6.48	117.11	104.80
1	A	737	LEU	CA-CB-CG	6.47	130.17	115.30
1	A	1192	LEU	CB-CA-C	-6.47	97.91	110.20
1	A	677	ARG	NE-CZ-NH1	6.46	123.53	120.30
2	B	691	GLU	CA-CB-CG	6.46	127.61	113.40
3	C	187	LYS	N-CA-CB	-6.46	98.97	110.60
3	C	240	VAL	N-CA-C	6.46	128.45	111.00
2	B	63	ILE	O-C-N	-6.46	112.36	122.70
2	B	569	TYR	CD1-CE1-CZ	-6.46	113.99	119.80
1	A	561	PRO	N-CD-CG	6.46	112.88	103.20
10	L	25	ALA	C-N-CA	6.46	137.84	121.70
1	A	361	LEU	CB-CA-C	-6.45	97.94	110.20
3	C	89	GLU	N-CA-C	-6.45	93.58	111.00
6	H	106	GLU	N-CA-C	-6.45	93.58	111.00
1	A	953	ASN	CB-CG-OD1	6.45	134.50	121.60
1	A	1050	GLU	O-C-N	-6.45	112.38	122.70
10	L	41	SER	N-CA-C	6.45	128.41	111.00
1	A	196	GLU	OE1-CD-OE2	-6.45	115.57	123.30
1	A	22	PHE	N-CA-C	-6.44	93.61	111.00
2	B	521	LEU	CA-CB-CG	-6.44	100.48	115.30
2	B	368	GLU	C-N-CA	-6.44	108.78	122.30
4	E	137	GLU	CG-CD-OE2	-6.44	105.42	118.30
4	E	131	THR	CA-C-N	-6.44	103.03	117.20
1	A	443	LEU	CA-CB-CG	6.43	130.10	115.30
7	I	109	ILE	CG1-CB-CG2	-6.43	97.25	111.40
7	I	96	SER	CA-CB-OG	6.43	128.57	111.20
1	A	1146	VAL	N-CA-CB	-6.43	97.35	111.50
2	B	424	LEU	CA-CB-CG	-6.43	100.51	115.30
2	B	526	GLU	OE1-CD-OE2	-6.43	115.58	123.30
1	A	508	PRO	N-CD-CG	6.43	112.85	103.20
2	B	788	ARG	C-N-CA	-6.43	105.63	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ASN	N-CA-C	6.43	128.36	111.00
1	A	411	ASP	N-CA-CB	6.43	122.17	110.60
2	B	944	THR	CB-CA-C	-6.43	94.24	111.60
3	C	172	PRO	CA-N-CD	-6.43	102.50	111.50
7	I	15	TYR	CE1-CZ-CE2	-6.43	109.52	119.80
8	J	7	CYS	CB-CA-C	-6.43	97.55	110.40
2	B	795	ILE	CB-CA-C	-6.42	98.76	111.60
1	A	298	PHE	CD1-CE1-CZ	6.42	127.80	120.10
2	B	249	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	777	PHE	CB-CG-CD2	6.42	125.29	120.80
1	A	1138	ILE	CG1-CB-CG2	-6.42	97.28	111.40
1	A	1157	ASP	CB-CG-OD2	6.42	124.08	118.30
8	J	60	PHE	CG-CD2-CE2	-6.42	113.74	120.80
1	A	99	ILE	CG1-CB-CG2	-6.42	97.29	111.40
2	B	914	LYS	CB-CA-C	-6.41	97.57	110.40
4	E	187	TYR	CA-CB-CG	6.41	125.59	113.40
4	E	71	LYS	CB-CA-C	-6.41	97.58	110.40
5	F	90	ARG	CB-CG-CD	6.41	128.27	111.60
7	I	30	ARG	NE-CZ-NH1	-6.41	117.09	120.30
1	A	152	VAL	CA-CB-CG1	6.41	120.51	110.90
6	H	60	ALA	CB-CA-C	-6.41	100.49	110.10
7	I	98	VAL	CG1-CB-CG2	-6.41	100.65	110.90
2	B	217	ARG	CG-CD-NE	-6.40	98.35	111.80
2	B	424	LEU	CB-CA-C	-6.40	98.04	110.20
2	B	661	LEU	CB-CG-CD2	6.40	121.89	111.00
1	A	536	LEU	N-CA-CB	-6.40	97.60	110.40
1	A	737	LEU	CB-CA-C	-6.40	98.04	110.20
2	B	556	THR	CA-CB-CG2	-6.40	103.44	112.40
3	C	40	GLU	N-CA-C	6.40	128.28	111.00
4	E	25	ASP	N-CA-CB	6.40	122.12	110.60
7	I	24	ARG	CB-CA-C	-6.40	97.60	110.40
2	B	810	GLU	CB-CA-C	6.40	123.20	110.40
1	A	126	LEU	CB-CG-CD1	-6.40	100.13	111.00
1	A	295	LEU	CB-CA-C	-6.39	98.05	110.20
2	B	1054	GLY	O-C-N	6.39	132.93	122.70
10	L	27	LEU	CB-CG-CD2	6.39	121.87	111.00
6	H	111	LEU	CA-CB-CG	6.39	130.00	115.30
10	L	70	ARG	CA-CB-CG	-6.39	99.34	113.40
3	C	229	TYR	CG-CD1-CE1	6.39	126.41	121.30
1	A	1166	ASP	CB-CG-OD2	-6.39	112.55	118.30
4	E	207	ARG	CG-CD-NE	-6.39	98.38	111.80
1	A	1309	ASP	CB-CA-C	-6.38	97.63	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1180	PHE	CB-CG-CD1	-6.38	116.33	120.80
1	A	1303	GLU	OE1-CD-OE2	6.38	130.95	123.30
1	A	1381	LEU	CB-CA-C	-6.38	98.08	110.20
2	B	612	GLU	N-CA-CB	-6.38	99.12	110.60
2	B	1049	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	1239	ARG	N-CA-CB	-6.38	99.12	110.60
2	B	780	VAL	CA-CB-CG2	-6.38	101.33	110.90
4	E	34	GLU	CG-CD-OE1	-6.38	105.55	118.30
2	B	589	VAL	O-C-N	-6.37	112.51	122.70
1	A	941	LYS	CB-CA-C	-6.37	97.66	110.40
3	C	150	GLY	CA-C-O	6.37	132.06	120.60
6	H	126	GLU	CG-CD-OE1	6.37	131.04	118.30
1	A	789	LYS	N-CA-C	6.37	128.19	111.00
1	A	827	THR	CA-C-N	6.37	131.21	117.20
1	A	778	GLY	N-CA-C	6.37	129.01	113.10
1	A	938	LYS	N-CA-CB	6.37	122.06	110.60
2	B	138	GLU	CG-CD-OE1	6.37	131.03	118.30
2	B	1110	PRO	CA-C-O	6.37	135.48	120.20
9	K	51	LEU	N-CA-CB	-6.37	97.67	110.40
2	B	812	LEU	CB-CG-CD2	6.36	121.81	111.00
2	B	178	ASN	CB-CA-C	-6.36	97.68	110.40
2	B	1059	LEU	CB-CG-CD2	-6.36	100.19	111.00
1	A	751	SER	O-C-N	6.36	132.87	122.70
2	B	568	ASP	CB-CG-OD1	-6.36	112.58	118.30
5	F	108	PHE	O-C-N	-6.36	112.53	122.70
10	L	63	ARG	CA-CB-CG	6.36	127.39	113.40
1	A	889	SER	N-CA-CB	6.36	120.03	110.50
2	B	1085	ILE	O-C-N	-6.36	112.53	122.70
1	A	934	LYS	N-CA-CB	6.35	122.04	110.60
1	A	1220	PHE	CD1-CE1-CZ	6.35	127.72	120.10
2	B	699	GLU	CB-CA-C	-6.35	97.69	110.40
3	C	147	LEU	CA-CB-CG	6.35	129.91	115.30
2	B	261	ARG	NE-CZ-NH1	6.35	123.48	120.30
2	B	431	TYR	CB-CA-C	-6.35	97.70	110.40
10	L	48	CYS	C-N-CA	6.35	137.58	121.70
2	B	223	VAL	CA-CB-CG2	6.35	120.42	110.90
2	B	904	ARG	NE-CZ-NH2	6.35	123.47	120.30
2	B	1167	GLY	N-CA-C	6.35	128.97	113.10
8	J	18	TRP	CD1-CG-CD2	-6.35	101.22	106.30
2	B	588	GLY	CA-C-O	-6.35	109.18	120.60
7	I	9	ASP	CB-CG-OD2	6.35	124.01	118.30
1	A	356	ASP	OD1-CG-OD2	6.34	135.35	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1015	VAL	CB-CA-C	6.34	123.45	111.40
2	B	646	LEU	N-CA-C	6.34	128.13	111.00
3	C	229	TYR	CG-CD2-CE2	-6.34	116.22	121.30
1	A	1144	LYS	CD-CE-NZ	6.34	126.28	111.70
1	A	556	TRP	CA-CB-CG	6.34	125.74	113.70
1	A	119	ASN	N-CA-C	6.34	128.11	111.00
2	B	130	VAL	CG1-CB-CG2	-6.34	100.76	110.90
2	B	990	ILE	CA-CB-CG1	6.34	123.04	111.00
2	B	1026	LEU	CB-CG-CD1	-6.34	100.23	111.00
3	C	186	LEU	N-CA-CB	-6.33	97.73	110.40
2	B	413	LEU	CB-CG-CD2	-6.33	100.23	111.00
2	B	634	TYR	CB-CG-CD2	6.33	124.80	121.00
2	B	1043	ASP	N-CA-CB	6.33	122.00	110.60
2	B	164	LYS	CA-C-N	6.33	131.13	117.20
2	B	650	GLU	CG-CD-OE1	-6.33	105.64	118.30
1	A	789	LYS	O-C-N	-6.33	112.58	122.70
2	B	787	VAL	N-CA-CB	-6.33	97.58	111.50
2	B	781	PHE	CG-CD2-CE2	-6.33	113.84	120.80
2	B	893	LEU	CB-CG-CD2	-6.33	100.25	111.00
2	B	1096	ARG	NH1-CZ-NH2	6.32	126.35	119.40
1	A	226	GLU	CG-CD-OE2	6.32	130.94	118.30
1	A	704	ALA	CA-C-O	-6.32	106.83	120.10
1	A	597	LEU	CB-CG-CD2	-6.31	100.27	111.00
2	B	1152	MET	CB-CG-SD	6.31	131.34	112.40
1	A	5	GLN	N-CA-CB	6.31	121.96	110.60
4	E	183	PRO	CA-N-CD	-6.31	102.67	111.50
6	H	45	GLU	CG-CD-OE2	-6.31	105.68	118.30
2	B	795	ILE	O-C-N	-6.31	112.61	122.70
9	K	83	PRO	N-CD-CG	-6.31	93.74	103.20
8	J	21	TYR	CB-CG-CD1	6.30	124.78	121.00
8	J	63	TYR	CB-CG-CD2	-6.30	117.22	121.00
1	A	144	THR	CA-CB-CG2	6.30	121.22	112.40
6	H	139	ASN	N-CA-CB	6.30	121.94	110.60
9	K	42	LEU	CB-CG-CD2	-6.30	100.29	111.00
9	K	78	THR	CA-CB-CG2	-6.30	103.59	112.40
1	A	920	LEU	C-N-CA	-6.29	109.08	122.30
7	I	75	CYS	CB-CA-C	-6.29	97.81	110.40
2	B	1004	GLU	OE1-CD-OE2	-6.29	115.75	123.30
1	A	268	ASP	CB-CA-C	6.29	122.98	110.40
1	A	579	SER	N-CA-CB	6.29	119.93	110.50
1	A	788	SER	CB-CA-C	6.29	122.05	110.10
6	H	110	ASP	C-N-CA	6.29	137.42	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1280	GLU	CG-CD-OE2	6.29	130.88	118.30
3	C	67	LEU	CB-CG-CD1	-6.29	100.31	111.00
1	A	673	GLY	CA-C-O	-6.29	109.28	120.60
2	B	307	ASP	CB-CG-OD1	-6.29	112.64	118.30
1	A	596	THR	CB-CA-C	-6.28	94.64	111.60
1	A	1062	GLU	CB-CG-CD	6.28	131.17	114.20
2	B	853	SER	CA-CB-OG	6.28	128.16	111.20
4	E	74	ASP	CA-C-O	6.28	133.29	120.10
7	I	26	LEU	CB-CG-CD2	-6.28	100.32	111.00
1	A	441	PRO	N-CA-CB	-6.28	95.69	102.60
1	A	552	TRP	CB-CG-CD1	-6.28	118.83	127.00
2	B	576	ASP	OD1-CG-OD2	-6.28	111.36	123.30
2	B	633	VAL	CA-CB-CG2	6.28	120.32	110.90
1	A	755	PHE	CB-CG-CD1	6.28	125.19	120.80
1	A	959	ASN	N-CA-C	-6.28	94.05	111.00
7	I	44	TYR	CA-C-N	-6.28	103.39	117.20
3	C	86	CYS	CB-CA-C	6.28	122.96	110.40
1	A	716	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	A	1094	VAL	CA-CB-CG2	-6.28	101.49	110.90
1	A	1122	PRO	C-N-CA	-6.28	109.12	122.30
2	B	530	GLY	N-CA-C	6.28	128.79	113.10
3	C	87	PHE	CG-CD1-CE1	-6.28	113.90	120.80
1	A	146	MET	CG-SD-CE	6.27	110.24	100.20
2	B	411	PRO	CA-N-CD	6.27	120.48	111.70
1	A	1207	LEU	CB-CG-CD1	-6.27	100.34	111.00
2	B	1206	GLU	OE1-CD-OE2	-6.27	115.77	123.30
7	I	22	ASN	O-C-N	6.27	132.74	122.70
2	B	1086	PHE	CG-CD2-CE2	6.27	127.70	120.80
1	A	651	LYS	CB-CA-C	6.27	122.94	110.40
2	B	736	THR	N-CA-CB	6.27	122.21	110.30
2	B	1132	GLU	CA-C-O	-6.27	106.94	120.10
1	A	98	LYS	CG-CD-CE	-6.27	93.10	111.90
1	A	1359	ASP	N-CA-CB	6.27	121.88	110.60
2	B	194	GLU	OE1-CD-OE2	6.26	130.82	123.30
3	C	260	LEU	CB-CG-CD1	6.26	121.65	111.00
6	H	3	ASN	C-N-CA	6.26	137.36	121.70
1	A	474	VAL	N-CA-CB	-6.26	97.72	111.50
4	E	77	SER	N-CA-C	-6.26	94.09	111.00
1	A	467	THR	CA-CB-CG2	-6.26	103.63	112.40
1	A	346	ASP	OD1-CG-OD2	-6.26	111.41	123.30
1	A	1214	GLU	O-C-N	6.26	132.71	122.70
2	B	995	ARG	CG-CD-NE	-6.26	98.66	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ASP	OD1-CG-OD2	-6.25	111.42	123.30
1	A	403	LYS	CA-CB-CG	6.25	127.16	113.40
2	B	337	ARG	NE-CZ-NH1	-6.25	117.17	120.30
2	B	738	PHE	CD1-CE1-CZ	-6.25	112.59	120.10
10	L	63	ARG	N-CA-CB	6.25	121.85	110.60
1	A	885	THR	OG1-CB-CG2	-6.25	95.63	110.00
4	E	135	PHE	CB-CG-CD1	6.25	125.17	120.80
1	A	1291	VAL	N-CA-CB	-6.25	97.76	111.50
2	B	407	ASP	OD1-CG-OD2	-6.24	111.44	123.30
1	A	856	THR	OG1-CB-CG2	-6.24	95.64	110.00
2	B	1217	TYR	CZ-CE2-CD2	-6.24	114.18	119.80
1	A	81	PHE	CB-CG-CD2	6.24	125.17	120.80
1	A	704	ALA	CB-CA-C	-6.24	100.74	110.10
1	A	1362	TYR	N-CA-CB	6.24	121.83	110.60
1	A	218	ASP	CB-CG-OD1	-6.24	112.69	118.30
5	F	92	ARG	CB-CG-CD	6.24	127.82	111.60
3	C	111	THR	CA-CB-CG2	-6.23	103.67	112.40
1	A	823	GLY	N-CA-C	6.23	128.68	113.10
2	B	1183	LYS	CG-CD-CE	6.23	130.60	111.90
2	B	857	ARG	NE-CZ-NH1	6.23	123.42	120.30
8	J	1	MET	CA-CB-CG	6.23	123.89	113.30
3	C	184	ASN	C-N-CA	-6.22	106.14	121.70
2	B	618	ASP	CB-CA-C	6.22	122.84	110.40
2	B	708	GLU	N-CA-CB	-6.22	99.40	110.60
4	E	170	LEU	CA-CB-CG	-6.22	100.99	115.30
3	C	153	LEU	N-CA-CB	-6.22	97.96	110.40
2	B	535	LEU	CB-CG-CD2	6.22	121.57	111.00
1	A	377	PRO	CA-N-CD	-6.22	102.79	111.50
3	C	4	GLU	N-CA-C	6.22	127.78	111.00
1	A	1001	ARG	O-C-N	-6.21	112.64	123.20
1	A	610	GLY	O-C-N	6.21	132.64	122.70
2	B	612	GLU	CB-CA-C	6.21	122.82	110.40
2	B	1224	PHE	CA-C-O	-6.21	107.06	120.10
3	C	239	PRO	CA-C-O	6.21	135.11	120.20
3	C	229	TYR	N-CA-C	6.21	127.77	111.00
1	A	830	LYS	CB-CA-C	-6.21	97.99	110.40
2	B	446	LEU	CB-CA-C	6.21	121.99	110.20
1	A	1345	ARG	CB-CA-C	-6.20	97.99	110.40
2	B	625	LYS	CD-CE-NZ	-6.20	97.43	111.70
6	H	56	THR	OG1-CB-CG2	-6.20	95.73	110.00
1	A	657	LEU	CB-CG-CD2	6.20	121.54	111.00
1	A	977	LYS	N-CA-C	-6.20	94.26	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	563	MET	CG-SD-CE	6.20	110.12	100.20
3	C	135	GLN	CA-CB-CG	6.20	127.04	113.40
3	C	215	GLU	N-CA-CB	6.20	121.75	110.60
1	A	905	ASP	CB-CG-OD1	-6.20	112.72	118.30
2	B	354	ASP	CB-CG-OD2	-6.20	112.72	118.30
3	C	133	ILE	O-C-N	6.20	132.61	122.70
6	H	6	PHE	CB-CG-CD1	-6.19	116.46	120.80
7	I	18	GLU	CG-CD-OE1	-6.19	105.92	118.30
2	B	208	SER	CB-CA-C	-6.19	98.34	110.10
1	A	379	VAL	CA-C-O	-6.19	107.10	120.10
2	B	603	LEU	CB-CG-CD1	6.19	121.52	111.00
4	E	117	THR	OG1-CB-CG2	-6.19	95.77	110.00
4	E	85	GLU	CG-CD-OE2	6.19	130.68	118.30
6	H	63	LEU	CB-CA-C	6.19	121.95	110.20
2	B	432	MET	CA-CB-CG	6.18	123.81	113.30
2	B	125	SER	CB-CA-C	6.18	121.84	110.10
2	B	606	LYS	N-CA-CB	-6.18	99.47	110.60
2	B	245	GLU	CA-CB-CG	6.18	127.00	113.40
3	C	34	ARG	CG-CD-NE	-6.18	98.83	111.80
1	A	1299	VAL	CG1-CB-CG2	6.18	120.78	110.90
2	B	642	ASP	CB-CG-OD2	6.17	123.86	118.30
1	A	1113	THR	N-CA-C	6.17	127.67	111.00
6	H	55	LEU	CB-CG-CD2	6.17	121.50	111.00
1	A	1277	GLU	CG-CD-OE2	6.17	130.64	118.30
2	B	662	MET	O-C-N	-6.17	112.83	122.70
2	B	879	ARG	CG-CD-NE	6.17	124.75	111.80
8	J	11	GLY	CA-C-O	-6.17	109.50	120.60
1	A	694	THR	OG1-CB-CG2	-6.17	95.82	110.00
1	A	918	GLU	CG-CD-OE2	6.17	130.63	118.30
1	A	947	PHE	CB-CG-CD1	6.17	125.12	120.80
3	C	24	ASN	CB-CA-C	-6.17	98.07	110.40
1	A	1064	VAL	CA-CB-CG1	6.16	120.14	110.90
1	A	1353	TYR	CA-CB-CG	6.16	125.11	113.40
2	B	1011	ILE	CB-CA-C	-6.16	99.27	111.60
2	B	1130	PHE	CZ-CE2-CD2	6.16	127.50	120.10
1	A	396	PRO	CA-CB-CG	-6.16	92.29	104.00
4	E	9	ILE	CG1-CB-CG2	-6.16	97.84	111.40
1	A	214	ILE	O-C-N	6.16	132.56	122.70
2	B	480	SER	CB-CA-C	-6.16	98.39	110.10
2	B	268	THR	CA-CB-CG2	6.16	121.02	112.40
10	L	61	THR	CA-CB-CG2	6.16	121.02	112.40
1	A	1373	ASP	OD1-CG-OD2	-6.16	111.61	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	942	ARG	CG-CD-NE	-6.16	98.87	111.80
6	H	95	TYR	CZ-CE2-CD2	6.15	125.34	119.80
7	I	22	ASN	CB-CA-C	-6.15	98.09	110.40
1	A	416	ARG	CB-CA-C	6.15	122.70	110.40
9	K	106	GLU	OE1-CD-OE2	-6.15	115.92	123.30
1	A	1304	TRP	CB-CA-C	-6.15	98.11	110.40
2	B	48	LEU	CA-CB-CG	-6.15	101.16	115.30
2	B	327	ARG	N-CA-CB	-6.15	99.54	110.60
2	B	522	VAL	N-CA-CB	-6.15	97.98	111.50
2	B	701	ILE	CG1-CB-CG2	-6.15	97.88	111.40
6	H	97	MET	N-CA-CB	-6.15	99.54	110.60
8	J	7	CYS	N-CA-CB	6.15	121.66	110.60
1	A	470	LEU	CB-CA-C	-6.15	98.52	110.20
3	C	35	ARG	CD-NE-CZ	6.14	132.20	123.60
6	H	42	ILE	N-CA-CB	-6.14	96.67	110.80
4	E	90	VAL	CG1-CB-CG2	6.14	120.73	110.90
9	K	61	TYR	CD1-CG-CD2	-6.14	111.14	117.90
1	A	419	LYS	CD-CE-NZ	-6.14	97.58	111.70
1	A	817	ALA	CB-CA-C	-6.14	100.89	110.10
2	B	666	TYR	CB-CG-CD2	-6.14	117.32	121.00
2	B	691	GLU	N-CA-CB	-6.14	99.55	110.60
3	C	173	ALA	CB-CA-C	-6.14	100.89	110.10
9	K	36	GLU	N-CA-CB	-6.14	99.55	110.60
4	E	186	LEU	CB-CG-CD1	6.14	121.44	111.00
2	B	414	ALA	CB-CA-C	6.14	119.31	110.10
1	A	439	ASN	CB-CG-OD1	6.13	133.87	121.60
1	A	677	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	912	LEU	CA-CB-CG	-6.13	101.19	115.30
1	A	1411	GLU	OE1-CD-OE2	-6.13	115.94	123.30
3	C	87	PHE	CZ-CE2-CD2	6.13	127.46	120.10
5	F	110	ASP	O-C-N	6.13	132.51	122.70
7	I	8	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	1259	MET	CB-CG-SD	-6.13	94.00	112.40
1	A	279	LEU	CA-CB-CG	6.13	129.40	115.30
9	K	15	GLY	O-C-N	-6.13	112.89	122.70
1	A	537	ARG	NH1-CZ-NH2	6.13	126.14	119.40
1	A	1275	GLY	O-C-N	6.13	132.50	122.70
4	E	123	LEU	CA-CB-CG	-6.13	101.21	115.30
8	J	25	LEU	CA-CB-CG	6.13	129.39	115.30
9	K	108	GLU	OE1-CD-OE2	-6.13	115.95	123.30
2	B	557	PHE	CB-CA-C	6.12	122.65	110.40
2	B	1009	ASP	CB-CG-OD2	-6.12	112.79	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	205	SER	CA-C-O	-6.12	107.24	120.10
3	C	11	ARG	NE-CZ-NH2	-6.12	117.24	120.30
2	B	414	ALA	N-CA-C	-6.12	94.48	111.00
3	C	183	TRP	CA-C-N	6.12	130.66	117.20
8	J	32	GLU	OE1-CD-OE2	-6.12	115.96	123.30
3	C	163	ILE	CA-CB-CG1	-6.11	99.39	111.00
4	E	172	GLU	CG-CD-OE2	6.11	130.52	118.30
5	F	79	ARG	CB-CG-CD	-6.11	95.72	111.60
1	A	396	PRO	CA-N-CD	6.11	120.25	111.70
1	A	782	ARG	CA-C-O	-6.11	107.28	120.10
1	A	947	PHE	CG-CD2-CE2	6.11	127.52	120.80
6	H	45	GLU	CG-CD-OE1	6.11	130.51	118.30
6	H	95	TYR	O-C-N	-6.11	112.93	122.70
7	I	75	CYS	N-CA-C	6.11	127.49	111.00
10	L	35	SER	N-CA-C	6.11	127.48	111.00
2	B	406	LEU	CB-CA-C	-6.10	98.61	110.20
1	A	956	LEU	CB-CG-CD1	6.10	121.37	111.00
2	B	994	TYR	CD1-CE1-CZ	6.10	125.29	119.80
3	C	34	ARG	CD-NE-CZ	6.10	132.14	123.60
10	L	70	ARG	N-CA-C	6.10	127.46	111.00
1	A	893	PHE	CD1-CE1-CZ	6.09	127.41	120.10
4	E	46	TYR	OH-CZ-CE2	6.09	136.55	120.10
5	F	116	ASP	CB-CG-OD2	6.09	123.78	118.30
7	I	94	ASP	CA-C-N	-6.09	103.79	117.20
2	B	652	LYS	CA-C-N	6.09	130.60	117.20
6	H	127	GLY	N-CA-C	6.09	128.33	113.10
4	E	168	TYR	CB-CG-CD1	-6.09	117.34	121.00
3	C	123	ASN	CB-CA-C	6.09	122.58	110.40
9	K	102	LYS	CD-CE-NZ	6.09	125.71	111.70
2	B	63	ILE	N-CA-CB	-6.09	96.80	110.80
2	B	1220	ARG	NH1-CZ-NH2	-6.09	112.70	119.40
2	B	593	PRO	CB-CG-CD	-6.08	82.78	106.50
6	H	19	ARG	NE-CZ-NH1	6.08	123.34	120.30
9	K	1	MET	CB-CA-C	-6.08	98.23	110.40
1	A	610	GLY	CA-C-N	-6.08	103.82	117.20
1	A	1199	ARG	CD-NE-CZ	-6.08	115.09	123.60
1	A	1370	LEU	CD1-CG-CD2	-6.08	92.26	110.50
2	B	96	TYR	CB-CG-CD2	-6.08	117.35	121.00
2	B	169	ARG	O-C-N	-6.08	112.97	122.70
2	B	657	HIS	C-N-CA	-6.08	106.50	121.70
2	B	408	LEU	N-CA-CB	-6.08	98.24	110.40
4	E	66	GLU	N-CA-C	-6.08	94.59	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	CYS	CA-CB-SG	6.08	124.94	114.00
2	B	989	THR	N-CA-CB	6.08	121.84	110.30
1	A	1287	TYR	CB-CG-CD2	-6.07	117.36	121.00
2	B	598	GLU	CG-CD-OE2	6.07	130.45	118.30
4	E	204	THR	N-CA-CB	-6.07	98.76	110.30
10	L	61	THR	N-CA-CB	6.07	121.84	110.30
1	A	749	ALA	N-CA-CB	-6.07	101.60	110.10
2	B	249	ARG	CD-NE-CZ	6.07	132.10	123.60
4	E	92	THR	OG1-CB-CG2	-6.07	96.04	110.00
1	A	907	THR	CB-CA-C	-6.07	95.22	111.60
1	A	177	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	889	SER	O-C-N	6.07	132.41	122.70
2	B	798	TYR	CE1-CZ-CE2	-6.07	110.09	119.80
2	B	1215	ARG	NE-CZ-NH1	6.07	123.33	120.30
4	E	148	GLU	N-CA-CB	6.07	121.52	110.60
2	B	549	THR	N-CA-CB	-6.06	98.78	110.30
9	K	33	ILE	N-CA-CB	-6.06	96.85	110.80
1	A	468	PHE	CG-CD2-CE2	6.06	127.47	120.80
2	B	934	LYS	CD-CE-NZ	-6.06	97.76	111.70
1	A	373	THR	N-CA-CB	-6.06	98.78	110.30
4	E	1	MET	CG-SD-CE	6.06	109.90	100.20
6	H	100	THR	OG1-CB-CG2	-6.06	96.06	110.00
7	I	119	THR	O-C-N	6.06	132.40	122.70
1	A	507	VAL	CG1-CB-CG2	-6.06	101.20	110.90
3	C	34	ARG	CB-CG-CD	-6.06	95.85	111.60
6	H	143	LEU	CB-CG-CD1	6.06	121.30	111.00
1	A	146	MET	CA-CB-CG	-6.06	103.00	113.30
1	A	141	LEU	CB-CG-CD2	-6.06	100.70	111.00
1	A	1385	THR	N-CA-CB	-6.05	98.80	110.30
2	B	874	PHE	N-CA-C	-6.05	94.66	111.00
1	A	591	PHE	CZ-CE2-CD2	6.05	127.36	120.10
1	A	953	ASN	O-C-N	-6.05	113.02	122.70
1	A	1325	THR	N-CA-CB	-6.05	98.81	110.30
2	B	25	ILE	CG1-CB-CG2	-6.05	98.10	111.40
1	A	130	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	A	326	ARG	CA-CB-CG	6.04	126.69	113.40
1	A	622	VAL	CA-CB-CG1	6.04	119.96	110.90
4	E	57	MET	CA-CB-CG	6.04	123.57	113.30
4	E	155	ARG	O-C-N	6.04	132.37	122.70
2	B	69	LEU	CB-CG-CD1	6.04	121.26	111.00
1	A	589	GLN	CA-C-O	-6.04	107.42	120.10
1	A	701	LEU	CB-CG-CD1	6.04	121.26	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	826	ASP	N-CA-C	-6.04	94.70	111.00
2	B	49	ASP	CB-CG-OD1	-6.03	112.87	118.30
1	A	698	GLN	CB-CA-C	-6.03	98.34	110.40
1	A	947	PHE	CE1-CZ-CE2	-6.03	109.15	120.00
1	A	925	LEU	CA-CB-CG	-6.03	101.44	115.30
1	A	1150	SER	N-CA-CB	-6.03	101.46	110.50
1	A	1315	GLU	OE1-CD-OE2	-6.03	116.07	123.30
7	I	37	GLU	N-CA-C	-6.03	94.73	111.00
2	B	133	LYS	CD-CE-NZ	-6.02	97.86	111.70
2	B	180	TYR	CE1-CZ-CE2	6.02	129.43	119.80
1	A	155	GLU	CA-CB-CG	6.02	126.64	113.40
4	E	12	LEU	CB-CA-C	6.02	121.63	110.20
2	B	131	ASP	CB-CG-OD1	-6.01	112.89	118.30
2	B	205	ILE	CG1-CB-CG2	-6.01	98.17	111.40
8	J	59	LYS	CD-CE-NZ	-6.01	97.87	111.70
1	A	825	ILE	CG1-CB-CG2	-6.01	98.18	111.40
2	B	735	ALA	O-C-N	6.01	132.32	122.70
3	C	43	THR	OG1-CB-CG2	-6.01	96.18	110.00
1	A	900	ASP	CA-C-N	-6.01	103.98	117.20
2	B	785	TYR	N-CA-CB	6.01	121.41	110.60
1	A	659	HIS	CB-CG-ND1	-6.01	108.18	123.20
1	A	839	ARG	CG-CD-NE	-6.01	99.19	111.80
1	A	548	ASN	CB-CG-ND2	-6.00	102.29	116.70
1	A	959	ASN	O-C-N	-6.00	113.10	122.70
2	B	935	ARG	CD-NE-CZ	6.00	132.01	123.60
1	A	1243	VAL	CA-CB-CG1	-6.00	101.90	110.90
1	A	886	ILE	CG1-CB-CG2	-6.00	98.20	111.40
6	H	82	PRO	N-CA-C	-6.00	96.50	112.10
2	B	951	GLN	CA-CB-CG	6.00	126.59	113.40
3	C	80	LEU	CB-CA-C	6.00	121.59	110.20
1	A	474	VAL	O-C-N	-5.99	113.11	122.70
2	B	213	ILE	CG1-CB-CG2	-5.99	98.21	111.40
3	C	180	TYR	CG-CD2-CE2	5.99	126.09	121.30
3	C	29	MET	CG-SD-CE	5.99	109.78	100.20
1	A	1352	VAL	CA-CB-CG2	5.99	119.88	110.90
4	E	40	GLU	O-C-N	5.99	132.28	122.70
8	J	49	MET	CA-CB-CG	-5.99	103.12	113.30
1	A	720	ARG	CD-NE-CZ	5.99	131.98	123.60
8	J	18	TRP	CG-CD1-NE1	5.99	116.08	110.10
1	A	477	PRO	CA-CB-CG	5.98	116.17	104.80
3	C	106	GLU	O-C-N	5.98	132.27	122.70
3	C	207	CYS	CB-CA-C	-5.98	98.44	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	17	ARG	CA-C-O	5.98	132.66	120.10
1	A	860	LEU	CB-CA-C	-5.98	98.84	110.20
2	B	709	ASP	N-CA-C	-5.98	94.85	111.00
7	I	3	THR	C-N-CA	5.98	136.65	121.70
6	H	17	PRO	N-CD-CG	-5.98	94.23	103.20
1	A	1029	ARG	NE-CZ-NH1	-5.98	117.31	120.30
4	E	131	THR	CA-CB-CG2	5.98	120.77	112.40
7	I	16	PRO	N-CD-CG	-5.97	94.24	103.20
2	B	1192	TYR	CG-CD1-CE1	5.97	126.08	121.30
3	C	263	THR	O-C-N	-5.97	113.15	122.70
6	H	20	TYR	N-CA-CB	-5.97	99.86	110.60
7	I	72	ASP	OD1-CG-OD2	-5.97	111.96	123.30
1	A	548	ASN	CB-CG-OD1	5.97	133.53	121.60
1	A	926	GLN	N-CA-CB	5.97	121.34	110.60
2	B	420	LEU	CB-CA-C	-5.97	98.86	110.20
9	K	81	TYR	CG-CD1-CE1	5.97	126.07	121.30
2	B	18	PHE	N-CA-CB	5.96	121.34	110.60
4	E	130	ALA	CB-CA-C	5.96	119.04	110.10
2	B	760	ASP	CB-CG-OD1	-5.96	112.94	118.30
2	B	789	MET	CB-CA-C	-5.96	98.48	110.40
6	H	53	ASP	C-N-CA	-5.96	106.80	121.70
1	A	456	MET	CG-SD-CE	-5.96	90.67	100.20
3	C	214	ASN	N-CA-CB	5.95	121.31	110.60
1	A	519	PRO	N-CD-CG	5.95	112.13	103.20
2	B	617	ARG	NH1-CZ-NH2	5.95	125.95	119.40
2	B	817	LEU	CB-CG-CD1	5.95	121.12	111.00
3	C	147	LEU	N-CA-CB	-5.95	98.50	110.40
4	E	17	ARG	CA-C-N	-5.95	104.11	117.20
1	A	1433	MET	N-CA-CB	5.95	121.30	110.60
3	C	68	GLY	C-N-CA	-5.95	106.84	121.70
3	C	261	ALA	N-CA-CB	5.94	118.42	110.10
1	A	207	ILE	CG1-CB-CG2	-5.94	98.33	111.40
4	E	123	LEU	CB-CG-CD2	5.94	121.10	111.00
10	L	66	GLN	N-CA-CB	-5.94	99.90	110.60
3	C	12	GLU	CB-CG-CD	-5.94	98.16	114.20
3	C	232	VAL	CG1-CB-CG2	5.94	120.40	110.90
4	E	168	TYR	CA-C-O	5.94	132.57	120.10
1	A	58	LEU	CB-CG-CD2	5.94	121.10	111.00
1	A	199	LEU	CB-CG-CD1	5.94	121.09	111.00
2	B	1052	VAL	CG1-CB-CG2	-5.94	101.40	110.90
3	C	49	VAL	CG1-CB-CG2	5.94	120.40	110.90
5	F	128	LYS	N-CA-CB	5.94	121.29	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	26	THR	CA-CB-CG2	5.94	120.71	112.40
2	B	212	LEU	CB-CG-CD1	-5.93	100.91	111.00
2	B	594	ALA	N-CA-CB	5.93	118.41	110.10
4	E	161	LYS	CA-CB-CG	5.93	126.45	113.40
1	A	1013	ASP	N-CA-CB	5.93	121.28	110.60
2	B	1103	ILE	CG1-CB-CG2	-5.93	98.35	111.40
6	H	98	TYR	CG-CD1-CE1	5.93	126.05	121.30
6	H	145	ARG	CA-C-N	-5.93	104.16	117.20
2	B	290	GLY	N-CA-C	5.93	127.92	113.10
3	C	95	CYS	CB-CA-C	5.92	122.25	110.40
1	A	393	ARG	CA-C-O	-5.92	107.67	120.10
1	A	895	LYS	N-CA-CB	5.92	121.25	110.60
2	B	660	LYS	CD-CE-NZ	5.92	125.31	111.70
2	B	806	THR	CA-CB-CG2	5.92	120.68	112.40
4	E	204	THR	CA-CB-OG1	5.92	121.43	109.00
1	A	1102	LYS	N-CA-CB	-5.92	99.95	110.60
2	B	297	ILE	CG1-CB-CG2	-5.91	98.39	111.40
6	H	87	ARG	CA-CB-CG	5.91	126.41	113.40
1	A	1430	LEU	C-N-CA	-5.91	109.89	122.30
1	A	992	ASP	N-CA-CB	-5.91	99.96	110.60
2	B	498	THR	CA-CB-OG1	5.91	121.41	109.00
2	B	781	PHE	CZ-CE2-CD2	5.91	127.19	120.10
2	B	1110	PRO	N-CD-CG	5.91	112.06	103.20
1	A	913	LEU	O-C-N	-5.91	113.25	122.70
4	E	55	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	A	922	ASP	N-CA-C	5.90	126.94	111.00
2	B	323	VAL	CG1-CB-CG2	-5.90	101.46	110.90
2	B	517	THR	N-CA-CB	5.90	121.51	110.30
2	B	586	TRP	O-C-N	-5.90	113.26	122.70
2	B	959	ASP	OD1-CG-OD2	-5.90	112.09	123.30
2	B	655	LYS	CA-C-O	5.90	132.49	120.10
2	B	1204	PHE	N-CA-CB	-5.90	99.98	110.60
3	C	147	LEU	CB-CG-CD2	5.90	121.03	111.00
2	B	753	ALA	N-CA-C	-5.90	95.08	111.00
1	A	722	LEU	CD1-CG-CD2	-5.89	92.82	110.50
2	B	369	GLY	CA-C-N	5.89	130.17	117.20
3	C	160	LYS	N-CA-CB	5.89	121.21	110.60
8	J	51	LEU	N-CA-C	5.89	126.91	111.00
1	A	843	LYS	CB-CG-CD	5.89	126.92	111.60
1	A	873	MET	CA-CB-CG	-5.89	103.28	113.30
1	A	1381	LEU	CB-CG-CD1	5.89	121.02	111.00
2	B	620	ARG	CA-CB-CG	5.89	126.36	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	536	LEU	CB-CG-CD2	5.89	121.01	111.00
1	A	547	LEU	CB-CG-CD1	5.89	121.01	111.00
1	A	586	ILE	CA-C-N	-5.89	104.25	117.20
2	B	368	GLU	CG-CD-OE1	5.89	130.08	118.30
4	E	205	SER	CA-C-N	5.89	127.98	116.20
6	H	58	THR	N-CA-CB	-5.89	99.11	110.30
6	H	115	TYR	O-C-N	-5.89	113.28	122.70
1	A	1012	ARG	CA-CB-CG	5.89	126.35	113.40
2	B	113	TYR	N-CA-CB	5.89	121.20	110.60
2	B	230	ALA	N-CA-C	5.89	126.89	111.00
4	E	197	LYS	CB-CA-C	-5.88	98.63	110.40
7	I	90	GLN	CA-C-N	5.88	130.14	117.20
1	A	894	GLU	OE1-CD-OE2	-5.88	116.24	123.30
8	J	28	ASP	CB-CA-C	-5.88	98.64	110.40
3	C	43	THR	N-CA-CB	-5.88	99.13	110.30
9	K	71	PHE	N-CA-CB	5.88	121.18	110.60
1	A	460	VAL	CG1-CB-CG2	-5.88	101.50	110.90
1	A	1267	MET	CA-CB-CG	-5.88	103.31	113.30
1	A	1445	ILE	O-C-N	5.88	132.10	122.70
2	B	31	TRP	CE3-CZ3-CH2	-5.88	114.74	121.20
2	B	1075	GLY	N-CA-C	5.88	127.79	113.10
8	J	45	CYS	O-C-N	-5.88	113.30	122.70
1	A	1005	GLU	CG-CD-OE2	-5.87	106.55	118.30
2	B	169	ARG	NH1-CZ-NH2	-5.87	112.94	119.40
2	B	204	ILE	CA-CB-CG1	5.87	122.16	111.00
2	B	1186	ASP	CB-CG-OD1	5.87	123.58	118.30
4	E	65	THR	C-N-CA	-5.87	107.02	121.70
4	E	72	PHE	CB-CG-CD1	-5.87	116.69	120.80
2	B	404	LYS	CD-CE-NZ	-5.87	98.20	111.70
3	C	20	PHE	CD1-CG-CD2	5.87	125.93	118.30
4	E	186	LEU	CB-CA-C	-5.87	99.05	110.20
5	F	119	ARG	O-C-N	5.87	132.09	122.70
4	E	190	LEU	CB-CG-CD1	-5.87	101.02	111.00
9	K	16	GLU	N-CA-CB	-5.87	100.04	110.60
1	A	475	THR	N-CA-CB	-5.87	99.15	110.30
1	A	1169	ILE	CG1-CB-CG2	-5.87	98.49	111.40
1	A	81	PHE	CB-CG-CD1	5.87	124.91	120.80
1	A	49	LYS	CD-CE-NZ	5.86	125.19	111.70
7	I	40	SER	CA-CB-OG	5.86	127.03	111.20
1	A	115	LEU	CD1-CG-CD2	-5.86	92.91	110.50
6	H	145	ARG	O-C-N	5.86	132.08	122.70
1	A	857	ARG	CB-CA-C	-5.86	98.68	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1062	GLU	CG-CD-OE1	-5.86	106.58	118.30
1	A	1368	MET	CA-CB-CG	5.86	123.26	113.30
2	B	786	ASN	N-CA-C	5.86	126.82	111.00
7	I	98	VAL	CA-CB-CG1	5.86	119.69	110.90
2	B	279	ASP	CB-CG-OD1	5.86	123.57	118.30
4	E	167	ARG	CG-CD-NE	-5.86	99.50	111.80
1	A	158	PRO	N-CA-C	5.85	127.32	112.10
2	B	388	CYS	O-C-N	-5.85	113.33	122.70
3	C	69	LEU	CD1-CG-CD2	-5.85	92.94	110.50
8	J	14	VAL	CA-CB-CG1	-5.85	102.12	110.90
1	A	159	THR	CB-CA-C	-5.85	95.80	111.60
1	A	261	ASP	CB-CG-OD1	5.85	123.56	118.30
3	C	33	LEU	CB-CA-C	5.85	121.31	110.20
3	C	192	TRP	O-C-N	-5.85	113.34	122.70
4	E	116	ILE	CG1-CB-CG2	-5.85	98.53	111.40
6	H	136	LYS	CB-CA-C	5.85	122.09	110.40
1	A	1098	VAL	CG1-CB-CG2	-5.84	101.55	110.90
4	E	28	TYR	CG-CD1-CE1	-5.84	116.62	121.30
1	A	537	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	1228	TRP	CA-CB-CG	5.84	124.80	113.70
1	A	736	ASN	C-N-CA	-5.84	107.09	121.70
3	C	105	GLY	N-CA-C	-5.84	98.50	113.10
2	B	953	LEU	CB-CG-CD1	5.84	120.93	111.00
2	B	1102	LYS	N-CA-CB	5.84	121.11	110.60
2	B	466	TRP	N-CA-CB	-5.84	100.09	110.60
1	A	110	CYS	CB-CA-C	-5.84	98.73	110.40
6	H	121	LEU	CD1-CG-CD2	-5.84	92.99	110.50
1	A	146	MET	N-CA-CB	-5.83	100.10	110.60
1	A	15	LYS	N-CA-CB	-5.83	100.10	110.60
1	A	26	GLU	OE1-CD-OE2	5.83	130.30	123.30
2	B	1151	LEU	O-C-N	-5.83	113.37	122.70
2	B	329	THR	CA-CB-CG2	-5.83	104.24	112.40
1	A	833	GLU	CG-CD-OE2	-5.83	106.64	118.30
2	B	436	VAL	CA-CB-CG1	5.83	119.64	110.90
3	C	239	PRO	CA-C-N	-5.83	104.38	117.20
2	B	807	ARG	NH1-CZ-NH2	5.83	125.81	119.40
3	C	142	VAL	N-CA-C	5.83	126.73	111.00
1	A	383	TYR	CB-CG-CD1	5.82	124.50	121.00
9	K	56	VAL	CA-C-O	5.82	132.33	120.10
1	A	521	MET	CG-SD-CE	5.82	109.52	100.20
6	H	118	PHE	CG-CD2-CE2	-5.82	114.39	120.80
1	A	123	ARG	O-C-N	5.82	132.01	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	111	LEU	CB-CG-CD1	-5.82	101.11	111.00
10	L	30	ILE	CG1-CB-CG2	-5.82	98.59	111.40
2	B	654	ARG	N-CA-CB	-5.82	100.13	110.60
2	B	686	ASN	O-C-N	5.82	132.01	122.70
4	E	103	LYS	CA-CB-CG	5.82	126.19	113.40
2	B	460	ALA	CB-CA-C	5.81	118.82	110.10
4	E	162	ARG	NE-CZ-NH1	5.81	123.21	120.30
9	K	41	THR	CA-CB-CG2	-5.81	104.26	112.40
1	A	85	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	399	HIS	CB-CA-C	-5.81	98.78	110.40
1	A	1071	SER	N-CA-CB	-5.81	101.78	110.50
2	B	1055	ILE	CA-CB-CG1	5.81	122.04	111.00
6	H	122	LEU	CB-CG-CD2	-5.81	101.12	111.00
2	B	539	LEU	CB-CG-CD1	-5.81	101.13	111.00
2	B	1041	GLU	CG-CD-OE2	-5.81	106.69	118.30
9	K	26	LYS	N-CA-CB	-5.81	100.14	110.60
2	B	254	LEU	CB-CG-CD1	5.80	120.87	111.00
9	K	79	GLU	N-CA-C	-5.80	95.33	111.00
1	A	182	VAL	O-C-N	-5.80	113.33	123.20
1	A	910	PRO	N-CD-CG	-5.80	94.50	103.20
2	B	642	ASP	N-CA-CB	5.80	121.05	110.60
3	C	39	ALA	N-CA-C	5.80	126.66	111.00
2	B	346	GLU	CA-C-O	-5.80	107.92	120.10
9	K	26	LYS	CG-CD-CE	5.80	129.30	111.90
1	A	616	VAL	O-C-N	-5.80	113.43	122.70
1	A	682	THR	CA-CB-CG2	-5.80	104.28	112.40
2	B	1172	ILE	CG1-CB-CG2	-5.80	98.65	111.40
1	A	131	SER	CB-CA-C	5.79	121.11	110.10
2	B	1082	MET	CG-SD-CE	-5.79	90.93	100.20
1	A	478	TYR	CG-CD1-CE1	5.79	125.93	121.30
2	B	461	LEU	CA-CB-CG	-5.79	101.98	115.30
4	E	150	VAL	CG1-CB-CG2	-5.79	101.63	110.90
7	I	106	CYS	C-N-CA	5.79	136.18	121.70
2	B	401	PHE	CB-CG-CD2	-5.79	116.75	120.80
2	B	613	VAL	CG1-CB-CG2	-5.79	101.64	110.90
3	C	157	CYS	CA-CB-SG	-5.79	103.58	114.00
3	C	220	ASP	CB-CG-OD2	-5.79	113.09	118.30
5	F	140	ASP	N-CA-C	5.79	126.63	111.00
7	I	18	GLU	CB-CA-C	5.79	121.97	110.40
1	A	11	LEU	CB-CG-CD1	-5.79	101.17	111.00
1	A	1234	GLU	CG-CD-OE2	-5.79	106.73	118.30
9	K	95	ILE	CG1-CB-CG2	-5.79	98.67	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	ASP	CB-CG-OD2	-5.78	113.09	118.30
1	A	1159	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	1418	LEU	CB-CG-CD2	-5.78	101.17	111.00
7	I	28	GLU	CA-CB-CG	5.78	126.12	113.40
7	I	114	GLN	CB-CA-C	5.78	121.97	110.40
5	F	99	LEU	CB-CG-CD1	-5.78	101.17	111.00
1	A	1286	LYS	CD-CE-NZ	-5.78	98.41	111.70
2	B	1012	ILE	CA-CB-CG1	5.78	121.98	111.00
2	B	136	THR	O-C-N	5.78	131.95	122.70
2	B	413	LEU	CB-CA-C	-5.78	99.22	110.20
2	B	1046	PRO	N-CD-CG	5.78	111.87	103.20
1	A	1256	GLU	N-CA-C	5.78	126.59	111.00
2	B	525	ALA	N-CA-C	5.78	126.59	111.00
1	A	853	ASP	CB-CG-OD2	5.77	123.50	118.30
2	B	882	THR	N-CA-C	5.77	126.59	111.00
9	K	88	LYS	C-N-CA	-5.77	107.27	121.70
1	A	575	LYS	CD-CE-NZ	-5.77	98.43	111.70
2	B	451	LYS	N-CA-CB	-5.77	100.22	110.60
2	B	834	ASN	CB-CG-OD1	-5.77	110.06	121.60
2	B	935	ARG	O-C-N	5.77	131.93	122.70
2	B	980	PHE	CZ-CE2-CD2	-5.77	113.18	120.10
7	I	35	VAL	CB-CA-C	-5.77	100.44	111.40
10	L	59	ALA	CB-CA-C	-5.77	101.45	110.10
2	B	617	ARG	NE-CZ-NH1	-5.77	117.42	120.30
3	C	170	TRP	CD1-NE1-CE2	-5.77	103.81	109.00
4	E	74	ASP	O-C-N	-5.77	113.47	122.70
1	A	218	ASP	CA-C-N	5.76	129.88	117.20
2	B	497	ARG	CG-CD-NE	-5.76	99.70	111.80
3	C	252	GLN	CA-CB-CG	5.76	126.08	113.40
4	E	165	LEU	CB-CG-CD1	-5.76	101.21	111.00
1	A	485	ASP	CB-CG-OD2	5.76	123.48	118.30
2	B	1162	ILE	CG1-CB-CG2	-5.76	98.73	111.40
3	C	39	ALA	CB-CA-C	-5.76	101.46	110.10
9	K	48	ALA	O-C-N	5.76	131.91	122.70
1	A	122	MET	N-CA-CB	-5.76	100.24	110.60
4	E	87	SER	CB-CA-C	5.76	121.04	110.10
1	A	1255	GLU	CG-CD-OE2	5.76	129.81	118.30
2	B	256	VAL	CG1-CB-CG2	-5.76	101.69	110.90
2	B	597	MET	N-CA-CB	-5.76	100.24	110.60
2	B	662	MET	CA-CB-CG	-5.76	103.51	113.30
1	A	1322	ILE	CG1-CB-CG2	-5.75	98.74	111.40
1	A	1443	VAL	CG1-CB-CG2	-5.75	101.69	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1135	ARG	O-C-N	-5.75	113.49	122.70
2	B	870	ILE	CA-CB-CG1	5.75	121.93	111.00
3	C	146	LYS	CD-CE-NZ	5.75	124.93	111.70
2	B	1190	ASP	CB-CG-OD2	5.75	123.48	118.30
3	C	35	ARG	CG-CD-NE	-5.75	99.72	111.80
8	J	1	MET	N-CA-CB	-5.75	100.25	110.60
1	A	566	ILE	CA-C-N	-5.75	104.55	117.20
1	A	709	THR	OG1-CB-CG2	-5.75	96.78	110.00
7	I	55	THR	CA-CB-CG2	5.75	120.45	112.40
2	B	66	ASP	CB-CG-OD2	5.75	123.47	118.30
2	B	323	VAL	O-C-N	-5.75	113.51	122.70
8	J	6	ARG	NH1-CZ-NH2	5.74	125.72	119.40
1	A	98	LYS	O-C-N	5.74	131.88	122.70
1	A	489	LEU	CB-CG-CD2	5.74	120.76	111.00
1	A	1238	ILE	CA-CB-CG1	5.74	121.90	111.00
10	L	50	ASP	N-CA-CB	5.74	120.93	110.60
10	L	64	LEU	CB-CG-CD1	5.74	120.75	111.00
1	A	1106	ASN	N-CA-C	5.73	126.48	111.00
4	E	1	MET	C-N-CA	5.73	136.03	121.70
1	A	430	TRP	CE3-CZ3-CH2	5.73	127.51	121.20
2	B	434	ARG	NE-CZ-NH2	-5.73	117.43	120.30
10	L	43	THR	CA-CB-CG2	5.73	120.43	112.40
1	A	109	HIS	CB-CA-C	5.73	121.86	110.40
1	A	505	CYS	CA-CB-SG	5.73	124.31	114.00
3	C	252	GLN	CB-CA-C	5.73	121.86	110.40
1	A	840	ARG	CA-C-O	-5.73	108.07	120.10
1	A	879	GLU	CG-CD-OE2	-5.73	106.85	118.30
3	C	36	VAL	CG1-CB-CG2	-5.73	101.74	110.90
7	I	21	GLU	OE1-CD-OE2	5.73	130.17	123.30
1	A	923	LEU	CB-CA-C	-5.73	99.32	110.20
8	J	47	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	57	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	542	GLU	OE1-CD-OE2	5.72	130.17	123.30
2	B	638	PHE	CD1-CE1-CZ	-5.72	113.23	120.10
2	B	845	SER	C-N-CA	-5.72	107.39	121.70
1	A	601	LYS	N-CA-CB	-5.72	100.31	110.60
1	A	796	SER	O-C-N	-5.72	113.55	122.70
1	A	905	ASP	N-CA-CB	-5.72	100.31	110.60
1	A	932	GLU	CA-CB-CG	5.72	125.98	113.40
2	B	1042	GLY	CA-C-O	-5.72	110.30	120.60
3	C	42	PRO	N-CA-CB	-5.72	96.31	102.60
2	B	320	ASP	OD1-CG-OD2	-5.72	112.44	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	47	ASP	CB-CG-OD2	5.72	123.45	118.30
3	C	170	TRP	C-N-CA	-5.72	110.29	122.30
1	A	1172	LEU	CA-C-O	-5.72	108.09	120.10
2	B	936	ASP	OD1-CG-OD2	-5.72	112.44	123.30
2	B	1219	ASP	OD1-CG-OD2	-5.71	112.44	123.30
2	B	531	GLN	CA-C-O	-5.71	108.10	120.10
1	A	901	LEU	CA-C-N	-5.71	104.63	117.20
1	A	1000	LEU	CD1-CG-CD2	-5.71	93.36	110.50
3	C	215	GLU	CB-CA-C	-5.71	98.98	110.40
2	B	701	ILE	N-CA-C	5.71	126.42	111.00
1	A	95	PHE	CZ-CE2-CD2	5.71	126.95	120.10
3	C	205	LYS	O-C-N	5.71	131.83	122.70
1	A	789	LYS	N-CA-CB	-5.71	100.33	110.60
4	E	192	ARG	CG-CD-NE	-5.71	99.82	111.80
10	L	69	ALA	CB-CA-C	-5.71	101.54	110.10
1	A	27	VAL	N-CA-C	5.70	126.40	111.00
1	A	636	GLU	CG-CD-OE2	5.70	129.71	118.30
5	F	72	LYS	C-N-CA	5.70	135.96	121.70
5	F	73	ALA	N-CA-C	5.70	126.40	111.00
1	A	1239	ARG	CG-CD-NE	-5.70	99.83	111.80
2	B	994	TYR	CG-CD2-CE2	-5.70	116.74	121.30
1	A	683	ILE	CG1-CB-CG2	-5.70	98.86	111.40
2	B	239	GLU	N-CA-CB	-5.70	100.34	110.60
5	F	108	PHE	CB-CG-CD2	-5.70	116.81	120.80
1	A	16	GLU	OE1-CD-OE2	5.70	130.13	123.30
1	A	595	THR	CA-CB-CG2	-5.70	104.43	112.40
10	L	70	ARG	CG-CD-NE	5.69	123.76	111.80
1	A	469	ARG	CA-CB-CG	5.69	125.92	113.40
2	B	698	GLU	OE1-CD-OE2	-5.69	116.47	123.30
6	H	118	PHE	CB-CG-CD1	-5.69	116.82	120.80
2	B	968	VAL	CA-CB-CG2	-5.69	102.36	110.90
2	B	1137	CYS	O-C-N	-5.69	113.60	122.70
1	A	566	ILE	CB-CA-C	-5.69	100.22	111.60
1	A	1209	MET	CB-CA-C	-5.69	99.02	110.40
1	A	61	ILE	N-CA-CB	5.69	123.88	110.80
2	B	171	PRO	CA-N-CD	5.69	119.66	111.70
2	B	987	LYS	CB-CG-CD	-5.69	96.81	111.60
1	A	964	ILE	CG1-CB-CG2	5.69	123.91	111.40
1	A	364	VAL	CA-CB-CG2	5.68	119.42	110.90
1	A	1239	ARG	CD-NE-CZ	-5.68	115.64	123.60
2	B	959	ASP	CB-CG-OD2	5.68	123.42	118.30
2	B	1005	GLY	N-CA-C	5.68	127.31	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1186	ASP	CB-CG-OD2	5.68	123.41	118.30
7	I	70	ARG	N-CA-CB	-5.68	100.37	110.60
7	I	118	ARG	N-CA-C	5.68	126.34	111.00
8	J	39	LEU	N-CA-CB	5.68	121.77	110.40
1	A	12	ARG	O-C-N	-5.68	113.61	122.70
3	C	85	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	1113	THR	OG1-CB-CG2	-5.68	96.94	110.00
2	B	994	TYR	CE1-CZ-CE2	-5.68	110.71	119.80
2	B	639	ILE	CG1-CB-CG2	-5.68	98.91	111.40
3	C	58	LEU	CB-CG-CD2	-5.68	101.35	111.00
1	A	18	GLN	O-C-N	5.68	131.78	122.70
1	A	465	TYR	CA-C-N	5.68	129.69	117.20
1	A	1045	VAL	CA-CB-CG1	-5.68	102.38	110.90
2	B	181	LEU	CB-CG-CD1	5.68	120.65	111.00
3	C	86	CYS	N-CA-CB	5.68	120.82	110.60
8	J	47	ARG	NE-CZ-NH2	-5.68	117.46	120.30
9	K	71	PHE	CB-CG-CD2	5.68	124.77	120.80
1	A	213	HIS	N-CA-C	5.67	126.32	111.00
2	B	135	ARG	NE-CZ-NH1	5.67	123.14	120.30
2	B	536	VAL	O-C-N	5.67	131.78	122.70
2	B	775	LYS	CB-CG-CD	-5.67	96.84	111.60
7	I	5	ARG	CB-CG-CD	5.67	126.36	111.60
1	A	496	GLU	CG-CD-OE1	5.67	129.65	118.30
2	B	904	ARG	CG-CD-NE	-5.67	99.89	111.80
1	A	914	GLU	CG-CD-OE2	-5.67	106.96	118.30
2	B	842	ASN	N-CA-C	-5.67	95.69	111.00
2	B	1002	THR	O-C-N	-5.67	113.63	122.70
1	A	293	GLU	N-CA-CB	5.67	120.80	110.60
1	A	635	ARG	CA-CB-CG	5.67	125.87	113.40
1	A	1020	CYS	CA-CB-SG	5.67	124.20	114.00
9	K	85	ASP	OD1-CG-OD2	-5.67	112.53	123.30
1	A	1103	GLU	N-CA-CB	-5.67	100.40	110.60
1	A	1259	MET	N-CA-C	-5.67	95.70	111.00
1	A	493	GLN	CB-CG-CD	5.66	126.32	111.60
2	B	488	TYR	CB-CG-CD1	5.66	124.40	121.00
6	H	146	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	1234	GLU	CA-CB-CG	5.66	125.85	113.40
1	A	1349	TYR	CG-CD1-CE1	5.66	125.83	121.30
10	L	42	ARG	NH1-CZ-NH2	-5.66	113.17	119.40
1	A	1006	ILE	CA-CB-CG1	5.66	121.75	111.00
1	A	179	LEU	CB-CA-C	-5.66	99.46	110.20
1	A	85	ASP	N-CA-C	-5.65	95.73	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	533	CYS	C-N-CA	-5.65	110.43	122.30
4	E	155	ARG	N-CA-CB	-5.65	100.42	110.60
1	A	261	ASP	CB-CG-OD2	5.65	123.39	118.30
7	I	8	ARG	CA-CB-CG	5.65	125.83	113.40
2	B	1175	LEU	CA-CB-CG	5.65	128.29	115.30
1	A	813	PHE	CB-CG-CD1	5.65	124.75	120.80
2	B	89	GLU	CA-CB-CG	5.65	125.83	113.40
2	B	131	ASP	O-C-N	5.65	131.74	122.70
2	B	910	VAL	CA-CB-CG2	-5.65	102.43	110.90
3	C	246	ARG	NH1-CZ-NH2	-5.65	113.19	119.40
1	A	476	SER	CA-CB-OG	-5.64	95.96	111.20
1	A	1277	GLU	N-CA-CB	5.64	120.76	110.60
7	I	80	SER	N-CA-C	5.64	126.24	111.00
2	B	1098	MET	CG-SD-CE	5.64	109.22	100.20
2	B	679	TYR	CG-CD2-CE2	-5.64	116.79	121.30
3	C	210	GLU	OE1-CD-OE2	5.64	130.07	123.30
1	A	1029	ARG	CB-CG-CD	5.64	126.26	111.60
4	E	100	ILE	CB-CA-C	-5.64	100.33	111.60
6	H	27	GLU	N-CA-CB	5.64	120.75	110.60
1	A	393	ARG	O-C-N	5.63	131.72	122.70
4	E	187	TYR	CE1-CZ-CE2	-5.63	110.79	119.80
6	H	145	ARG	NE-CZ-NH2	-5.63	117.48	120.30
3	C	127	ARG	NH1-CZ-NH2	-5.63	113.20	119.40
7	I	3	THR	CA-CB-CG2	-5.63	104.51	112.40
1	A	1046	LEU	CA-C-O	5.63	131.93	120.10
3	C	114	TYR	CG-CD2-CE2	5.63	125.80	121.30
7	I	92	ARG	CA-CB-CG	5.63	125.78	113.40
2	B	624	LEU	CB-CA-C	-5.63	99.51	110.20
1	A	1383	SER	CA-CB-OG	-5.62	96.01	111.20
2	B	446	LEU	C-N-CA	5.62	135.76	121.70
1	A	691	LEU	CB-CG-CD2	-5.62	101.44	111.00
1	A	1017	LEU	C-N-CA	-5.62	107.64	121.70
2	B	436	VAL	CB-CA-C	5.62	122.08	111.40
1	A	751	SER	N-CA-CB	-5.62	102.07	110.50
1	A	154	SER	CB-CA-C	5.62	120.78	110.10
2	B	42	GLY	N-CA-C	5.62	127.14	113.10
2	B	983	ARG	N-CA-CB	-5.62	100.49	110.60
4	E	48	ASP	OD1-CG-OD2	-5.62	112.62	123.30
4	E	106	GLN	CB-CA-C	5.62	121.64	110.40
5	F	138	LEU	CD1-CG-CD2	-5.62	93.64	110.50
8	J	36	LEU	CB-CG-CD2	-5.62	101.45	111.00
4	E	137	GLU	O-C-N	-5.62	113.71	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	773	MET	CG-SD-CE	5.62	109.19	100.20
1	A	922	ASP	OD1-CG-OD2	-5.61	112.63	123.30
9	K	85	ASP	N-CA-CB	5.61	120.70	110.60
10	L	47	ARG	NH1-CZ-NH2	-5.61	113.22	119.40
1	A	994	GLN	O-C-N	-5.61	113.72	122.70
2	B	891	ASP	CB-CG-OD2	5.61	123.35	118.30
2	B	997	GLU	CA-CB-CG	-5.61	101.05	113.40
1	A	326	ARG	NE-CZ-NH1	5.61	123.11	120.30
2	B	23	ALA	CB-CA-C	-5.61	101.68	110.10
2	B	947	GLY	CA-C-O	-5.61	110.50	120.60
2	B	981	ALA	N-CA-C	5.61	126.15	111.00
4	E	168	TYR	CA-C-N	-5.61	104.86	117.20
1	A	371	ALA	CB-CA-C	-5.61	101.69	110.10
1	A	714	PHE	CD1-CE1-CZ	-5.61	113.37	120.10
1	A	999	VAL	CA-CB-CG1	-5.61	102.49	110.90
4	E	49	SER	N-CA-C	5.61	126.14	111.00
4	E	123	LEU	CB-CG-CD1	-5.61	101.47	111.00
1	A	592	ASP	CB-CG-OD1	5.61	123.34	118.30
1	A	1257	ASP	CB-CA-C	-5.61	99.19	110.40
1	A	280	GLU	CA-CB-CG	5.60	125.72	113.40
3	C	230	MET	N-CA-CB	-5.60	100.52	110.60
1	A	561	PRO	CB-CG-CD	-5.60	84.67	106.50
2	B	367	LEU	CA-CB-CG	5.60	128.18	115.30
4	E	197	LYS	N-CA-C	-5.60	95.89	111.00
6	H	37	LYS	CD-CE-NZ	5.60	124.57	111.70
2	B	217	ARG	CB-CG-CD	5.60	126.15	111.60
1	A	794	PRO	N-CD-CG	-5.59	94.81	103.20
2	B	743	ILE	CA-CB-CG1	5.59	121.63	111.00
2	B	224	GLN	CA-CB-CG	-5.59	101.10	113.40
2	B	423	LYS	CD-CE-NZ	-5.59	98.84	111.70
2	B	1053	GLU	N-CA-CB	5.59	120.67	110.60
1	A	605	MET	CA-CB-CG	5.59	122.81	113.30
7	I	17	ARG	CB-CG-CD	5.59	126.14	111.60
1	A	1436	ILE	CG1-CB-CG2	-5.59	99.11	111.40
2	B	655	LYS	CD-CE-NZ	5.59	124.55	111.70
1	A	104	GLU	OE1-CD-OE2	-5.59	116.60	123.30
1	A	1289	ARG	N-CA-C	-5.59	95.91	111.00
3	C	201	TRP	CE3-CZ3-CH2	-5.59	115.06	121.20
4	E	79	TRP	CA-C-N	5.59	129.49	117.20
6	H	146	ARG	CD-NE-CZ	5.59	131.42	123.60
9	K	110	ASN	N-CA-C	-5.59	95.92	111.00
1	A	915	SER	C-N-CA	-5.58	110.57	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	553	VAL	CA-CB-CG2	5.58	119.27	110.90
1	A	1029	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	1238	ILE	CA-CB-CG2	-5.58	99.74	110.90
2	B	1206	GLU	CG-CD-OE1	5.58	129.46	118.30
8	J	38	ARG	N-CA-C	-5.58	95.93	111.00
4	E	158	SER	CB-CA-C	5.58	120.70	110.10
1	A	1204	ASP	OD1-CG-OD2	-5.58	112.70	123.30
2	B	198	ASP	OD1-CG-OD2	-5.58	112.70	123.30
2	B	457	LEU	CB-CG-CD2	5.58	120.48	111.00
2	B	1154	ALA	N-CA-CB	5.58	117.91	110.10
5	F	120	ILE	CA-CB-CG1	5.58	121.60	111.00
8	J	50	ILE	CB-CA-C	5.58	122.76	111.60
1	A	230	ARG	CG-CD-NE	-5.58	100.09	111.80
2	B	962	LYS	CD-CE-NZ	5.58	124.53	111.70
1	A	596	THR	CA-CB-OG1	5.58	120.71	109.00
1	A	739	ASP	CB-CG-OD1	5.58	123.32	118.30
2	B	608	ASP	N-CA-C	-5.58	95.94	111.00
6	H	26	ILE	O-C-N	5.58	131.62	122.70
1	A	1208	THR	CB-CA-C	-5.57	96.55	111.60
2	B	328	GLU	CA-CB-CG	-5.57	101.14	113.40
2	B	1085	ILE	CG1-CB-CG2	-5.57	99.14	111.40
6	H	2	SER	CB-CA-C	5.57	120.69	110.10
5	F	75	PRO	N-CA-C	5.57	126.59	112.10
1	A	121	LEU	CA-CB-CG	5.57	128.11	115.30
1	A	1374	VAL	CA-CB-CG2	-5.57	102.54	110.90
1	A	305	ASP	N-CA-C	5.57	126.04	111.00
1	A	837	ILE	CA-CB-CG1	-5.57	100.42	111.00
9	K	12	LEU	CB-CG-CD1	5.57	120.47	111.00
1	A	1196	GLU	CA-CB-CG	-5.57	101.15	113.40
1	A	1442	ASP	CB-CA-C	-5.57	99.27	110.40
9	K	11	LEU	CB-CA-C	-5.57	99.62	110.20
1	A	1406	VAL	CG1-CB-CG2	5.57	119.81	110.90
3	C	168	ALA	N-CA-CB	-5.57	102.31	110.10
4	E	75	MET	CA-CB-CG	5.57	122.76	113.30
2	B	446	LEU	CB-CG-CD1	5.56	120.46	111.00
9	K	18	LYS	N-CA-CB	5.56	120.62	110.60
1	A	509	LEU	CB-CG-CD2	5.56	120.46	111.00
1	A	656	TRP	CE3-CZ3-CH2	5.56	127.32	121.20
2	B	364	ILE	CA-C-N	5.56	129.44	117.20
2	B	597	MET	CB-CA-C	5.56	121.52	110.40
4	E	215	MET	N-CA-C	5.56	126.01	111.00
1	A	1004	ASN	N-CA-C	5.56	126.01	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	515	HIS	CB-CA-C	-5.56	99.28	110.40
1	A	578	LEU	CB-CG-CD1	-5.56	101.55	111.00
1	A	44	THR	N-CA-CB	5.55	120.85	110.30
1	A	777	PHE	CD1-CG-CD2	-5.55	111.08	118.30
3	C	106	GLU	OE1-CD-OE2	5.55	129.97	123.30
3	C	221	TYR	N-CA-C	5.55	126.00	111.00
8	J	29	GLU	CG-CD-OE1	-5.55	107.19	118.30
3	C	108	GLU	CA-C-N	-5.55	104.98	117.20
1	A	672	ASP	CB-CA-C	-5.55	99.30	110.40
4	E	38	PRO	O-C-N	5.55	131.58	122.70
1	A	353	ILE	CB-CA-C	-5.55	100.50	111.60
1	A	709	THR	CA-CB-CG2	5.55	120.17	112.40
8	J	52	THR	CA-CB-CG2	-5.55	104.63	112.40
2	B	1073	TYR	OH-CZ-CE2	5.55	135.07	120.10
7	I	6	PHE	C-N-CA	5.54	135.56	121.70
1	A	1317	MET	CB-CA-C	5.54	121.49	110.40
3	C	263	THR	CA-CB-CG2	5.54	120.16	112.40
2	B	1020	ARG	CG-CD-NE	-5.54	100.17	111.80
1	A	999	VAL	N-CA-CB	-5.54	99.31	111.50
2	B	453	ILE	N-CA-C	-5.54	96.05	111.00
2	B	1197	PRO	CA-C-O	5.54	133.49	120.20
4	E	98	ILE	CB-CA-C	5.54	122.67	111.60
2	B	378	LEU	CB-CG-CD1	-5.53	101.59	111.00
5	F	82	THR	CB-CA-C	-5.53	96.66	111.60
5	F	154	ASP	CB-CA-C	5.53	121.47	110.40
9	K	46	ILE	O-C-N	-5.53	113.84	122.70
2	B	412	LEU	N-CA-C	-5.53	96.07	111.00
4	E	167	ARG	NE-CZ-NH2	5.53	123.06	120.30
7	I	44	TYR	CZ-CE2-CD2	-5.53	114.82	119.80
1	A	416	ARG	NH1-CZ-NH2	-5.53	113.32	119.40
1	A	708	MET	N-CA-C	-5.53	96.07	111.00
1	A	497	THR	CA-CB-CG2	-5.53	104.66	112.40
6	H	93	TYR	OH-CZ-CE2	-5.53	105.18	120.10
1	A	1407	GLU	CA-CB-CG	5.52	125.55	113.40
2	B	537	LYS	CB-CG-CD	5.52	125.96	111.60
1	A	1268	LEU	CB-CG-CD2	5.52	120.39	111.00
2	B	523	CYS	CB-CA-C	-5.52	99.35	110.40
2	B	642	ASP	C-N-CA	-5.52	107.89	121.70
1	A	792	TYR	OH-CZ-CE2	-5.52	105.19	120.10
1	A	368	LYS	O-C-N	-5.52	113.87	122.70
1	A	858	ASN	CB-CG-OD1	-5.52	110.56	121.60
2	B	986	GLN	CA-CB-CG	-5.52	101.26	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	68	GLU	CB-CG-CD	5.52	129.10	114.20
1	A	850	VAL	CG1-CB-CG2	-5.52	102.07	110.90
2	B	39	ARG	NE-CZ-NH1	5.52	123.06	120.30
2	B	351	TYR	CG-CD1-CE1	5.52	125.71	121.30
2	B	723	VAL	N-CA-CB	5.52	123.64	111.50
1	A	66	LYS	CA-CB-CG	5.51	125.53	113.40
2	B	841	MET	CG-SD-CE	5.51	109.02	100.20
1	A	644	LYS	CB-CA-C	-5.51	99.37	110.40
1	A	755	PHE	CD1-CE1-CZ	5.51	126.72	120.10
2	B	265	SER	CB-CA-C	5.51	120.57	110.10
6	H	57	VAL	O-C-N	-5.51	113.88	122.70
2	B	1010	LEU	CB-CA-C	-5.51	99.73	110.20
1	A	630	ILE	CG1-CB-CG2	-5.51	99.28	111.40
3	C	209	TYR	CD1-CE1-CZ	5.51	124.76	119.80
2	B	796	LEU	CB-CG-CD1	-5.51	101.64	111.00
1	A	1260	LEU	O-C-N	-5.50	113.89	122.70
2	B	33	VAL	CG1-CB-CG2	-5.50	102.09	110.90
2	B	763	GLN	CB-CA-C	-5.50	99.39	110.40
1	A	992	ASP	OD1-CG-OD2	-5.50	112.84	123.30
2	B	197	PHE	CB-CG-CD2	5.50	124.65	120.80
2	B	692	TYR	CG-CD2-CE2	5.50	125.70	121.30
4	E	141	VAL	CA-CB-CG1	5.50	119.16	110.90
10	L	62	LYS	CD-CE-NZ	5.50	124.36	111.70
1	A	938	LYS	CG-CD-CE	-5.50	95.40	111.90
1	A	962	ARG	O-C-N	-5.50	113.90	122.70
2	B	615	MET	CA-CB-CG	5.50	122.65	113.30
1	A	1077	THR	CA-C-N	5.50	129.30	117.20
2	B	612	GLU	CB-CG-CD	5.50	129.04	114.20
4	E	160	GLU	OE1-CD-OE2	-5.50	116.70	123.30
5	F	154	ASP	CB-CG-OD2	-5.50	113.35	118.30
6	H	77	ARG	CA-CB-CG	5.50	125.50	113.40
1	A	96	ILE	CA-CB-CG1	5.50	121.44	111.00
1	A	777	PHE	CG-CD2-CE2	5.50	126.85	120.80
2	B	654	ARG	CB-CA-C	-5.50	99.41	110.40
3	C	140	ASN	CB-CA-C	5.50	121.39	110.40
2	B	415	GLN	N-CA-CB	5.49	120.49	110.60
2	B	634	TYR	CZ-CE2-CD2	5.49	124.75	119.80
2	B	879	ARG	O-C-N	5.49	131.49	122.70
2	B	210	LYS	CB-CG-CD	5.49	125.88	111.60
2	B	434	ARG	CB-CA-C	5.49	121.38	110.40
2	B	513	GLN	O-C-N	5.49	131.49	122.70
4	E	181	ALA	N-CA-C	5.49	125.83	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	SER	N-CA-CB	-5.49	102.27	110.50
1	A	708	MET	N-CA-CB	-5.49	100.72	110.60
3	C	183	TRP	NE1-CE2-CZ2	-5.49	124.36	130.40
9	K	88	LYS	N-CA-C	-5.49	96.18	111.00
2	B	367	LEU	CB-CA-C	5.49	120.63	110.20
1	A	225	ASN	O-C-N	5.49	131.48	122.70
1	A	873	MET	CB-CG-SD	5.49	128.86	112.40
2	B	317	CYS	N-CA-CB	5.49	120.47	110.60
2	B	1073	TYR	CE1-CZ-CE2	-5.49	111.02	119.80
6	H	99	GLY	O-C-N	5.48	131.47	122.70
1	A	1021	LEU	CA-C-O	5.48	131.61	120.10
1	A	1295	THR	OG1-CB-CG2	-5.48	97.39	110.00
4	E	192	ARG	CB-CG-CD	5.48	125.86	111.60
1	A	601	LYS	CD-CE-NZ	-5.48	99.10	111.70
3	C	60	ASP	CB-CG-OD1	5.48	123.23	118.30
4	E	61	GLN	N-CA-C	-5.48	96.20	111.00
5	F	77	ASP	C-N-CA	-5.48	108.00	121.70
2	B	879	ARG	N-CA-CB	5.48	120.46	110.60
1	A	285	PRO	O-C-N	5.48	131.46	122.70
8	J	28	ASP	N-CA-CB	5.48	120.46	110.60
1	A	382	PRO	CA-C-O	-5.48	107.06	120.20
2	B	1183	LYS	CA-CB-CG	5.48	125.45	113.40
10	L	42	ARG	N-CA-CB	5.48	120.46	110.60
1	A	357	PRO	N-CD-CG	5.47	111.41	103.20
1	A	671	ALA	CB-CA-C	-5.47	101.89	110.10
2	B	274	PRO	CA-N-CD	-5.47	103.84	111.50
2	B	1186	ASP	OD1-CG-OD2	-5.47	112.90	123.30
4	E	20	LYS	N-CA-CB	-5.47	100.75	110.60
1	A	189	ARG	NE-CZ-NH2	5.47	123.04	120.30
2	B	943	SER	O-C-N	-5.47	113.94	122.70
1	A	853	ASP	CB-CG-OD1	-5.47	113.38	118.30
1	A	174	ILE	CA-CB-CG1	5.47	121.39	111.00
1	A	465	TYR	O-C-N	-5.47	113.95	122.70
2	B	967	ARG	CB-CA-C	-5.47	99.46	110.40
1	A	1058	VAL	CG1-CB-CG2	5.47	119.65	110.90
3	C	93	ASP	N-CA-CB	-5.47	100.76	110.60
1	A	866	PHE	N-CA-CB	-5.47	100.76	110.60
1	A	900	ASP	CB-CA-C	-5.47	99.47	110.40
2	B	1155	SER	CA-CB-OG	5.47	125.96	111.20
3	C	50	GLU	N-CA-C	-5.47	96.24	111.00
4	E	210	SER	N-CA-CB	-5.47	102.30	110.50
1	A	686	ALA	N-CA-CB	5.46	117.75	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	396	ASP	O-C-N	5.46	131.44	122.70
1	A	400	PRO	CB-CA-C	5.46	125.65	112.00
1	A	1424	VAL	CG1-CB-CG2	5.46	119.64	110.90
6	H	9	ILE	CG1-CB-CG2	-5.46	99.39	111.40
7	I	84	VAL	CB-CA-C	5.46	121.78	111.40
1	A	552	TRP	CB-CG-CD2	5.46	133.69	126.60
1	A	870	GLU	N-CA-CB	5.46	120.42	110.60
2	B	231	PRO	CB-CG-CD	-5.46	85.21	106.50
2	B	275	TYR	CD1-CE1-CZ	5.46	124.71	119.80
2	B	961	LEU	CB-CG-CD1	5.46	120.28	111.00
2	B	1211	ASN	CB-CA-C	-5.46	99.48	110.40
5	F	82	THR	CA-CB-CG2	5.46	120.04	112.40
9	K	101	LEU	N-CA-CB	-5.46	99.48	110.40
10	L	54	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	A	502	SER	O-C-N	-5.46	113.97	122.70
2	B	598	GLU	CB-CG-CD	5.46	128.93	114.20
1	A	86	LEU	N-CA-CB	5.45	121.31	110.40
1	A	1298	TYR	CG-CD1-CE1	-5.45	116.94	121.30
2	B	1103	ILE	N-CA-CB	5.45	123.34	110.80
1	A	740	LEU	CB-CG-CD1	5.45	120.27	111.00
2	B	613	VAL	CA-CB-CG2	5.45	119.08	110.90
2	B	969	ARG	CB-CA-C	-5.45	99.50	110.40
9	K	75	ILE	CA-CB-CG1	5.45	121.36	111.00
1	A	88	LYS	CG-CD-CE	-5.45	95.55	111.90
1	A	349	ALA	CB-CA-C	-5.45	101.93	110.10
2	B	1020	ARG	CA-CB-CG	5.45	125.39	113.40
3	C	136	ASP	OD1-CG-OD2	-5.45	112.95	123.30
3	C	232	VAL	C-N-CA	-5.45	108.08	121.70
5	F	143	PHE	N-CA-C	5.45	125.71	111.00
2	B	351	TYR	CB-CG-CD1	5.45	124.27	121.00
2	B	1047	PHE	N-CA-C	5.45	125.70	111.00
2	B	1198	TYR	CE1-CZ-CE2	-5.45	111.09	119.80
9	K	32	VAL	CA-CB-CG2	-5.45	102.73	110.90
9	K	93	SER	CB-CA-C	-5.45	99.75	110.10
2	B	1020	ARG	NE-CZ-NH1	-5.44	117.58	120.30
2	B	1223	ASP	C-N-CA	5.44	135.31	121.70
1	A	771	GLU	CG-CD-OE1	-5.44	107.42	118.30
1	A	1116	LEU	O-C-N	-5.44	113.99	122.70
2	B	65	GLU	CB-CA-C	5.44	121.28	110.40
1	A	376	TYR	CB-CA-C	-5.44	99.52	110.40
1	A	1021	LEU	O-C-N	-5.44	114.00	122.70
1	A	1449	SER	CB-CA-C	5.44	120.43	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1159	ARG	NE-CZ-NH1	5.44	123.02	120.30
4	E	186	LEU	CB-CG-CD2	-5.44	101.76	111.00
9	K	37	LYS	CD-CE-NZ	5.44	124.21	111.70
1	A	411	ASP	O-C-N	5.44	131.40	122.70
2	B	633	VAL	CB-CA-C	-5.44	101.07	111.40
1	A	1060	PRO	O-C-N	5.43	132.44	123.20
1	A	1450	LEU	CB-CG-CD2	5.43	120.24	111.00
1	A	831	THR	C-N-CA	-5.43	108.12	121.70
1	A	1135	ARG	CG-CD-NE	-5.43	100.39	111.80
3	C	249	ASP	CB-CA-C	5.43	121.26	110.40
8	J	10	CYS	CB-CA-C	5.43	121.26	110.40
1	A	931	GLU	OE1-CD-OE2	-5.43	116.78	123.30
4	E	192	ARG	CD-NE-CZ	5.43	131.20	123.60
6	H	41	ASP	OD1-CG-OD2	-5.43	112.98	123.30
7	I	44	TYR	CA-CB-CG	5.43	123.72	113.40
2	B	990	ILE	CG1-CB-CG2	-5.43	99.46	111.40
10	L	48	CYS	CA-CB-SG	5.43	123.77	114.00
1	A	1028	THR	OG1-CB-CG2	-5.42	97.53	110.00
1	A	1296	GLY	N-CA-C	5.42	126.66	113.10
1	A	1325	THR	CA-CB-CG2	5.42	119.99	112.40
2	B	888	GLY	CA-C-O	-5.42	110.83	120.60
3	C	54	ASN	CA-C-N	-5.42	105.27	117.20
6	H	128	ASN	N-CA-C	5.42	125.64	111.00
2	B	616	ILE	C-N-CA	-5.42	108.14	121.70
9	K	79	GLU	CA-CB-CG	5.42	125.33	113.40
1	A	830	LYS	CD-CE-NZ	5.42	124.17	111.70
2	B	206	ASN	N-CA-CB	5.42	120.36	110.60
2	B	1150	ARG	CB-CA-C	-5.42	99.56	110.40
4	E	79	TRP	CA-CB-CG	-5.42	103.40	113.70
1	A	649	ILE	CG1-CB-CG2	-5.42	99.48	111.40
1	A	1168	GLU	CA-CB-CG	5.42	125.32	113.40
2	B	463	THR	OG1-CB-CG2	-5.42	97.54	110.00
2	B	798	TYR	CB-CG-CD2	5.42	124.25	121.00
2	B	855	PHE	CA-C-O	-5.42	108.73	120.10
2	B	1192	TYR	OH-CZ-CE2	5.42	134.72	120.10
10	L	63	ARG	NH1-CZ-NH2	-5.42	113.44	119.40
1	A	373	THR	OG1-CB-CG2	-5.42	97.55	110.00
1	A	1042	PHE	CD1-CE1-CZ	-5.42	113.60	120.10
2	B	137	TYR	N-CA-CB	5.42	120.35	110.60
7	I	24	ARG	N-CA-CB	5.42	120.35	110.60
1	A	380	VAL	CG1-CB-CG2	-5.41	102.24	110.90
1	A	468	PHE	N-CA-C	-5.41	96.38	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	827	THR	O-C-N	-5.41	114.04	122.70
1	A	1013	ASP	CA-C-N	5.41	129.11	117.20
2	B	165	VAL	N-CA-CB	5.41	123.41	111.50
2	B	294	ASP	OD1-CG-OD2	-5.41	113.01	123.30
2	B	890	TYR	CB-CG-CD2	-5.41	117.75	121.00
6	H	121	LEU	N-CA-CB	-5.41	99.58	110.40
9	K	110	ASN	N-CA-CB	5.41	120.34	110.60
1	A	1283	VAL	N-CA-CB	-5.41	99.60	111.50
2	B	90	ILE	N-CA-C	5.41	125.61	111.00
2	B	1104	HIS	N-CA-C	-5.41	96.39	111.00
1	A	527	THR	N-CA-CB	-5.41	100.02	110.30
1	A	655	PHE	C-N-CA	-5.41	108.18	121.70
6	H	37	LYS	CA-C-N	-5.41	105.30	117.20
9	K	11	LEU	CA-CB-CG	5.41	127.74	115.30
1	A	836	TYR	CG-CD1-CE1	-5.41	116.97	121.30
1	A	1043	ASP	CB-CA-C	-5.41	99.59	110.40
2	B	124	TYR	CZ-CE2-CD2	5.41	124.67	119.80
6	H	93	TYR	CD1-CE1-CZ	-5.41	114.93	119.80
8	J	56	LEU	CD1-CG-CD2	-5.41	94.28	110.50
2	B	741	CYS	CA-CB-SG	5.41	123.73	114.00
10	L	40	LEU	CA-C-O	-5.41	108.75	120.10
1	A	909	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	1154	TYR	OH-CZ-CE2	5.40	134.69	120.10
2	B	586	TRP	CB-CA-C	5.40	121.21	110.40
6	H	42	ILE	CA-CB-CG1	-5.40	100.74	111.00
1	A	206	GLU	N-CA-CB	5.40	120.32	110.60
1	A	900	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	1280	GLU	O-C-N	-5.40	114.06	122.70
2	B	1064	TYR	C-N-CA	-5.40	108.20	121.70
2	B	849	GLY	CA-C-O	-5.40	110.88	120.60
6	H	7	ASP	OD1-CG-OD2	-5.40	113.04	123.30
1	A	186	LYS	CB-CG-CD	5.40	125.63	111.60
2	B	390	LEU	CB-CG-CD1	-5.40	101.83	111.00
1	A	32	VAL	CB-CA-C	5.40	121.65	111.40
1	A	84	ILE	CG1-CB-CG2	-5.40	99.53	111.40
1	A	261	ASP	OD1-CG-OD2	-5.40	113.05	123.30
2	B	1062	HIS	N-CA-C	5.39	125.57	111.00
1	A	228	PHE	CB-CG-CD2	5.39	124.58	120.80
2	B	212	LEU	CB-CG-CD2	5.39	120.17	111.00
9	K	74	ARG	CB-CG-CD	5.39	125.62	111.60
1	A	241	VAL	CG1-CB-CG2	-5.39	102.28	110.90
1	A	920	LEU	CD1-CG-CD2	5.39	126.67	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	974	ASP	O-C-N	5.39	131.32	122.70
2	B	764	SER	N-CA-CB	-5.39	102.42	110.50
2	B	962	LYS	N-CA-CB	5.39	120.30	110.60
1	A	1226	VAL	CA-CB-CG1	-5.39	102.82	110.90
3	C	193	TYR	CD1-CE1-CZ	5.39	124.65	119.80
6	H	115	TYR	CA-C-N	5.39	129.05	117.20
1	A	874	ASP	OD1-CG-OD2	5.38	133.53	123.30
3	C	157	CYS	CB-CA-C	-5.38	99.63	110.40
2	B	1106	ARG	CD-NE-CZ	5.38	131.14	123.60
10	L	65	VAL	CG1-CB-CG2	5.38	119.51	110.90
4	E	109	ILE	O-C-N	5.38	131.31	122.70
9	K	113	THR	C-N-CA	5.38	135.15	121.70
1	A	347	PHE	CG-CD2-CE2	5.38	126.72	120.80
9	K	5	ASP	CB-CA-C	-5.38	99.64	110.40
1	A	1328	TYR	CB-CG-CD1	5.38	124.23	121.00
9	K	75	ILE	CA-C-O	5.38	131.40	120.10
1	A	173	THR	OG1-CB-CG2	-5.38	97.63	110.00
1	A	893	PHE	CB-CG-CD1	5.38	124.56	120.80
2	B	370	PHE	CG-CD2-CE2	5.38	126.71	120.80
2	B	1043	ASP	N-CA-C	-5.38	96.48	111.00
1	A	151	ASP	N-CA-C	-5.38	96.49	111.00
2	B	66	ASP	C-N-CA	5.38	135.14	121.70
8	J	36	LEU	C-N-CA	-5.38	108.26	121.70
1	A	871	ASP	N-CA-CB	-5.37	100.93	110.60
2	B	593	PRO	N-CD-CG	5.37	111.26	103.20
1	A	472	LEU	CD1-CG-CD2	5.37	126.61	110.50
1	A	646	PHE	C-N-CA	-5.37	111.03	122.30
2	B	1148	LYS	CA-CB-CG	5.37	125.21	113.40
1	A	448	PRO	N-CD-CG	5.37	111.25	103.20
1	A	1421	CYS	O-C-N	-5.37	114.11	122.70
2	B	341	LEU	CB-CG-CD2	-5.37	101.88	111.00
2	B	1069	PHE	CB-CG-CD1	5.37	124.56	120.80
2	B	1199	ALA	CB-CA-C	-5.37	102.05	110.10
1	A	544	ASP	OD1-CG-OD2	-5.36	113.11	123.30
1	A	578	LEU	CB-CG-CD2	5.36	120.12	111.00
1	A	381	THR	CB-CA-C	-5.36	97.13	111.60
2	B	857	ARG	CA-CB-CG	-5.36	101.61	113.40
8	J	10	CYS	O-C-N	-5.36	114.09	123.20
2	B	452	THR	CA-CB-CG2	5.36	119.90	112.40
2	B	645	SER	N-CA-C	5.36	125.47	111.00
2	B	1086	PHE	CG-CD1-CE1	-5.36	114.91	120.80
2	B	492	LEU	CB-CG-CD2	-5.36	101.89	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	52	ILE	CA-C-O	5.36	131.34	120.10
1	A	247	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	1294	PRO	CB-CG-CD	-5.35	85.62	106.50
1	A	693	VAL	CA-CB-CG1	-5.35	102.87	110.90
1	A	905	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	1274	ARG	CG-CD-NE	-5.35	100.56	111.80
5	F	80	ALA	N-CA-CB	-5.35	102.61	110.10
2	B	339	THR	CA-CB-OG1	5.35	120.24	109.00
2	B	436	VAL	CA-CB-CG2	5.35	118.93	110.90
6	H	14	GLU	CA-CB-CG	-5.35	101.63	113.40
6	H	19	ARG	CD-NE-CZ	5.35	131.09	123.60
2	B	39	ARG	NE-CZ-NH2	5.35	122.97	120.30
2	B	1034	VAL	CA-CB-CG1	5.35	118.92	110.90
4	E	57	MET	CG-SD-CE	5.35	108.76	100.20
4	E	198	ILE	O-C-N	-5.35	114.14	122.70
1	A	25	GLU	CG-CD-OE1	5.35	129.00	118.30
4	E	215	MET	CB-CA-C	-5.35	99.70	110.40
1	A	81	PHE	CA-C-N	-5.35	105.51	116.20
1	A	1414	ALA	CB-CA-C	-5.35	102.08	110.10
1	A	182	VAL	N-CA-C	5.34	125.43	111.00
1	A	379	VAL	CA-C-N	5.34	128.96	117.20
1	A	501	LEU	C-N-CA	-5.34	108.34	121.70
1	A	737	LEU	CD1-CG-CD2	5.34	126.53	110.50
2	B	872	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	A	76	GLU	C-N-CA	5.34	135.05	121.70
2	B	1029	CYS	CB-CA-C	5.34	121.08	110.40
7	I	92	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	A	375	THR	N-CA-CB	5.34	120.44	110.30
2	B	269	ILE	CG1-CB-CG2	-5.34	99.65	111.40
2	B	463	THR	CB-CA-C	-5.34	97.18	111.60
2	B	1020	ARG	N-CA-CB	-5.34	100.99	110.60
6	H	25	ARG	CG-CD-NE	-5.34	100.59	111.80
9	K	15	GLY	CA-C-N	5.34	128.95	117.20
1	A	439	ASN	O-C-N	-5.34	114.16	122.70
1	A	972	HIS	CB-CA-C	5.34	121.07	110.40
2	B	1108	ARG	CG-CD-NE	-5.34	100.59	111.80
4	E	16	PHE	CB-CA-C	5.34	121.07	110.40
4	E	181	ALA	N-CA-CB	-5.34	102.63	110.10
8	J	21	TYR	CG-CD1-CE1	5.34	125.57	121.30
1	A	1024	SER	CA-CB-OG	5.33	125.60	111.20
3	C	127	ARG	CG-CD-NE	-5.33	100.60	111.80
6	H	102	TYR	CA-C-N	-5.33	105.46	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	A	1438	THR	CA-CB-CG2	5.33	119.87	112.40
2	B	792	MET	CG-SD-CE	-5.33	91.67	100.20
2	B	1061	GLU	CG-CD-OE1	5.33	128.97	118.30
3	C	169	LYS	O-C-N	5.33	131.23	122.70
8	J	26	GLN	CB-CA-C	5.33	121.07	110.40
2	B	603	LEU	O-C-N	-5.33	114.17	122.70
7	I	45	ARG	CB-CA-C	-5.33	99.74	110.40
1	A	285	PRO	C-N-CA	5.33	135.02	121.70
6	H	91	ASP	CA-C-O	5.33	131.29	120.10
1	A	884	ASP	CA-C-O	-5.33	108.91	120.10
3	C	168	ALA	N-CA-C	5.33	125.38	111.00
1	A	285	PRO	N-CA-CB	5.33	109.69	103.30
1	A	438	ASP	CB-CG-OD1	5.33	123.09	118.30
2	B	1198	TYR	CG-CD1-CE1	-5.33	117.04	121.30
3	C	164	ALA	CB-CA-C	-5.33	102.11	110.10
1	A	423	ASP	N-CA-CB	-5.32	101.02	110.60
2	B	303	TYR	CD1-CG-CD2	-5.32	112.04	117.90
4	E	57	MET	N-CA-CB	5.32	120.18	110.60
6	H	14	GLU	O-C-N	5.32	131.22	122.70
1	A	1373	ASP	CB-CG-OD1	5.32	123.09	118.30
2	B	538	ASN	CB-CG-OD1	-5.32	110.96	121.60
3	C	210	GLU	CG-CD-OE1	5.32	128.94	118.30
10	L	31	CYS	CA-CB-SG	5.32	123.58	114.00
1	A	237	THR	OG1-CB-CG2	5.32	122.23	110.00
1	A	506	ALA	O-C-N	5.32	131.21	122.70
2	B	446	LEU	CA-C-N	-5.32	105.50	117.20
2	B	539	LEU	CA-C-N	-5.32	105.50	117.20
7	I	4	PHE	O-C-N	5.32	131.20	122.70
9	K	75	ILE	CA-C-N	-5.32	105.51	117.20
1	A	50	ILE	N-CA-C	5.31	125.35	111.00
1	A	364	VAL	CG1-CB-CG2	-5.31	102.40	110.90
1	A	474	VAL	CG1-CB-CG2	5.31	119.40	110.90
1	A	974	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	980	ASP	N-CA-C	5.31	125.35	111.00
2	B	549	THR	CA-CB-OG1	5.31	120.16	109.00
9	K	19	LEU	CB-CG-CD1	-5.31	101.97	111.00
1	A	244	PRO	CA-C-O	-5.31	107.45	120.20
2	B	164	LYS	CD-CE-NZ	5.31	123.92	111.70
2	B	411	PRO	O-C-N	-5.31	114.20	122.70
2	B	1129	ARG	CG-CD-NE	-5.31	100.64	111.80
1	A	1025	ARG	N-CA-CB	5.31	120.16	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	698	GLU	CG-CD-OE1	5.31	128.91	118.30
2	B	706	GLN	CG-CD-OE1	-5.31	110.99	121.60
3	C	166	GLU	OE1-CD-OE2	5.31	129.67	123.30
2	B	1080	LYS	O-C-N	5.31	131.19	122.70
1	A	81	PHE	CD1-CE1-CZ	5.30	126.47	120.10
2	B	199	MET	C-N-CA	-5.30	111.16	122.30
2	B	663	ALA	CB-CA-C	-5.30	102.14	110.10
2	B	788	ARG	CG-CD-NE	-5.30	100.66	111.80
2	B	1213	THR	CB-CA-C	-5.30	97.28	111.60
7	I	30	ARG	CB-CA-C	-5.30	99.79	110.40
1	A	824	LEU	C-N-CA	-5.30	108.45	121.70
1	A	920	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	182	VAL	C-N-CA	-5.30	111.17	122.30
2	B	1210	MET	CG-SD-CE	5.29	108.67	100.20
1	A	801	GLU	CB-CA-C	5.29	120.99	110.40
3	C	233	GLU	OE1-CD-OE2	5.29	129.65	123.30
7	I	70	ARG	NH1-CZ-NH2	5.29	125.22	119.40
1	A	941	LYS	CA-CB-CG	-5.29	101.76	113.40
7	I	84	VAL	CA-CB-CG1	-5.29	102.96	110.90
2	B	781	PHE	N-CA-C	5.29	125.28	111.00
1	A	492	PRO	O-C-N	5.29	131.16	122.70
1	A	748	MET	C-N-CA	-5.29	108.48	121.70
1	A	114	LEU	CA-CB-CG	5.29	127.45	115.30
1	A	1206	ASP	CB-CG-OD2	5.29	123.06	118.30
8	J	58	GLU	CB-CG-CD	5.29	128.47	114.20
1	A	619	LYS	CG-CD-CE	5.28	127.75	111.90
3	C	114	TYR	CB-CG-CD1	5.28	124.17	121.00
9	K	14	GLU	N-CA-C	-5.28	96.73	111.00
2	B	1096	ARG	C-N-CA	-5.28	108.49	121.70
1	A	301	ALA	N-CA-C	5.28	125.26	111.00
1	A	393	ARG	NH1-CZ-NH2	5.28	125.21	119.40
1	A	766	GLY	N-CA-C	5.28	126.30	113.10
2	B	336	ARG	CG-CD-NE	-5.28	100.71	111.80
7	I	58	VAL	N-CA-C	-5.28	96.74	111.00
1	A	49	LYS	CA-CB-CG	-5.28	101.79	113.40
1	A	1428	VAL	CA-CB-CG2	-5.28	102.98	110.90
2	B	833	TYR	CA-C-O	-5.28	109.02	120.10
4	E	100	ILE	O-C-N	5.28	131.14	122.70
9	K	70	ARG	CB-CA-C	5.28	120.95	110.40
1	A	4	GLN	N-CA-CB	-5.27	101.11	110.60
6	H	103	LYS	CB-CG-CD	5.27	125.31	111.60
1	A	193	ASP	CB-CG-OD2	-5.27	113.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1334	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	A	1358	SER	N-CA-CB	5.27	118.41	110.50
2	B	303	TYR	CD1-CE1-CZ	-5.27	115.06	119.80
2	B	1073	TYR	CB-CG-CD2	5.27	124.16	121.00
1	A	526	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	A	111	GLY	CA-C-N	-5.27	105.61	117.20
1	A	841	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	1406	VAL	CA-CB-CG2	-5.27	103.00	110.90
2	B	978	ASP	N-CA-CB	-5.27	101.11	110.60
3	C	15	LYS	CG-CD-CE	5.27	127.71	111.90
3	C	68	GLY	N-CA-C	-5.27	99.93	113.10
2	B	225	VAL	N-CA-CB	-5.27	99.91	111.50
2	B	1220	ARG	CG-CD-NE	5.27	122.86	111.80
1	A	770	VAL	CA-CB-CG1	-5.27	103.00	110.90
2	B	415	GLN	O-C-N	5.27	131.13	122.70
9	K	108	GLU	CG-CD-OE2	5.27	128.83	118.30
1	A	764	CYS	N-CA-CB	-5.26	101.12	110.60
1	A	465	TYR	CB-CA-C	-5.26	99.88	110.40
1	A	592	ASP	CA-C-N	5.26	128.78	117.20
1	A	866	PHE	CB-CG-CD1	-5.26	117.12	120.80
2	B	1094	ARG	CB-CG-CD	5.26	125.28	111.60
6	H	116	TYR	CB-CA-C	-5.26	99.88	110.40
1	A	106	VAL	CA-CB-CG1	5.26	118.79	110.90
2	B	484	ASN	N-CA-C	5.26	125.20	111.00
2	B	644	GLU	N-CA-CB	-5.26	101.13	110.60
3	C	133	ILE	CB-CA-C	-5.26	101.08	111.60
10	L	42	ARG	CD-NE-CZ	5.26	130.96	123.60
1	A	572	TRP	CD1-NE1-CE2	-5.26	104.27	109.00
1	A	1209	MET	C-N-CA	-5.26	111.26	122.30
9	K	53	ASP	CB-CG-OD1	-5.26	113.57	118.30
4	E	75	MET	N-CA-C	-5.26	96.81	111.00
2	B	668	ASP	OD1-CG-OD2	-5.25	113.31	123.30
1	A	646	PHE	CD1-CE1-CZ	-5.25	113.80	120.10
1	A	1154	TYR	CB-CG-CD2	5.25	124.15	121.00
1	A	666	ILE	C-N-CA	-5.25	111.27	122.30
3	C	228	PHE	CB-CA-C	-5.25	99.90	110.40
1	A	30	ILE	C-N-CA	-5.25	108.58	121.70
1	A	914	GLU	O-C-N	5.25	131.10	122.70
1	A	1418	LEU	CB-CA-C	-5.25	100.23	110.20
2	B	965	LYS	CG-CD-CE	5.25	127.65	111.90
2	B	1018	PRO	CB-CA-C	-5.25	98.88	112.00
2	B	393	LYS	CA-CB-CG	5.25	124.94	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	840	ILE	CA-CB-CG2	-5.25	100.40	110.90
3	C	21	ILE	CG1-CB-CG2	-5.25	99.85	111.40
1	A	931	GLU	CA-CB-CG	5.25	124.94	113.40
1	A	1004	ASN	N-CA-CB	-5.25	101.16	110.60
2	B	885	MET	CG-SD-CE	5.25	108.59	100.20
3	C	85	ASP	N-CA-CB	-5.25	101.16	110.60
4	E	212	ARG	NH1-CZ-NH2	-5.25	113.63	119.40
1	A	172	PRO	N-CD-CG	5.24	111.06	103.20
1	A	486	GLU	CA-CB-CG	5.24	124.93	113.40
2	B	1086	PHE	CB-CG-CD1	5.24	124.47	120.80
1	A	1443	VAL	CA-CB-CG2	5.24	118.76	110.90
3	C	153	LEU	CB-CG-CD2	5.24	119.91	111.00
2	B	1203	LEU	CA-C-O	5.24	131.10	120.10
1	A	696	GLU	CB-CA-C	5.24	120.87	110.40
2	B	1156	ASP	N-CA-CB	5.24	120.03	110.60
1	A	1000	LEU	CA-CB-CG	5.24	127.34	115.30
2	B	1073	TYR	CB-CG-CD1	-5.24	117.86	121.00
4	E	137	GLU	N-CA-CB	-5.24	101.18	110.60
1	A	982	THR	OG1-CB-CG2	-5.23	97.96	110.00
7	I	70	ARG	CB-CA-C	-5.23	99.93	110.40
7	I	92	ARG	CG-CD-NE	-5.23	100.81	111.80
2	B	502	ILE	CG1-CB-CG2	5.23	122.91	111.40
3	C	202	PRO	CA-C-O	-5.23	107.64	120.20
9	K	46	ILE	CA-CB-CG1	5.23	120.94	111.00
1	A	361	LEU	N-CA-C	5.23	125.12	111.00
1	A	876	ALA	N-CA-C	5.23	125.12	111.00
1	A	1298	TYR	N-CA-C	-5.23	96.88	111.00
2	B	1132	GLU	CG-CD-OE2	-5.23	107.84	118.30
3	C	108	GLU	CA-C-O	5.23	131.08	120.10
6	H	92	ASP	OD1-CG-OD2	-5.23	113.37	123.30
9	K	37	LYS	CA-C-N	-5.23	105.70	117.20
1	A	751	SER	CA-CB-OG	5.22	125.31	111.20
1	A	873	MET	N-CA-CB	-5.22	101.19	110.60
1	A	1302	PRO	O-C-N	5.22	131.06	122.70
1	A	839	ARG	C-N-CA	-5.22	108.64	121.70
2	B	974	PRO	N-CD-CG	5.22	111.03	103.20
3	C	227	THR	N-CA-CB	-5.22	100.38	110.30
1	A	939	ASP	OD1-CG-OD2	5.22	133.22	123.30
1	A	222	LEU	CB-CG-CD2	5.22	119.88	111.00
1	A	633	VAL	O-C-N	-5.22	114.35	122.70
1	A	676	MET	CA-CB-CG	5.22	122.17	113.30
6	H	132	LEU	CB-CG-CD1	-5.22	102.13	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	111	THR	OG1-CB-CG2	-5.22	98.00	110.00
2	B	579	ARG	NH1-CZ-NH2	5.22	125.14	119.40
2	B	893	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	182	VAL	CA-CB-CG1	-5.22	103.08	110.90
1	A	469	ARG	NH1-CZ-NH2	-5.22	113.66	119.40
2	B	463	THR	N-CA-C	5.22	125.08	111.00
3	C	253	LYS	CD-CE-NZ	-5.22	99.70	111.70
7	I	35	VAL	CA-CB-CG2	-5.22	103.08	110.90
1	A	179	LEU	CB-CG-CD1	5.21	119.86	111.00
1	A	883	LEU	N-CA-CB	-5.21	99.97	110.40
2	B	384	ARG	O-C-N	-5.21	114.36	122.70
7	I	103	CYS	CB-CA-C	-5.21	99.97	110.40
8	J	55	ASP	CB-CG-OD1	5.21	122.99	118.30
10	L	28	LYS	CA-C-N	5.21	128.67	117.20
1	A	927	VAL	CA-CB-CG2	-5.21	103.08	110.90
2	B	350	GLN	N-CA-CB	-5.21	101.22	110.60
2	B	403	LYS	CA-CB-CG	-5.21	101.93	113.40
3	C	166	GLU	CG-CD-OE1	-5.21	107.88	118.30
4	E	174	GLN	CG-CD-OE1	5.21	132.02	121.60
2	B	655	LYS	C-N-CA	-5.21	111.36	122.30
9	K	84	LYS	CA-CB-CG	5.21	124.86	113.40
1	A	302	THR	N-CA-CB	-5.21	100.40	110.30
6	H	99	GLY	CA-C-N	-5.21	105.74	117.20
1	A	425	GLN	CB-CA-C	-5.21	99.99	110.40
1	A	717	ASN	N-CA-C	5.21	125.06	111.00
1	A	855	THR	N-CA-CB	5.21	120.19	110.30
2	B	214	ALA	CB-CA-C	5.21	117.91	110.10
2	B	257	LYS	CD-CE-NZ	-5.21	99.73	111.70
2	B	358	LYS	CB-CG-CD	5.21	125.14	111.60
1	A	496	GLU	CA-CB-CG	5.21	124.85	113.40
2	B	181	LEU	N-CA-C	-5.21	96.95	111.00
2	B	963	PHE	CD1-CG-CD2	5.21	125.07	118.30
9	K	42	LEU	C-N-CA	-5.21	111.37	122.30
1	A	1429	ILE	CA-CB-CG2	5.20	121.31	110.90
10	L	26	THR	N-CA-CB	5.20	120.19	110.30
1	A	129	LYS	CA-C-N	-5.20	105.75	117.20
5	F	139	PRO	CA-CB-CG	5.20	114.69	104.80
1	A	378	GLU	OE1-CD-OE2	5.20	129.54	123.30
1	A	844	ALA	O-C-N	-5.20	114.38	122.70
1	A	1154	TYR	CE1-CZ-OH	-5.20	106.06	120.10
2	B	242	SER	O-C-N	-5.20	114.38	122.70
1	A	656	TRP	CA-CB-CG	5.20	123.58	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	804	TYR	CD1-CE1-CZ	5.20	124.48	119.80
2	B	583	ASN	C-N-CA	-5.20	111.38	122.30
2	B	612	GLU	CG-CD-OE1	-5.20	107.90	118.30
3	C	52	GLU	CG-CD-OE2	-5.20	107.90	118.30
1	A	1018	PHE	CG-CD1-CE1	5.20	126.52	120.80
1	A	1042	PHE	CG-CD1-CE1	5.20	126.52	120.80
1	A	599	SER	CB-CA-C	-5.20	100.23	110.10
7	I	97	MET	CA-C-O	5.19	131.01	120.10
1	A	127	ALA	C-N-CA	5.19	134.68	121.70
1	A	616	VAL	N-CA-CB	-5.19	100.08	111.50
1	A	728	LYS	CB-CG-CD	5.19	125.10	111.60
2	B	312	GLU	CG-CD-OE2	-5.19	107.91	118.30
2	B	749	LEU	CB-CG-CD1	-5.19	102.17	111.00
2	B	847	ASP	CB-CG-OD2	5.19	122.97	118.30
6	H	22	LYS	CD-CE-NZ	-5.19	99.76	111.70
1	A	535	THR	N-CA-CB	-5.19	100.44	110.30
1	A	1114	PRO	O-C-N	5.19	131.00	122.70
1	A	1264	GLU	CG-CD-OE2	5.19	128.68	118.30
2	B	40	GLU	OE1-CD-OE2	5.19	129.53	123.30
2	B	90	ILE	CA-CB-CG2	5.19	121.28	110.90
3	C	185	LYS	CD-CE-NZ	-5.19	99.76	111.70
1	A	1169	ILE	CA-C-N	-5.19	105.78	117.20
10	L	67	PHE	N-CA-CB	5.19	119.94	110.60
1	A	303	TYR	CD1-CE1-CZ	-5.19	115.13	119.80
1	A	1103	GLU	CA-CB-CG	5.19	124.81	113.40
2	B	104	GLU	N-CA-C	5.19	125.00	111.00
3	C	129	ILE	CA-CB-CG1	5.19	120.85	111.00
1	A	896	ARG	CD-NE-CZ	-5.18	116.34	123.60
2	B	1158	PHE	N-CA-C	5.18	124.99	111.00
9	K	78	THR	O-C-N	5.18	130.99	122.70
9	K	105	PHE	CG-CD1-CE1	5.18	126.50	120.80
1	A	494	SER	CB-CA-C	-5.18	100.26	110.10
1	A	1381	LEU	O-C-N	-5.18	114.41	122.70
2	B	1216	LEU	CB-CG-CD1	5.18	119.81	111.00
2	B	48	LEU	CB-CG-CD1	5.18	119.81	111.00
2	B	244	LEU	CD1-CG-CD2	5.18	126.04	110.50
2	B	276	ILE	CA-CB-CG2	-5.18	100.54	110.90
1	A	701	LEU	CB-CG-CD2	-5.18	102.20	111.00
9	K	4	PRO	CA-C-O	-5.18	107.77	120.20
1	A	158	PRO	C-N-CA	-5.18	108.76	121.70
1	A	219	PHE	CB-CG-CD1	-5.18	117.18	120.80
4	E	7	ARG	NE-CZ-NH1	5.18	122.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	118	ARG	N-CA-CB	-5.18	101.28	110.60
1	A	228	PHE	O-C-N	5.17	130.98	122.70
3	C	75	MET	CG-SD-CE	-5.17	91.92	100.20
7	I	47	GLU	O-C-N	-5.17	114.42	122.70
1	A	52	GLY	CA-C-O	-5.17	111.29	120.60
1	A	1438	THR	O-C-N	-5.17	114.41	123.20
1	A	590	ARG	CB-CA-C	5.17	120.74	110.40
1	A	675	THR	CA-CB-CG2	5.17	119.64	112.40
9	K	44	ASN	O-C-N	-5.17	114.43	122.70
1	A	234	MET	CA-C-O	-5.17	109.25	120.10
2	B	359	GLU	CB-CA-C	-5.17	100.06	110.40
1	A	995	GLU	CA-C-N	5.17	128.57	117.20
1	A	1118	VAL	N-CA-CB	5.17	122.86	111.50
2	B	1171	VAL	CG1-CB-CG2	-5.17	102.64	110.90
1	A	304	MET	CG-SD-CE	-5.16	91.94	100.20
1	A	1440	ALA	N-CA-CB	-5.16	102.87	110.10
1	A	296	LEU	CA-CB-CG	-5.16	103.43	115.30
2	B	624	LEU	CB-CG-CD2	-5.16	102.23	111.00
7	I	120	GLN	N-CA-C	5.16	124.93	111.00
1	A	1199	ARG	O-C-N	5.16	130.95	122.70
2	B	591	ARG	O-C-N	5.16	130.96	122.70
2	B	745	PRO	O-C-N	5.16	130.95	122.70
9	K	95	ILE	C-N-CA	5.16	134.60	121.70
4	E	82	PHE	CG-CD2-CE2	-5.16	115.13	120.80
1	A	104	GLU	N-CA-C	5.16	124.92	111.00
1	A	219	PHE	CB-CG-CD2	5.16	124.41	120.80
2	B	482	VAL	CA-CB-CG1	5.16	118.63	110.90
2	B	884	ARG	NE-CZ-NH2	-5.16	117.72	120.30
4	E	128	PRO	N-CD-CG	5.16	110.93	103.20
2	B	697	GLU	OE1-CD-OE2	5.15	129.48	123.30
1	A	893	PHE	CD1-CG-CD2	-5.15	111.61	118.30
2	B	942	ARG	CD-NE-CZ	5.15	130.81	123.60
2	B	518	HIS	CA-CB-CG	5.15	122.35	113.60
6	H	53	ASP	O-C-N	-5.15	114.46	122.70
7	I	39	GLY	O-C-N	-5.15	114.46	122.70
1	A	496	GLU	CA-C-N	-5.15	105.88	117.20
1	A	950	GLY	CA-C-O	-5.15	111.34	120.60
1	A	1371	LEU	CB-CG-CD2	5.15	119.75	111.00
6	H	136	LYS	CA-CB-CG	5.15	124.72	113.40
1	A	1133	LEU	CD1-CG-CD2	5.15	125.94	110.50
4	E	21	GLU	CG-CD-OE1	5.14	128.59	118.30
4	E	107	THR	OG1-CB-CG2	-5.14	98.17	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	566	LEU	O-C-N	-5.14	114.47	122.70
3	C	66	ARG	CD-NE-CZ	-5.14	116.40	123.60
7	I	59	VAL	N-CA-CB	-5.14	100.19	111.50
1	A	1409	LEU	CB-CG-CD2	-5.14	102.27	111.00
2	B	649	LYS	N-CA-C	-5.14	97.13	111.00
9	K	49	GLU	CA-C-N	5.14	128.50	117.20
1	A	1450	LEU	CB-CA-C	5.14	119.96	110.20
2	B	452	THR	C-N-CA	5.14	134.54	121.70
6	H	118	PHE	CZ-CE2-CD2	5.14	126.26	120.10
9	K	28	PRO	N-CA-CB	-5.14	96.95	102.60
2	B	878	GLN	O-C-N	5.13	130.91	122.70
2	B	1074	ASN	C-N-CA	-5.13	111.52	122.30
3	C	52	GLU	CB-CA-C	5.13	120.67	110.40
1	A	725	ALA	CB-CA-C	-5.13	102.40	110.10
2	B	895	ASP	OD1-CG-OD2	-5.13	113.55	123.30
3	C	101	LEU	CA-CB-CG	-5.13	103.50	115.30
1	A	64	ASN	C-N-CA	5.13	134.52	121.70
2	B	772	ALA	N-CA-C	5.13	124.85	111.00
1	A	555	ASP	OD1-CG-OD2	-5.13	113.56	123.30
1	A	298	PHE	CG-CD1-CE1	-5.13	115.16	120.80
1	A	1120	LEU	CB-CG-CD1	5.13	119.72	111.00
2	B	370	PHE	CB-CG-CD1	-5.13	117.21	120.80
2	B	136	THR	OG1-CB-CG2	-5.12	98.21	110.00
7	I	61	ASP	OD1-CG-OD2	-5.12	113.56	123.30
1	A	68	GLN	CA-CB-CG	5.12	124.67	113.40
1	A	93	VAL	CA-C-N	-5.12	105.95	116.20
1	A	853	ASP	N-CA-C	5.12	124.83	111.00
4	E	80	VAL	N-CA-C	-5.12	97.16	111.00
2	B	479	VAL	CA-CB-CG2	5.12	118.58	110.90
2	B	804	GLY	N-CA-C	5.12	125.91	113.10
10	L	65	VAL	CB-CA-C	-5.12	101.67	111.40
1	A	877	HIS	O-C-N	-5.12	114.51	122.70
2	B	517	THR	CB-CA-C	-5.12	97.78	111.60
2	B	1074	ASN	CA-C-O	5.12	130.85	120.10
2	B	1080	LYS	CA-C-N	-5.12	105.94	117.20
1	A	637	LYS	CD-CE-NZ	5.12	123.47	111.70
3	C	181	ASP	N-CA-C	5.12	124.81	111.00
7	I	35	VAL	C-N-CA	5.11	134.48	121.70
1	A	1220	PHE	CE1-CZ-CE2	-5.11	110.80	120.00
2	B	638	PHE	CB-CG-CD2	5.11	124.38	120.80
7	I	94	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	841	LEU	CB-CG-CD2	-5.11	102.31	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	GLU	N-CA-C	5.11	124.79	111.00
1	A	244	PRO	N-CD-CG	-5.11	95.54	103.20
1	A	883	LEU	CD1-CG-CD2	-5.11	95.18	110.50
1	A	994	GLN	N-CA-CB	5.11	119.79	110.60
4	E	154	ILE	CB-CA-C	-5.11	101.39	111.60
7	I	107	SER	N-CA-C	5.11	124.79	111.00
2	B	973	ILE	CG1-CB-CG2	-5.11	100.17	111.40
3	C	161	LYS	N-CA-CB	-5.11	101.41	110.60
7	I	5	ARG	NH1-CZ-NH2	-5.11	113.78	119.40
1	A	230	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	1255	GLU	OE1-CD-OE2	-5.10	117.18	123.30
2	B	1078	GLY	N-CA-C	5.10	125.85	113.10
8	J	18	TRP	CE2-CD2-CG	5.10	111.38	107.30
8	J	36	LEU	N-CA-CB	5.10	120.60	110.40
1	A	619	LYS	O-C-N	-5.10	114.54	122.70
1	A	1256	GLU	O-C-N	-5.10	114.54	122.70
2	B	376	PHE	N-CA-CB	5.10	119.78	110.60
10	L	38	LEU	CB-CA-C	5.10	119.89	110.20
3	C	99	LEU	CA-CB-CG	-5.10	103.58	115.30
3	C	205	LYS	CB-CG-CD	5.10	124.86	111.60
7	I	30	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	955	PRO	N-CD-CG	5.10	110.84	103.20
4	E	35	VAL	CA-CB-CG2	5.10	118.54	110.90
1	A	522	GLY	O-C-N	5.09	130.85	122.70
2	B	680	THR	CA-CB-CG2	5.09	119.53	112.40
3	C	194	GLU	CG-CD-OE2	-5.09	108.11	118.30
4	E	24	LYS	CG-CD-CE	-5.09	96.62	111.90
2	B	168	GLY	CA-C-O	5.09	129.76	120.60
4	E	72	PHE	CG-CD2-CE2	-5.09	115.20	120.80
5	F	143	PHE	CB-CG-CD2	-5.09	117.23	120.80
7	I	92	ARG	O-C-N	5.09	130.85	122.70
9	K	64	GLU	O-C-N	-5.09	114.56	122.70
1	A	58	LEU	N-CA-CB	5.09	120.58	110.40
2	B	164	LYS	CG-CD-CE	5.09	127.17	111.90
1	A	504	LEU	CA-C-O	-5.09	109.42	120.10
4	E	46	TYR	CB-CG-CD1	-5.09	117.95	121.00
5	F	138	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	A	109	HIS	C-N-CA	5.08	134.41	121.70
1	A	413	ILE	CB-CA-C	-5.08	101.43	111.60
2	B	737	THR	CA-CB-OG1	5.08	119.67	109.00
2	B	981	ALA	N-CA-CB	-5.08	102.98	110.10
1	A	591	PHE	CG-CD1-CE1	5.08	126.39	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	32	VAL	CA-CB-CG1	5.08	118.52	110.90
1	A	1382	THR	CA-CB-CG2	-5.08	105.29	112.40
7	I	97	MET	O-C-N	-5.08	114.57	122.70
1	A	701	LEU	CA-CB-CG	5.08	126.98	115.30
2	B	730	ARG	O-C-N	-5.08	114.57	122.70
1	A	25	GLU	O-C-N	-5.08	114.58	122.70
2	B	1077	THR	O-C-N	-5.08	114.57	123.20
1	A	923	LEU	N-CA-CB	5.08	120.55	110.40
1	A	1116	LEU	N-CA-C	-5.08	97.30	111.00
2	B	249	ARG	C-N-CA	5.08	134.39	121.70
1	A	789	LYS	CB-CA-C	-5.07	100.25	110.40
1	A	851	HIS	C-N-CA	-5.07	109.01	121.70
2	B	96	TYR	C-N-CA	-5.07	109.01	121.70
4	E	75	MET	CB-CA-C	5.07	120.55	110.40
1	A	1153	TYR	CG-CD2-CE2	5.07	125.36	121.30
4	E	82	PHE	N-CA-CB	5.07	119.73	110.60
4	E	148	GLU	OE1-CD-OE2	-5.07	117.21	123.30
2	B	964	VAL	N-CA-CB	-5.07	100.35	111.50
2	B	1084	GLN	C-N-CA	5.07	134.37	121.70
2	B	1213	THR	CA-CB-CG2	-5.07	105.31	112.40
3	C	183	TRP	CD1-NE1-CE2	-5.07	104.44	109.00
1	A	453	MET	CG-SD-CE	-5.07	92.10	100.20
2	B	198	ASP	CB-CA-C	-5.07	100.27	110.40
2	B	684	LEU	O-C-N	-5.07	114.59	122.70
2	B	895	ASP	N-CA-C	-5.07	97.32	111.00
6	H	141	TYR	CB-CG-CD2	5.07	124.04	121.00
8	J	55	ASP	CB-CA-C	5.07	120.53	110.40
1	A	1281	ARG	NH1-CZ-NH2	-5.06	113.83	119.40
3	C	189	THR	N-CA-C	-5.06	97.33	111.00
7	I	118	ARG	CA-CB-CG	5.06	124.54	113.40
1	A	160	GLN	CA-CB-CG	5.06	124.54	113.40
1	A	1119	TYR	CD1-CE1-CZ	5.06	124.36	119.80
2	B	587	HIS	CA-C-O	-5.06	109.47	120.10
2	B	904	ARG	N-CA-C	5.06	124.67	111.00
4	E	28	TYR	CD1-CG-CD2	-5.06	112.33	117.90
1	A	99	ILE	CA-CB-CG2	-5.06	100.78	110.90
1	A	994	GLN	CB-CA-C	-5.06	100.28	110.40
2	B	644	GLU	C-N-CA	-5.06	109.05	121.70
2	B	911	ILE	CG1-CB-CG2	-5.06	100.27	111.40
3	C	27	LEU	C-N-CA	-5.06	109.05	121.70
4	E	133	GLU	C-N-CA	-5.06	109.05	121.70
5	F	84	TYR	CZ-CE2-CD2	5.06	124.35	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	595	ARG	NE-CZ-NH1	5.06	122.83	120.30
6	H	85	GLY	N-CA-C	5.06	125.74	113.10
7	I	29	CYS	O-C-N	5.06	130.79	122.70
2	B	485	ARG	CD-NE-CZ	5.06	130.68	123.60
1	A	394	ASN	CB-CA-C	-5.05	100.29	110.40
1	A	566	ILE	C-N-CA	5.05	134.34	121.70
1	A	576	GLN	O-C-N	-5.05	114.61	122.70
1	A	976	THR	O-C-N	-5.05	114.61	122.70
2	B	69	LEU	CB-CG-CD2	-5.05	102.41	111.00
2	B	381	MET	CB-CA-C	-5.05	100.29	110.40
2	B	520	GLY	O-C-N	-5.05	114.61	122.70
1	A	226	GLU	CA-C-N	5.05	128.32	117.20
1	A	272	ALA	CB-CA-C	5.05	117.68	110.10
4	E	110	PHE	N-CA-CB	-5.05	101.50	110.60
4	E	82	PHE	CG-CD1-CE1	5.05	126.36	120.80
7	I	107	SER	CA-CB-OG	-5.05	97.56	111.20
1	A	1053	PHE	C-N-CA	-5.05	109.08	121.70
1	A	1433	MET	CB-CA-C	-5.05	100.30	110.40
2	B	56	ASP	CA-C-N	5.05	128.31	117.20
1	A	949	ASP	OD1-CG-OD2	-5.05	113.71	123.30
1	A	991	LYS	CA-CB-CG	5.04	124.50	113.40
1	A	1215	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	A	958	VAL	N-CA-C	5.04	124.62	111.00
1	A	1172	LEU	CB-CA-C	-5.04	100.62	110.20
3	C	193	TYR	CB-CG-CD2	5.04	124.03	121.00
1	A	1281	ARG	CB-CA-C	-5.04	100.32	110.40
2	B	485	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	B	895	ASP	CA-C-O	-5.04	109.52	120.10
2	B	848	ARG	N-CA-C	5.04	124.61	111.00
2	B	1188	LYS	CD-CE-NZ	-5.04	100.11	111.70
4	E	37	LEU	CB-CA-C	5.04	119.77	110.20
4	E	112	TYR	CZ-CE2-CD2	5.04	124.33	119.80
4	E	4	GLU	OE1-CD-OE2	-5.04	117.26	123.30
9	K	113	THR	O-C-N	5.04	130.76	122.70
1	A	894	GLU	CG-CD-OE2	5.03	128.37	118.30
1	A	1239	ARG	C-N-CA	5.03	134.28	121.70
4	E	129	PRO	O-C-N	5.03	130.75	122.70
2	B	398	ARG	CG-CD-NE	-5.03	101.23	111.80
3	C	24	ASN	N-CA-C	5.03	124.58	111.00
1	A	725	ALA	N-CA-C	5.03	124.58	111.00
2	B	486	TYR	CB-CG-CD2	-5.03	117.98	121.00
7	I	34	TYR	N-CA-C	5.03	124.58	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	331	LEU	N-CA-CB	5.03	120.46	110.40
4	E	62	ALA	N-CA-CB	-5.03	103.06	110.10
5	F	117	PRO	O-C-N	-5.03	114.66	122.70
6	H	121	LEU	N-CA-C	-5.03	97.43	111.00
2	B	38	PHE	O-C-N	-5.02	114.66	122.70
9	K	63	VAL	CG1-CB-CG2	5.02	118.94	110.90
7	I	71	SER	N-CA-CB	5.02	118.03	110.50
8	J	6	ARG	O-C-N	5.02	130.73	122.70
1	A	122	MET	CG-SD-CE	5.02	108.23	100.20
1	A	399	HIS	C-N-CA	5.02	143.09	122.00
1	A	922	ASP	CB-CA-C	-5.02	100.36	110.40
2	B	405	ARG	NH1-CZ-NH2	-5.02	113.88	119.40
2	B	550	ASP	CB-CG-OD2	-5.02	113.78	118.30
2	B	620	ARG	CA-C-N	-5.02	106.16	117.20
6	H	40	LEU	O-C-N	5.02	130.73	122.70
1	A	220	THR	CA-C-N	-5.02	106.16	117.20
1	A	295	LEU	N-CA-C	-5.02	97.45	111.00
1	A	465	TYR	CE1-CZ-CE2	-5.02	111.77	119.80
1	A	1026	LEU	O-C-N	-5.02	114.67	122.70
2	B	466	TRP	N-CA-C	5.02	124.54	111.00
8	J	47	ARG	CA-CB-CG	-5.02	102.36	113.40
1	A	738	LYS	CA-C-O	-5.01	109.57	120.10
2	B	1077	THR	CA-C-O	5.01	130.63	120.10
7	I	52	ILE	CB-CA-C	-5.01	101.57	111.60
1	A	630	ILE	N-CA-C	-5.01	97.47	111.00
2	B	512	ARG	NE-CZ-NH2	5.01	122.81	120.30
5	F	97	ARG	CD-NE-CZ	5.01	130.62	123.60
2	B	68	THR	OG1-CB-CG2	-5.01	98.48	110.00
1	A	774	ARG	N-CA-CB	5.01	119.61	110.60
1	A	1092	LYS	CD-CE-NZ	5.01	123.22	111.70
1	A	1170	ILE	CG1-CB-CG2	-5.01	100.38	111.40
2	B	635	ARG	NE-CZ-NH1	5.01	122.80	120.30
4	E	66	GLU	CB-CA-C	5.01	120.42	110.40
6	H	32	THR	N-CA-C	-5.01	97.48	111.00
2	B	165	VAL	N-CA-C	5.01	124.52	111.00
2	B	411	PRO	N-CA-CB	-5.01	97.09	102.60
1	A	164	ARG	O-C-N	-5.00	114.69	123.20
5	F	106	PRO	CA-N-CD	5.00	118.71	111.70
1	A	1407	GLU	CG-CD-OE2	5.00	128.30	118.30
2	B	823	ALA	CB-CA-C	-5.00	102.60	110.10

There are no chirality outliers.

All (191) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1035	TYR	Sidechain
1	A	1046	LEU	Mainchain
1	A	1093	LYS	Peptide
1	A	1111	MET	Mainchain
1	A	1117	THR	Mainchain
1	A	1119	TYR	Sidechain
1	A	1123	GLY	Peptide
1	A	1160	SER	Peptide
1	A	120	GLU	Peptide
1	A	1208	THR	Mainchain
1	A	1220	PHE	Peptide
1	A	1232	ASN	Peptide
1	A	1278	ASN	Sidechain
1	A	128	ILE	Peptide
1	A	1298	TYR	Sidechain
1	A	1301	GLU	Mainchain
1	A	1306	LEU	Mainchain
1	A	1328	TYR	Sidechain
1	A	1361	SER	Mainchain
1	A	1365	TYR	Peptide
1	A	1366	ARG	Sidechain
1	A	1375	MET	Mainchain
1	A	1384	VAL	Peptide
1	A	150	THR	Peptide
1	A	158	PRO	Mainchain,Peptide
1	A	159	THR	Mainchain,Peptide
1	A	165	GLY	Peptide
1	A	191	THR	Peptide
1	A	194	ALA	Peptide
1	A	261	ASP	Peptide
1	A	325	ILE	Peptide
1	A	377	PRO	Mainchain
1	A	399	HIS	Mainchain,Peptide
1	A	434	ARG	Sidechain
1	A	44	THR	Peptide
1	A	441	PRO	Mainchain
1	A	464	PRO	Mainchain,Peptide
1	A	478	TYR	Sidechain
1	A	484	GLY	Mainchain
1	A	504	LEU	Mainchain
1	A	52	GLY	Peptide
1	A	537	ARG	Mainchain

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Mol	Chain	Res	Type	Group
1	A	545	GLN	Mainchain
1	A	555	ASP	Peptide
1	A	556	TRP	Peptide
1	A	60	SER	Peptide
1	A	65	LEU	Peptide
1	A	650	GLN	Sidechain
1	A	659	HIS	Sidechain
1	A	705	LYS	Peptide
1	A	706	HIS	Peptide
1	A	74	MET	Peptide
1	A	741	ASN	Mainchain
1	A	78	PRO	Mainchain
1	A	852	TYR	Sidechain
1	A	870	GLU	Mainchain
1	A	884	ASP	Mainchain
1	A	897	TYR	Sidechain
1	A	900	ASP	Mainchain
1	A	907	THR	Mainchain
1	A	936	LEU	Mainchain
1	A	952	ALA	Mainchain
1	A	966	ASN	Mainchain
1	A	992	ASP	Mainchain
1	A	998	LEU	Mainchain
2	B	1020	ARG	Sidechain
2	B	1025	HIS	Sidechain
2	B	104	GLU	Peptide
2	B	1062	HIS	Sidechain,Mainchain
2	B	107	GLY	Peptide
2	B	1086	PHE	Mainchain
2	B	109	THR	Peptide
2	B	1097	HIS	Sidechain
2	B	1101	ASP	Peptide
2	B	1108	ARG	Peptide
2	B	1109	GLY	Peptide
2	B	1141	HIS	Sidechain
2	B	1152	MET	Peptide
2	B	1153	GLU	Peptide
2	B	1157	ALA	Peptide
2	B	1166	CYS	Mainchain
2	B	1181	GLU	Peptide
2	B	1198	TYR	Sidechain
2	B	1217	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	B	1221	SER	Peptide
2	B	1222	ARG	Peptide
2	B	124	TYR	Sidechain
2	B	133	LYS	Peptide
2	B	180	TYR	Peptide
2	B	202	TYR	Sidechain
2	B	203	PHE	Sidechain
2	B	23	ALA	Mainchain
2	B	238	ALA	Mainchain
2	B	248	SER	Peptide
2	B	259	TYR	Sidechain
2	B	351	TYR	Sidechain
2	B	369	GLY	Peptide
2	B	408	LEU	Mainchain
2	B	431	TYR	Peptide
2	B	501	PRO	Peptide
2	B	518	HIS	Sidechain
2	B	546	SER	Mainchain
2	B	616	ILE	Mainchain
2	B	620	ARG	Mainchain
2	B	627	PHE	Sidechain
2	B	64	CYS	Peptide
2	B	642	ASP	Peptide
2	B	643	ASP	Peptide
2	B	644	GLU	Peptide
2	B	648	HIS	Sidechain
2	B	692	TYR	Sidechain
2	B	732	SER	Peptide
2	B	769	TYR	Sidechain
2	B	808	ALA	Mainchain
2	B	849	GLY	Mainchain
2	B	851	PHE	Sidechain
2	B	860	MET	Peptide
2	B	882	THR	Peptide
2	B	915	THR	Peptide
2	B	967	ARG	Mainchain
2	B	975	GLN	Mainchain
2	B	984	HIS	Sidechain
2	B	990	ILE	Mainchain
3	C	127	ARG	Mainchain
3	C	140	ASN	Peptide
3	C	156	THR	Mainchain

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Mol	Chain	Res	Type	Group
3	C	163	ILE	Mainchain
3	C	171	GLY	Mainchain
3	C	184	ASN	Peptide
3	C	186	LEU	Mainchain
3	C	190	ASP	Peptide
3	C	20	PHE	Sidechain
3	C	200	GLU	Sidechain
3	C	214	ASN	Peptide
3	C	227	THR	Mainchain
3	C	240	VAL	Mainchain
3	C	261	ALA	Peptide
3	C	267	GLN	Peptide
3	C	34	ARG	Sidechain
3	C	4	GLU	Peptide
3	C	62	PHE	Sidechain
3	C	96	SER	Peptide
4	E	119	SER	Peptide
4	E	125	PRO	Peptide
4	E	135	PHE	Sidechain
4	E	147	HIS	Sidechain
4	E	170	LEU	Peptide
4	E	212	ARG	Sidechain
4	E	56	LYS	Peptide
4	E	61	GLN	Mainchain
4	E	77	SER	Peptide
6	H	102	TYR	Peptide
6	H	103	LYS	Peptide
6	H	127	GLY	Peptide
6	H	131	ASN	Peptide
6	H	135	LEU	Peptide
6	H	136	LYS	Peptide
6	H	17	PRO	Peptide
6	H	29	ALA	Peptide
6	H	3	ASN	Peptide
6	H	54	SER	Peptide
6	H	61	SER	Peptide
6	H	62	SER	Peptide
6	H	86	ASP	Peptide
6	H	87	ARG	Peptide
6	H	88	SER	Peptide
7	I	100	PHE	Mainchain
7	I	111	THR	Peptide

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Mol	Chain	Res	Type	Group
7	I	15	TYR	Sidechain
7	I	3	THR	Peptide
7	I	33	SER	Mainchain
7	I	39	GLY	Mainchain
7	I	43	VAL	Mainchain
7	I	45	ARG	Sidechain
7	I	84	VAL	Mainchain
8	J	49	MET	Mainchain
8	J	9	SER	Mainchain
9	K	111	LEU	Peptide
9	K	40	HIS	Mainchain
9	K	58	PHE	Sidechain
9	K	70	ARG	Mainchain
9	K	71	PHE	Mainchain
10	L	27	LEU	Peptide
10	L	35	SER	Peptide
10	L	49	LYS	Peptide
10	L	59	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	10606	0	10660	1097	0
2	B	8690	0	8709	1000	2
3	C	2095	0	2053	264	0
4	E	1760	0	1788	203	1
5	F	670	0	690	70	0
6	H	1068	0	1040	223	0
7	I	990	0	948	109	0
8	J	525	0	538	60	0
9	K	919	0	927	122	0
10	L	364	0	389	108	0
11	A	2	0	0	0	0
12	A	2	0	0	1	0
12	B	1	0	0	0	0
12	C	1	0	0	1	0
12	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	J	1	0	0	2	0
12	L	1	0	0	2	0
13	B	29	0	11	13	0
14	A	2	0	0	0	0
14	B	3	0	0	7	0
All	All	27731	0	27753	3079	2

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 56.

All (3079) 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)
2:B:226:PHE:CD1	2:B:226:PHE:CE1	1.77	1.67
2:B:370:PHE:CD1	2:B:370:PHE:CE1	1.78	1.67
3:C:165:LYS:CD	3:C:165:LYS:CG	1.74	1.65
2:B:18:PHE:CG	2:B:18:PHE:CB	1.79	1.65
4:E:79:TRP:CB	4:E:79:TRP:CG	1.78	1.65
4:E:95:THR:CB	4:E:95:THR:CG2	1.75	1.65
10:L:40:LEU:CB	10:L:40:LEU:CG	1.75	1.65
1:A:302:THR:CG2	1:A:302:THR:CB	1.75	1.64
2:B:606:LYS:CD	2:B:606:LYS:CE	1.75	1.64
8:J:43:ARG:CG	8:J:43:ARG:CD	1.75	1.64
1:A:426:LEU:CG	1:A:426:LEU:CD1	1.74	1.64
4:E:194:GLU:CB	4:E:194:GLU:CG	1.75	1.64
4:E:212:ARG:CG	4:E:212:ARG:CD	1.76	1.64
1:A:1315:GLU:CG	1:A:1315:GLU:CB	1.75	1.64
1:A:1164:PRO:CD	1:A:1164:PRO:CG	1.76	1.64
1:A:1409:LEU:CG	1:A:1409:LEU:CD1	1.74	1.64
1:A:469:ARG:CG	1:A:469:ARG:CB	1.76	1.63
1:A:975:HIS:CA	1:A:975:HIS:CB	1.75	1.63
2:B:706:GLN:CG	2:B:706:GLN:CB	1.76	1.63
2:B:137:TYR:CG	2:B:137:TYR:CB	1.78	1.63
2:B:241:ARG:CG	2:B:241:ARG:CD	1.75	1.63
2:B:813:LYS:CD	2:B:813:LYS:CG	1.75	1.63
2:B:212:LEU:CD2	2:B:212:LEU:CG	1.75	1.63
2:B:723:VAL:CB	2:B:723:VAL:CA	1.76	1.63
4:E:98:ILE:CA	4:E:98:ILE:CB	1.76	1.62
6:H:104:PHE:CZ	6:H:104:PHE:CE2	1.82	1.62
1:A:69:THR:CA	1:A:69:THR:CB	1.74	1.62
2:B:502:ILE:CB	2:B:502:ILE:CG2	1.76	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:31:THR:CB	4:E:31:THR:CG2	1.76	1.62
2:B:620:ARG:CG	2:B:620:ARG:CD	1.75	1.62
2:B:883:LEU:CD2	2:B:883:LEU:CG	1.78	1.62
1:A:1225:PHE:CG	1:A:1225:PHE:CB	1.75	1.62
4:E:157:SER:CB	4:E:157:SER:CA	1.75	1.62
1:A:1194:ARG:CB	1:A:1194:ARG:CG	1.76	1.62
4:E:180:ARG:CB	4:E:180:ARG:CG	1.74	1.62
1:A:1445:ILE:CG2	1:A:1445:ILE:CB	1.76	1.62
4:E:180:ARG:CG	4:E:180:ARG:CD	1.75	1.62
2:B:654:ARG:CG	2:B:654:ARG:CB	1.77	1.62
3:C:245:VAL:CB	3:C:245:VAL:CG1	1.76	1.62
1:A:889:SER:CA	1:A:889:SER:CB	1.77	1.62
2:B:41:LYS:CE	2:B:41:LYS:CD	1.76	1.62
1:A:1286:LYS:CG	1:A:1286:LYS:CB	1.75	1.62
2:B:787:VAL:CB	2:B:787:VAL:CG1	1.74	1.62
9:K:72:LYS:CE	9:K:72:LYS:CD	1.76	1.62
1:A:1236:LEU:CG	1:A:1236:LEU:CD2	1.79	1.61
1:A:843:LYS:CE	1:A:843:LYS:CD	1.74	1.61
7:I:34:TYR:CB	7:I:34:TYR:CG	1.79	1.61
10:L:27:LEU:CG	10:L:27:LEU:CB	1.74	1.61
1:A:202:LEU:CD2	1:A:202:LEU:CG	1.76	1.61
2:B:883:LEU:CG	2:B:883:LEU:CD1	1.78	1.61
5:F:72:LYS:CG	5:F:72:LYS:CD	1.79	1.61
2:B:1198:TYR:CB	2:B:1198:TYR:CA	1.74	1.61
2:B:883:LEU:CG	2:B:883:LEU:CB	1.78	1.61
2:B:937:ALA:CB	2:B:937:ALA:CA	1.75	1.61
1:A:110:CYS:CB	1:A:110:CYS:CA	1.74	1.61
1:A:213:HIS:CB	1:A:213:HIS:CA	1.76	1.61
5:F:72:LYS:CE	5:F:72:LYS:CD	1.76	1.61
10:L:61:THR:CG2	10:L:61:THR:CB	1.77	1.61
1:A:264:PHE:CG	1:A:264:PHE:CB	1.80	1.60
1:A:934:LYS:CG	1:A:934:LYS:CD	1.77	1.60
2:B:509:ALA:CA	2:B:509:ALA:CB	1.76	1.60
2:B:870:ILE:CB	2:B:870:ILE:CG2	1.77	1.60
3:C:218:PRO:CB	3:C:218:PRO:CG	1.77	1.60
1:A:61:ILE:CB	1:A:61:ILE:CG2	1.77	1.60
2:B:1185:CYS:CA	2:B:1185:CYS:CB	1.78	1.60
4:E:43:LYS:CB	4:E:43:LYS:CG	1.78	1.60
6:H:22:LYS:CD	6:H:22:LYS:CG	1.75	1.60
1:A:1176:LEU:CD2	1:A:1176:LEU:CG	1.76	1.60
1:A:1225:PHE:CA	1:A:1225:PHE:CB	1.79	1.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:660:LYS:CG	2:B:660:LYS:CD	1.76	1.60
10:L:40:LEU:CD2	10:L:40:LEU:CG	1.74	1.60
2:B:425:THR:CG2	2:B:425:THR:CB	1.77	1.60
4:E:45:LYS:CE	4:E:45:LYS:CD	1.78	1.60
1:A:720:ARG:CG	1:A:720:ARG:CB	1.76	1.60
2:B:1154:ALA:CA	2:B:1154:ALA:CB	1.77	1.60
3:C:94:LYS:CG	3:C:94:LYS:CB	1.77	1.60
2:B:961:LEU:CG	2:B:961:LEU:CB	1.74	1.60
4:E:37:LEU:CD1	4:E:37:LEU:CG	1.75	1.60
4:E:61:GLN:CB	4:E:61:GLN:CG	1.75	1.60
1:A:46:THR:CA	1:A:46:THR:CB	1.78	1.59
4:E:57:MET:CB	4:E:57:MET:CG	1.77	1.59
10:L:47:ARG:CB	10:L:47:ARG:CG	1.76	1.59
1:A:744:LYS:CE	1:A:744:LYS:CD	1.80	1.59
1:A:635:ARG:CG	1:A:635:ARG:CD	1.80	1.59
4:E:12:LEU:CG	4:E:12:LEU:CD1	1.79	1.59
4:E:54:GLN:CG	4:E:54:GLN:CB	1.76	1.59
9:K:54:ARG:CG	9:K:54:ARG:CD	1.78	1.59
1:A:368:LYS:CE	1:A:368:LYS:CD	1.76	1.59
9:K:94:ILE:CA	9:K:94:ILE:CB	1.75	1.59
2:B:238:ALA:CB	2:B:238:ALA:CA	1.79	1.59
1:A:1350:LYS:CD	1:A:1350:LYS:CE	1.79	1.59
2:B:167:ILE:CG2	2:B:167:ILE:CB	1.75	1.59
6:H:63:LEU:CD2	6:H:63:LEU:CG	1.76	1.59
1:A:1235:LYS:CE	1:A:1235:LYS:CD	1.78	1.59
1:A:415:LEU:CD1	1:A:415:LEU:CG	1.78	1.59
7:I:42:LEU:CG	7:I:42:LEU:CD1	1.76	1.59
1:A:237:THR:CB	1:A:237:THR:CG2	1.81	1.58
1:A:976:THR:CB	1:A:976:THR:CA	1.75	1.58
2:B:934:LYS:CB	2:B:934:LYS:CG	1.75	1.58
1:A:1319:VAL:CB	1:A:1319:VAL:CG1	1.77	1.58
1:A:1432:GLN:CG	1:A:1432:GLN:CB	1.75	1.58
1:A:274:ILE:CA	1:A:274:ILE:CB	1.75	1.58
2:B:632:ARG:CD	2:B:632:ARG:CG	1.77	1.58
2:B:617:ARG:CG	2:B:617:ARG:CD	1.78	1.58
1:A:1290:LYS:CD	1:A:1290:LYS:CE	1.81	1.58
1:A:1363:VAL:CB	1:A:1363:VAL:CG1	1.80	1.58
2:B:137:TYR:CB	2:B:137:TYR:CA	1.75	1.58
2:B:98:THR:CB	2:B:98:THR:CA	1.74	1.58
3:C:199:LYS:CD	3:C:199:LYS:CG	1.76	1.58
9:K:113:THR:CG2	9:K:113:THR:CB	1.80	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:43:THR:CA	10:L:43:THR:CB	1.74	1.58
1:A:1385:THR:CB	1:A:1385:THR:CG2	1.79	1.58
2:B:217:ARG:CG	2:B:217:ARG:CD	1.74	1.58
2:B:895:ASP:CA	2:B:895:ASP:CB	1.76	1.58
1:A:1003:LYS:CG	1:A:1003:LYS:CB	1.80	1.58
7:I:46:HIS:CB	7:I:46:HIS:CA	1.76	1.58
2:B:1132:GLU:CB	2:B:1132:GLU:CG	1.76	1.58
6:H:107:VAL:CB	6:H:107:VAL:CA	1.80	1.58
1:A:123:ARG:CB	1:A:123:ARG:CG	1.78	1.58
1:A:427:GLN:CB	1:A:427:GLN:CG	1.80	1.58
2:B:965:LYS:CE	2:B:965:LYS:CD	1.75	1.58
1:A:1112:LYS:CB	1:A:1112:LYS:CG	1.79	1.58
6:H:22:LYS:CB	6:H:22:LYS:CG	1.78	1.58
2:B:871:THR:CA	2:B:871:THR:CB	1.78	1.58
10:L:27:LEU:CA	10:L:27:LEU:CB	1.79	1.58
6:H:131:ASN:CA	6:H:131:ASN:CB	1.78	1.57
7:I:1:MET:CA	7:I:1:MET:CB	1.74	1.57
1:A:1092:LYS:CB	1:A:1092:LYS:CG	1.76	1.57
1:A:1109:LYS:CG	1:A:1109:LYS:CD	1.78	1.57
1:A:1282:VAL:CG2	1:A:1282:VAL:CB	1.77	1.57
1:A:4:GLN:CG	1:A:4:GLN:CB	1.80	1.57
2:B:249:ARG:CD	2:B:249:ARG:CG	1.82	1.57
9:K:54:ARG:CG	9:K:54:ARG:CB	1.75	1.57
1:A:387:ARG:CG	1:A:387:ARG:CD	1.80	1.57
3:C:166:GLU:CB	3:C:166:GLU:CG	1.77	1.57
4:E:197:LYS:CD	4:E:197:LYS:CG	1.75	1.57
9:K:88:LYS:CG	9:K:88:LYS:CD	1.81	1.57
1:A:186:LYS:CB	1:A:186:LYS:CG	1.82	1.57
1:A:279:LEU:CD2	1:A:279:LEU:CG	1.76	1.57
6:H:77:ARG:CB	6:H:77:ARG:CG	1.80	1.57
7:I:77:LYS:CG	7:I:77:LYS:CD	1.80	1.57
9:K:12:LEU:CG	9:K:12:LEU:CD1	1.80	1.57
1:A:720:ARG:CG	1:A:720:ARG:CD	1.74	1.57
1:A:983:ILE:N	1:A:983:ILE:CA	1.68	1.57
1:A:1176:LEU:CD1	1:A:1176:LEU:CG	1.78	1.57
3:C:70:ILE:CG2	3:C:70:ILE:CB	1.82	1.57
3:C:86:CYS:CA	3:C:86:CYS:CB	1.83	1.57
2:B:418:LYS:CE	2:B:418:LYS:CD	1.82	1.57
4:E:91:LYS:CG	4:E:91:LYS:CB	1.78	1.57
8:J:30:LEU:CD2	8:J:30:LEU:CG	1.76	1.57
10:L:49:LYS:CD	10:L:49:LYS:CG	1.80	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:56:THR:CA	6:H:56:THR:CB	1.76	1.57
9:K:111:LEU:CD2	9:K:111:LEU:CG	1.76	1.57
1:A:670:ILE:CB	1:A:670:ILE:CG2	1.79	1.57
2:B:193:LYS:CD	2:B:193:LYS:CG	1.78	1.57
9:K:26:LYS:CE	9:K:26:LYS:CD	1.78	1.57
1:A:431:LYS:CD	1:A:431:LYS:CG	1.76	1.56
2:B:1002:THR:CB	2:B:1002:THR:CG2	1.77	1.56
2:B:108:VAL:CG2	2:B:108:VAL:CB	1.77	1.56
3:C:94:LYS:CG	3:C:94:LYS:CD	1.78	1.56
1:A:129:LYS:CG	1:A:129:LYS:CB	1.80	1.56
1:A:147:VAL:CB	1:A:147:VAL:CG1	1.76	1.56
2:B:230:ALA:CA	2:B:230:ALA:CB	1.75	1.56
2:B:451:LYS:CG	2:B:451:LYS:CB	1.75	1.56
2:B:726:ALA:CA	2:B:726:ALA:CB	1.79	1.56
2:B:883:LEU:CB	2:B:883:LEU:CA	1.82	1.56
6:H:32:THR:CA	6:H:32:THR:CB	1.77	1.56
2:B:227:LYS:CD	2:B:227:LYS:CG	1.78	1.56
1:A:1162:VAL:CG1	1:A:1162:VAL:CB	1.77	1.56
1:A:1176:LEU:CB	1:A:1176:LEU:CA	1.76	1.56
1:A:619:LYS:NZ	1:A:619:LYS:CE	1.69	1.56
2:B:118:ARG:CA	2:B:118:ARG:CB	1.74	1.56
2:B:418:LYS:CG	2:B:418:LYS:CD	1.79	1.56
2:B:1165:ILE:CB	2:B:1165:ILE:CA	1.81	1.56
2:B:367:LEU:CD1	2:B:367:LEU:CG	1.79	1.56
9:K:111:LEU:CD1	9:K:111:LEU:CG	1.83	1.56
10:L:58:LYS:NZ	10:L:58:LYS:CE	1.67	1.56
2:B:192:LEU:CD2	2:B:192:LEU:CG	1.82	1.56
1:A:144:THR:CB	1:A:144:THR:CA	1.76	1.56
1:A:806:ARG:CG	1:A:806:ARG:CB	1.79	1.56
2:B:136:THR:CA	2:B:136:THR:CB	1.78	1.56
2:B:228:LYS:CD	2:B:228:LYS:CG	1.78	1.56
2:B:25:ILE:CB	2:B:25:ILE:CG2	1.78	1.56
2:B:712:PRO:CB	2:B:712:PRO:CG	1.80	1.56
4:E:44:ALA:CB	4:E:44:ALA:CA	1.75	1.56
1:A:711:ARG:CB	1:A:711:ARG:CG	1.80	1.56
2:B:249:ARG:CA	2:B:249:ARG:C	1.74	1.56
3:C:199:LYS:CE	3:C:199:LYS:CD	1.81	1.56
3:C:35:ARG:CD	3:C:35:ARG:CG	1.83	1.56
2:B:1148:LYS:CE	2:B:1148:LYS:CD	1.81	1.56
2:B:639:ILE:CB	2:B:639:ILE:CG2	1.77	1.56
2:B:622:LYS:CB	2:B:622:LYS:CG	1.81	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:735:ALA:CA	2:B:735:ALA:N	1.68	1.56
6:H:136:LYS:CA	6:H:136:LYS:CB	1.77	1.56
3:C:160:LYS:CG	3:C:160:LYS:CD	1.78	1.55
5:F:123:LYS:CE	5:F:123:LYS:NZ	1.68	1.55
1:A:123:ARG:CD	1:A:123:ARG:CG	1.80	1.55
7:I:45:ARG:CD	7:I:45:ARG:CG	1.81	1.55
1:A:843:LYS:CB	1:A:843:LYS:CG	1.76	1.55
1:A:952:ALA:CA	1:A:952:ALA:CB	1.85	1.55
2:B:1101:ASP:CB	2:B:1101:ASP:CG	1.75	1.55
2:B:434:ARG:CG	2:B:434:ARG:CD	1.84	1.55
2:B:451:LYS:CD	2:B:451:LYS:CG	1.80	1.55
8:J:38:ARG:CG	8:J:38:ARG:CB	1.85	1.55
2:B:996:ARG:CD	2:B:996:ARG:CG	1.77	1.55
3:C:163:ILE:CB	3:C:163:ILE:CG2	1.84	1.55
4:E:131:THR:CA	4:E:131:THR:CB	1.77	1.55
1:A:217:LYS:CE	1:A:217:LYS:CD	1.81	1.55
1:A:737:LEU:CD2	1:A:737:LEU:CG	1.81	1.55
9:K:26:LYS:CB	9:K:26:LYS:CG	1.78	1.55
2:B:1061:GLU:CG	2:B:1061:GLU:CB	1.81	1.55
10:L:54:ARG:CG	10:L:54:ARG:CD	1.80	1.55
1:A:1094:VAL:CB	1:A:1094:VAL:CG1	1.84	1.55
1:A:1102:LYS:CG	1:A:1102:LYS:CB	1.77	1.55
1:A:1221:LYS:CB	1:A:1221:LYS:CG	1.79	1.55
1:A:1350:LYS:CD	1:A:1350:LYS:CG	1.78	1.55
1:A:31:SER:CA	1:A:31:SER:C	1.75	1.55
1:A:601:LYS:CG	1:A:601:LYS:CD	1.81	1.55
2:B:712:PRO:CG	2:B:712:PRO:CD	1.80	1.55
2:B:90:ILE:N	2:B:90:ILE:CA	1.69	1.55
2:B:933:SER:C	2:B:933:SER:CA	1.74	1.55
2:B:961:LEU:CG	2:B:961:LEU:CD2	1.82	1.55
6:H:111:LEU:CD1	6:H:111:LEU:CG	1.80	1.55
1:A:379:VAL:CB	1:A:379:VAL:CG2	1.80	1.55
4:E:20:LYS:CB	4:E:20:LYS:CG	1.74	1.55
7:I:49:ILE:CG2	7:I:49:ILE:CB	1.81	1.55
1:A:34:LYS:CB	1:A:34:LYS:CG	1.76	1.54
1:A:1133:LEU:CG	1:A:1133:LEU:CD2	1.78	1.54
2:B:106:ASP:CA	2:B:106:ASP:C	1.76	1.54
2:B:916:THR:CG2	2:B:916:THR:CB	1.85	1.54
10:L:49:LYS:CB	10:L:49:LYS:CG	1.75	1.54
1:A:205:GLU:CD	1:A:205:GLU:CG	1.76	1.54
1:A:695:LYS:CG	1:A:695:LYS:CD	1.80	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ALA:CA	1:A:9:ALA:CB	1.81	1.54
3:C:124:LEU:CD2	3:C:124:LEU:CG	1.77	1.54
10:L:27:LEU:CG	10:L:27:LEU:CD2	1.79	1.54
1:A:191:THR:CG2	1:A:191:THR:CB	1.78	1.54
2:B:935:ARG:CG	2:B:935:ARG:CD	1.79	1.54
3:C:205:LYS:CD	3:C:205:LYS:CE	1.75	1.54
4:E:50:MET:CA	4:E:50:MET:C	1.74	1.54
9:K:95:ILE:CB	9:K:95:ILE:CG2	1.74	1.54
1:A:49:LYS:CD	1:A:49:LYS:CG	1.79	1.54
2:B:723:VAL:CB	2:B:723:VAL:CG2	1.79	1.54
4:E:162:ARG:CG	4:E:162:ARG:CD	1.86	1.54
6:H:9:ILE:CB	6:H:9:ILE:CA	1.85	1.54
1:A:1055:ARG:CD	1:A:1055:ARG:CG	1.82	1.54
1:A:1203:ASN:C	1:A:1203:ASN:CA	1.75	1.54
1:A:1235:LYS:CB	1:A:1235:LYS:CG	1.82	1.54
3:C:147:LEU:CG	3:C:147:LEU:CB	1.75	1.54
3:C:154:LYS:CG	3:C:154:LYS:CD	1.83	1.54
1:A:1221:LYS:CG	1:A:1221:LYS:CD	1.81	1.54
1:A:965:GLN:CG	1:A:965:GLN:CD	1.75	1.54
2:B:1188:LYS:CG	2:B:1188:LYS:CD	1.76	1.54
3:C:205:LYS:CG	3:C:205:LYS:CD	1.85	1.54
4:E:152:LYS:CB	4:E:152:LYS:CG	1.85	1.54
1:A:15:LYS:CG	1:A:15:LYS:CB	1.79	1.54
1:A:795:GLU:CD	1:A:795:GLU:CG	1.76	1.54
13:B:3008:CTP:C1'	13:B:3008:CTP:N1	1.69	1.54
1:A:830:LYS:CD	1:A:830:LYS:CE	1.79	1.54
2:B:420:LEU:CD1	2:B:420:LEU:CG	1.80	1.54
1:A:1080:THR:C	1:A:1080:THR:CA	1.76	1.53
2:B:115:GLN:CD	2:B:115:GLN:CG	1.76	1.53
2:B:951:GLN:CB	2:B:951:GLN:CG	1.77	1.53
1:A:1222:ASN:CB	1:A:1222:ASN:CA	1.82	1.53
2:B:1102:LYS:CG	2:B:1102:LYS:CB	1.78	1.53
7:I:120:GLN:CG	7:I:120:GLN:CB	1.84	1.53
9:K:16:GLU:CG	9:K:16:GLU:CD	1.74	1.53
10:L:38:LEU:CD2	10:L:38:LEU:CG	1.79	1.53
10:L:46:VAL:CG2	10:L:46:VAL:CB	1.86	1.53
1:A:24:PRO:C	1:A:24:PRO:CA	1.74	1.53
2:B:1057:LYS:CE	2:B:1057:LYS:CD	1.86	1.53
2:B:344:LYS:CB	2:B:344:LYS:CG	1.83	1.53
6:H:11:GLN:CG	6:H:11:GLN:CB	1.82	1.53
7:I:93:LYS:CE	7:I:93:LYS:CD	1.85	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1132:LYS:CD	1:A:1132:LYS:CG	1.80	1.53
1:A:74:MET:CG	1:A:74:MET:CB	1.84	1.53
2:B:434:ARG:CG	2:B:434:ARG:CB	1.85	1.53
10:L:49:LYS:NZ	10:L:49:LYS:CE	1.70	1.53
2:B:1153:GLU:CG	2:B:1153:GLU:CD	1.76	1.53
2:B:1221:SER:CA	2:B:1221:SER:C	1.74	1.53
2:B:458:LYS:CD	2:B:458:LYS:CG	1.83	1.53
3:C:15:LYS:CE	3:C:15:LYS:CD	1.80	1.53
7:I:20:LYS:CD	7:I:20:LYS:CE	1.81	1.53
3:C:267:GLN:C	3:C:267:GLN:CA	1.76	1.53
1:A:180:LYS:CD	1:A:180:LYS:CG	1.85	1.53
2:B:243:ALA:CA	2:B:243:ALA:CB	1.84	1.53
2:B:41:LYS:CE	2:B:41:LYS:NZ	1.71	1.53
1:A:1080:THR:CB	1:A:1080:THR:CA	1.78	1.53
4:E:31:THR:CB	4:E:31:THR:CA	1.85	1.53
9:K:55:LYS:CG	9:K:55:LYS:CD	1.82	1.53
1:A:867:ILE:CG2	1:A:867:ILE:CB	1.85	1.53
3:C:146:LYS:CG	3:C:146:LYS:CB	1.86	1.53
7:I:3:THR:CG2	7:I:3:THR:CB	1.85	1.53
1:A:248:PRO:CG	1:A:248:PRO:CB	1.83	1.52
1:A:295:LEU:CG	1:A:295:LEU:CD2	1.83	1.52
2:B:882:THR:CB	2:B:882:THR:CG2	1.83	1.52
3:C:15:LYS:CD	3:C:15:LYS:CG	1.84	1.52
5:F:87:LYS:CE	5:F:87:LYS:CD	1.83	1.52
1:A:571:LEU:CD2	1:A:571:LEU:CG	1.84	1.52
7:I:115:LYS:NZ	7:I:115:LYS:CE	1.72	1.52
9:K:54:ARG:CD	9:K:54:ARG:NE	1.69	1.52
1:A:1176:LEU:CB	1:A:1176:LEU:CG	1.83	1.52
1:A:289:ILE:CA	1:A:289:ILE:CB	1.79	1.52
1:A:508:PRO:CG	1:A:508:PRO:CD	1.80	1.52
2:B:622:LYS:CD	2:B:622:LYS:CG	1.83	1.52
1:A:1128:GLN:CA	1:A:1128:GLN:C	1.77	1.52
4:E:129:PRO:CD	4:E:129:PRO:CG	1.85	1.52
8:J:42:LYS:CD	8:J:42:LYS:CG	1.85	1.52
1:A:1261:LYS:CD	1:A:1261:LYS:CE	1.86	1.52
1:A:1280:GLU:CD	1:A:1280:GLU:CG	1.78	1.52
2:B:595:ARG:CG	2:B:595:ARG:CD	1.87	1.52
2:B:70:ILE:CA	2:B:70:ILE:CB	1.87	1.52
2:B:962:LYS:CE	2:B:962:LYS:CD	1.88	1.52
9:K:89:ASN:CB	9:K:89:ASN:CG	1.78	1.52
1:A:1187:GLN:CG	1:A:1187:GLN:CB	1.85	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:GLU:CD	1:A:681:GLU:CG	1.77	1.52
1:A:705:LYS:CB	1:A:705:LYS:CA	1.84	1.52
2:B:1183:LYS:CG	2:B:1183:LYS:CB	1.79	1.52
2:B:63:ILE:CA	2:B:63:ILE:C	1.77	1.52
2:B:951:GLN:CD	2:B:951:GLN:CG	1.77	1.52
9:K:11:LEU:CG	9:K:11:LEU:CD1	1.83	1.52
2:B:415:GLN:CB	2:B:415:GLN:CG	1.86	1.52
7:I:72:ASP:CB	7:I:72:ASP:CG	1.77	1.52
2:B:416:LEU:CD2	2:B:416:LEU:CG	1.87	1.52
4:E:152:LYS:CG	4:E:152:LYS:CD	1.82	1.52
6:H:41:ASP:CG	6:H:41:ASP:CB	1.77	1.52
3:C:15:LYS:CB	3:C:15:LYS:CG	1.84	1.52
1:A:1003:LYS:CD	1:A:1003:LYS:CG	1.82	1.52
1:A:132:LYS:CG	1:A:132:LYS:CD	1.80	1.52
1:A:133:LYS:NZ	1:A:133:LYS:CE	1.70	1.52
1:A:393:ARG:CG	1:A:393:ARG:CD	1.86	1.52
1:A:984:LYS:CE	1:A:984:LYS:NZ	1.72	1.52
3:C:214:ASN:CB	3:C:214:ASN:CG	1.75	1.52
1:A:1099:PRO:CB	1:A:1099:PRO:CG	1.79	1.51
1:A:44:THR:CB	1:A:44:THR:CA	1.88	1.51
2:B:1029:CYS:C	2:B:1029:CYS:CA	1.79	1.51
6:H:139:ASN:CA	6:H:139:ASN:CB	1.84	1.51
1:A:173:THR:CB	1:A:173:THR:CG2	1.86	1.51
2:B:1097:HIS:CB	2:B:1097:HIS:CA	1.88	1.51
2:B:510:LYS:NZ	2:B:510:LYS:CE	1.72	1.51
1:A:389:THR:CG2	1:A:389:THR:CB	1.86	1.51
2:B:733:HIS:CA	2:B:733:HIS:C	1.77	1.51
2:B:99:LYS:NZ	2:B:99:LYS:CE	1.71	1.51
2:B:477:ALA:CA	2:B:477:ALA:CB	1.88	1.51
9:K:26:LYS:CG	9:K:26:LYS:CD	1.83	1.51
1:A:199:LEU:CG	1:A:199:LEU:CD1	1.85	1.51
2:B:227:LYS:CE	2:B:227:LYS:NZ	1.70	1.51
2:B:1057:LYS:CD	2:B:1057:LYS:CG	1.88	1.51
2:B:353:LYS:CD	2:B:353:LYS:CG	1.84	1.51
5:F:100:GLN:CD	5:F:100:GLN:CG	1.76	1.51
1:A:121:LEU:CG	1:A:121:LEU:CD1	1.86	1.51
1:A:1411:GLU:CG	1:A:1411:GLU:CD	1.76	1.51
2:B:384:ARG:CD	2:B:384:ARG:CG	1.85	1.51
6:H:19:ARG:CB	6:H:19:ARG:CG	1.85	1.51
1:A:1093:LYS:CD	1:A:1093:LYS:CG	1.88	1.51
1:A:217:LYS:CD	1:A:217:LYS:CG	1.84	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:LYS:CD	1:A:601:LYS:CE	1.89	1.51
7:I:117:LYS:CE	7:I:117:LYS:NZ	1.69	1.51
1:A:978:PRO:CB	1:A:978:PRO:CG	1.79	1.51
3:C:116:LYS:CE	3:C:116:LYS:CD	1.88	1.51
1:A:1102:LYS:CG	1:A:1102:LYS:CD	1.89	1.51
2:B:622:LYS:NZ	2:B:622:LYS:CE	1.74	1.51
2:B:655:LYS:CG	2:B:655:LYS:CD	1.86	1.51
2:B:959:ASP:CG	2:B:959:ASP:CB	1.79	1.51
1:A:104:GLU:C	1:A:104:GLU:CA	1.76	1.50
1:A:1132:LYS:CE	1:A:1132:LYS:CD	1.89	1.50
1:A:1281:ARG:CD	1:A:1281:ARG:CG	1.86	1.50
1:A:143:LYS:NZ	1:A:143:LYS:CE	1.71	1.50
2:B:191:LYS:CG	2:B:191:LYS:CB	1.84	1.50
2:B:465:ASN:CG	2:B:465:ASN:CB	1.79	1.50
4:E:165:LEU:CG	4:E:165:LEU:CD1	1.84	1.50
10:L:64:LEU:CD1	10:L:64:LEU:CG	1.84	1.50
1:A:5:GLN:CG	1:A:5:GLN:CB	1.89	1.50
2:B:1163:CYS:CA	2:B:1163:CYS:CB	1.89	1.50
2:B:882:THR:C	2:B:882:THR:CA	1.76	1.50
3:C:205:LYS:CG	3:C:205:LYS:CB	1.86	1.50
2:B:233:PRO:CB	2:B:233:PRO:CG	1.76	1.50
9:K:4:PRO:CD	9:K:4:PRO:CG	1.75	1.50
1:A:843:LYS:CD	1:A:843:LYS:CG	1.85	1.50
4:E:43:LYS:CE	4:E:43:LYS:CD	1.87	1.50
2:B:1189:ILE:CB	2:B:1189:ILE:CG2	1.86	1.50
2:B:245:GLU:C	2:B:245:GLU:CA	1.76	1.50
4:E:161:LYS:CD	4:E:161:LYS:CE	1.89	1.50
1:A:860:LEU:CG	1:A:860:LEU:CD1	1.88	1.50
7:I:1:MET:CG	7:I:1:MET:CB	1.90	1.50
1:A:1450:LEU:CG	1:A:1450:LEU:CD2	1.86	1.50
1:A:698:GLN:CG	1:A:698:GLN:CD	1.79	1.50
2:B:115:GLN:CB	2:B:115:GLN:CG	1.89	1.50
2:B:916:THR:CA	2:B:916:THR:C	1.80	1.50
2:B:344:LYS:CD	2:B:344:LYS:CE	1.86	1.49
2:B:531:GLN:CG	2:B:531:GLN:CB	1.89	1.49
1:A:157:ASP:CB	1:A:157:ASP:CG	1.81	1.49
1:A:196:GLU:CG	1:A:196:GLU:CD	1.80	1.49
1:A:938:LYS:CD	1:A:938:LYS:CG	1.90	1.49
1:A:567:LYS:NZ	1:A:567:LYS:CE	1.74	1.49
1:A:830:LYS:CD	1:A:830:LYS:CG	1.87	1.49
2:B:408:LEU:CG	2:B:408:LEU:CD1	1.87	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:CB	1:A:61:ILE:CA	1.89	1.49
9:K:20:LYS:CB	9:K:20:LYS:CG	1.91	1.49
1:A:992:ASP:CG	1:A:992:ASP:CB	1.81	1.49
2:B:593:PRO:CG	2:B:593:PRO:CB	1.87	1.49
5:F:87:LYS:CE	5:F:87:LYS:NZ	1.74	1.49
10:L:38:LEU:CD1	10:L:38:LEU:CG	1.86	1.49
5:F:76:LYS:CE	5:F:76:LYS:NZ	1.71	1.49
9:K:102:LYS:CE	9:K:102:LYS:CD	1.91	1.49
2:B:227:LYS:CE	2:B:227:LYS:CD	1.89	1.48
2:B:592:ASN:CG	2:B:592:ASN:CB	1.79	1.48
6:H:52:GLN:CD	6:H:52:GLN:CG	1.78	1.48
1:A:566:ILE:CB	1:A:566:ILE:CG2	1.88	1.48
2:B:915:THR:CA	2:B:915:THR:CB	1.85	1.48
10:L:48:CYS:CA	10:L:48:CYS:C	1.79	1.48
10:L:62:LYS:NZ	10:L:62:LYS:CE	1.72	1.48
1:A:110:CYS:CB	1:A:110:CYS:SG	2.02	1.48
1:A:1122:PRO:CG	1:A:1122:PRO:CB	1.77	1.48
5:F:111:LEU:CD2	5:F:111:LEU:CG	1.89	1.48
6:H:91:ASP:C	6:H:91:ASP:CA	1.81	1.48
10:L:26:THR:CB	10:L:26:THR:CA	1.91	1.48
10:L:45:ALA:CA	10:L:45:ALA:CB	1.87	1.48
1:A:1290:LYS:NZ	1:A:1290:LYS:CE	1.72	1.48
2:B:180:TYR:C	2:B:180:TYR:CA	1.81	1.48
2:B:646:LEU:CD1	2:B:646:LEU:CG	1.90	1.48
4:E:152:LYS:CE	4:E:152:LYS:CD	1.88	1.48
10:L:26:THR:CG2	10:L:26:THR:CB	1.90	1.48
4:E:84:ASP:CB	4:E:84:ASP:CG	1.78	1.48
1:A:1285:MET:CG	1:A:1285:MET:SD	2.02	1.48
2:B:432:MET:SD	2:B:432:MET:CE	2.02	1.48
2:B:556:THR:CB	2:B:556:THR:CG2	1.89	1.48
2:B:1080:LYS:CE	2:B:1080:LYS:NZ	1.76	1.47
2:B:270:LYS:NZ	2:B:270:LYS:CE	1.71	1.47
1:A:1109:LYS:CG	1:A:1109:LYS:CB	1.89	1.47
2:B:239:GLU:CG	2:B:239:GLU:CD	1.80	1.47
1:A:620:LYS:NZ	1:A:620:LYS:CE	1.75	1.47
2:B:171:PRO:CG	2:B:171:PRO:CB	1.82	1.47
2:B:502:ILE:CB	2:B:502:ILE:CA	1.90	1.47
6:H:3:ASN:CG	6:H:3:ASN:CB	1.81	1.47
4:E:103:LYS:CE	4:E:103:LYS:NZ	1.73	1.47
4:E:131:THR:CG2	4:E:131:THR:CB	1.86	1.47
4:E:162:ARG:CB	4:E:162:ARG:CG	1.90	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1:MET:CG	4:E:1:MET:SD	2.02	1.47
7:I:20:LYS:NZ	7:I:20:LYS:CE	1.75	1.47
10:L:62:LYS:CD	10:L:62:LYS:CE	1.90	1.47
9:K:55:LYS:CE	9:K:55:LYS:CD	1.93	1.47
1:A:291:GLU:CD	1:A:291:GLU:CG	1.80	1.47
6:H:2:SER:CA	6:H:2:SER:C	1.82	1.47
1:A:49:LYS:CD	1:A:49:LYS:CE	1.89	1.46
2:B:106:ASP:CG	2:B:106:ASP:CB	1.84	1.46
2:B:164:LYS:CE	2:B:164:LYS:CD	1.89	1.46
2:B:646:LEU:CD2	2:B:646:LEU:CG	1.93	1.46
3:C:50:GLU:CG	3:C:50:GLU:CD	1.82	1.46
9:K:26:LYS:CE	9:K:26:LYS:NZ	1.74	1.46
1:A:1262:LYS:CD	1:A:1262:LYS:CG	1.91	1.46
1:A:1350:LYS:NZ	1:A:1350:LYS:CE	1.75	1.46
1:A:66:LYS:CG	1:A:66:LYS:CB	1.94	1.46
2:B:368:GLU:CD	2:B:368:GLU:CG	1.79	1.46
2:B:668:ASP:CB	2:B:668:ASP:CG	1.82	1.46
4:E:201:LYS:CG	4:E:201:LYS:CD	1.91	1.46
4:E:41:ASP:CB	4:E:41:ASP:CG	1.84	1.46
1:A:1144:LYS:CE	1:A:1144:LYS:CD	1.89	1.46
3:C:124:LEU:CG	3:C:124:LEU:CD1	1.91	1.46
4:E:129:PRO:CG	4:E:129:PRO:CB	1.93	1.46
2:B:1002:THR:C	2:B:1002:THR:CA	1.83	1.46
3:C:137:LYS:CG	3:C:137:LYS:CB	1.94	1.46
7:I:120:GLN:CG	7:I:120:GLN:CD	1.80	1.46
4:E:43:LYS:CE	4:E:43:LYS:NZ	1.76	1.45
6:H:123:MET:SD	6:H:123:MET:CG	2.04	1.45
2:B:723:VAL:CB	2:B:723:VAL:CG1	1.95	1.45
7:I:17:ARG:CG	7:I:17:ARG:CD	1.93	1.45
9:K:20:LYS:CD	9:K:20:LYS:CG	1.92	1.45
3:C:135:GLN:CD	3:C:135:GLN:CG	1.80	1.45
1:A:188:ASP:C	1:A:188:ASP:CA	1.83	1.45
1:A:703:THR:CG2	1:A:703:THR:CB	1.92	1.44
1:A:938:LYS:CE	1:A:938:LYS:CD	1.94	1.44
2:B:1020:ARG:CA	2:B:1020:ARG:C	1.84	1.44
2:B:1098:MET:SD	2:B:1098:MET:CE	2.06	1.44
7:I:34:TYR:OH	7:I:34:TYR:CZ	1.67	1.44
1:A:69:THR:CA	1:A:69:THR:C	1.86	1.44
2:B:103:ASN:CB	2:B:103:ASN:CG	1.85	1.44
5:F:129:LYS:CE	5:F:129:LYS:CD	1.95	1.44
1:A:1277:GLU:CD	1:A:1277:GLU:CG	1.85	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:531:GLN:CG	2:B:531:GLN:CD	1.83	1.44
9:K:110:ASN:CG	9:K:110:ASN:CB	1.83	1.44
3:C:260:LEU:CD1	3:C:260:LEU:CG	1.92	1.44
1:A:1130:GLN:CG	1:A:1130:GLN:CD	1.86	1.44
2:B:961:LEU:CG	2:B:961:LEU:CD1	1.95	1.44
8:J:42:LYS:CD	8:J:42:LYS:CE	1.96	1.44
1:A:705:LYS:CE	1:A:705:LYS:NZ	1.77	1.44
2:B:527:THR:OG1	2:B:527:THR:CB	1.63	1.44
2:B:901:PRO:CG	2:B:901:PRO:CD	1.79	1.44
6:H:136:LYS:C	6:H:136:LYS:CA	1.83	1.44
2:B:1097:HIS:ND1	2:B:1097:HIS:HA	1.24	1.44
4:E:1:MET:CE	4:E:1:MET:SD	2.06	1.44
1:A:24:PRO:CG	1:A:24:PRO:CB	1.86	1.43
2:B:436:VAL:CB	2:B:436:VAL:CA	1.94	1.43
1:A:748:MET:CG	1:A:748:MET:SD	2.05	1.43
1:A:752:LYS:CD	1:A:752:LYS:CE	1.96	1.43
1:A:910:PRO:CB	1:A:910:PRO:CG	1.78	1.43
2:B:895:ASP:CB	2:B:895:ASP:CG	1.86	1.43
6:H:104:PHE:C	6:H:104:PHE:CA	1.85	1.43
7:I:13:MET:CE	7:I:13:MET:SD	2.04	1.43
5:F:106:PRO:CB	5:F:106:PRO:CG	1.82	1.43
7:I:93:LYS:CE	7:I:93:LYS:NZ	1.80	1.43
1:A:941:LYS:CD	1:A:941:LYS:CE	1.97	1.43
1:A:991:LYS:CE	1:A:991:LYS:NZ	1.79	1.42
2:B:868:MET:CE	2:B:868:MET:SD	2.08	1.42
2:B:246:LYS:C	2:B:246:LYS:CA	1.83	1.42
3:C:35:ARG:CB	3:C:35:ARG:CG	1.94	1.42
2:B:199:MET:SD	2:B:199:MET:CE	2.08	1.42
1:A:1132:LYS:CE	1:A:1132:LYS:NZ	1.79	1.42
1:A:162:VAL:CB	1:A:162:VAL:CG2	1.97	1.42
1:A:448:PRO:CB	1:A:448:PRO:CG	1.78	1.42
2:B:1156:ASP:CG	2:B:1156:ASP:CB	1.85	1.42
3:C:73:GLN:CG	3:C:73:GLN:CD	1.84	1.42
1:A:518:LYS:CD	1:A:518:LYS:CE	1.97	1.42
1:A:56:PRO:O	1:A:57:ARG:CD	1.65	1.42
2:B:1210:MET:CE	2:B:1210:MET:SD	2.08	1.42
2:B:346:GLU:CG	2:B:346:GLU:CD	1.85	1.42
1:A:695:LYS:CD	1:A:695:LYS:CE	1.95	1.42
1:A:1187:GLN:CG	1:A:1187:GLN:CD	1.85	1.41
2:B:1219:ASP:CG	2:B:1219:ASP:CB	1.87	1.41
2:B:736:THR:CG2	2:B:736:THR:CB	1.99	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:122:SER:OG	3:C:122:SER:CB	1.69	1.41
2:B:315:LYS:CE	2:B:315:LYS:NZ	1.82	1.41
1:A:1110:ASN:CB	1:A:1110:ASN:CG	1.88	1.41
4:E:24:LYS:CE	4:E:24:LYS:NZ	1.84	1.41
1:A:1222:ASN:CG	1:A:1222:ASN:CB	1.87	1.40
4:E:121:MET:SD	4:E:121:MET:CG	2.10	1.40
1:A:934:LYS:CE	1:A:934:LYS:CD	1.99	1.40
1:A:941:LYS:CG	1:A:941:LYS:CD	1.99	1.40
2:B:775:LYS:CB	2:B:775:LYS:CG	1.99	1.40
3:C:154:LYS:CG	3:C:154:LYS:CB	1.99	1.40
1:A:122:MET:SD	1:A:122:MET:CE	2.08	1.40
1:A:941:LYS:CE	1:A:941:LYS:NZ	1.82	1.40
1:A:1358:SER:OG	1:A:1358:SER:CB	1.70	1.40
2:B:641:GLU:CD	2:B:641:GLU:CG	1.88	1.40
2:B:870:ILE:CA	2:B:870:ILE:CB	2.00	1.40
1:A:620:LYS:CD	1:A:620:LYS:CE	1.99	1.40
3:C:102:GLN:CG	3:C:102:GLN:CB	1.96	1.40
3:C:154:LYS:CE	3:C:154:LYS:CD	1.99	1.40
1:A:346:ASP:CB	1:A:346:ASP:CG	1.88	1.39
2:B:962:LYS:CG	2:B:962:LYS:CD	2.00	1.39
1:A:1235:LYS:CE	1:A:1235:LYS:NZ	1.83	1.39
1:A:423:ASP:CG	1:A:423:ASP:CB	1.88	1.39
2:B:975:GLN:CD	2:B:975:GLN:NE2	1.72	1.39
4:E:50:MET:CG	4:E:50:MET:SD	2.09	1.39
1:A:895:LYS:CD	1:A:895:LYS:CE	1.99	1.39
2:B:986:GLN:CG	2:B:986:GLN:CD	1.91	1.39
1:A:70:CYS:SG	1:A:80:HIS:NE2	1.94	1.39
1:A:1446:ASP:CB	1:A:1446:ASP:CG	1.90	1.39
2:B:987:LYS:NZ	2:B:987:LYS:CE	1.85	1.39
1:A:1232:ASN:CG	1:A:1232:ASN:CB	1.89	1.38
5:F:129:LYS:CE	5:F:129:LYS:NZ	1.84	1.38
1:A:1135:ARG:CD	1:A:1135:ARG:CG	2.00	1.38
4:E:73:PRO:CG	4:E:73:PRO:CB	1.75	1.38
10:L:68:GLU:CD	10:L:68:GLU:CG	1.91	1.38
6:H:131:ASN:CG	6:H:131:ASN:CB	1.91	1.38
2:B:305:VAL:CB	2:B:305:VAL:CG1	2.01	1.38
2:B:598:GLU:CD	2:B:598:GLU:CG	1.92	1.38
2:B:652:LYS:NZ	2:B:652:LYS:CE	1.87	1.37
4:E:93:MET:CE	4:E:93:MET:SD	2.12	1.37
1:A:555:ASP:CG	1:A:555:ASP:CB	1.92	1.37
1:A:368:LYS:CD	1:A:368:LYS:CG	2.01	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:53:PRO:CB	4:E:53:PRO:CG	1.89	1.36
4:E:106:GLN:CD	4:E:106:GLN:CG	1.91	1.36
1:A:676:MET:CG	1:A:676:MET:SD	2.14	1.35
2:B:789:MET:SD	2:B:789:MET:CE	2.14	1.35
1:A:382:PRO:CB	1:A:382:PRO:CG	1.81	1.35
6:H:139:ASN:CB	6:H:139:ASN:CG	1.95	1.35
1:A:369:SER:OG	9:K:2:ASN:ND2	1.60	1.35
1:A:437:MET:CE	1:A:437:MET:SD	2.15	1.34
6:H:19:ARG:CD	6:H:19:ARG:CG	2.03	1.34
7:I:1:MET:CE	7:I:1:MET:SD	2.15	1.34
1:A:1272:THR:CG2	1:A:1272:THR:CB	2.04	1.34
1:A:728:LYS:CD	1:A:728:LYS:CG	2.03	1.33
1:A:761:MET:SD	1:A:761:MET:CE	2.15	1.33
2:B:347:LYS:CD	2:B:347:LYS:CG	2.04	1.33
7:I:55:THR:CG2	7:I:55:THR:CB	2.06	1.33
1:A:705:LYS:CG	1:A:705:LYS:CB	2.06	1.32
1:A:1259:MET:CE	1:A:1259:MET:SD	2.18	1.32
1:A:186:LYS:CD	1:A:186:LYS:CG	2.06	1.32
1:A:1294:PRO:CG	1:A:1294:PRO:CB	1.93	1.31
3:C:260:LEU:CD2	3:C:260:LEU:CG	2.06	1.31
13:B:3008:CTP:C2'	14:B:3010:HOH:O	1.65	1.31
3:C:165:LYS:NZ	3:C:165:LYS:CE	1.92	1.30
2:B:705:MET:CE	2:B:705:MET:CG	2.08	1.29
1:A:1259:MET:CG	1:A:1259:MET:SD	2.21	1.28
2:B:231:PRO:CB	2:B:231:PRO:CG	2.12	1.28
2:B:313:MET:SD	2:B:313:MET:CE	1.18	1.27
2:B:705:MET:SD	2:B:705:MET:CE	1.18	1.27
1:A:156:ASP:O	1:A:158:PRO:HD3	1.28	1.25
1:A:708:MET:SD	1:A:708:MET:CE	2.24	1.25
1:A:1202:MET:SD	1:A:1202:MET:CE	2.24	1.25
2:B:999:MET:SD	2:B:999:MET:CE	1.16	1.25
2:B:313:MET:CG	2:B:313:MET:CE	2.16	1.24
1:A:752:LYS:NZ	1:A:752:LYS:CE	2.02	1.23
2:B:766:ARG:NH2	13:B:3008:CTP:H5'2	1.52	1.22
4:E:20:LYS:CE	4:E:20:LYS:NZ	2.00	1.22
7:I:16:PRO:O	7:I:17:ARG:HD3	1.39	1.22
13:B:3008:CTP:C3'	14:B:3010:HOH:O	1.74	1.22
1:A:1285:MET:SD	1:A:1285:MET:CE	2.29	1.21
2:B:999:MET:CG	2:B:999:MET:CE	2.19	1.21
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	1.57	1.20
1:A:41:MET:SD	1:A:41:MET:CE	2.29	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:LYS:CE	1:A:728:LYS:CD	2.19	1.18
1:A:752:LYS:HE2	2:B:1019:SER:OG	1.43	1.17
2:B:1097:HIS:ND1	2:B:1097:HIS:CA	2.05	1.17
5:F:103:MET:CE	5:F:103:MET:SD	2.32	1.17
4:E:50:MET:CE	4:E:50:MET:SD	2.32	1.16
3:C:125:MET:SD	3:C:125:MET:CE	2.33	1.16
1:A:56:PRO:O	1:A:57:ARG:HD2	1.24	1.15
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.03	1.15
1:A:487:MET:SD	1:A:487:MET:CE	1.05	1.15
7:I:4:PHE:HE1	7:I:13:MET:HE2	1.09	1.14
3:C:75:MET:SD	3:C:75:MET:CE	2.36	1.14
6:H:128:ASN:O	6:H:131:ASN:ND2	1.82	1.13
2:B:269:ILE:HD13	2:B:317:CYS:SG	1.90	1.12
2:B:662:MET:CE	2:B:662:MET:SD	2.37	1.12
1:A:1176:LEU:CB	1:A:1176:LEU:HG	1.73	1.11
6:H:138:GLU:O	6:H:139:ASN:C	1.87	1.11
1:A:42:ASP:OD2	1:A:47:ARG:N	1.84	1.11
2:B:705:MET:SD	2:B:705:MET:HE1	1.76	1.11
10:L:58:LYS:O	10:L:59:ALA:HB3	1.51	1.11
2:B:999:MET:HE1	2:B:999:MET:SD	1.74	1.10
2:B:313:MET:HE2	2:B:313:MET:SD	1.76	1.10
2:B:705:MET:SD	2:B:705:MET:HE2	1.76	1.10
2:B:999:MET:SD	2:B:999:MET:HE2	1.74	1.10
2:B:705:MET:SD	2:B:705:MET:HE3	1.76	1.09
2:B:885:MET:CE	2:B:885:MET:SD	2.40	1.09
2:B:999:MET:HE3	2:B:999:MET:SD	1.74	1.09
1:A:1233:ASP:O	1:A:1234:GLU:HB3	1.42	1.09
1:A:304:MET:CE	1:A:304:MET:SD	2.40	1.09
1:A:487:MET:CE	1:A:487:MET:CG	2.31	1.09
2:B:313:MET:SD	2:B:313:MET:HE3	1.76	1.08
6:H:103:LYS:HB3	6:H:105:GLU:OE1	1.51	1.08
7:I:4:PHE:HE1	7:I:13:MET:CE	1.65	1.08
1:A:487:MET:SD	1:A:487:MET:HE2	1.65	1.07
2:B:313:MET:SD	2:B:313:MET:HE1	1.76	1.07
2:B:552:MET:SD	2:B:552:MET:CG	2.41	1.07
1:A:487:MET:HE1	1:A:487:MET:SD	1.65	1.07
1:A:901:LEU:H	1:A:926:GLN:NE2	1.54	1.06
7:I:45:ARG:HG2	7:I:45:ARG:HH11	1.17	1.06
1:A:1151:GLU:CG	7:I:45:ARG:HD2	1.86	1.06
1:A:487:MET:HE3	1:A:487:MET:SD	1.65	1.05
3:C:242:GLN:O	3:C:246:ARG:HB2	1.56	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:ASP:OD1	9:K:26:LYS:NZ	1.89	1.05
10:L:31:CYS:SG	10:L:34:CYS:SG	2.55	1.05
1:A:567:LYS:HE2	6:H:95:TYR:CE2	1.91	1.05
1:A:247:ARG:NH1	1:A:263:THR:HG23	1.73	1.04
3:C:265:MET:SD	3:C:265:MET:CE	2.46	1.04
4:E:24:LYS:NZ	4:E:24:LYS:CD	2.20	1.04
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.21	1.03
2:B:364:ILE:HD13	2:B:585:VAL:HG13	1.32	1.03
1:A:1385:THR:HG22	1:A:1385:THR:O	1.56	1.03
2:B:58:THR:O	2:B:62:ILE:HG12	1.60	1.02
2:B:114:PRO:HD3	2:B:124:TYR:CE1	1.94	1.02
2:B:270:LYS:CD	2:B:270:LYS:NZ	2.22	1.02
1:A:1133:LEU:CB	1:A:1133:LEU:CD2	2.37	1.02
1:A:1079:MET:HG2	1:A:1359:ASP:OD2	1.60	1.01
2:B:1077:THR:HG22	2:B:1079:LYS:H	1.26	1.01
5:F:77:ASP:O	5:F:78:GLN:HB2	1.58	1.00
4:E:169:ARG:HD3	5:F:140:ASP:OD2	1.60	1.00
1:A:1055:ARG:CG	1:A:1055:ARG:NE	2.24	1.00
2:B:424:LEU:O	2:B:424:LEU:HG	1.61	1.00
10:L:58:LYS:O	10:L:59:ALA:CB	2.08	1.00
1:A:56:PRO:O	1:A:57:ARG:HD3	1.58	0.99
6:H:55:LEU:HD22	6:H:144:ILE:HD12	1.43	0.99
2:B:792:MET:CE	2:B:792:MET:SD	2.49	0.99
1:A:110:CYS:SG	1:A:148:CYS:SG	2.60	0.99
7:I:4:PHE:CE1	7:I:13:MET:CE	2.45	0.99
1:A:566:ILE:HD13	6:H:96:VAL:HG12	1.45	0.98
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.46	0.98
2:B:25:ILE:CG2	2:B:658:ILE:HD11	1.93	0.98
3:C:71:PRO:HB2	3:C:133:ILE:HD12	1.46	0.98
3:C:152:GLU:OE2	3:C:154:LYS:HD2	1.64	0.97
2:B:424:LEU:O	2:B:424:LEU:CG	2.13	0.97
9:K:1:MET:SD	9:K:1:MET:CE	2.53	0.97
2:B:660:LYS:CE	2:B:660:LYS:CG	2.41	0.97
1:A:379:VAL:CG1	1:A:379:VAL:CG2	2.43	0.96
1:A:579:SER:HA	1:A:582:ILE:HD13	1.47	0.96
2:B:643:ASP:O	2:B:644:GLU:HB2	1.62	0.96
8:J:2:ILE:CD1	8:J:57:ILE:HG21	1.95	0.96
1:A:380:VAL:HG13	1:A:385:ILE:HD13	1.44	0.96
6:H:106:GLU:O	6:H:107:VAL:O	1.82	0.96
6:H:22:LYS:CE	6:H:22:LYS:CG	2.42	0.96
9:K:95:ILE:CG2	9:K:95:ILE:CG1	2.44	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:THR:HG21	1:A:617:VAL:H	1.31	0.96
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	1.63	0.96
1:A:903:ASN:C	1:A:903:ASN:HD22	1.65	0.95
2:B:1148:LYS:NZ	2:B:1148:LYS:CD	2.27	0.95
3:C:172:PRO:O	3:C:235:VAL:HG12	1.64	0.95
4:E:31:THR:OG1	4:E:34:GLU:HB2	1.66	0.95
1:A:752:LYS:HE2	2:B:1019:SER:CB	1.96	0.95
2:B:955:THR:HG21	10:L:55:ILE:HD13	1.49	0.95
2:B:1051:THR:HG22	2:B:1053:GLU:N	1.80	0.94
1:A:567:LYS:CD	6:H:95:TYR:HA	1.96	0.94
1:A:55:ASP:O	1:A:57:ARG:N	1.99	0.94
6:H:103:LYS:O	6:H:115:TYR:HD1	1.51	0.94
2:B:620:ARG:NE	2:B:620:ARG:CG	2.29	0.94
7:I:4:PHE:CE1	7:I:13:MET:HE2	2.02	0.94
1:A:567:LYS:HG3	1:A:568:PRO:CD	1.97	0.94
1:A:55:ASP:OD1	1:A:55:ASP:O	1.84	0.94
1:A:752:LYS:CE	2:B:1019:SER:OG	2.15	0.94
1:A:187:LYS:HB2	1:A:194:ALA:HB3	1.48	0.94
3:C:54:ASN:OD1	3:C:56:THR:HB	1.66	0.94
2:B:1220:ARG:O	2:B:1222:ARG:HD3	1.68	0.93
8:J:2:ILE:HD13	8:J:57:ILE:HG21	1.48	0.93
2:B:1190:ASP:O	2:B:1191:ILE:HG12	1.65	0.93
2:B:552:MET:SD	2:B:552:MET:CE	2.57	0.93
2:B:712:PRO:N	2:B:712:PRO:CG	2.32	0.93
2:B:542:MET:HG3	2:B:747:MET:CE	1.98	0.93
2:B:498:THR:CG2	2:B:537:LYS:HB2	1.99	0.93
7:I:45:ARG:HH11	7:I:45:ARG:CG	1.82	0.93
2:B:766:ARG:HH22	13:B:3008:CTP:H5'2	1.26	0.93
9:K:111:LEU:CD2	9:K:111:LEU:HG	1.99	0.92
10:L:34:CYS:HG	12:L:3005:ZN:ZN	0.65	0.92
3:C:86:CYS:HA	3:C:86:CYS:CB	1.99	0.92
1:A:567:LYS:HD3	6:H:95:TYR:CG	2.04	0.92
9:K:110:ASN:O	9:K:112:GLN:N	2.01	0.92
2:B:955:THR:HG22	10:L:54:ARG:O	1.69	0.92
2:B:1166:CYS:O	2:B:1168:LEU:N	2.01	0.92
6:H:89:LEU:O	6:H:91:ASP:N	2.02	0.92
8:J:43:ARG:CG	8:J:43:ARG:NE	2.32	0.92
1:A:567:LYS:CE	6:H:95:TYR:CE1	2.53	0.92
10:L:40:LEU:HG	10:L:40:LEU:CB	1.97	0.92
7:I:16:PRO:O	7:I:17:ARG:CD	2.18	0.91
1:A:1176:LEU:CB	1:A:1176:LEU:HA	1.99	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:103:LYS:HG2	6:H:105:GLU:OE2	1.70	0.91
2:B:916:THR:N	2:B:935:ARG:O	2.03	0.91
2:B:25:ILE:CG1	2:B:25:ILE:CG2	2.48	0.91
1:A:1079:MET:SD	1:A:1359:ASP:OD2	2.29	0.91
3:C:99:LEU:HD12	3:C:99:LEU:N	1.86	0.91
1:A:1203:ASN:HA	1:A:1203:ASN:C	1.90	0.91
10:L:26:THR:CG2	10:L:27:LEU:H	1.81	0.91
2:B:766:ARG:HH22	13:B:3008:CTP:C5'	1.83	0.91
1:A:156:ASP:O	1:A:158:PRO:CD	2.19	0.90
6:H:130:ARG:C	6:H:130:ARG:HD2	1.90	0.90
1:A:108:MET:H	1:A:171:GLN:HE22	1.15	0.90
3:C:163:ILE:CG2	3:C:163:ILE:HB	1.98	0.90
1:A:567:LYS:HD3	6:H:95:TYR:CA	2.01	0.90
1:A:1079:MET:CG	1:A:1359:ASP:OD2	2.18	0.90
1:A:567:LYS:CD	6:H:95:TYR:CG	2.55	0.90
1:A:1161:THR:CG2	1:A:1163:ILE:H	1.84	0.90
6:H:63:LEU:C	6:H:90:ALA:HB3	1.91	0.90
4:E:79:TRP:HB2	4:E:105:PHE:CD1	2.06	0.90
2:B:1198:TYR:CB	2:B:1198:TYR:HA	2.02	0.89
2:B:639:ILE:CG2	2:B:639:ILE:CG1	2.49	0.89
1:A:148:CYS:HG	12:A:3006:ZN:ZN	0.62	0.89
3:C:95:CYS:HG	12:C:3002:ZN:ZN	0.71	0.89
2:B:766:ARG:NH2	13:B:3008:CTP:C5'	2.35	0.89
6:H:6:PHE:CD2	6:H:7:ASP:N	2.40	0.89
3:C:116:LYS:NZ	3:C:116:LYS:CD	2.36	0.89
1:A:901:LEU:HB2	1:A:926:GLN:HE21	1.37	0.89
1:A:679:ILE:HD11	1:A:732:LEU:HB2	1.55	0.89
5:F:81:THR:CG2	5:F:136:ARG:HH11	1.85	0.89
1:A:1194:ARG:CD	1:A:1194:ARG:CB	2.51	0.89
2:B:217:ARG:NE	2:B:217:ARG:CG	2.36	0.89
6:H:63:LEU:H	6:H:63:LEU:HD12	1.35	0.88
7:I:4:PHE:CE1	7:I:13:MET:HE1	2.08	0.88
2:B:895:ASP:CB	2:B:895:ASP:HA	2.03	0.88
1:A:567:LYS:CE	6:H:95:TYR:CZ	2.55	0.88
7:I:45:ARG:NH1	7:I:45:ARG:HG2	1.89	0.88
1:A:31:SER:HB3	1:A:83:HIS:HD2	1.39	0.88
6:H:93:TYR:HB3	6:H:144:ILE:O	1.74	0.88
10:L:34:CYS:CB	10:L:51:CYS:HB3	2.03	0.88
2:B:1002:THR:CG2	2:B:1002:THR:OG1	2.22	0.88
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.39	0.87
1:A:555:ASP:OD1	9:K:26:LYS:CE	2.23	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:916:THR:C	2:B:916:THR:HA	1.90	0.87
2:B:98:THR:C	2:B:98:THR:CB	2.43	0.87
4:E:36:GLU:O	4:E:37:LEU:C	2.12	0.87
8:J:7:CYS:HG	8:J:45:CYS:HG	0.91	0.87
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.15	0.87
1:A:567:LYS:HD3	6:H:95:TYR:HA	1.56	0.87
1:A:1286:LYS:CD	1:A:1286:LYS:CB	2.52	0.87
8:J:7:CYS:HG	12:J:3001:ZN:ZN	0.59	0.87
2:B:101:MET:SD	2:B:101:MET:CE	2.63	0.86
2:B:498:THR:HG21	2:B:537:LYS:HB2	1.56	0.86
1:A:1151:GLU:HG2	7:I:45:ARG:HD2	1.55	0.86
2:B:424:LEU:HD23	2:B:424:LEU:C	1.96	0.86
4:E:83:CYS:O	4:E:113:GLN:NE2	2.07	0.86
1:A:567:LYS:HB3	6:H:96:VAL:H	1.40	0.86
1:A:567:LYS:HD3	6:H:95:TYR:CD2	2.11	0.86
4:E:79:TRP:HB2	4:E:105:PHE:CE1	2.11	0.86
5:F:123:LYS:NZ	5:F:123:LYS:CD	2.39	0.86
7:I:42:LEU:CD2	7:I:42:LEU:CD1	2.54	0.86
1:A:187:LYS:HG3	1:A:194:ALA:CB	2.05	0.86
1:A:503:GLN:NE2	5:F:90:ARG:NH2	2.24	0.86
7:I:51:ASN:HB2	7:I:118:ARG:CZ	2.06	0.85
2:B:1097:HIS:CA	2:B:1097:HIS:CG	2.57	0.85
2:B:515:HIS:H	2:B:518:HIS:HD2	1.25	0.85
10:L:34:CYS:SG	10:L:36:SER:OG	2.34	0.85
2:B:294:ASP:H	7:I:12:ASN:HD22	1.18	0.85
1:A:567:LYS:HB3	6:H:96:VAL:N	1.91	0.85
1:A:1298:TYR:O	1:A:1299:VAL:HG23	1.77	0.85
2:B:593:PRO:HG2	2:B:617:ARG:NH2	1.92	0.85
1:A:752:LYS:CG	1:A:752:LYS:CE	2.53	0.85
1:A:351:THR:CG2	2:B:1103:ILE:HG13	2.07	0.85
2:B:212:LEU:CD1	2:B:212:LEU:CD2	2.54	0.85
2:B:502:ILE:HB	2:B:502:ILE:CG2	2.04	0.85
1:A:155:GLU:OE2	4:E:125:PRO:HB2	1.76	0.84
1:A:55:ASP:N	1:A:56:PRO:CD	2.40	0.84
6:H:123:MET:HE1	6:H:142:LEU:HD13	1.58	0.84
8:J:7:CYS:SG	8:J:45:CYS:SG	2.75	0.84
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.60	0.84
2:B:723:VAL:CB	2:B:723:VAL:HA	2.02	0.84
6:H:106:GLU:O	6:H:107:VAL:C	2.16	0.84
4:E:71:LYS:NZ	4:E:160:GLU:OE2	2.10	0.84
1:A:184:SER:HB2	1:A:199:LEU:HD23	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:CE	6:H:95:TYR:CE2	2.60	0.84
2:B:169:ARG:HG3	2:B:454:THR:CG2	2.07	0.84
2:B:294:ASP:H	7:I:12:ASN:ND2	1.75	0.84
4:E:6:GLU:OE2	4:E:43:LYS:NZ	2.11	0.83
6:H:5:LEU:O	6:H:133:ASN:ND2	2.11	0.83
1:A:711:ARG:HE	7:I:95:THR:HG22	1.43	0.83
2:B:615:MET:HG2	2:B:626:ILE:HD12	1.60	0.83
2:B:691:GLU:HG2	2:B:693:ILE:HD11	1.59	0.83
9:K:111:LEU:CB	9:K:111:LEU:CD1	2.57	0.83
10:L:51:CYS:SG	10:L:53:HIS:HB2	2.19	0.83
1:A:1385:THR:C	1:A:1385:THR:CG2	2.47	0.83
1:A:503:GLN:NE2	5:F:90:ARG:HH21	1.76	0.83
1:A:571:LEU:CD2	1:A:571:LEU:CD1	2.56	0.83
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.14	0.83
2:B:90:ILE:N	2:B:90:ILE:HA	1.92	0.83
1:A:849:MET:HE2	1:A:1061:GLY:HA2	1.58	0.83
3:C:40:GLU:HA	3:C:163:ILE:HD12	1.60	0.83
6:H:138:GLU:O	6:H:140:ALA:N	2.11	0.83
7:I:34:TYR:CA	7:I:34:TYR:CG	2.61	0.83
4:E:157:SER:CB	4:E:157:SER:C	2.47	0.83
1:A:247:ARG:HH11	1:A:263:THR:HG23	1.41	0.82
10:L:64:LEU:CD1	10:L:64:LEU:HG	2.06	0.82
3:C:245:VAL:CG2	3:C:245:VAL:CG1	2.57	0.82
9:K:24:ASP:OD1	9:K:74:ARG:NH1	2.13	0.82
10:L:34:CYS:HB3	10:L:51:CYS:CB	2.08	0.82
1:A:889:SER:CB	1:A:889:SER:C	2.47	0.82
10:L:38:LEU:CD1	10:L:38:LEU:HG	2.06	0.82
1:A:1364:ASN:HD22	1:A:1366:ARG:H	1.25	0.82
1:A:711:ARG:CA	1:A:711:ARG:CG	2.58	0.82
1:A:1118:VAL:HB	1:A:1327:ILE:HD12	1.60	0.82
2:B:680:THR:HG22	2:B:682:SER:H	1.42	0.82
1:A:145:LYS:HE3	1:A:149:GLU:CD	1.99	0.82
1:A:73:GLY:O	1:A:75:ASN:N	2.12	0.82
2:B:130:VAL:H	2:B:167:ILE:HD11	1.44	0.82
2:B:431:TYR:O	2:B:431:TYR:CD2	2.32	0.82
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.14	0.82
2:B:114:PRO:HD3	2:B:124:TYR:HE1	1.41	0.82
2:B:561:TRP:O	2:B:590:HIS:HE1	1.62	0.82
1:A:110:CYS:C	1:A:110:CYS:CB	2.47	0.82
2:B:884:ARG:O	2:B:936:ASP:HB3	1.80	0.82
9:K:18:LYS:O	9:K:19:LEU:HD23	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:53:ASP:OD2	9:K:81:TYR:OH	1.97	0.82
2:B:1163:CYS:HA	2:B:1191:ILE:HD13	1.62	0.81
13:B:3008:CTP:H3'	14:B:3010:HOH:O	1.57	0.81
1:A:1198:ASP:OD1	1:A:1200:ALA:HB3	1.80	0.81
1:A:472:LEU:O	1:A:475:THR:HB	1.81	0.81
2:B:169:ARG:HG3	2:B:454:THR:HG21	1.61	0.81
4:E:100:ILE:HG22	4:E:101:GLN:N	1.92	0.81
2:B:1198:TYR:CA	2:B:1198:TYR:CG	2.62	0.81
2:B:1221:SER:HA	2:B:1221:SER:C	1.96	0.81
1:A:1409:LEU:CD1	1:A:1409:LEU:HG	2.05	0.81
2:B:820:GLY:HA3	2:B:1091:TYR:CZ	2.15	0.81
3:C:245:VAL:HB	3:C:245:VAL:CG1	2.05	0.81
2:B:1051:THR:CG2	2:B:1053:GLU:H	1.91	0.81
2:B:261:ARG:O	2:B:264:SER:N	2.12	0.81
1:A:952:ALA:N	1:A:952:ALA:CB	2.44	0.81
6:H:57:VAL:HG22	6:H:144:ILE:HD11	1.63	0.81
2:B:104:GLU:OE1	10:L:54:ARG:NE	2.13	0.81
1:A:1445:ILE:CG2	1:A:1445:ILE:CA	2.59	0.81
1:A:636:GLU:OE2	1:A:962:ARG:CD	2.28	0.81
2:B:643:ASP:O	2:B:644:GLU:CB	2.29	0.80
10:L:47:ARG:HG2	10:L:48:CYS:H	1.46	0.80
1:A:64:ASN:OD1	1:A:64:ASN:O	1.98	0.80
2:B:813:LYS:CE	2:B:813:LYS:CG	2.59	0.80
1:A:69:THR:C	1:A:69:THR:HA	1.98	0.80
2:B:754:SER:O	2:B:806:THR:HG21	1.81	0.80
1:A:1350:LYS:CB	1:A:1350:LYS:CD	2.59	0.80
2:B:712:PRO:CA	2:B:712:PRO:CG	2.59	0.80
6:H:2:SER:HA	6:H:2:SER:C	1.98	0.80
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.16	0.80
1:A:1162:VAL:CG1	1:A:1162:VAL:CA	2.59	0.80
1:A:901:LEU:H	1:A:926:GLN:HE22	1.26	0.80
4:E:165:LEU:CB	4:E:165:LEU:CD1	2.60	0.80
1:A:104:GLU:C	1:A:104:GLU:CB	2.51	0.79
2:B:424:LEU:CD2	2:B:424:LEU:O	2.30	0.79
4:E:98:ILE:HA	4:E:98:ILE:CB	2.06	0.79
1:A:748:MET:CB	1:A:748:MET:SD	2.70	0.79
13:B:3008:CTP:H2'	14:B:3010:HOH:O	1.47	0.79
4:E:147:HIS:HD2	4:E:149:LEU:H	1.25	0.79
1:A:1161:THR:HG22	1:A:1163:ILE:N	1.97	0.79
1:A:1385:THR:CG2	1:A:1385:THR:O	2.31	0.79
1:A:23:SER:O	1:A:27:VAL:HG23	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:55:ARG:O	4:E:56:LYS:C	2.16	0.79
1:A:1120:LEU:HD21	1:A:1131:ALA:HB2	1.64	0.79
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.64	0.79
1:A:636:GLU:OE2	1:A:962:ARG:HD2	1.83	0.79
1:A:487:MET:HE2	1:A:487:MET:CG	2.02	0.79
6:H:97:MET:HE3	6:H:118:PHE:CG	2.16	0.79
1:A:42:ASP:OD2	1:A:46:THR:C	2.21	0.79
2:B:1185:CYS:HA	2:B:1185:CYS:CB	2.10	0.78
2:B:952:VAL:HG22	2:B:966:VAL:HG22	1.65	0.78
5:F:105:ALA:HB1	5:F:106:PRO:HD2	1.65	0.78
1:A:567:LYS:CG	1:A:568:PRO:CD	2.61	0.78
2:B:1065:GLN:HE22	2:B:1067:ARG:HB2	1.47	0.78
1:A:1148:ILE:HD11	1:A:1198:ASP:HB2	1.65	0.78
2:B:63:ILE:HA	2:B:63:ILE:C	2.03	0.78
1:A:1003:LYS:CG	1:A:1003:LYS:CA	2.61	0.78
1:A:587:HIS:CE1	1:A:969:GLN:HG2	2.19	0.78
2:B:1128:LEU:O	2:B:1128:LEU:HG	1.84	0.78
1:A:1072:ILE:HD11	1:A:1368:MET:HG3	1.66	0.78
2:B:357:GLN:NE2	2:B:368:GLU:HG2	1.99	0.78
9:K:82:ASP:OD1	9:K:83:PRO:HG2	1.82	0.78
2:B:243:ALA:HB2	2:B:251:ILE:HD13	1.64	0.78
3:C:167:HIS:HD2	3:C:169:LYS:H	1.30	0.78
6:H:103:LYS:CB	6:H:105:GLU:OE1	2.30	0.78
2:B:227:LYS:CB	2:B:227:LYS:CD	2.63	0.77
6:H:32:THR:HB	6:H:32:THR:CA	2.10	0.77
1:A:1282:VAL:CA	1:A:1282:VAL:CG2	2.62	0.77
1:A:61:ILE:CB	1:A:61:ILE:HA	2.10	0.77
4:E:37:LEU:CD1	4:E:37:LEU:HG	2.06	0.77
7:I:13:MET:CE	7:I:13:MET:CG	2.61	0.77
1:A:1233:ASP:O	1:A:1234:GLU:CB	2.26	0.77
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.67	0.77
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.66	0.77
2:B:509:ALA:N	2:B:509:ALA:CB	2.48	0.77
3:C:70:ILE:CG2	3:C:70:ILE:CA	2.63	0.77
2:B:136:THR:HA	2:B:136:THR:CB	2.10	0.77
6:H:89:LEU:C	6:H:91:ASP:H	1.86	0.77
1:A:31:SER:CB	1:A:83:HIS:HD2	1.97	0.77
3:C:146:LYS:CD	3:C:146:LYS:CB	2.62	0.77
1:A:247:ARG:NH1	1:A:263:THR:CG2	2.47	0.77
1:A:351:THR:CG2	2:B:1103:ILE:CG1	2.63	0.77
2:B:242:SER:HG	2:B:363:HIS:HD1	1.29	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1222:ARG:NH1	2:B:1222:ARG:HG2	1.99	0.77
3:C:35:ARG:NE	3:C:35:ARG:CG	2.48	0.77
1:A:555:ASP:OD1	9:K:26:LYS:HE3	1.83	0.77
1:A:32:VAL:HG23	1:A:33:ALA:H	1.49	0.76
2:B:841:MET:SD	2:B:846:ILE:HD11	2.25	0.76
3:C:86:CYS:SG	3:C:95:CYS:HB3	2.25	0.76
2:B:617:ARG:CB	2:B:617:ARG:CD	2.60	0.76
3:C:239:PRO:O	3:C:242:GLN:HB2	1.85	0.76
1:A:55:ASP:N	1:A:56:PRO:HD2	2.01	0.76
1:A:806:ARG:CD	1:A:806:ARG:CB	2.63	0.76
1:A:752:LYS:HZ3	2:B:1019:SER:N	1.82	0.76
13:B:3008:CTP:C1'	13:B:3008:CTP:C6	2.67	0.76
2:B:916:THR:HB	2:B:935:ARG:HB2	1.67	0.76
3:C:147:LEU:HG	3:C:147:LEU:CB	2.09	0.76
10:L:27:LEU:HG	10:L:27:LEU:CB	2.07	0.76
2:B:268:THR:C	2:B:269:ILE:HD12	2.06	0.76
1:A:1151:GLU:OE2	7:I:45:ARG:HD3	1.85	0.76
1:A:752:LYS:HZ3	2:B:1019:SER:H	1.32	0.76
10:L:31:CYS:SG	10:L:51:CYS:SG	2.83	0.76
1:A:1363:VAL:CA	1:A:1363:VAL:CG1	2.62	0.76
5:F:114:GLU:HB2	5:F:120:ILE:HD13	1.65	0.76
1:A:567:LYS:CE	6:H:95:TYR:CD1	2.69	0.76
1:A:670:ILE:CG2	1:A:670:ILE:CA	2.64	0.76
9:K:78:THR:HG22	9:K:79:GLU:H	1.50	0.76
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.21	0.75
10:L:38:LEU:O	10:L:39:SER:HB2	1.84	0.75
1:A:42:ASP:OD1	1:A:45:GLN:HA	1.87	0.75
1:A:867:ILE:CG2	1:A:867:ILE:CG1	2.63	0.75
9:K:23:PRO:O	9:K:23:PRO:HD2	1.86	0.75
3:C:55:THR:HB	3:C:152:GLU:H	1.52	0.75
6:H:77:ARG:O	6:H:78:SER:O	2.04	0.75
1:A:518:LYS:CD	1:A:518:LYS:NZ	2.50	0.75
7:I:45:ARG:NH1	7:I:45:ARG:CG	2.48	0.75
9:K:65:HIS:HD2	9:K:67:PHE:H	1.31	0.75
1:A:1281:ARG:CD	1:A:1281:ARG:CB	2.64	0.75
2:B:1222:ARG:HH11	2:B:1222:ARG:CG	2.00	0.75
2:B:1163:CYS:HB2	2:B:1182:CYS:SG	2.26	0.75
2:B:639:ILE:CA	2:B:639:ILE:CG2	2.65	0.75
2:B:915:THR:CA	2:B:915:THR:HB	2.09	0.75
2:B:961:LEU:HG	2:B:961:LEU:CB	2.12	0.75
2:B:999:MET:CG	2:B:999:MET:HE3	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:169:ARG:CD	5:F:140:ASP:OD2	2.35	0.75
2:B:1161:HIS:C	2:B:1162:ILE:HD12	2.06	0.75
4:E:12:LEU:HD21	4:E:58:MET:SD	2.27	0.75
6:H:63:LEU:H	6:H:63:LEU:CD1	1.99	0.75
4:E:131:THR:CA	4:E:131:THR:HB	2.11	0.75
5:F:77:ASP:O	5:F:78:GLN:CB	2.22	0.75
1:A:1364:ASN:ND2	1:A:1366:ARG:H	1.83	0.74
2:B:134:LYS:O	2:B:135:ARG:HG3	1.87	0.74
6:H:123:MET:HE1	6:H:142:LEU:CD1	2.16	0.74
1:A:582:ILE:HD12	1:A:582:ILE:H	1.52	0.74
1:A:886:ILE:HD12	1:A:943:LEU:HB3	1.69	0.74
2:B:705:MET:CE	2:B:705:MET:HG3	2.12	0.74
6:H:32:THR:CB	6:H:32:THR:HA	2.10	0.74
1:A:567:LYS:HE2	6:H:95:TYR:CZ	2.19	0.74
1:A:676:MET:CB	1:A:676:MET:SD	2.75	0.74
2:B:1154:ALA:HA	2:B:1154:ALA:CB	2.11	0.74
2:B:417:PHE:CD2	2:B:417:PHE:C	2.60	0.74
1:A:1242:VAL:HG11	1:A:1259:MET:CE	2.17	0.74
2:B:90:ILE:HD12	2:B:432:MET:SD	2.27	0.74
6:H:105:GLU:H	6:H:105:GLU:CD	1.90	0.74
7:I:4:PHE:CZ	7:I:13:MET:HE1	2.23	0.74
1:A:426:LEU:HG	1:A:426:LEU:CD1	2.12	0.74
1:A:567:LYS:CG	1:A:568:PRO:HD3	2.17	0.74
6:H:138:GLU:HG2	6:H:139:ASN:N	2.01	0.74
2:B:477:ALA:CB	2:B:477:ALA:HA	2.14	0.74
1:A:202:LEU:CD2	1:A:202:LEU:CD1	2.66	0.74
1:A:50:ILE:HG22	1:A:52:GLY:H	1.52	0.74
2:B:420:LEU:CD1	2:B:420:LEU:HG	2.13	0.74
2:B:25:ILE:HG21	2:B:658:ILE:HD11	1.69	0.74
6:H:107:VAL:CG2	6:H:107:VAL:CA	2.64	0.74
1:A:120:GLU:HG2	1:A:123:ARG:HH22	1.53	0.73
2:B:106:ASP:HA	2:B:106:ASP:C	2.02	0.73
9:K:102:LYS:O	9:K:106:GLU:HB2	1.89	0.73
1:A:1176:LEU:CD2	1:A:1176:LEU:CD1	2.66	0.73
1:A:431:LYS:CE	1:A:431:LYS:CG	2.64	0.73
1:A:596:THR:HG22	1:A:597:LEU:H	1.52	0.73
2:B:408:LEU:CB	2:B:408:LEU:CD1	2.67	0.73
10:L:26:THR:HG22	10:L:27:LEU:H	1.52	0.73
1:A:389:THR:CG2	1:A:389:THR:OG1	2.37	0.73
1:A:858:ASN:HD22	1:A:858:ASN:C	1.92	0.73
2:B:890:TYR:OH	2:B:936:ASP:OD1	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:152:GLU:OE2	3:C:154:LYS:CD	2.36	0.73
4:E:12:LEU:CD1	4:E:12:LEU:CD2	2.66	0.73
1:A:187:LYS:CB	1:A:194:ALA:HB3	2.18	0.73
2:B:130:VAL:HG22	2:B:167:ILE:HD11	1.70	0.73
1:A:567:LYS:CB	6:H:96:VAL:H	2.02	0.73
9:K:35:PHE:HE1	9:K:73:LEU:HD12	1.52	0.73
4:E:91:LYS:CB	4:E:91:LYS:CD	2.67	0.73
8:J:45:CYS:HG	12:J:3001:ZN:ZN	0.40	0.73
1:A:1259:MET:CB	1:A:1259:MET:SD	2.76	0.73
1:A:503:GLN:HE21	5:F:90:ARG:HH21	1.35	0.73
1:A:903:ASN:C	1:A:903:ASN:ND2	2.35	0.73
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.71	0.73
4:E:20:LYS:CB	4:E:20:LYS:CD	2.66	0.73
4:E:98:ILE:CA	4:E:98:ILE:HB	2.15	0.73
1:A:1133:LEU:CD2	1:A:1133:LEU:HB3	2.18	0.72
1:A:279:LEU:CD1	1:A:279:LEU:CD2	2.64	0.72
2:B:313:MET:CG	2:B:313:MET:HE2	1.99	0.72
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.70	0.72
2:B:167:ILE:CG2	2:B:167:ILE:CG1	2.66	0.72
2:B:624:LEU:HD11	2:B:626:ILE:HD11	1.71	0.72
6:H:103:LYS:O	6:H:115:TYR:CD1	2.40	0.72
9:K:94:ILE:CG2	9:K:94:ILE:CA	2.64	0.72
2:B:137:TYR:CB	2:B:137:TYR:HA	2.13	0.72
6:H:47:PHE:CZ	6:H:146:ARG:HD2	2.25	0.72
7:I:3:THR:CG2	7:I:3:THR:CA	2.67	0.72
1:A:1265:ASN:O	1:A:1266:THR:C	2.23	0.72
2:B:1002:THR:CG2	2:B:1002:THR:CA	2.65	0.72
4:E:212:ARG:CG	4:E:212:ARG:NE	2.52	0.72
8:J:30:LEU:CD2	8:J:30:LEU:CD1	2.64	0.72
4:E:31:THR:CA	4:E:31:THR:HB	2.13	0.72
6:H:17:PRO:HB3	6:H:24:CYS:SG	2.29	0.72
1:A:1138:ILE:HD11	1:A:1319:VAL:HG21	1.71	0.72
1:A:511:ILE:HD13	1:A:521:MET:SD	2.29	0.72
1:A:596:THR:HG22	1:A:597:LEU:HD12	1.71	0.72
2:B:1097:HIS:CG	2:B:1097:HIS:HA	2.19	0.72
1:A:1151:GLU:OE2	7:I:45:ARG:CD	2.38	0.72
4:E:29:PHE:O	4:E:30:ILE:HD13	1.89	0.72
10:L:27:LEU:HG	10:L:27:LEU:CD2	2.15	0.72
2:B:1020:ARG:HA	2:B:1020:ARG:C	2.07	0.72
2:B:424:LEU:HD23	2:B:424:LEU:O	1.89	0.72
4:E:79:TRP:CA	4:E:79:TRP:CG	2.73	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1319:VAL:CG2	1:A:1319:VAL:CG1	2.65	0.72
2:B:556:THR:CG2	2:B:556:THR:CA	2.67	0.72
9:K:94:ILE:HA	9:K:94:ILE:CB	2.13	0.72
1:A:595:THR:HG22	1:A:596:THR:N	2.04	0.71
1:A:752:LYS:HE2	2:B:1019:SER:HG	1.52	0.71
2:B:701:ILE:HD13	2:B:703:ILE:HG13	1.72	0.71
2:B:999:MET:HE3	2:B:999:MET:HG2	1.70	0.71
2:B:435:THR:HG23	2:B:437:GLU:HB2	1.70	0.71
2:B:933:SER:CA	2:B:934:LYS:N	2.53	0.71
6:H:103:LYS:CG	6:H:105:GLU:OE2	2.38	0.71
1:A:415:LEU:CD1	1:A:415:LEU:CB	2.68	0.71
2:B:238:ALA:CB	2:B:238:ALA:N	2.52	0.71
1:A:54:ASN:C	1:A:56:PRO:HD2	2.10	0.71
1:A:567:LYS:CE	6:H:95:TYR:CD2	2.74	0.71
7:I:32:CYS:HB2	7:I:34:TYR:H	1.54	0.71
9:K:72:LYS:CE	9:K:72:LYS:CG	2.66	0.71
1:A:1222:ASN:HA	1:A:1222:ASN:CB	2.14	0.71
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.72	0.71
13:B:3008:CTP:C1'	14:B:3010:HOH:O	2.18	0.71
7:I:98:VAL:HG22	7:I:99:LEU:N	2.04	0.71
1:A:1385:THR:CA	1:A:1385:THR:CG2	2.68	0.71
1:A:266:LEU:HA	1:A:269:ILE:HD12	1.71	0.71
2:B:99:LYS:NZ	2:B:183:GLU:OE1	2.24	0.71
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.25	0.71
1:A:369:SER:CB	9:K:2:ASN:ND2	2.52	0.71
1:A:147:VAL:CG2	1:A:147:VAL:CG1	2.69	0.71
1:A:385:ILE:HD11	1:A:426:LEU:HB2	1.72	0.71
2:B:431:TYR:O	2:B:431:TYR:HD2	1.73	0.71
4:E:36:GLU:O	4:E:38:PRO:N	2.23	0.71
1:A:720:ARG:CG	1:A:720:ARG:CA	2.69	0.70
2:B:237:VAL:HG12	2:B:238:ALA:N	2.04	0.70
3:C:163:ILE:CG1	3:C:163:ILE:CG2	2.65	0.70
5:F:101:ILE:HD12	5:F:107:VAL:HG22	1.73	0.70
2:B:1221:SER:OG	5:F:141:GLY:HA3	1.91	0.70
6:H:139:ASN:HA	6:H:139:ASN:CB	2.14	0.70
2:B:251:ILE:HG22	2:B:251:ILE:O	1.92	0.70
2:B:70:ILE:CA	2:B:70:ILE:HB	2.17	0.70
6:H:107:VAL:CA	6:H:107:VAL:HB	2.15	0.70
1:A:1072:ILE:HD13	1:A:1363:VAL:HG11	1.73	0.70
1:A:356:ASP:OD2	1:A:469:ARG:HD3	1.90	0.70
1:A:237:THR:CG2	1:A:237:THR:HB	2.11	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1077:THR:HG22	2:B:1079:LYS:N	2.05	0.70
2:B:1166:CYS:O	2:B:1167:GLY:C	2.23	0.70
2:B:663:ALA:O	2:B:667:GLN:HG3	1.92	0.70
1:A:567:LYS:HE2	6:H:95:TYR:CD2	2.27	0.70
2:B:775:LYS:CD	2:B:775:LYS:CB	2.70	0.70
2:B:98:THR:N	2:B:98:THR:CB	2.54	0.70
6:H:56:THR:N	6:H:56:THR:CB	2.50	0.70
2:B:955:THR:HG23	10:L:55:ILE:HA	1.73	0.70
1:A:107:CYS:SG	1:A:148:CYS:SG	2.90	0.70
3:C:162:GLY:HA3	3:C:170:TRP:CD2	2.26	0.70
2:B:1162:ILE:CD1	2:B:1194:ILE:HG12	2.22	0.70
2:B:498:THR:HG22	2:B:537:LYS:HB2	1.72	0.70
6:H:6:PHE:CG	6:H:7:ASP:N	2.58	0.70
8:J:42:LYS:HG3	8:J:43:ARG:N	2.07	0.70
1:A:1364:ASN:HD22	1:A:1366:ARG:HD2	1.54	0.69
1:A:380:VAL:CG1	1:A:385:ILE:HD13	2.21	0.69
2:B:1077:THR:CG2	2:B:1079:LYS:H	2.04	0.69
2:B:592:ASN:O	2:B:593:PRO:C	2.24	0.69
3:C:19:ASP:C	3:C:19:ASP:OD1	2.30	0.69
5:F:75:PRO:O	5:F:77:ASP:O	2.10	0.69
1:A:295:LEU:CB	1:A:295:LEU:CD2	2.68	0.69
2:B:724:ASP:O	2:B:726:ALA:N	2.25	0.69
6:H:113:ALA:HA	6:H:125:LEU:O	1.92	0.69
1:A:837:ILE:HD11	1:A:1102:LYS:HG2	1.73	0.69
1:A:1225:PHE:HA	1:A:1225:PHE:CB	2.15	0.69
2:B:1163:CYS:SG	2:B:1165:ILE:HG12	2.33	0.69
3:C:120:ILE:H	3:C:120:ILE:HD12	1.56	0.69
7:I:13:MET:HE2	7:I:13:MET:HG3	1.74	0.69
1:A:703:THR:CG2	1:A:703:THR:CA	2.69	0.69
2:B:757:PRO:HD2	2:B:984:HIS:HE1	1.58	0.69
7:I:46:HIS:CG	7:I:46:HIS:CA	2.72	0.69
1:A:1138:ILE:HD12	1:A:1316:VAL:HG22	1.75	0.69
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.23	0.69
2:B:357:GLN:HE21	2:B:368:GLU:HG2	1.56	0.69
2:B:550:ASP:OD1	2:B:551:PRO:HD2	1.93	0.69
2:B:877:PRO:O	2:B:878:GLN:HG2	1.92	0.69
3:C:41:ILE:C	3:C:163:ILE:HD11	2.12	0.69
2:B:1166:CYS:CB	2:B:1185:CYS:SG	2.78	0.69
2:B:487:THR:HG22	2:B:490:SER:H	1.57	0.69
3:C:25:VAL:HG11	3:C:29:MET:HG2	1.73	0.69
8:J:51:LEU:O	8:J:51:LEU:HG	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:THR:HG22	1:A:712:GLU:H	1.57	0.69
2:B:1222:ARG:HH11	2:B:1222:ARG:CB	2.06	0.69
6:H:103:LYS:NZ	6:H:105:GLU:OE2	2.16	0.69
2:B:955:THR:CG2	10:L:55:ILE:HD13	2.20	0.69
1:A:46:THR:HB	1:A:46:THR:CA	2.13	0.69
2:B:128:LEU:O	2:B:167:ILE:HD12	1.92	0.69
2:B:655:LYS:CB	2:B:655:LYS:CD	2.69	0.69
1:A:567:LYS:CG	6:H:96:VAL:H	2.06	0.69
8:J:7:CYS:CB	8:J:10:CYS:HG	2.06	0.69
1:A:636:GLU:OE2	1:A:962:ARG:HD3	1.93	0.68
2:B:787:VAL:CA	2:B:787:VAL:CG1	2.69	0.68
3:C:267:GLN:C	3:C:267:GLN:HA	2.05	0.68
6:H:89:LEU:C	6:H:91:ASP:N	2.44	0.68
1:A:351:THR:HG23	2:B:1103:ILE:CG1	2.23	0.68
2:B:705:MET:HE3	2:B:705:MET:CG	2.04	0.68
3:C:124:LEU:HD23	3:C:124:LEU:N	2.09	0.68
1:A:144:THR:CA	1:A:144:THR:HB	2.12	0.68
5:F:97:ARG:NH2	5:F:101:ILE:HD11	2.09	0.68
1:A:4:GLN:CG	1:A:4:GLN:N	2.56	0.68
2:B:1025:HIS:HE1	2:B:1090:THR:HG21	1.56	0.68
1:A:72:GLU:OE2	2:B:1175:LEU:HD11	1.92	0.68
2:B:1222:ARG:HH11	2:B:1222:ARG:HB2	1.58	0.68
2:B:283:VAL:HG22	2:B:297:ILE:HD13	1.76	0.68
7:I:34:TYR:CB	7:I:34:TYR:CD2	2.62	0.68
2:B:1190:ASP:O	2:B:1191:ILE:CG1	2.42	0.68
2:B:225:VAL:O	2:B:226:PHE:CD2	2.46	0.68
2:B:643:ASP:HB3	2:B:644:GLU:C	2.14	0.68
1:A:715:GLU:OE1	1:A:774:ARG:HD3	1.92	0.68
2:B:883:LEU:HG	2:B:883:LEU:CB	2.11	0.68
3:C:15:LYS:O	3:C:240:VAL:CG2	2.41	0.68
3:C:50:GLU:HB3	10:L:64:LEU:HD13	1.75	0.68
1:A:1259:MET:HB2	1:A:1259:MET:SD	2.33	0.68
1:A:1364:ASN:HD21	1:A:1366:ARG:HD2	1.53	0.68
1:A:567:LYS:CB	6:H:95:TYR:HA	2.24	0.68
2:B:243:ALA:C	2:B:244:LEU:HG	2.13	0.68
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.27	0.67
3:C:33:LEU:HD13	3:C:248:ILE:HD13	1.75	0.67
1:A:385:ILE:HD11	1:A:426:LEU:CB	2.23	0.67
1:A:503:GLN:HE21	5:F:90:ARG:NH2	1.90	0.67
2:B:118:ARG:HH22	2:B:194:GLU:CG	2.06	0.67
2:B:787:VAL:C	2:B:787:VAL:CG1	2.61	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:18:VAL:HG23	3:C:240:VAL:HG11	1.75	0.67
8:J:10:CYS:SG	8:J:45:CYS:SG	2.92	0.67
10:L:27:LEU:CG	10:L:27:LEU:HB3	2.15	0.67
1:A:469:ARG:CD	1:A:469:ARG:CB	2.70	0.67
2:B:26:THR:O	2:B:27:ALA:C	2.29	0.67
1:A:107:CYS:SG	1:A:167:CYS:SG	2.93	0.67
1:A:679:ILE:HD12	1:A:729:ALA:HA	1.77	0.67
2:B:1002:THR:CG2	2:B:1006:ILE:HB	2.24	0.67
2:B:654:ARG:CB	2:B:654:ARG:CD	2.69	0.67
6:H:111:LEU:CD2	6:H:111:LEU:CD1	2.71	0.67
6:H:123:MET:CB	6:H:123:MET:SD	2.82	0.67
6:H:96:VAL:HG22	6:H:143:LEU:HD23	1.75	0.67
1:A:1224:LEU:HG	1:A:1225:PHE:N	2.09	0.67
1:A:744:LYS:HD3	1:A:748:MET:SD	2.35	0.67
2:B:549:THR:HG22	2:B:628:THR:HB	1.77	0.67
2:B:879:ARG:NH2	2:B:885:MET:CE	2.57	0.67
6:H:135:LEU:HD13	6:H:139:ASN:O	1.95	0.67
1:A:289:ILE:CA	1:A:289:ILE:CG1	2.71	0.67
2:B:293:PRO:O	2:B:294:ASP:C	2.31	0.67
3:C:205:LYS:CG	3:C:205:LYS:CA	2.71	0.67
6:H:123:MET:HE1	6:H:142:LEU:HD22	1.76	0.67
8:J:2:ILE:HD11	8:J:57:ILE:HG21	1.76	0.67
1:A:531:ILE:HD11	1:A:578:LEU:CD2	2.25	0.67
2:B:68:THR:HG23	2:B:91:SER:HB3	1.77	0.67
9:K:35:PHE:CE1	9:K:73:LEU:HD12	2.29	0.67
1:A:1072:ILE:CD1	1:A:1363:VAL:HG11	2.25	0.67
1:A:347:PHE:H	2:B:1107:ALA:HA	1.60	0.67
1:A:741:ASN:HD22	1:A:741:ASN:C	1.96	0.67
2:B:1020:ARG:CA	2:B:1021:MET:N	2.55	0.67
2:B:864:LYS:O	2:B:961:LEU:CD2	2.43	0.67
1:A:31:SER:CA	1:A:32:VAL:N	2.57	0.67
1:A:857:ARG:HA	1:A:864:ILE:HD13	1.76	0.67
4:E:98:ILE:O	4:E:101:GLN:HB3	1.94	0.67
9:K:113:THR:CG2	9:K:113:THR:CA	2.69	0.67
3:C:252:GLN:HE22	9:K:99:GLY:HA2	1.59	0.67
1:A:426:LEU:CD2	1:A:426:LEU:CD1	2.73	0.67
1:A:741:ASN:ND2	1:A:741:ASN:C	2.48	0.67
2:B:542:MET:HG3	2:B:747:MET:HE3	1.75	0.67
2:B:217:ARG:HD3	2:B:407:ASP:OD2	1.94	0.66
10:L:31:CYS:HG	10:L:34:CYS:HG	1.26	0.66
1:A:123:ARG:CA	1:A:123:ARG:CG	2.73	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:9:ILE:HB	6:H:9:ILE:CA	2.16	0.66
1:A:834:THR:HG21	1:A:1077:THR:CA	2.25	0.66
2:B:795:ILE:HD13	2:B:856:PHE:HE1	1.59	0.66
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.25	0.66
2:B:1222:ARG:NH1	2:B:1222:ARG:CG	2.56	0.66
2:B:705:MET:CG	2:B:705:MET:HE2	2.09	0.66
2:B:806:THR:HG23	2:B:808:ALA:H	1.61	0.66
9:K:12:LEU:CD1	9:K:12:LEU:CD2	2.72	0.66
10:L:38:LEU:HD13	10:L:48:CYS:HA	1.77	0.66
2:B:120:ARG:HG2	10:L:55:ILE:HD11	1.75	0.66
1:A:119:ASN:O	1:A:120:GLU:HB2	1.94	0.66
1:A:587:HIS:HD2	1:A:966:ASN:OD1	1.78	0.66
8:J:2:ILE:HD13	8:J:57:ILE:CG2	2.24	0.66
1:A:965:GLN:CB	1:A:965:GLN:CD	2.58	0.66
2:B:417:PHE:CD2	2:B:417:PHE:O	2.48	0.66
2:B:25:ILE:HD11	2:B:651:LEU:HD12	1.77	0.66
1:A:379:VAL:CG2	1:A:379:VAL:CA	2.74	0.66
2:B:882:THR:C	2:B:882:THR:HA	2.09	0.66
2:B:882:THR:HG1	2:B:933:SER:N	1.94	0.66
3:C:86:CYS:SG	3:C:95:CYS:CB	2.83	0.66
6:H:25:ARG:NH2	6:H:41:ASP:OD2	2.29	0.66
6:H:76:THR:HG22	6:H:76:THR:O	1.96	0.66
1:A:1432:GLN:CG	1:A:1432:GLN:CA	2.71	0.66
1:A:11:LEU:HD11	2:B:1195:HIS:CD2	2.31	0.66
2:B:451:LYS:HA	2:B:454:THR:HB	1.77	0.66
1:A:666:ILE:HG13	2:B:1027:ILE:HD13	1.75	0.66
2:B:864:LYS:O	2:B:961:LEU:HD23	1.96	0.66
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.44	0.65
1:A:34:LYS:HG2	1:A:83:HIS:HE1	1.61	0.65
2:B:542:MET:HG3	2:B:747:MET:HE2	1.77	0.65
6:H:111:LEU:CD1	6:H:111:LEU:HG	2.16	0.65
8:J:7:CYS:SG	8:J:46:CYS:SG	2.94	0.65
1:A:1055:ARG:CB	1:A:1055:ARG:CD	2.73	0.65
2:B:118:ARG:HH22	2:B:194:GLU:CD	1.98	0.65
1:A:1224:LEU:HD23	1:A:1226:VAL:CG2	2.26	0.65
1:A:567:LYS:CD	6:H:95:TYR:CD2	2.77	0.65
1:A:934:LYS:CB	1:A:934:LYS:CD	2.70	0.65
2:B:787:VAL:O	2:B:787:VAL:CG1	2.44	0.65
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.26	0.65
4:E:61:GLN:HB2	4:E:79:TRP:CE3	2.32	0.65
6:H:22:LYS:HE2	6:H:22:LYS:CG	2.24	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:13:MET:CE	7:I:13:MET:HG3	2.24	0.65
1:A:1151:GLU:CG	7:I:45:ARG:CD	2.70	0.65
1:A:672:ASP:HB3	1:A:674:PRO:HG2	1.79	0.65
2:B:484:ASN:OD1	2:B:486:TYR:CE1	2.49	0.65
3:C:196:ASP:HB3	3:C:199:LYS:HG3	1.77	0.65
4:E:63:ASN:O	4:E:64:PRO:O	2.15	0.65
2:B:118:ARG:CA	2:B:118:ARG:CG	2.70	0.65
9:K:29:ASN:HB3	9:K:77:THR:O	1.96	0.65
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.95	0.65
2:B:25:ILE:HG22	2:B:658:ILE:HD11	1.78	0.65
7:I:16:PRO:HG3	7:I:27:PHE:CE2	2.32	0.65
1:A:69:THR:HB	1:A:69:THR:CA	2.16	0.65
2:B:1002:THR:HG21	2:B:1006:ILE:HB	1.78	0.65
2:B:1171:VAL:HG21	2:B:1191:ILE:HD12	1.78	0.65
2:B:344:LYS:O	2:B:347:LYS:N	2.29	0.65
1:A:156:ASP:OD2	1:A:156:ASP:N	2.29	0.65
1:A:919:ILE:HD13	1:A:983:ILE:HD13	1.79	0.65
2:B:1191:ILE:CG2	2:B:1192:TYR:N	2.59	0.65
2:B:883:LEU:HA	2:B:883:LEU:CB	2.18	0.65
1:A:1004:ASN:CG	4:E:167:ARG:HG3	2.16	0.65
1:A:1132:LYS:CB	1:A:1132:LYS:CD	2.73	0.65
3:C:169:LYS:NZ	10:L:69:ALA:O	2.27	0.65
4:E:78:LEU:HG	4:E:79:TRP:N	2.10	0.65
1:A:1151:GLU:HG2	7:I:45:ARG:CD	2.26	0.65
1:A:1162:VAL:CG2	1:A:1162:VAL:CG1	2.75	0.64
1:A:1425:SER:O	1:A:1429:ILE:HD12	1.98	0.64
1:A:211:PHE:HA	1:A:214:ILE:HD12	1.79	0.64
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.79	0.64
1:A:566:ILE:HD12	1:A:566:ILE:N	2.11	0.64
2:B:169:ARG:CB	2:B:454:THR:HG23	2.23	0.64
8:J:4:PRO:HD3	8:J:53:HIS:HD2	1.62	0.64
1:A:446:ARG:HG2	1:A:446:ARG:HH11	1.60	0.64
1:A:550:LEU:HD13	1:A:556:TRP:CZ2	2.32	0.64
2:B:136:THR:CA	2:B:136:THR:HB	2.15	0.64
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.80	0.64
5:F:81:THR:HG23	5:F:136:ARG:HH11	1.58	0.64
2:B:282:ILE:HD12	2:B:283:VAL:N	2.13	0.64
2:B:655:LYS:CG	2:B:655:LYS:CE	2.74	0.64
3:C:133:ILE:HD11	3:C:237:SER:HA	1.79	0.64
1:A:19:PHE:HB2	1:A:1417:GLU:O	1.97	0.64
1:A:901:LEU:HB2	1:A:926:GLN:NE2	2.09	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:653:VAL:O	2:B:654:ARG:HD3	1.97	0.64
4:E:197:LYS:CG	4:E:197:LYS:CE	2.70	0.64
1:A:50:ILE:HG22	1:A:52:GLY:N	2.12	0.64
2:B:191:LYS:CA	2:B:191:LYS:CG	2.75	0.64
2:B:883:LEU:CG	2:B:883:LEU:HB3	2.16	0.64
2:B:986:GLN:CD	2:B:1020:ARG:HH21	2.01	0.64
3:C:208:GLU:O	3:C:210:GLU:N	2.31	0.64
10:L:48:CYS:HB3	10:L:51:CYS:O	1.98	0.64
1:A:737:LEU:CB	1:A:737:LEU:CD2	2.76	0.64
3:C:8:VAL:HG12	3:C:9:LYS:H	1.62	0.64
1:A:132:LYS:CB	1:A:132:LYS:CD	2.75	0.64
1:A:567:LYS:HB3	6:H:96:VAL:HG23	1.79	0.64
1:A:843:LYS:NZ	1:A:843:LYS:CD	2.59	0.64
1:A:587:HIS:NE2	1:A:969:GLN:HG2	2.13	0.64
2:B:770:GLN:HG2	2:B:983:ARG:O	1.98	0.64
2:B:63:ILE:HD12	2:B:92:PHE:HB2	1.80	0.64
4:E:2:ASP:HB3	4:E:6:GLU:HB2	1.78	0.64
6:H:6:PHE:C	6:H:6:PHE:CD2	2.71	0.64
7:I:120:GLN:O	7:I:121:PHE:HB2	1.96	0.64
1:A:120:GLU:CG	1:A:123:ARG:HH22	2.10	0.64
1:A:199:LEU:CD2	1:A:199:LEU:CD1	2.74	0.64
1:A:535:THR:HG21	1:A:617:VAL:N	2.09	0.64
1:A:908:LEU:O	1:A:909:ASP:C	2.35	0.64
3:C:209:TYR:N	3:C:209:TYR:CD1	2.64	0.64
10:L:43:THR:HB	10:L:43:THR:CA	2.12	0.64
1:A:1118:VAL:HB	1:A:1327:ILE:CD1	2.26	0.64
1:A:1363:VAL:CG2	1:A:1363:VAL:CG1	2.75	0.64
1:A:172:PRO:HG2	1:A:174:ILE:CD1	2.28	0.64
1:A:56:PRO:O	1:A:57:ARG:CG	2.46	0.64
2:B:527:THR:HG1	2:B:527:THR:CB	2.07	0.64
2:B:654:ARG:H	2:B:657:HIS:HD2	1.45	0.64
6:H:111:LEU:HB3	6:H:127:GLY:O	1.98	0.64
8:J:42:LYS:CB	8:J:42:LYS:CD	2.72	0.64
1:A:1242:VAL:HG11	1:A:1259:MET:HE2	1.79	0.63
2:B:516:ASN:H	2:B:516:ASN:HD22	1.46	0.63
3:C:255:VAL:HG12	3:C:255:VAL:O	1.97	0.63
1:A:1151:GLU:HG3	7:I:45:ARG:HD2	1.76	0.63
1:A:138:ILE:HG13	1:A:139:TRP:N	2.12	0.63
2:B:30:SER:O	2:B:34:ILE:HD12	1.98	0.63
2:B:1158:PHE:CE2	2:B:1159:ARG:O	2.50	0.63
4:E:59:SER:O	4:E:60:PHE:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:56:THR:CA	6:H:56:THR:HB	2.14	0.63
2:B:1152:MET:CE	2:B:1152:MET:HA	2.27	0.63
2:B:419:THR:HG22	2:B:419:THR:O	1.98	0.63
2:B:364:ILE:CD1	2:B:585:VAL:HG13	2.18	0.63
3:C:124:LEU:CA	3:C:124:LEU:CD2	2.76	0.63
1:A:571:LEU:HG	1:A:571:LEU:CD2	2.15	0.63
5:F:101:ILE:CD1	5:F:107:VAL:HG22	2.28	0.63
1:A:846:GLU:HA	1:A:1066:VAL:HG23	1.81	0.63
1:A:533:LYS:NZ	1:A:745:GLN:HE22	1.97	0.63
1:A:752:LYS:CE	2:B:1019:SER:CB	2.72	0.63
2:B:293:PRO:HB3	7:I:11:ASN:HB3	1.80	0.63
2:B:67:SER:O	2:B:91:SER:HA	1.98	0.63
3:C:11:ARG:O	3:C:12:GLU:HG3	1.98	0.63
3:C:40:GLU:OE1	3:C:254:LYS:NZ	2.32	0.63
4:E:31:THR:CB	4:E:31:THR:C	2.65	0.63
6:H:104:PHE:C	6:H:104:PHE:HA	2.11	0.63
6:H:91:ASP:HA	6:H:91:ASP:C	2.08	0.63
1:A:55:ASP:C	1:A:57:ARG:H	1.99	0.63
2:B:98:THR:OG1	2:B:127:GLY:O	2.17	0.63
2:B:429:PHE:CE2	2:B:433:GLN:NE2	2.66	0.63
1:A:1055:ARG:HE	1:A:1055:ARG:CG	2.10	0.63
1:A:1242:VAL:HG11	1:A:1259:MET:HE3	1.80	0.63
1:A:689:LYS:O	1:A:693:VAL:HG23	1.99	0.63
1:A:752:LYS:HE2	2:B:1019:SER:HB2	1.78	0.63
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.11	0.63
2:B:515:HIS:H	2:B:518:HIS:CD2	2.13	0.63
6:H:4:THR:O	6:H:5:LEU:HD23	1.99	0.63
1:A:351:THR:HG21	2:B:1103:ILE:CG1	2.29	0.62
2:B:1002:THR:O	2:B:1003:ALA:C	2.35	0.62
2:B:115:GLN:CA	2:B:115:GLN:CG	2.76	0.62
2:B:246:LYS:C	2:B:246:LYS:HA	2.11	0.62
2:B:937:ALA:C	2:B:937:ALA:CB	2.65	0.62
3:C:124:LEU:CB	3:C:124:LEU:CD2	2.77	0.62
3:C:183:TRP:NE1	3:C:207:CYS:HB3	2.14	0.62
1:A:1072:ILE:CD1	1:A:1368:MET:HG3	2.29	0.62
1:A:444:PHE:CE2	1:A:470:LEU:HD21	2.34	0.62
1:A:744:LYS:CE	1:A:744:LYS:CG	2.75	0.62
2:B:121:ASN:HD21	2:B:965:LYS:NZ	1.97	0.62
4:E:23:VAL:HG11	4:E:30:ILE:HD11	1.80	0.62
5:F:81:THR:CG2	5:F:136:ARG:NH1	2.61	0.62
6:H:105:GLU:HB3	6:H:107:VAL:HG23	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1225:PHE:CD1	1:A:1225:PHE:CB	2.73	0.62
1:A:1319:VAL:CA	1:A:1319:VAL:CG1	2.72	0.62
1:A:42:ASP:OD2	1:A:47:ARG:CA	2.46	0.62
1:A:70:CYS:SG	1:A:80:HIS:CD2	2.89	0.62
2:B:1084:GLN:HE22	3:C:192:TRP:H	1.47	0.62
3:C:66:ARG:CG	3:C:66:ARG:HH11	2.04	0.62
5:F:100:GLN:CG	5:F:100:GLN:NE2	2.58	0.62
6:H:32:THR:CA	6:H:32:THR:CG2	2.68	0.62
1:A:121:LEU:HG	1:A:121:LEU:CD1	2.19	0.62
1:A:216:VAL:HA	1:A:219:PHE:CZ	2.35	0.62
2:B:729:ILE:H	2:B:729:ILE:HD12	1.64	0.62
2:B:871:THR:HA	2:B:871:THR:CB	2.18	0.62
4:E:43:LYS:O	4:E:47:CYS:CB	2.48	0.62
6:H:91:ASP:CA	6:H:92:ASP:N	2.58	0.62
1:A:605:MET:CE	1:A:607:ILE:HG13	2.28	0.62
1:A:535:THR:CG2	1:A:616:VAL:HA	2.29	0.62
3:C:66:ARG:CG	3:C:66:ARG:NH1	2.56	0.62
4:E:43:LYS:CB	4:E:43:LYS:CD	2.76	0.62
4:E:50:MET:HG3	4:E:50:MET:C	2.19	0.62
9:K:65:HIS:CD2	9:K:67:PHE:H	2.16	0.62
1:A:270:LEU:O	1:A:274:ILE:HD12	1.99	0.62
1:A:752:LYS:HG2	1:A:752:LYS:CE	2.29	0.62
9:K:95:ILE:CG2	9:K:95:ILE:CA	2.71	0.62
10:L:40:LEU:CD1	10:L:40:LEU:CD2	2.75	0.62
1:A:282:ASN:C	1:A:283:GLY:O	2.38	0.62
1:A:698:GLN:CG	1:A:698:GLN:NE2	2.60	0.62
2:B:879:ARG:NH2	2:B:885:MET:HE1	2.13	0.62
6:H:47:PHE:CG	6:H:95:TYR:HD1	2.17	0.62
8:J:30:LEU:CD2	8:J:30:LEU:CB	2.72	0.62
1:A:1194:ARG:HG2	1:A:1194:ARG:HH11	1.65	0.62
1:A:869:GLY:O	4:E:204:THR:HG21	2.00	0.62
2:B:999:MET:HB3	2:B:1000:PRO:HD2	1.81	0.62
4:E:161:LYS:CG	4:E:161:LYS:CE	2.67	0.62
1:A:1436:ILE:O	1:A:1436:ILE:HD12	2.00	0.62
1:A:387:ARG:O	1:A:388:LEU:C	2.37	0.62
3:C:178:PHE:C	3:C:178:PHE:CD2	2.72	0.62
4:E:147:HIS:CD2	4:E:149:LEU:H	2.12	0.62
1:A:635:ARG:CD	1:A:635:ARG:CB	2.73	0.61
2:B:270:LYS:CD	2:B:270:LYS:HZ3	2.12	0.61
6:H:97:MET:CE	6:H:118:PHE:CD1	2.83	0.61
1:A:535:THR:O	1:A:575:LYS:HE2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:ILE:CG2	2:B:167:ILE:CA	2.76	0.61
3:C:148:ARG:NH1	8:J:64:ASN:HA	2.16	0.61
4:E:57:MET:SD	4:E:57:MET:CE	2.88	0.61
5:F:87:LYS:CD	5:F:87:LYS:NZ	2.63	0.61
10:L:27:LEU:CG	10:L:27:LEU:HB2	2.15	0.61
1:A:834:THR:HG21	1:A:1077:THR:HA	1.80	0.61
1:A:265:LYS:CE	1:A:302:THR:HG22	2.29	0.61
2:B:118:ARG:CB	2:B:118:ARG:N	2.58	0.61
2:B:824:ILE:HD12	8:J:9:SER:OG	2.01	0.61
3:C:40:GLU:OE2	3:C:254:LYS:NZ	2.34	0.61
4:E:78:LEU:HD11	4:E:109:ILE:HD13	1.83	0.61
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	1.82	0.61
1:A:154:SER:O	1:A:155:GLU:O	2.18	0.61
1:A:274:ILE:CA	1:A:274:ILE:CG1	2.73	0.61
1:A:326:ARG:O	1:A:327:ALA:HB2	2.00	0.61
1:A:567:LYS:HD2	1:A:568:PRO:HD3	1.82	0.61
1:A:636:GLU:OE1	1:A:966:ASN:ND2	2.33	0.61
2:B:789:MET:CE	2:B:965:LYS:HB3	2.29	0.61
2:B:94:LYS:HG3	2:B:95:ILE:N	2.14	0.61
3:C:74:SER:HB2	3:C:238:ILE:HD12	1.83	0.61
8:J:6:ARG:HD2	8:J:11:GLY:O	2.00	0.61
1:A:265:LYS:CD	1:A:302:THR:HG22	2.30	0.61
1:A:938:LYS:CD	1:A:938:LYS:CB	2.77	0.61
6:H:63:LEU:HB2	6:H:90:ALA:HB2	1.83	0.61
1:A:1112:LYS:CA	1:A:1112:LYS:CG	2.74	0.61
1:A:265:LYS:NZ	1:A:302:THR:HG21	2.15	0.61
1:A:361:LEU:HD21	1:A:511:ILE:HD11	1.82	0.61
2:B:1020:ARG:CB	2:B:1020:ARG:C	2.65	0.61
2:B:1165:ILE:HB	2:B:1165:ILE:CA	2.17	0.61
3:C:124:LEU:O	3:C:127:ARG:HG3	2.00	0.61
9:K:55:LYS:HB2	9:K:81:TYR:CE1	2.36	0.61
2:B:313:MET:CE	2:B:313:MET:CB	2.79	0.61
2:B:431:TYR:CE1	2:B:447:ALA:HB1	2.36	0.61
2:B:653:VAL:HG23	2:B:653:VAL:O	1.99	0.61
1:A:804:TYR:O	2:B:761:HIS:ND1	2.33	0.61
2:B:788:ARG:O	2:B:789:MET:HG2	2.00	0.61
8:J:14:VAL:HG13	8:J:50:ILE:HD11	1.82	0.61
1:A:1112:LYS:CB	1:A:1112:LYS:CD	2.74	0.61
1:A:1282:VAL:HG22	1:A:1308:THR:HG22	1.82	0.61
1:A:187:LYS:CG	1:A:194:ALA:CB	2.79	0.61
1:A:523:ILE:HD12	1:A:622:VAL:CG2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:603:LEU:HB3	2:B:609:ILE:HD13	1.81	0.61
2:B:98:THR:HB	2:B:98:THR:CA	2.13	0.61
4:E:85:GLU:OE2	4:E:92:THR:OG1	2.15	0.61
7:I:45:ARG:CD	7:I:45:ARG:CB	2.69	0.61
2:B:436:VAL:CA	2:B:436:VAL:HB	2.20	0.61
2:B:795:ILE:HD12	2:B:795:ILE:N	2.15	0.61
1:A:844:ALA:CB	1:A:1384:VAL:HG12	2.30	0.61
1:A:46:THR:O	1:A:48:ALA:N	2.34	0.61
1:A:752:LYS:HZ2	2:B:1018:PRO:HD2	1.63	0.61
2:B:660:LYS:HE3	2:B:660:LYS:CG	2.30	0.61
3:C:20:PHE:N	3:C:20:PHE:CD2	2.69	0.61
6:H:97:MET:HE3	6:H:118:PHE:CD1	2.35	0.61
1:A:275:SER:O	1:A:279:LEU:HG	2.01	0.60
1:A:415:LEU:CD2	1:A:415:LEU:CD1	2.70	0.60
3:C:3:GLU:OE1	9:K:103:THR:HG22	2.00	0.60
1:A:84:ILE:HG22	1:A:241:VAL:CG2	2.32	0.60
2:B:245:GLU:C	2:B:245:GLU:N	2.51	0.60
2:B:871:THR:CA	2:B:871:THR:HB	2.15	0.60
3:C:209:TYR:N	3:C:209:TYR:HD1	1.99	0.60
4:E:65:THR:O	4:E:69:ILE:CG1	2.49	0.60
4:E:65:THR:O	4:E:69:ILE:HG12	2.00	0.60
10:L:40:LEU:HD22	10:L:44:ASP:OD1	2.00	0.60
1:A:132:LYS:CE	1:A:132:LYS:CG	2.75	0.60
1:A:216:VAL:HA	1:A:219:PHE:CE2	2.35	0.60
1:A:72:GLU:OE2	2:B:1175:LEU:CD1	2.47	0.60
2:B:46:GLN:HG3	2:B:47:GLN:H	1.65	0.60
2:B:593:PRO:CG	2:B:617:ARG:NH2	2.63	0.60
2:B:773:MET:O	2:B:774:GLY:C	2.36	0.60
2:B:899:ILE:HG22	2:B:900:ALA:H	1.65	0.60
7:I:111:THR:HG22	7:I:113:ASP:H	1.64	0.60
9:K:88:LYS:O	9:K:89:ASN:C	2.37	0.60
1:A:1080:THR:CB	1:A:1080:THR:N	2.62	0.60
1:A:1155:ASP:OD1	1:A:1162:VAL:CG2	2.43	0.60
1:A:567:LYS:CE	6:H:95:TYR:CG	2.85	0.60
1:A:31:SER:HB3	1:A:83:HIS:CD2	2.29	0.60
1:A:46:THR:C	1:A:46:THR:CB	2.69	0.60
3:C:53:THR:O	3:C:154:LYS:N	2.35	0.60
6:H:107:VAL:CB	6:H:107:VAL:HA	2.18	0.60
1:A:144:THR:C	1:A:144:THR:CB	2.68	0.60
1:A:353:ILE:HD12	1:A:482:PHE:CE2	2.37	0.60
1:A:737:LEU:HG	1:A:737:LEU:CD2	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:516:ASN:ND2	2:B:516:ASN:H	2.00	0.60
2:B:744:HIS:HD2	2:B:746:SER:H	1.48	0.60
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.32	0.60
9:K:78:THR:HG22	9:K:79:GLU:N	2.17	0.60
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.83	0.60
1:A:1236:LEU:CD2	1:A:1236:LEU:CB	2.74	0.60
1:A:1134:ILE:HG22	1:A:1306:LEU:HD11	1.83	0.60
2:B:1152:MET:HE2	2:B:1152:MET:HA	1.83	0.60
2:B:879:ARG:HH21	2:B:885:MET:HE1	1.67	0.60
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.36	0.60
1:A:351:THR:HG23	2:B:1103:ILE:HG13	1.82	0.60
2:B:645:SER:OG	2:B:646:LEU:N	2.33	0.60
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.00	0.60
3:C:26:ASP:O	3:C:27:LEU:C	2.38	0.60
1:A:148:CYS:SG	1:A:167:CYS:SG	3.00	0.60
1:A:213:HIS:CB	1:A:213:HIS:C	2.69	0.60
1:A:901:LEU:N	1:A:926:GLN:NE2	2.38	0.60
2:B:684:LEU:HD23	2:B:689:LEU:HD12	1.84	0.60
7:I:111:THR:HG21	7:I:113:ASP:HB2	1.84	0.60
1:A:1148:ILE:CD1	1:A:1198:ASP:HB2	2.32	0.60
1:A:1450:LEU:HG	1:A:1450:LEU:CD2	2.16	0.60
1:A:145:LYS:HE3	1:A:149:GLU:OE2	2.02	0.60
1:A:173:THR:CA	1:A:173:THR:CG2	2.76	0.60
1:A:200:ARG:NH2	1:A:206:GLU:OE2	2.35	0.60
1:A:976:THR:CB	1:A:976:THR:HA	2.18	0.60
2:B:249:ARG:CD	2:B:249:ARG:CB	2.79	0.60
2:B:46:GLN:HG3	2:B:47:GLN:N	2.17	0.60
2:B:620:ARG:CG	2:B:620:ARG:HE	2.14	0.60
4:E:61:GLN:HB2	4:E:79:TRP:HE3	1.66	0.60
6:H:138:GLU:CG	6:H:139:ASN:N	2.61	0.60
2:B:120:ARG:CG	10:L:55:ILE:HD11	2.31	0.59
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.84	0.59
3:C:260:LEU:O	3:C:260:LEU:HD12	2.02	0.59
1:A:1055:ARG:HG3	1:A:1055:ARG:NE	2.17	0.59
1:A:150:THR:HA	1:A:166:GLY:HA2	1.84	0.59
1:A:494:SER:OG	1:A:497:THR:HB	2.02	0.59
2:B:192:LEU:CD2	2:B:192:LEU:HG	2.17	0.59
3:C:124:LEU:HG	3:C:124:LEU:CD2	2.18	0.59
3:C:56:THR:HG23	3:C:57:VAL:N	2.16	0.59
5:F:123:LYS:HD2	5:F:123:LYS:NZ	2.18	0.59
2:B:1163:CYS:HB3	2:B:1166:CYS:SG	2.41	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:THR:CA	2:B:136:THR:CG2	2.77	0.59
2:B:455:SER:O	2:B:459:TYR:HB3	2.01	0.59
2:B:984:HIS:CD2	2:B:1025:HIS:HA	2.37	0.59
3:C:73:GLN:HE21	3:C:75:MET:H	1.49	0.59
3:C:97:VAL:HG12	3:C:98:VAL:N	2.16	0.59
4:E:47:CYS:SG	4:E:52:ARG:O	2.60	0.59
7:I:46:HIS:CB	7:I:46:HIS:C	2.65	0.59
2:B:365:THR:HG22	2:B:367:LEU:H	1.67	0.59
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.85	0.59
2:B:864:LYS:HB2	2:B:871:THR:HA	1.84	0.59
10:L:54:ARG:NE	10:L:54:ARG:CG	2.62	0.59
3:C:5:GLY:C	3:C:24:ASN:HD22	2.05	0.59
6:H:93:TYR:N	6:H:93:TYR:CD1	2.70	0.59
9:K:46:ILE:O	9:K:47:ARG:C	2.36	0.59
1:A:1055:ARG:HG3	1:A:1055:ARG:HE	1.68	0.59
1:A:33:ALA:HB2	1:A:56:PRO:HB2	1.84	0.59
2:B:1027:ILE:HD12	2:B:1052:VAL:CG2	2.32	0.59
3:C:242:GLN:NE2	3:C:246:ARG:HE	2.00	0.59
3:C:86:CYS:SG	3:C:92:CYS:SG	3.01	0.59
1:A:1127:ASP:HB3	1:A:1130:GLN:H	1.67	0.59
3:C:180:TYR:CD1	3:C:180:TYR:C	2.76	0.59
3:C:40:GLU:CD	3:C:254:LYS:NZ	2.56	0.59
1:A:1445:ILE:HD12	1:A:1445:ILE:H	1.67	0.59
1:A:507:VAL:HB	1:A:508:PRO:HD3	1.84	0.59
1:A:975:HIS:N	1:A:975:HIS:CB	2.60	0.59
2:B:424:LEU:HD23	2:B:425:THR:N	2.17	0.59
9:K:23:PRO:CD	9:K:23:PRO:O	2.49	0.59
1:A:120:GLU:HG2	1:A:123:ARG:NH2	2.18	0.58
1:A:356:ASP:OD2	1:A:469:ARG:CD	2.51	0.58
1:A:1208:THR:O	1:A:1209:MET:C	2.35	0.58
1:A:230:ARG:NH1	1:A:232:GLU:OE2	2.35	0.58
3:C:124:LEU:HG	3:C:124:LEU:CD1	2.23	0.58
2:B:294:ASP:N	7:I:12:ASN:HD22	1.97	0.58
3:C:66:ARG:NH2	8:J:3:VAL:O	2.34	0.58
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.03	0.58
1:A:982:THR:HG22	1:A:984:LYS:N	2.18	0.58
3:C:209:TYR:H	3:C:209:TYR:HD1	1.49	0.58
1:A:213:HIS:CG	1:A:213:HIS:CA	2.84	0.58
1:A:40:THR:HG23	1:A:54:ASN:ND2	2.18	0.58
1:A:534:LEU:O	1:A:574:GLY:HA3	2.04	0.58
1:A:34:LYS:HG2	1:A:83:HIS:CE1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:ASN:HD21	1:A:905:ASP:HB2	1.68	0.58
2:B:1191:ILE:HG22	2:B:1192:TYR:N	2.17	0.58
10:L:49:LYS:CE	10:L:49:LYS:CG	2.77	0.58
1:A:903:ASN:ND2	1:A:905:ASP:N	2.52	0.58
1:A:91:PHE:CD1	1:A:99:ILE:HD13	2.38	0.58
9:K:94:ILE:CA	9:K:94:ILE:CG1	2.75	0.58
1:A:172:PRO:HG2	1:A:174:ILE:HD11	1.86	0.58
2:B:1020:ARG:O	2:B:1021:MET:HB2	1.96	0.58
2:B:167:ILE:CG2	2:B:424:LEU:HD13	2.33	0.58
1:A:134:ARG:HD2	1:A:221:SER:O	2.03	0.58
1:A:567:LYS:HD3	6:H:96:VAL:N	2.18	0.58
1:A:537:ARG:NH2	1:A:600:PRO:O	2.36	0.58
4:E:36:GLU:O	4:E:38:PRO:CD	2.52	0.58
2:B:1162:ILE:HD11	2:B:1194:ILE:HG12	1.85	0.58
2:B:273:LEU:HD12	2:B:276:ILE:HD13	1.86	0.58
2:B:953:LEU:C	2:B:953:LEU:HD23	2.24	0.58
9:K:28:PRO:O	9:K:29:ASN:HB2	2.03	0.58
2:B:98:THR:C	2:B:98:THR:HB	2.23	0.58
1:A:693:VAL:HG21	1:A:721:PHE:CE1	2.30	0.58
1:A:976:THR:CB	1:A:976:THR:C	2.68	0.58
2:B:1222:ARG:HH11	2:B:1222:ARG:HG2	1.63	0.58
13:B:3008:CTP:O3A	14:B:3010:HOH:O	2.17	0.58
2:B:870:ILE:HA	2:B:870:ILE:CB	2.22	0.58
4:E:197:LYS:CD	4:E:197:LYS:CB	2.75	0.58
2:B:955:THR:CG2	10:L:54:ARG:O	2.49	0.58
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.86	0.57
2:B:691:GLU:HG2	2:B:693:ILE:CD1	2.32	0.57
5:F:114:GLU:HB2	5:F:120:ILE:CD1	2.34	0.57
5:F:81:THR:HG23	5:F:136:ARG:NH1	2.19	0.57
1:A:1080:THR:HB	1:A:1080:THR:CA	2.18	0.57
1:A:84:ILE:HD13	1:A:270:LEU:CD1	2.34	0.57
1:A:920:LEU:HD22	1:A:921:GLY:N	2.19	0.57
2:B:25:ILE:HB	2:B:29:ASP:OD2	2.04	0.57
2:B:249:ARG:CZ	2:B:415:GLN:HG3	2.33	0.57
2:B:898:LEU:C	2:B:899:ILE:O	2.30	0.57
4:E:129:PRO:CG	4:E:129:PRO:CA	2.79	0.57
6:H:138:GLU:CG	6:H:139:ASN:H	2.17	0.57
1:A:860:LEU:CD2	1:A:860:LEU:CD1	2.76	0.57
2:B:733:HIS:CA	2:B:734:HIS:N	2.62	0.57
3:C:5:GLY:O	3:C:24:ASN:ND2	2.37	0.57
1:A:858:ASN:ND2	1:A:858:ASN:C	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:LYS:NZ	3:C:15:LYS:CD	2.66	0.57
10:L:38:LEU:CD2	10:L:38:LEU:CB	2.79	0.57
1:A:173:THR:OG1	1:A:173:THR:CG2	2.50	0.57
1:A:351:THR:CG2	2:B:1103:ILE:HG12	2.34	0.57
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.85	0.57
1:A:567:LYS:HD3	6:H:95:TYR:C	2.24	0.57
2:B:137:TYR:CG	2:B:137:TYR:HB2	2.22	0.57
1:A:567:LYS:HD2	6:H:95:TYR:HA	1.84	0.57
1:A:120:GLU:HG2	1:A:123:ARG:HH12	1.70	0.57
3:C:53:THR:O	3:C:153:LEU:HA	2.04	0.57
5:F:111:LEU:O	5:F:113:GLY:N	2.35	0.57
1:A:670:ILE:HD13	2:B:1067:ARG:CZ	2.34	0.57
1:A:786:HIS:HE1	2:B:742:GLU:OE2	1.87	0.57
1:A:882:SER:HB3	1:A:953:ASN:OD1	2.03	0.57
2:B:1188:LYS:CB	2:B:1188:LYS:CD	2.78	0.57
7:I:42:LEU:CB	7:I:42:LEU:CD1	2.74	0.57
1:A:914:GLU:C	1:A:916:GLY:H	2.08	0.57
2:B:1008:PRO:HG2	2:B:1011:ILE:HD11	1.85	0.57
2:B:863:GLU:OE1	2:B:962:LYS:HD3	2.04	0.57
3:C:56:THR:CG2	3:C:57:VAL:N	2.63	0.57
5:F:109:VAL:HG22	5:F:127:GLU:OE1	2.04	0.57
10:L:46:VAL:N	10:L:46:VAL:CG2	2.68	0.57
1:A:492:PRO:HG3	1:A:501:LEU:HD12	1.86	0.57
3:C:41:ILE:N	3:C:163:ILE:HD11	2.19	0.57
3:C:88:CYS:SG	3:C:95:CYS:SG	3.02	0.57
8:J:53:HIS:ND1	8:J:53:HIS:C	2.58	0.57
1:A:867:ILE:HD12	1:A:1000:LEU:HD21	1.85	0.57
2:B:243:ALA:C	2:B:243:ALA:CB	2.69	0.57
2:B:639:ILE:HD11	2:B:691:GLU:CD	2.25	0.57
9:K:110:ASN:ND2	9:K:110:ASN:CB	2.65	0.57
1:A:1122:PRO:O	1:A:1123:GLY:C	2.41	0.56
1:A:91:PHE:HD1	1:A:99:ILE:HD13	1.70	0.56
2:B:1148:LYS:CD	2:B:1148:LYS:HZ2	2.16	0.56
2:B:886:LYS:O	2:B:888:GLY:N	2.38	0.56
2:B:906:SER:O	2:B:907:GLY:C	2.41	0.56
3:C:93:ASP:O	3:C:127:ARG:NH2	2.36	0.56
1:A:679:ILE:CD1	1:A:732:LEU:HB2	2.31	0.56
2:B:1084:GLN:HE22	3:C:192:TRP:N	2.03	0.56
2:B:296:GLU:O	2:B:300:HIS:CD2	2.58	0.56
6:H:9:ILE:CB	6:H:9:ILE:HA	2.22	0.56
9:K:18:LYS:HE3	9:K:36:GLU:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:252:GLN:HE22	9:K:99:GLY:CA	2.17	0.56
1:A:1383:SER:OG	1:A:1384:VAL:N	2.38	0.56
1:A:1445:ILE:CG2	1:A:1445:ILE:HA	2.34	0.56
1:A:162:VAL:CA	1:A:162:VAL:CG2	2.78	0.56
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.05	0.56
2:B:603:LEU:CB	2:B:609:ILE:HD13	2.35	0.56
2:B:98:THR:CG2	2:B:98:THR:CA	2.79	0.56
5:F:147:SER:O	5:F:148:VAL:C	2.40	0.56
7:I:16:PRO:HG3	7:I:27:PHE:HE2	1.68	0.56
7:I:48:LEU:N	7:I:48:LEU:HD23	2.20	0.56
1:A:243:PRO:O	1:A:243:PRO:HG2	2.04	0.56
1:A:567:LYS:CD	6:H:95:TYR:CA	2.69	0.56
1:A:982:THR:HG22	1:A:984:LYS:H	1.70	0.56
2:B:1128:LEU:HD12	2:B:1128:LEU:C	2.26	0.56
2:B:1163:CYS:HA	2:B:1191:ILE:CD1	2.33	0.56
2:B:1165:ILE:CB	2:B:1165:ILE:N	2.66	0.56
2:B:169:ARG:HG3	2:B:454:THR:OG1	2.05	0.56
2:B:458:LYS:O	2:B:459:TYR:C	2.43	0.56
4:E:80:VAL:HG12	4:E:81:GLU:N	2.20	0.56
6:H:57:VAL:HG22	6:H:144:ILE:CD1	2.35	0.56
1:A:446:ARG:CG	1:A:446:ARG:HH11	2.14	0.56
1:A:589:GLN:HB2	1:A:961:ARG:HH22	1.70	0.56
2:B:238:ALA:CB	2:B:238:ALA:C	2.66	0.56
3:C:9:LYS:HG2	3:C:9:LYS:O	2.06	0.56
4:E:213:ILE:O	4:E:213:ILE:HG23	2.06	0.56
6:H:3:ASN:CB	6:H:3:ASN:ND2	2.63	0.56
6:H:56:THR:HA	6:H:56:THR:CB	2.18	0.56
2:B:100:PRO:HD2	2:B:180:TYR:CZ	2.41	0.56
2:B:259:TYR:HB2	2:B:268:THR:HG22	1.87	0.56
2:B:169:ARG:CG	2:B:454:THR:CG2	2.82	0.56
2:B:723:VAL:HB	2:B:723:VAL:CG1	2.24	0.56
3:C:133:ILE:O	3:C:134:ILE:HD13	2.05	0.56
3:C:255:VAL:HB	9:K:95:ILE:HD11	1.86	0.56
10:L:61:THR:CG2	10:L:61:THR:HB	2.18	0.56
2:B:775:LYS:CB	2:B:775:LYS:HD2	2.36	0.56
2:B:883:LEU:CG	2:B:883:LEU:HB2	2.16	0.56
4:E:180:ARG:CA	4:E:180:ARG:CG	2.78	0.56
4:E:213:ILE:O	4:E:213:ILE:CG2	2.53	0.56
1:A:1138:ILE:CD1	1:A:1319:VAL:HG21	2.36	0.56
1:A:466:SER:HB2	2:B:1103:ILE:HD11	1.87	0.56
1:A:596:THR:HG22	1:A:597:LEU:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:938:LYS:CE	1:A:938:LYS:CG	2.84	0.56
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.55	0.56
2:B:875:GLU:O	2:B:876:LYS:C	2.38	0.56
6:H:81:PRO:HB2	6:H:82:PRO:HD3	1.87	0.56
1:A:119:ASN:OD1	1:A:119:ASN:C	2.44	0.56
1:A:187:LYS:HG3	1:A:194:ALA:HB2	1.86	0.56
1:A:566:ILE:HD12	1:A:566:ILE:H	1.69	0.56
2:B:417:PHE:C	2:B:417:PHE:HD2	2.07	0.56
2:B:723:VAL:HB	2:B:723:VAL:CG2	2.19	0.56
6:H:136:LYS:C	6:H:136:LYS:HA	2.13	0.56
9:K:26:LYS:CB	9:K:26:LYS:CD	2.84	0.56
1:A:1176:LEU:HB2	1:A:1176:LEU:CA	2.18	0.56
1:A:247:ARG:HH11	1:A:263:THR:CG2	2.13	0.56
2:B:1002:THR:C	2:B:1002:THR:HA	2.14	0.56
1:A:351:THR:HG21	2:B:1103:ILE:HG13	1.88	0.56
2:B:1162:ILE:HD13	2:B:1194:ILE:HG12	1.88	0.56
1:A:566:ILE:HD13	6:H:96:VAL:O	2.05	0.56
1:A:1315:GLU:CB	1:A:1315:GLU:CD	2.72	0.55
2:B:108:VAL:CG2	2:B:108:VAL:CG1	2.81	0.55
3:C:142:VAL:HG12	3:C:142:VAL:O	2.03	0.55
1:A:1004:ASN:HD21	1:A:1007:ILE:HD12	1.71	0.55
1:A:523:ILE:HD12	1:A:622:VAL:CG1	2.36	0.55
1:A:567:LYS:CD	1:A:568:PRO:HD3	2.36	0.55
2:B:556:THR:C	2:B:556:THR:CG2	2.75	0.55
2:B:882:THR:CG2	2:B:882:THR:HB	2.21	0.55
3:C:73:GLN:HB3	3:C:131:HIS:H	1.71	0.55
5:F:129:LYS:CE	5:F:129:LYS:CG	2.84	0.55
9:K:106:GLU:O	9:K:110:ASN:ND2	2.39	0.55
1:A:187:LYS:CG	1:A:194:ALA:HB3	2.36	0.55
1:A:630:ILE:HD13	1:A:645:LEU:HD23	1.88	0.55
2:B:841:MET:HB2	2:B:990:ILE:HD12	1.88	0.55
4:E:13:TRP:CE3	4:E:39:LEU:HD13	2.41	0.55
10:L:26:THR:HB	10:L:26:THR:CA	2.19	0.55
10:L:40:LEU:HB2	10:L:40:LEU:CG	2.19	0.55
1:A:125:ALA:O	1:A:126:LEU:C	2.42	0.55
1:A:1282:VAL:CG1	1:A:1282:VAL:CG2	2.78	0.55
1:A:4:GLN:CG	1:A:4:GLN:H	2.19	0.55
1:A:597:LEU:H	1:A:597:LEU:HD12	1.71	0.55
1:A:599:SER:HB2	1:A:602:ASP:H	1.72	0.55
1:A:679:ILE:HD12	1:A:729:ALA:CA	2.36	0.55
2:B:654:ARG:CG	2:B:654:ARG:CA	2.68	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:55:LYS:HB3	9:K:81:TYR:HD1	1.72	0.55
1:A:431:LYS:CB	1:A:431:LYS:CD	2.80	0.55
2:B:59:LEU:O	2:B:60:GLN:C	2.37	0.55
6:H:130:ARG:HB2	6:H:133:ASN:CB	2.37	0.55
1:A:1102:LYS:CA	1:A:1102:LYS:CG	2.78	0.55
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.41	0.55
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.41	0.55
2:B:118:ARG:NH2	2:B:194:GLU:CG	2.69	0.55
3:C:131:HIS:O	3:C:132:PRO:C	2.36	0.55
2:B:37:PHE:HB2	2:B:681:TRP:CE3	2.42	0.55
3:C:15:LYS:CB	3:C:15:LYS:CD	2.85	0.55
6:H:105:GLU:HG2	6:H:136:LYS:HZ1	1.71	0.55
7:I:120:GLN:O	7:I:121:PHE:CB	2.55	0.55
7:I:14:LEU:HB3	7:I:27:PHE:HB3	1.89	0.55
1:A:611:GLN:O	1:A:613:ILE:HD12	2.07	0.55
2:B:120:ARG:HG2	10:L:55:ILE:CD1	2.36	0.55
2:B:360:PHE:O	2:B:361:LEU:C	2.43	0.55
2:B:660:LYS:CB	2:B:660:LYS:CD	2.82	0.55
6:H:96:VAL:HA	6:H:142:LEU:O	2.07	0.55
1:A:369:SER:H	9:K:2:ASN:ND2	2.04	0.55
2:B:1221:SER:CA	2:B:1222:ARG:N	2.63	0.55
4:E:52:ARG:HG3	4:E:53:PRO:HD3	1.89	0.55
6:H:63:LEU:CD2	6:H:63:LEU:CB	2.79	0.55
6:H:8:ASP:OD2	6:H:9:ILE:N	2.37	0.55
9:K:11:LEU:CD1	9:K:11:LEU:CB	2.78	0.55
1:A:144:THR:O	1:A:146:MET:HG2	2.07	0.55
1:A:4:GLN:CG	1:A:4:GLN:CA	2.78	0.55
1:A:610:GLY:C	1:A:611:GLN:HG2	2.27	0.55
1:A:73:GLY:C	1:A:75:ASN:N	2.58	0.55
2:B:227:LYS:CE	2:B:227:LYS:CG	2.85	0.55
2:B:692:TYR:C	2:B:693:ILE:HD12	2.26	0.55
4:E:165:LEU:CD2	4:E:165:LEU:CD1	2.82	0.55
5:F:75:PRO:O	5:F:77:ASP:N	2.40	0.55
5:F:82:THR:HB	5:F:84:TYR:H	1.72	0.54
1:A:365:GLY:HA2	1:A:461:LYS:O	2.08	0.54
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.36	0.54
1:A:982:THR:HB	1:A:985:ASP:OD2	2.07	0.54
1:A:666:ILE:HG13	2:B:1027:ILE:CD1	2.36	0.54
4:E:43:LYS:O	4:E:47:CYS:HB3	2.06	0.54
6:H:142:LEU:HG	6:H:143:LEU:N	2.21	0.54
2:B:269:ILE:N	2:B:269:ILE:HD12	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:ASP:CB	2:B:658:ILE:HD13	2.37	0.54
2:B:384:ARG:CG	2:B:384:ARG:NE	2.67	0.54
2:B:425:THR:HA	2:B:428:ILE:HD12	1.89	0.54
3:C:181:ASP:OD2	3:C:185:LYS:N	2.39	0.54
3:C:25:VAL:CG1	3:C:29:MET:HG2	2.36	0.54
1:A:279:LEU:CB	1:A:279:LEU:CD2	2.79	0.54
2:B:956:THR:HA	2:B:961:LEU:O	2.08	0.54
3:C:166:GLU:CB	3:C:166:GLU:CD	2.75	0.54
7:I:111:THR:CG2	7:I:113:ASP:H	2.19	0.54
1:A:1004:ASN:ND2	4:E:167:ARG:HG3	2.23	0.54
1:A:230:ARG:HD2	1:A:233:TRP:CZ2	2.43	0.54
1:A:265:LYS:NZ	1:A:302:THR:CG2	2.71	0.54
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.89	0.54
2:B:1174:LYS:O	2:B:1178:ASN:N	2.41	0.54
2:B:63:ILE:C	2:B:63:ILE:CG2	2.75	0.54
4:E:44:ALA:C	4:E:44:ALA:CB	2.71	0.54
4:E:95:THR:HB	4:E:95:THR:CG2	2.18	0.54
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.43	0.54
1:A:180:LYS:CE	1:A:180:LYS:CG	2.82	0.54
1:A:26:GLU:HA	1:A:29:ALA:HB3	1.89	0.54
2:B:269:ILE:N	2:B:269:ILE:CD1	2.71	0.54
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.88	0.54
5:F:119:ARG:HG2	5:F:119:ARG:HH11	1.71	0.54
6:H:100:THR:O	6:H:116:TYR:HA	2.07	0.54
6:H:95:TYR:C	6:H:96:VAL:CG2	2.76	0.54
1:A:155:GLU:OE2	4:E:125:PRO:CB	2.54	0.54
1:A:346:ASP:O	1:A:347:PHE:HB2	2.06	0.54
2:B:632:ARG:CG	2:B:632:ARG:NE	2.65	0.54
6:H:123:MET:CE	6:H:142:LEU:HD22	2.37	0.54
7:I:120:GLN:O	7:I:121:PHE:CD1	2.61	0.54
8:J:53:HIS:HD1	8:J:53:HIS:C	2.10	0.54
1:A:1176:LEU:CA	1:A:1176:LEU:HB3	2.18	0.54
1:A:1406:VAL:C	1:A:1408:ILE:N	2.58	0.54
1:A:523:ILE:HD12	1:A:622:VAL:HG13	1.90	0.54
2:B:883:LEU:HG	2:B:883:LEU:CD1	2.17	0.54
4:E:45:LYS:CG	4:E:45:LYS:CE	2.82	0.54
6:H:37:LYS:O	6:H:125:LEU:HA	2.07	0.54
1:A:601:LYS:CD	1:A:601:LYS:CB	2.81	0.54
2:B:353:LYS:CG	2:B:353:LYS:CE	2.84	0.54
2:B:940:PRO:O	2:B:941:LEU:C	2.44	0.54
4:E:180:ARG:NE	4:E:180:ARG:CG	2.66	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:50:MET:CG	4:E:50:MET:C	2.76	0.54
6:H:4:THR:OG1	6:H:5:LEU:N	2.40	0.54
9:K:94:ILE:C	9:K:94:ILE:CB	2.70	0.54
1:A:302:THR:CG2	1:A:302:THR:OG1	2.52	0.54
1:A:711:ARG:CB	1:A:711:ARG:CD	2.82	0.54
2:B:813:LYS:CB	2:B:813:LYS:CD	2.80	0.54
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.09	0.53
1:A:909:ASP:OD1	1:A:911:SER:N	2.27	0.53
2:B:294:ASP:O	2:B:297:ILE:HB	2.08	0.53
2:B:206:ASN:OD1	2:B:458:LYS:CE	2.56	0.53
3:C:74:SER:HB2	3:C:237:SER:O	2.08	0.53
6:H:113:ALA:CB	6:H:124:ARG:HH21	2.21	0.53
7:I:58:VAL:O	7:I:58:VAL:HG12	2.05	0.53
1:A:1283:VAL:HG12	1:A:1284:MET:O	2.08	0.53
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.73	0.53
1:A:895:LYS:CD	1:A:895:LYS:NZ	2.71	0.53
2:B:353:LYS:CD	2:B:353:LYS:CB	2.81	0.53
2:B:705:MET:HG3	2:B:705:MET:HE3	1.81	0.53
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.91	0.53
3:C:7:GLN:OE1	9:K:104:ASN:ND2	2.42	0.53
4:E:16:PHE:O	4:E:20:LYS:HG2	2.08	0.53
5:F:72:LYS:CB	5:F:72:LYS:CD	2.82	0.53
1:A:119:ASN:O	1:A:120:GLU:CB	2.56	0.53
2:B:599:THR:O	2:B:600:LEU:C	2.44	0.53
3:C:94:LYS:CE	3:C:94:LYS:CG	2.81	0.53
4:E:127:ILE:N	4:E:128:PRO:CD	2.71	0.53
9:K:89:ASN:ND2	9:K:89:ASN:CB	2.65	0.53
1:A:247:ARG:HH12	1:A:263:THR:HG23	1.70	0.53
1:A:528:LEU:HD23	1:A:751:SER:HA	1.91	0.53
2:B:1084:GLN:C	2:B:1085:ILE:HG13	2.28	0.53
2:B:1153:GLU:HA	2:B:1153:GLU:CD	2.29	0.53
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.37	0.53
2:B:735:ALA:CB	2:B:735:ALA:N	2.63	0.53
6:H:105:GLU:C	6:H:107:VAL:N	2.58	0.53
7:I:51:ASN:HB2	7:I:118:ARG:NH2	2.24	0.53
1:A:203:SER:O	1:A:204:THR:C	2.45	0.53
2:B:1194:ILE:O	2:B:1194:ILE:HG13	2.07	0.53
2:B:792:MET:SD	2:B:857:ARG:NH2	2.81	0.53
2:B:877:PRO:HB3	2:B:915:THR:HG22	1.91	0.53
3:C:41:ILE:O	3:C:163:ILE:HD11	2.08	0.53
2:B:969:ARG:NH2	3:C:61:GLU:OE1	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:43:LYS:O	4:E:47:CYS:HB2	2.08	0.53
10:L:34:CYS:HB3	10:L:51:CYS:SG	2.49	0.53
1:A:516:SER:O	1:A:517:ASN:CG	2.47	0.53
1:A:595:THR:CG2	1:A:596:THR:N	2.71	0.53
2:B:1004:GLU:HB2	2:B:1006:ILE:HD13	1.90	0.53
2:B:269:ILE:HD13	2:B:317:CYS:HG	1.70	0.53
2:B:367:LEU:CD1	2:B:367:LEU:CD2	2.83	0.53
3:C:124:LEU:CD2	3:C:124:LEU:N	2.72	0.53
3:C:11:ARG:NE	3:C:209:TYR:CE2	2.67	0.53
3:C:240:VAL:C	3:C:242:GLN:N	2.60	0.53
6:H:138:GLU:C	6:H:140:ALA:N	2.59	0.53
2:B:827:ILE:HG12	2:B:1012:ILE:HD11	1.89	0.53
2:B:416:LEU:CD1	2:B:466:TRP:CZ2	2.92	0.53
2:B:712:PRO:HA	2:B:733:HIS:NE2	2.23	0.53
2:B:809:MET:O	2:B:810:GLU:C	2.42	0.53
4:E:71:LYS:CE	4:E:160:GLU:OE2	2.57	0.53
9:K:111:LEU:CD2	9:K:111:LEU:CB	2.77	0.53
10:L:27:LEU:CA	10:L:27:LEU:HB2	2.20	0.53
1:A:274:ILE:CG2	1:A:274:ILE:CA	2.83	0.53
1:A:886:ILE:HD12	1:A:943:LEU:CB	2.36	0.53
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.39	0.53
2:B:642:ASP:HB2	2:B:643:ASP:OD1	2.08	0.53
2:B:25:ILE:HG22	2:B:658:ILE:CD1	2.39	0.53
2:B:95:ILE:HG22	2:B:96:TYR:N	2.23	0.53
3:C:46:ILE:HD13	3:C:67:LEU:HB3	1.90	0.53
9:K:77:THR:OG1	9:K:83:PRO:HD3	2.09	0.53
1:A:110:CYS:N	1:A:110:CYS:CB	2.67	0.53
1:A:608:ILE:HG22	1:A:609:ASP:N	2.24	0.53
2:B:1185:CYS:N	2:B:1185:CYS:CB	2.68	0.53
2:B:266:ALA:HB1	2:B:316:PRO:HB3	1.91	0.53
3:C:113:VAL:HG12	3:C:144:ILE:HD12	1.91	0.53
10:L:40:LEU:CG	10:L:40:LEU:HB3	2.19	0.53
1:A:69:THR:CB	1:A:69:THR:N	2.67	0.53
2:B:209:GLU:OE1	2:B:788:ARG:NH2	2.40	0.53
2:B:213:ILE:HD12	2:B:481:GLN:NE2	2.24	0.53
6:H:105:GLU:N	6:H:105:GLU:CD	2.61	0.53
2:B:305:VAL:CG1	2:B:305:VAL:CA	2.83	0.52
2:B:961:LEU:CG	2:B:961:LEU:HB2	2.19	0.52
3:C:19:ASP:OD1	3:C:20:PHE:N	2.42	0.52
1:A:27:VAL:HG12	1:A:27:VAL:O	2.09	0.52
2:B:104:GLU:HB2	2:B:108:VAL:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:844:SER:O	2:B:847:ASP:HB2	2.09	0.52
3:C:214:ASN:CB	3:C:214:ASN:ND2	2.65	0.52
8:J:16:ASP:OD1	8:J:17:LYS:CG	2.58	0.52
1:A:1358:SER:HG	1:A:1358:SER:CB	2.13	0.52
2:B:280:ILE:HD12	2:B:280:ILE:N	2.24	0.52
3:C:148:ARG:HH11	8:J:64:ASN:HA	1.74	0.52
6:H:138:GLU:O	6:H:139:ASN:O	2.27	0.52
1:A:35:ILE:HD13	1:A:241:VAL:HG21	1.90	0.52
2:B:1128:LEU:O	2:B:1128:LEU:CG	2.56	0.52
3:C:101:LEU:HB3	3:C:155:LEU:HB2	1.92	0.52
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.91	0.52
6:H:123:MET:HE1	6:H:142:LEU:CD2	2.38	0.52
1:A:104:GLU:C	1:A:104:GLU:HB3	2.30	0.52
1:A:57:ARG:HB3	1:A:68:GLN:HG3	1.92	0.52
2:B:775:LYS:CA	2:B:775:LYS:CG	2.86	0.52
4:E:161:LYS:CE	4:E:172:GLU:OE2	2.57	0.52
1:A:1004:ASN:ND2	1:A:1007:ILE:HD12	2.25	0.52
1:A:147:VAL:CG1	1:A:147:VAL:CA	2.84	0.52
1:A:567:LYS:CB	1:A:568:PRO:CD	2.87	0.52
1:A:858:ASN:ND2	1:A:862:ASN:H	2.07	0.52
1:A:913:LEU:HD12	1:A:913:LEU:C	2.25	0.52
2:B:137:TYR:HB3	2:B:137:TYR:CA	2.19	0.52
2:B:830:TYR:O	2:B:831:SER:CB	2.55	0.52
4:E:176:PRO:O	4:E:212:ARG:HA	2.10	0.52
7:I:86:PHE:N	7:I:86:PHE:CD2	2.76	0.52
9:K:11:LEU:HG	9:K:11:LEU:CD1	2.20	0.52
1:A:752:LYS:NZ	2:B:1019:SER:H	2.06	0.52
1:A:806:ARG:CZ	2:B:729:ILE:HD11	2.39	0.52
2:B:846:ILE:HD12	2:B:974:PRO:HB2	1.91	0.52
3:C:40:GLU:C	3:C:163:ILE:CD1	2.77	0.52
6:H:123:MET:CE	6:H:123:MET:CG	2.88	0.52
6:H:56:THR:O	6:H:144:ILE:HA	2.10	0.52
1:A:1151:GLU:HA	7:I:44:TYR:O	2.09	0.52
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.09	0.52
1:A:752:LYS:NZ	2:B:1018:PRO:HD2	2.25	0.52
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.49	0.52
2:B:376:PHE:HB3	2:B:586:TRP:CZ3	2.45	0.52
2:B:821:GLN:OE1	2:B:850:LEU:HD12	2.10	0.52
2:B:875:GLU:O	2:B:877:PRO:HD3	2.09	0.52
2:B:899:ILE:HD12	2:B:911:ILE:HG13	1.92	0.52
6:H:11:GLN:HB3	6:H:29:ALA:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:LYS:CG	1:A:1003:LYS:HA	2.40	0.52
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.45	0.52
1:A:601:LYS:CD	1:A:601:LYS:NZ	2.69	0.52
1:A:69:THR:O	2:B:1174:LYS:HG2	2.10	0.52
2:B:883:LEU:HB3	2:B:883:LEU:CA	2.20	0.52
10:L:28:LYS:O	10:L:59:ALA:HB3	2.08	0.52
1:A:35:ILE:HD13	1:A:241:VAL:HG11	1.92	0.52
1:A:33:ALA:CB	1:A:56:PRO:HB2	2.39	0.52
2:B:764:SER:HB3	2:B:765:PRO:HD3	1.90	0.52
1:A:1325:THR:O	4:E:148:GLU:HG2	2.09	0.52
1:A:568:PRO:HG2	6:H:46:LEU:O	2.10	0.52
10:L:47:ARG:CG	10:L:48:CYS:H	2.19	0.52
1:A:636:GLU:CD	1:A:962:ARG:HD3	2.31	0.51
1:A:784:LEU:HB3	1:A:785:PRO:HD2	1.91	0.51
2:B:23:ALA:HB3	2:B:655:LYS:HG3	1.92	0.51
10:L:48:CYS:HG	12:L:3005:ZN:ZN	1.19	0.51
10:L:46:VAL:CG2	10:L:46:VAL:CA	2.81	0.51
1:A:1098:VAL:N	1:A:1099:PRO:CD	2.73	0.51
1:A:1259:MET:O	1:A:1263:ILE:HG12	2.10	0.51
1:A:1287:TYR:O	1:A:1302:PRO:HA	2.11	0.51
1:A:735:VAL:HG12	1:A:736:ASN:N	2.24	0.51
1:A:941:LYS:CD	1:A:941:LYS:NZ	2.73	0.51
2:B:616:ILE:HD12	2:B:616:ILE:N	2.25	0.51
2:B:578:THR:HG23	2:B:622:LYS:O	2.09	0.51
5:F:83:PRO:HA	5:F:146:TRP:CZ3	2.45	0.51
1:A:1146:VAL:O	1:A:1146:VAL:HG13	2.10	0.51
1:A:635:ARG:CG	1:A:635:ARG:NE	2.64	0.51
2:B:384:ARG:O	2:B:385:LEU:C	2.44	0.51
2:B:640:VAL:HG22	2:B:651:LEU:CD2	2.40	0.51
2:B:726:ALA:C	2:B:726:ALA:CB	2.75	0.51
2:B:883:LEU:CA	2:B:883:LEU:HB2	2.20	0.51
6:H:111:LEU:CB	6:H:127:GLY:O	2.58	0.51
6:H:47:PHE:CB	6:H:95:TYR:HD1	2.23	0.51
6:H:63:LEU:CD2	6:H:63:LEU:CD1	2.82	0.51
10:L:48:CYS:CA	10:L:49:LYS:N	2.68	0.51
1:A:304:MET:HB2	1:A:304:MET:HE2	1.91	0.51
1:A:378:GLU:OE1	1:A:434:ARG:HD3	2.11	0.51
1:A:844:ALA:HB2	1:A:1384:VAL:HG12	1.92	0.51
3:C:233:GLU:OE1	8:J:12:LYS:HE2	2.11	0.51
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.57	0.51
5:F:107:VAL:HG12	5:F:109:VAL:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:902:GLY:O	10:L:65:VAL:HG11	2.10	0.51
1:A:265:LYS:HD3	1:A:302:THR:HG22	1.92	0.51
1:A:958:VAL:O	1:A:960:ILE:HD12	2.10	0.51
2:B:1102:LYS:CD	2:B:1102:LYS:CB	2.81	0.51
2:B:224:GLN:HB3	2:B:226:PHE:CZ	2.45	0.51
4:E:52:ARG:CG	4:E:53:PRO:HD3	2.41	0.51
5:F:82:THR:HB	5:F:84:TYR:N	2.25	0.51
8:J:3:VAL:HA	8:J:53:HIS:CD2	2.45	0.51
1:A:1094:VAL:HB	1:A:1094:VAL:CG1	2.21	0.51
1:A:1164:PRO:O	1:A:1167:GLU:HG2	2.10	0.51
1:A:1318:THR:HG23	4:E:11:ARG:HH12	1.75	0.51
1:A:24:PRO:CA	1:A:25:GLU:N	2.67	0.51
1:A:666:ILE:O	1:A:666:ILE:HD13	2.10	0.51
1:A:692:ASP:O	1:A:696:GLU:HB3	2.11	0.51
1:A:664:THR:HG21	1:A:746:MET:HE2	1.91	0.51
1:A:830:LYS:CD	1:A:830:LYS:CB	2.79	0.51
2:B:90:ILE:HA	2:B:133:LYS:O	2.10	0.51
2:B:89:GLU:HB2	2:B:137:TYR:HB2	1.92	0.51
3:C:112:ASN:CB	3:C:114:TYR:CE1	2.94	0.51
3:C:133:ILE:CD1	3:C:237:SER:HA	2.41	0.51
1:A:567:LYS:CD	6:H:95:TYR:CD1	2.94	0.51
1:A:982:THR:HG22	1:A:985:ASP:H	1.74	0.51
2:B:350:GLN:O	2:B:350:GLN:HG3	2.10	0.51
2:B:622:LYS:CD	2:B:622:LYS:CB	2.88	0.51
9:K:105:PHE:C	9:K:107:THR:N	2.63	0.51
9:K:55:LYS:CB	9:K:81:TYR:CD1	2.93	0.51
1:A:1027:ALA:O	1:A:1030:ARG:HB2	2.10	0.51
1:A:122:MET:CE	1:A:138:ILE:HD13	2.41	0.51
1:A:15:LYS:CA	1:A:15:LYS:CG	2.82	0.51
1:A:265:LYS:CE	1:A:302:THR:CG2	2.88	0.51
1:A:511:ILE:HD13	1:A:521:MET:CE	2.40	0.51
1:A:771:GLU:OE2	2:B:510:LYS:NZ	2.41	0.51
2:B:795:ILE:HD13	2:B:856:PHE:CE1	2.44	0.51
3:C:214:ASN:O	3:C:217:ASP:HB2	2.10	0.51
3:C:4:GLU:HG2	3:C:5:GLY:H	1.75	0.51
1:A:283:GLY:O	1:A:284:ALA:HB2	2.11	0.51
1:A:843:LYS:CE	1:A:843:LYS:CG	2.88	0.51
2:B:1059:LEU:HD11	2:B:1064:TYR:HB2	1.93	0.51
7:I:51:ASN:CB	7:I:118:ARG:CZ	2.86	0.51
1:A:1166:ASP:O	1:A:1167:GLU:C	2.47	0.51
1:A:1203:ASN:O	1:A:1205:LYS:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:LYS:CD	1:A:984:LYS:NZ	2.67	0.51
2:B:113:TYR:CG	2:B:192:LEU:HD22	2.46	0.51
2:B:137:TYR:CG	2:B:137:TYR:HB3	2.22	0.51
2:B:595:ARG:CB	2:B:595:ARG:CD	2.84	0.51
2:B:98:THR:OG1	2:B:127:GLY:N	2.44	0.51
4:E:23:VAL:CG1	4:E:30:ILE:HD11	2.41	0.51
4:E:45:LYS:NZ	4:E:45:LYS:CD	2.69	0.51
7:I:117:LYS:CD	7:I:117:LYS:NZ	2.70	0.51
7:I:75:CYS:HB2	7:I:77:LYS:H	1.75	0.51
9:K:18:LYS:HE2	9:K:38:GLU:OE2	2.10	0.51
1:A:1428:VAL:O	1:A:1429:ILE:C	2.50	0.50
1:A:265:LYS:HZ2	1:A:302:THR:HG21	1.76	0.50
1:A:84:ILE:HG22	1:A:241:VAL:HG23	1.92	0.50
2:B:879:ARG:NH2	2:B:885:MET:HE2	2.25	0.50
2:B:899:ILE:HD12	2:B:911:ILE:HA	1.92	0.50
2:B:59:LEU:HG	2:B:95:ILE:HD13	1.93	0.50
2:B:98:THR:HB	2:B:99:LYS:O	2.11	0.50
3:C:112:ASN:HB3	3:C:114:TYR:CE1	2.46	0.50
5:F:114:GLU:OE1	5:F:119:ARG:NE	2.43	0.50
1:A:1080:THR:C	1:A:1080:THR:HA	2.13	0.50
1:A:1135:ARG:CG	1:A:1135:ARG:NE	2.71	0.50
1:A:551:TYR:CD2	9:K:62:LYS:HD3	2.46	0.50
1:A:533:LYS:HZ2	1:A:745:GLN:HE22	1.59	0.50
1:A:884:ASP:O	1:A:886:ILE:N	2.44	0.50
2:B:1027:ILE:HD12	2:B:1052:VAL:HG22	1.93	0.50
2:B:206:ASN:OD1	2:B:458:LYS:HE2	2.12	0.50
3:C:71:PRO:C	3:C:133:ILE:HD12	2.32	0.50
1:A:1004:ASN:OD1	4:E:167:ARG:HG3	2.10	0.50
10:L:54:ARG:CB	10:L:54:ARG:CD	2.78	0.50
1:A:144:THR:CB	1:A:144:THR:N	2.66	0.50
2:B:112:LEU:C	2:B:112:LEU:HD12	2.31	0.50
1:A:72:GLU:HG2	2:B:1175:LEU:HD11	1.94	0.50
2:B:180:TYR:CA	2:B:181:LEU:N	2.65	0.50
2:B:273:LEU:HB3	2:B:274:PRO:HD2	1.92	0.50
2:B:212:LEU:HD23	2:B:480:SER:HB2	1.93	0.50
9:K:88:LYS:CG	9:K:88:LYS:CE	2.85	0.50
1:A:296:LEU:HD12	1:A:296:LEU:C	2.31	0.50
2:B:518:HIS:O	2:B:519:TRP:C	2.48	0.50
2:B:592:ASN:CA	2:B:592:ASN:CG	2.73	0.50
2:B:976:ILE:HD12	2:B:976:ILE:H	1.76	0.50
3:C:43:THR:O	3:C:161:LYS:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:56:THR:CG2	6:H:56:THR:CA	2.83	0.50
6:H:95:TYR:C	6:H:96:VAL:HG23	2.30	0.50
8:J:56:LEU:O	8:J:57:ILE:C	2.47	0.50
1:A:247:ARG:HH12	1:A:263:THR:CG2	2.24	0.50
2:B:192:LEU:CB	2:B:192:LEU:CD2	2.81	0.50
2:B:898:LEU:O	10:L:58:LYS:HE3	2.11	0.50
4:E:178:ILE:O	4:E:214:CYS:HA	2.12	0.50
6:H:56:THR:O	6:H:144:ILE:HD13	2.12	0.50
1:A:1436:ILE:HD12	2:B:1144:ALA:HB2	1.94	0.50
1:A:518:LYS:CG	1:A:518:LYS:CE	2.88	0.50
1:A:511:ILE:CD1	1:A:521:MET:SD	3.00	0.50
1:A:567:LYS:HD3	6:H:95:TYR:CB	2.39	0.50
2:B:1029:CYS:HB2	2:B:1090:THR:OG1	2.12	0.50
1:A:466:SER:CB	2:B:1103:ILE:HD11	2.40	0.50
2:B:35:SER:HA	2:B:811:TYR:CE2	2.46	0.50
4:E:93:MET:CE	4:E:116:ILE:HG21	2.42	0.50
1:A:1163:ILE:HD12	1:A:1163:ILE:N	2.26	0.50
1:A:1341:ILE:HD13	1:A:1379:GLY:O	2.10	0.50
1:A:754:SER:H	1:A:757:ASN:HD22	1.60	0.50
2:B:1165:ILE:CG2	2:B:1165:ILE:CA	2.83	0.50
2:B:273:LEU:CD1	2:B:276:ILE:HD13	2.42	0.50
2:B:453:ILE:HG22	2:B:454:THR:N	2.24	0.50
2:B:528:PRO:HG2	2:B:532:ALA:HB3	1.94	0.50
7:I:49:ILE:HG22	7:I:49:ILE:O	2.12	0.50
8:J:2:ILE:HD11	8:J:57:ILE:HD13	1.94	0.50
1:A:565:ILE:HG22	1:A:569:LYS:O	2.11	0.50
1:A:72:GLU:HG2	2:B:1175:LEU:CD1	2.42	0.50
3:C:56:THR:CG2	3:C:58:LEU:H	2.24	0.50
4:E:178:ILE:HD11	4:E:182:ASP:CG	2.32	0.50
6:H:105:GLU:HG2	6:H:136:LYS:NZ	2.27	0.50
7:I:75:CYS:SG	7:I:106:CYS:SG	3.10	0.50
1:A:107:CYS:HB2	1:A:148:CYS:HB2	1.92	0.50
1:A:110:CYS:C	1:A:110:CYS:HB2	2.31	0.50
1:A:191:THR:CG2	1:A:191:THR:HB	2.20	0.50
1:A:679:ILE:HD13	1:A:732:LEU:HD12	1.94	0.50
2:B:705:MET:CE	2:B:745:PRO:HG3	2.42	0.50
10:L:26:THR:HG22	10:L:28:LYS:H	1.76	0.50
1:A:1150:SER:OG	7:I:46:HIS:HB3	2.12	0.49
1:A:31:SER:CB	1:A:83:HIS:CD2	2.87	0.49
2:B:408:LEU:O	2:B:411:PRO:HD2	2.12	0.49
2:B:431:TYR:CE1	2:B:447:ALA:CB	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:78:LEU:HD21	4:E:80:VAL:CG2	2.42	0.49
1:A:551:TYR:O	9:K:62:LYS:NZ	2.45	0.49
1:A:1127:ASP:OD2	1:A:1130:GLN:HB2	2.12	0.49
1:A:84:ILE:HD13	1:A:270:LEU:HD11	1.93	0.49
1:A:523:ILE:HD12	1:A:622:VAL:HG22	1.93	0.49
1:A:786:HIS:H	1:A:786:HIS:CD2	2.29	0.49
2:B:933:SER:C	2:B:933:SER:HA	2.12	0.49
3:C:122:SER:CB	3:C:122:SER:HG	2.12	0.49
6:H:10:PHE:O	6:H:54:SER:HB2	2.11	0.49
8:J:16:ASP:OD1	8:J:17:LYS:HG2	2.12	0.49
1:A:1349:TYR:C	1:A:1349:TYR:CD2	2.83	0.49
1:A:531:ILE:HD11	1:A:578:LEU:HD21	1.94	0.49
1:A:3:GLY:N	1:A:76:GLU:OE2	2.45	0.49
2:B:1097:HIS:CE1	2:B:1102:LYS:HG3	2.47	0.49
2:B:1189:ILE:CA	2:B:1189:ILE:CG2	2.87	0.49
2:B:25:ILE:CG2	2:B:658:ILE:CD1	2.79	0.49
3:C:147:LEU:CD1	3:C:147:LEU:CB	2.85	0.49
1:A:1235:LYS:CG	1:A:1235:LYS:CA	2.85	0.49
1:A:1446:ASP:HB3	5:F:131:PRO:O	2.13	0.49
1:A:901:LEU:N	1:A:926:GLN:HE22	2.04	0.49
1:A:9:ALA:N	1:A:9:ALA:CB	2.66	0.49
2:B:114:PRO:HD3	2:B:124:TYR:CZ	2.42	0.49
2:B:510:LYS:N	2:B:511:PRO:CD	2.74	0.49
2:B:899:ILE:CD1	2:B:911:ILE:HG13	2.41	0.49
3:C:48:SER:HB3	3:C:158:VAL:HB	1.94	0.49
4:E:131:THR:C	4:E:131:THR:CB	2.69	0.49
4:E:36:GLU:O	4:E:38:PRO:HD3	2.12	0.49
6:H:98:TYR:C	6:H:118:PHE:HD2	2.15	0.49
1:A:353:ILE:HD12	1:A:482:PHE:CD2	2.47	0.49
1:A:50:ILE:CG2	1:A:51:GLY:N	2.72	0.49
1:A:961:ARG:O	1:A:965:GLN:HG3	2.12	0.49
2:B:48:LEU:HD23	2:B:48:LEU:N	2.27	0.49
6:H:97:MET:HE1	6:H:118:PHE:CD1	2.47	0.49
2:B:217:ARG:NE	2:B:217:ARG:HG3	2.26	0.49
3:C:135:GLN:NE2	3:C:135:GLN:CG	2.65	0.49
4:E:61:GLN:CG	4:E:61:GLN:CA	2.85	0.49
7:I:10:CYS:SG	7:I:29:CYS:SG	3.10	0.49
7:I:55:THR:HG21	7:I:121:PHE:O	2.11	0.49
10:L:48:CYS:HA	10:L:48:CYS:C	2.11	0.49
1:A:567:LYS:HB2	6:H:95:TYR:HA	1.95	0.49
2:B:544:CYS:HB2	2:B:634:TYR:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:162:GLY:HA3	3:C:170:TRP:CD1	2.48	0.49
7:I:1:MET:C	7:I:1:MET:CB	2.73	0.49
1:A:387:ARG:CB	1:A:387:ARG:CD	2.87	0.49
1:A:605:MET:HE3	1:A:607:ILE:HG13	1.93	0.49
1:A:69:THR:CA	1:A:69:THR:CG2	2.82	0.49
1:A:967:ALA:HB2	1:A:1044:TRP:CZ3	2.48	0.49
2:B:127:GLY:HA2	2:B:168:GLY:O	2.13	0.49
2:B:899:ILE:HG22	2:B:900:ALA:N	2.27	0.49
9:K:55:LYS:HB2	9:K:81:TYR:CD1	2.47	0.49
1:A:1267:MET:HE3	1:A:1267:MET:HB3	1.47	0.49
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.12	0.49
1:A:176:LYS:NZ	1:A:178:GLY:O	2.36	0.49
2:B:1052:VAL:HA	2:B:1055:ILE:HD12	1.94	0.49
2:B:581:PHE:HA	2:B:585:VAL:O	2.13	0.49
3:C:40:GLU:C	3:C:163:ILE:HD11	2.33	0.49
8:J:7:CYS:SG	8:J:46:CYS:N	2.86	0.49
9:K:111:LEU:HB3	9:K:111:LEU:CD1	2.42	0.49
9:K:18:LYS:HE3	9:K:38:GLU:HG2	1.95	0.49
1:A:58:LEU:HB3	1:A:80:HIS:O	2.12	0.49
1:A:965:GLN:OE1	1:A:965:GLN:CG	2.52	0.49
2:B:170:LEU:HD12	2:B:457:LEU:HD13	1.94	0.49
2:B:43:LEU:HD11	2:B:811:TYR:O	2.13	0.49
3:C:9:LYS:O	3:C:10:ILE:C	2.51	0.49
6:H:130:ARG:HB2	6:H:133:ASN:HB3	1.94	0.49
1:A:427:GLN:CD	1:A:427:GLN:CB	2.75	0.48
2:B:416:LEU:HD12	2:B:466:TRP:CZ2	2.47	0.48
2:B:648:HIS:HE2	2:B:711:GLU:HA	1.77	0.48
3:C:216:GLY:O	3:C:217:ASP:C	2.51	0.48
4:E:78:LEU:HD21	4:E:80:VAL:HG23	1.95	0.48
6:H:24:CYS:SG	6:H:44:VAL:HG21	2.53	0.48
7:I:49:ILE:CA	7:I:49:ILE:CG2	2.86	0.48
9:K:47:ARG:HD2	9:K:47:ARG:O	2.13	0.48
1:A:1094:VAL:CA	1:A:1094:VAL:CG1	2.81	0.48
1:A:62:ASP:C	1:A:64:ASN:H	2.16	0.48
2:B:230:ALA:CB	2:B:230:ALA:N	2.70	0.48
2:B:167:ILE:CG2	2:B:424:LEU:CD1	2.92	0.48
8:J:7:CYS:HB3	8:J:10:CYS:H	1.78	0.48
1:A:588:LEU:HD23	1:A:588:LEU:C	2.34	0.48
1:A:84:ILE:CG2	1:A:241:VAL:CG2	2.91	0.48
1:A:903:ASN:ND2	1:A:905:ASP:H	2.12	0.48
2:B:167:ILE:HG21	2:B:424:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:ALA:HB2	2:B:251:ILE:CD1	2.40	0.48
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.42	0.48
2:B:296:GLU:O	2:B:300:HIS:HD2	1.95	0.48
2:B:603:LEU:HD13	2:B:609:ILE:HD11	1.96	0.48
2:B:617:ARG:NE	2:B:617:ARG:CG	2.69	0.48
9:K:43:GLY:HA2	9:K:71:PHE:CZ	2.48	0.48
1:A:1232:ASN:ND2	1:A:1232:ASN:CB	2.70	0.48
1:A:296:LEU:HD12	1:A:296:LEU:O	2.13	0.48
2:B:137:TYR:HB2	2:B:137:TYR:CA	2.19	0.48
2:B:566:LEU:HD13	2:B:588:GLY:HA2	1.95	0.48
2:B:621:GLU:O	2:B:622:LYS:HB2	2.12	0.48
2:B:615:MET:CG	2:B:626:ILE:HD12	2.39	0.48
2:B:735:ALA:HA	2:B:735:ALA:N	2.06	0.48
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.78	0.48
4:E:5:ASN:O	4:E:9:ILE:HG13	2.14	0.48
8:J:43:ARG:O	8:J:47:ARG:HG3	2.14	0.48
1:A:60:SER:C	1:A:61:ILE:O	2.48	0.48
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.79	0.48
2:B:273:LEU:CD1	2:B:276:ILE:CD1	2.91	0.48
2:B:520:GLY:O	2:B:521:LEU:HD23	2.13	0.48
3:C:92:CYS:SG	3:C:95:CYS:SG	3.11	0.48
9:K:82:ASP:OD1	9:K:83:PRO:CG	2.58	0.48
1:A:1151:GLU:O	1:A:1193:LEU:HA	2.13	0.48
1:A:535:THR:HG23	1:A:616:VAL:HA	1.96	0.48
1:A:630:ILE:HD12	1:A:642:CYS:SG	2.54	0.48
1:A:901:LEU:HA	1:A:907:THR:HG23	1.95	0.48
2:B:70:ILE:HA	2:B:70:ILE:CB	2.22	0.48
2:B:724:ASP:O	2:B:725:PRO:C	2.49	0.48
2:B:733:HIS:C	2:B:733:HIS:CB	2.78	0.48
2:B:789:MET:HE3	2:B:965:LYS:HB3	1.95	0.48
2:B:121:ASN:ND2	2:B:965:LYS:NZ	2.61	0.48
3:C:244:VAL:O	3:C:248:ILE:HG12	2.14	0.48
1:A:983:ILE:HD12	1:A:983:ILE:N	2.28	0.48
2:B:1006:ILE:HG22	2:B:1007:VAL:N	2.29	0.48
2:B:1153:GLU:HA	2:B:1153:GLU:OE1	2.14	0.48
2:B:237:VAL:CG1	2:B:238:ALA:N	2.72	0.48
2:B:210:LYS:HE3	2:B:461:LEU:O	2.13	0.48
2:B:509:ALA:HA	2:B:509:ALA:CB	2.19	0.48
2:B:642:ASP:HB3	2:B:649:LYS:HG3	1.95	0.48
2:B:701:ILE:HD13	2:B:703:ILE:CG1	2.42	0.48
2:B:953:LEU:HD23	2:B:954:VAL:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:8:VAL:CG1	3:C:9:LYS:H	2.27	0.48
4:E:112:TYR:CD1	4:E:112:TYR:C	2.86	0.48
1:A:1362:TYR:CD2	1:A:1362:TYR:C	2.86	0.48
1:A:786:HIS:CD2	1:A:786:HIS:N	2.81	0.48
1:A:867:ILE:CG2	1:A:867:ILE:CA	2.84	0.48
1:A:868:TYR:CE1	1:A:1064:VAL:HG13	2.48	0.48
1:A:913:LEU:HD12	1:A:914:GLU:N	2.29	0.48
1:A:926:GLN:O	1:A:926:GLN:HG3	2.13	0.48
2:B:251:ILE:O	2:B:251:ILE:CG2	2.54	0.48
2:B:314:LEU:O	2:B:315:LYS:C	2.51	0.48
2:B:408:LEU:O	2:B:409:ALA:C	2.47	0.48
2:B:779:GLY:C	2:B:780:VAL:CG2	2.77	0.48
3:C:43:THR:C	3:C:77:ILE:HD13	2.34	0.48
6:H:103:LYS:HD3	6:H:105:GLU:CD	2.34	0.48
7:I:50:THR:CG2	7:I:50:THR:O	2.59	0.48
8:J:38:ARG:CD	8:J:38:ARG:CB	2.85	0.48
10:L:27:LEU:CA	10:L:27:LEU:HB3	2.19	0.48
1:A:1172:LEU:O	1:A:1173:HIS:CD2	2.67	0.48
1:A:217:LYS:O	1:A:221:SER:HB2	2.14	0.48
1:A:351:THR:HG21	2:B:1103:ILE:HG12	1.94	0.48
1:A:41:MET:O	1:A:50:ILE:HD11	2.14	0.48
1:A:524:VAL:O	1:A:525:GLN:C	2.49	0.48
1:A:709:THR:HG22	1:A:711:ARG:N	2.29	0.48
2:B:167:ILE:O	2:B:167:ILE:HG22	2.13	0.48
2:B:545:ILE:O	2:B:546:SER:C	2.49	0.48
2:B:724:ASP:C	2:B:726:ALA:H	2.17	0.48
2:B:789:MET:HE2	2:B:965:LYS:HB3	1.94	0.48
2:B:845:SER:O	2:B:846:ILE:C	2.50	0.48
1:A:1120:LEU:HD21	1:A:1131:ALA:CB	2.41	0.48
1:A:1132:LYS:O	1:A:1133:LEU:C	2.49	0.48
1:A:531:ILE:HD11	1:A:578:LEU:HD22	1.93	0.48
1:A:57:ARG:HB3	1:A:68:GLN:CG	2.44	0.48
1:A:606:LEU:HG	1:A:613:ILE:HD13	1.95	0.48
2:B:1198:TYR:HA	2:B:1198:TYR:CG	2.41	0.48
6:H:136:LYS:CA	6:H:137:GLN:N	2.68	0.48
6:H:22:LYS:HG2	6:H:22:LYS:HE2	1.96	0.48
1:A:1164:PRO:O	1:A:1167:GLU:CG	2.62	0.47
2:B:192:LEU:O	2:B:193:LYS:HB2	2.13	0.47
2:B:830:TYR:O	2:B:831:SER:OG	2.27	0.47
2:B:956:THR:HG22	2:B:960:GLY:HA2	1.95	0.47
2:B:367:LEU:CD1	2:B:367:LEU:HG	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:35:ARG:CB	3:C:35:ARG:CD	2.92	0.47
4:E:80:VAL:HA	4:E:109:ILE:O	2.14	0.47
5:F:117:PRO:O	5:F:118:LEU:C	2.49	0.47
6:H:128:ASN:O	6:H:128:ASN:OD1	2.32	0.47
7:I:65:ASP:C	7:I:65:ASP:OD1	2.52	0.47
7:I:71:SER:OG	7:I:83:ASN:ND2	2.47	0.47
1:A:1067:LEU:O	1:A:1071:SER:OG	2.25	0.47
1:A:1209:MET:O	1:A:1210:GLY:C	2.49	0.47
2:B:99:LYS:HB3	2:B:100:PRO:HD3	1.96	0.47
2:B:642:ASP:HB3	2:B:649:LYS:HE2	1.96	0.47
2:B:820:GLY:HA3	2:B:1091:TYR:CE2	2.48	0.47
2:B:859:TYR:CD1	2:B:859:TYR:N	2.83	0.47
2:B:897:GLY:O	2:B:898:LEU:HD23	2.15	0.47
5:F:109:VAL:CG1	5:F:110:ASP:N	2.77	0.47
7:I:43:VAL:O	7:I:43:VAL:CG1	2.61	0.47
10:L:43:THR:HA	10:L:43:THR:CB	2.19	0.47
1:A:237:THR:CG2	1:A:237:THR:CA	2.81	0.47
1:A:446:ARG:CG	1:A:446:ARG:NH1	2.74	0.47
1:A:498:ARG:HD3	1:A:498:ARG:HH11	1.23	0.47
2:B:1161:HIS:HA	2:B:1192:TYR:O	2.14	0.47
2:B:122:LEU:O	2:B:207:GLY:N	2.38	0.47
2:B:249:ARG:CA	2:B:250:PHE:N	2.68	0.47
2:B:555:ILE:HD12	2:B:587:HIS:CE1	2.50	0.47
4:E:31:THR:OG1	4:E:31:THR:CG2	2.56	0.47
9:K:111:LEU:N	9:K:111:LEU:HD23	2.29	0.47
10:L:46:VAL:CG2	10:L:46:VAL:CG1	2.85	0.47
1:A:146:MET:HA	1:A:171:GLN:HB2	1.96	0.47
1:A:381:THR:C	1:A:383:TYR:N	2.64	0.47
2:B:1160:VAL:HG12	2:B:1161:HIS:O	2.14	0.47
2:B:190:TYR:O	2:B:191:LYS:C	2.50	0.47
4:E:127:ILE:N	4:E:128:PRO:HD3	2.29	0.47
4:E:164:LEU:HD12	4:E:168:TYR:HD1	1.79	0.47
5:F:75:PRO:CG	5:F:78:GLN:OE1	2.63	0.47
9:K:55:LYS:CB	9:K:81:TYR:HD1	2.28	0.47
1:A:867:ILE:HD12	1:A:1000:LEU:HD11	1.97	0.47
1:A:1127:ASP:O	1:A:1128:GLN:C	2.52	0.47
1:A:1146:VAL:O	1:A:1146:VAL:CG1	2.60	0.47
1:A:50:ILE:HG22	1:A:51:GLY:N	2.22	0.47
1:A:578:LEU:O	1:A:582:ILE:HD12	2.15	0.47
1:A:633:VAL:HG21	1:A:645:LEU:HD22	1.96	0.47
1:A:793:SER:O	1:A:794:PRO:C	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1163:CYS:HB2	2:B:1182:CYS:HB2	1.96	0.47
2:B:877:PRO:O	2:B:878:GLN:CG	2.63	0.47
3:C:33:LEU:CD1	3:C:248:ILE:HD13	2.42	0.47
4:E:59:SER:O	4:E:60:PHE:CB	2.59	0.47
6:H:7:ASP:C	6:H:7:ASP:OD1	2.52	0.47
9:K:88:LYS:CD	9:K:88:LYS:CB	2.88	0.47
1:A:1221:LYS:CG	1:A:1221:LYS:CE	2.76	0.47
1:A:14:VAL:H	1:A:1432:GLN:NE2	2.11	0.47
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.96	0.47
1:A:862:ASN:OD1	4:E:174:GLN:HA	2.14	0.47
1:A:982:THR:HB	1:A:985:ASP:CG	2.35	0.47
2:B:1006:ILE:HD12	2:B:1006:ILE:H	1.79	0.47
2:B:1185:CYS:CA	2:B:1185:CYS:HB2	2.21	0.47
2:B:458:LYS:CE	2:B:458:LYS:CG	2.80	0.47
2:B:566:LEU:HA	2:B:566:LEU:HD12	1.66	0.47
6:H:56:THR:HG21	6:H:145:ARG:NE	2.30	0.47
1:A:1100:ARG:O	1:A:1104:ILE:HG13	2.14	0.47
1:A:1194:ARG:CB	1:A:1194:ARG:HD2	2.42	0.47
2:B:101:MET:HA	2:B:110:HIS:O	2.15	0.47
2:B:1163:CYS:CB	2:B:1163:CYS:HA	2.23	0.47
2:B:369:GLY:C	2:B:370:PHE:CD1	2.88	0.47
2:B:416:LEU:CD2	2:B:416:LEU:CB	2.82	0.47
2:B:880:THR:O	2:B:933:SER:OG	2.28	0.47
5:F:119:ARG:NH1	5:F:119:ARG:HG2	2.29	0.47
5:F:75:PRO:O	5:F:76:LYS:C	2.53	0.47
3:C:57:VAL:HG21	8:J:60:PHE:HB3	1.96	0.47
3:C:241:ASP:HB3	9:K:109:TRP:CD2	2.49	0.47
10:L:49:LYS:NZ	10:L:49:LYS:HG2	2.30	0.47
1:A:1163:ILE:O	1:A:1164:PRO:C	2.51	0.47
1:A:110:CYS:SG	1:A:167:CYS:CB	3.02	0.47
1:A:679:ILE:HD11	1:A:729:ALA:O	2.15	0.47
2:B:1174:LYS:O	2:B:1179:GLN:N	2.40	0.47
2:B:185:THR:HG23	2:B:188:ASP:OD2	2.14	0.47
2:B:274:PRO:HG3	2:B:359:GLU:O	2.15	0.47
1:A:771:GLU:CD	2:B:510:LYS:NZ	2.68	0.47
6:H:118:PHE:N	6:H:121:LEU:O	2.33	0.47
7:I:92:ARG:HB3	7:I:94:ASP:H	1.80	0.47
10:L:26:THR:CB	10:L:27:LEU:H	2.27	0.47
1:A:93:VAL:HA	1:A:96:ILE:CD1	2.45	0.47
2:B:875:GLU:O	2:B:877:PRO:CD	2.62	0.47
3:C:24:ASN:ND2	3:C:24:ASN:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:100:ILE:CG2	4:E:101:GLN:N	2.59	0.47
4:E:93:MET:HE3	4:E:116:ILE:HG21	1.97	0.47
1:A:852:TYR:CD2	5:F:136:ARG:HD3	2.50	0.47
8:J:53:HIS:ND1	8:J:54:VAL:N	2.62	0.47
1:A:421:ALA:HA	1:A:424:ILE:HD11	1.97	0.47
1:A:535:THR:O	1:A:535:THR:HG23	2.14	0.47
1:A:913:LEU:O	1:A:914:GLU:C	2.52	0.47
2:B:112:LEU:HD12	2:B:113:TYR:N	2.30	0.47
3:C:135:GLN:CB	3:C:135:GLN:CD	2.71	0.47
9:K:100:ALA:O	9:K:103:THR:HB	2.15	0.47
1:A:967:ALA:HB2	1:A:1044:TRP:CE3	2.50	0.46
1:A:1259:MET:O	1:A:1260:LEU:C	2.52	0.46
1:A:573:SER:O	1:A:574:GLY:C	2.51	0.46
2:B:123:THR:OG1	2:B:458:LYS:HE3	2.15	0.46
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.97	0.46
2:B:883:LEU:CD2	2:B:883:LEU:HG	2.21	0.46
3:C:98:VAL:C	3:C:99:LEU:HD12	2.36	0.46
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.31	0.46
1:A:399:HIS:CD2	1:A:400:PRO:HD3	2.50	0.46
2:B:102:VAL:O	2:B:109:THR:HA	2.15	0.46
2:B:1080:LYS:CD	2:B:1080:LYS:NZ	2.76	0.46
2:B:284:ILE:HD13	2:B:333:PHE:CE2	2.50	0.46
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.30	0.46
3:C:154:LYS:CG	3:C:154:LYS:CA	2.88	0.46
3:C:207:CYS:O	3:C:208:GLU:C	2.53	0.46
3:C:74:SER:CB	3:C:238:ILE:HD12	2.43	0.46
4:E:50:MET:CA	4:E:51:GLY:N	2.68	0.46
1:A:698:GLN:CB	1:A:698:GLN:CD	2.71	0.46
1:A:693:VAL:CG2	1:A:721:PHE:HE1	2.19	0.46
2:B:450:ALA:O	2:B:451:LYS:C	2.52	0.46
6:H:113:ALA:CB	6:H:124:ARG:NH2	2.78	0.46
6:H:27:GLU:OE1	6:H:39:THR:CG2	2.63	0.46
1:A:385:ILE:HD12	1:A:385:ILE:O	2.16	0.46
1:A:546:VAL:O	1:A:547:LEU:C	2.51	0.46
1:A:837:ILE:O	1:A:838:GLN:C	2.49	0.46
2:B:1020:ARG:O	2:B:1021:MET:C	2.51	0.46
2:B:639:ILE:C	2:B:639:ILE:CG2	2.84	0.46
2:B:900:ALA:O	2:B:903:VAL:HG23	2.16	0.46
2:B:950:ASP:O	2:B:951:GLN:CB	2.64	0.46
3:C:116:LYS:CD	3:C:116:LYS:HZ3	2.25	0.46
5:F:74:ILE:HD12	5:F:143:PHE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:18:GLY:O	6:H:19:ARG:HB2	2.15	0.46
6:H:14:GLU:O	6:H:26:ILE:HA	2.16	0.46
10:L:34:CYS:SG	10:L:51:CYS:HB3	2.54	0.46
1:A:1030:ARG:O	1:A:1034:GLU:HB2	2.15	0.46
1:A:138:ILE:HD12	1:A:142:CYS:SG	2.55	0.46
1:A:304:MET:CE	1:A:304:MET:HB2	2.45	0.46
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.97	0.46
2:B:425:THR:CG2	2:B:425:THR:CA	2.85	0.46
5:F:75:PRO:HG2	5:F:78:GLN:OE1	2.15	0.46
8:J:20:SER:O	8:J:24:LEU:HG	2.14	0.46
1:A:834:THR:HG21	1:A:1077:THR:OG1	2.16	0.46
1:A:1151:GLU:CD	7:I:45:ARG:CD	2.84	0.46
1:A:1111:MET:HE1	1:A:1331:SER:HA	1.98	0.46
1:A:42:ASP:OD2	1:A:47:ARG:HA	2.15	0.46
1:A:562:THR:HG22	6:H:98:TYR:CD2	2.51	0.46
1:A:512:VAL:HG11	1:A:635:ARG:HH21	1.81	0.46
1:A:903:ASN:HD22	1:A:904:THR:N	2.09	0.46
2:B:1171:VAL:HG21	2:B:1191:ILE:CD1	2.46	0.46
2:B:862:GLN:HE22	2:B:961:LEU:HD13	1.79	0.46
4:E:55:ARG:O	4:E:57:MET:N	2.48	0.46
4:E:95:THR:CG2	4:E:95:THR:CA	2.87	0.46
5:F:81:THR:HB	5:F:144:GLU:OE1	2.16	0.46
6:H:135:LEU:CD1	6:H:139:ASN:O	2.64	0.46
6:H:91:ASP:C	6:H:91:ASP:OD1	2.54	0.46
9:K:95:ILE:HD12	9:K:95:ILE:HG23	1.97	0.46
1:A:377:PRO:O	1:A:377:PRO:CD	2.64	0.46
1:A:406:ILE:N	1:A:406:ILE:HD12	2.30	0.46
1:A:474:VAL:O	1:A:475:THR:C	2.51	0.46
1:A:566:ILE:CD1	6:H:96:VAL:O	2.62	0.46
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.98	0.46
1:A:896:ARG:HD3	1:A:897:TYR:CZ	2.50	0.46
2:B:1165:ILE:HD13	2:B:1165:ILE:N	2.31	0.46
2:B:841:MET:CE	2:B:990:ILE:HD11	2.46	0.46
9:K:18:LYS:CE	9:K:38:GLU:OE2	2.63	0.46
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.31	0.46
1:A:326:ARG:O	1:A:327:ALA:CB	2.64	0.46
1:A:672:ASP:H	1:A:736:ASN:ND2	2.13	0.46
1:A:763:ALA:O	1:A:764:CYS:HB2	2.15	0.46
1:A:914:GLU:C	1:A:916:GLY:N	2.69	0.46
1:A:983:ILE:C	1:A:983:ILE:N	2.53	0.46
2:B:451:LYS:O	2:B:453:ILE:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:455:SER:O	2:B:459:TYR:CB	2.63	0.46
2:B:556:THR:C	2:B:556:THR:HG22	2.36	0.46
2:B:64:CYS:HA	2:B:67:SER:HB2	1.98	0.46
5:F:128:LYS:HA	5:F:128:LYS:HD3	1.80	0.46
6:H:13:SER:O	6:H:14:GLU:HG3	2.16	0.46
8:J:53:HIS:HE1	8:J:55:ASP:CA	2.29	0.46
9:K:20:LYS:CE	9:K:20:LYS:CG	2.90	0.46
10:L:47:ARG:HG2	10:L:48:CYS:N	2.22	0.46
1:A:1039:LYS:HE3	1:A:1043:ASP:OD2	2.16	0.46
1:A:270:LEU:C	1:A:274:ILE:HD12	2.35	0.46
1:A:605:MET:CE	1:A:607:ILE:CG1	2.93	0.46
1:A:587:HIS:HE2	1:A:969:GLN:HG2	1.80	0.46
2:B:416:LEU:HD11	2:B:466:TRP:CZ2	2.50	0.46
2:B:639:ILE:CG2	2:B:639:ILE:HG13	2.43	0.46
2:B:94:LYS:HG2	2:B:96:TYR:CE1	2.51	0.46
3:C:145:CYS:SG	3:C:146:LYS:N	2.89	0.46
1:A:243:PRO:CB	1:A:245:PRO:HD2	2.43	0.46
1:A:605:MET:HE2	1:A:607:ILE:CD1	2.46	0.46
1:A:72:GLU:CG	2:B:1175:LEU:CD1	2.94	0.46
1:A:909:ASP:CG	1:A:910:PRO:HD2	2.36	0.46
1:A:964:ILE:HD13	1:A:1045:VAL:HG21	1.97	0.46
2:B:1031:LEU:O	2:B:1031:LEU:HG	2.16	0.46
2:B:1035:ALA:HB1	2:B:1040:ASN:O	2.16	0.46
2:B:189:LEU:HA	2:B:189:LEU:HD23	1.79	0.46
2:B:561:TRP:O	2:B:590:HIS:CE1	2.54	0.46
2:B:912:ILE:O	2:B:938:SER:HB2	2.16	0.46
3:C:218:PRO:O	3:C:219:PHE:C	2.55	0.46
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.46	0.46
5:F:111:LEU:CD1	5:F:120:ILE:HD12	2.46	0.46
7:I:17:ARG:NE	7:I:17:ARG:CG	2.75	0.46
1:A:1226:VAL:HG12	1:A:1227:ILE:N	2.28	0.45
1:A:1336:MET:HE2	1:A:1381:LEU:H	1.81	0.45
1:A:444:PHE:HE2	1:A:470:LEU:HD21	1.79	0.45
1:A:531:ILE:O	1:A:535:THR:HB	2.15	0.45
1:A:58:LEU:HA	1:A:80:HIS:HB2	1.98	0.45
1:A:633:VAL:O	1:A:634:THR:C	2.50	0.45
1:A:982:THR:C	1:A:983:ILE:CA	2.73	0.45
2:B:113:TYR:CD2	2:B:192:LEU:CD2	2.99	0.45
2:B:276:ILE:HG21	2:B:280:ILE:HD11	1.98	0.45
2:B:999:MET:CG	2:B:999:MET:HE2	2.30	0.45
3:C:106:GLU:O	3:C:149:LYS:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:THR:HG22	3:C:58:LEU:H	1.81	0.45
1:A:1151:GLU:CD	7:I:45:ARG:HD2	2.36	0.45
1:A:1194:ARG:HG2	1:A:1194:ARG:NH1	2.31	0.45
1:A:130:ASP:O	1:A:131:SER:C	2.53	0.45
1:A:1417:GLU:OE1	1:A:1419:ASP:OD1	2.33	0.45
1:A:31:SER:N	1:A:31:SER:C	2.58	0.45
2:B:29:ASP:CG	2:B:658:ILE:HD13	2.37	0.45
2:B:41:LYS:CE	2:B:41:LYS:CG	2.82	0.45
2:B:451:LYS:O	2:B:454:THR:N	2.49	0.45
2:B:557:PHE:O	2:B:560:GLU:HB2	2.16	0.45
2:B:566:LEU:O	2:B:567:GLU:C	2.54	0.45
2:B:806:THR:HG22	2:B:809:MET:H	1.81	0.45
2:B:835:GLN:O	2:B:838:SER:HB3	2.16	0.45
3:C:196:ASP:CB	3:C:199:LYS:HG3	2.44	0.45
4:E:31:THR:O	4:E:32:GLN:C	2.54	0.45
1:A:300:VAL:O	1:A:303:TYR:HB3	2.16	0.45
1:A:531:ILE:HD11	1:A:578:LEU:HD11	1.98	0.45
1:A:711:ARG:N	1:A:711:ARG:CG	2.78	0.45
1:A:9:ALA:C	1:A:9:ALA:CB	2.72	0.45
2:B:1002:THR:CA	2:B:1003:ALA:N	2.66	0.45
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.51	0.45
3:C:181:ASP:CG	3:C:181:ASP:O	2.44	0.45
4:E:132:ILE:HG22	4:E:133:GLU:N	2.29	0.45
6:H:52:GLN:O	6:H:53:ASP:O	2.35	0.45
10:L:26:THR:CG2	10:L:28:LYS:H	2.29	0.45
10:L:29:TYR:O	10:L:30:ILE:HG13	2.16	0.45
1:A:122:MET:HE3	1:A:138:ILE:HD13	1.97	0.45
2:B:408:LEU:HD11	2:B:545:ILE:HD13	1.98	0.45
2:B:420:LEU:CD1	2:B:420:LEU:CD2	2.83	0.45
2:B:555:ILE:HD13	2:B:582:VAL:HG21	1.97	0.45
2:B:758:PHE:N	2:B:759:PRO:CD	2.79	0.45
2:B:35:SER:HA	2:B:811:TYR:HE2	1.81	0.45
2:B:956:THR:CG2	2:B:960:GLY:HA2	2.47	0.45
3:C:146:LYS:CB	3:C:146:LYS:HD3	2.44	0.45
3:C:205:LYS:CD	3:C:205:LYS:NZ	2.74	0.45
3:C:27:LEU:O	3:C:30:ALA:HB3	2.16	0.45
6:H:15:VAL:CG2	6:H:26:ILE:HG13	2.46	0.45
8:J:43:ARG:HH11	8:J:43:ARG:HD3	1.36	0.45
9:K:55:LYS:CB	9:K:55:LYS:CD	2.82	0.45
1:A:1187:GLN:CG	1:A:1187:GLN:N	2.79	0.45
1:A:289:ILE:CA	1:A:289:ILE:CG2	2.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:PRO:CG	2:B:359:GLU:HB3	2.47	0.45
2:B:779:GLY:C	2:B:780:VAL:HG23	2.26	0.45
2:B:806:THR:CG2	2:B:808:ALA:H	2.26	0.45
5:F:114:GLU:CB	5:F:120:ILE:HD13	2.40	0.45
8:J:2:ILE:O	8:J:3:VAL:C	2.50	0.45
8:J:38:ARG:CA	8:J:38:ARG:CG	2.85	0.45
9:K:65:HIS:CD2	9:K:66:PRO:N	2.84	0.45
1:A:1169:ILE:HD11	1:A:1229:SER:HB2	1.98	0.45
2:B:1074:ASN:O	2:B:1075:GLY:C	2.52	0.45
1:A:1438:THR:HB	2:B:1142:GLY:O	2.16	0.45
2:B:1163:CYS:CA	2:B:1163:CYS:SG	3.02	0.45
2:B:387:LEU:HD12	2:B:387:LEU:HA	1.66	0.45
2:B:436:VAL:CB	2:B:436:VAL:HA	2.27	0.45
2:B:590:HIS:CD2	2:B:591:ARG:N	2.85	0.45
2:B:951:GLN:NE2	2:B:951:GLN:CG	2.68	0.45
6:H:52:GLN:O	6:H:53:ASP:C	2.55	0.45
1:A:1436:ILE:CD1	2:B:1144:ALA:HB2	2.46	0.45
2:B:121:ASN:HA	2:B:207:GLY:CA	2.47	0.45
2:B:299:GLU:HG2	2:B:571:PRO:HD2	1.98	0.45
13:B:3008:CTP:C4'	14:B:3010:HOH:O	2.33	0.45
3:C:11:ARG:HE	3:C:209:TYR:HE2	1.55	0.45
4:E:118:PRO:O	4:E:122:LYS:HG3	2.17	0.45
8:J:49:MET:HB3	8:J:50:ILE:HD12	1.99	0.45
1:A:262:LEU:HD22	1:A:325:ILE:CD1	2.47	0.45
2:B:129:PHE:CD2	2:B:166:PHE:HA	2.52	0.45
9:K:104:ASN:OD1	9:K:104:ASN:N	2.48	0.45
1:A:184:SER:CB	1:A:199:LEU:HD23	2.39	0.45
1:A:377:PRO:O	1:A:377:PRO:HD2	2.16	0.45
1:A:550:LEU:HD13	1:A:556:TRP:HZ2	1.81	0.45
2:B:123:THR:O	2:B:125:SER:N	2.50	0.45
2:B:311:LEU:O	2:B:312:GLU:C	2.55	0.45
2:B:875:GLU:O	2:B:877:PRO:N	2.50	0.45
2:B:957:ASN:HB3	2:B:961:LEU:H	1.82	0.45
3:C:116:LYS:NZ	3:C:116:LYS:HD3	2.26	0.45
3:C:44:LEU:HG	3:C:45:ALA:N	2.31	0.45
4:E:117:THR:O	4:E:119:SER:N	2.50	0.45
4:E:127:ILE:HD12	4:E:130:ALA:HB3	1.99	0.45
6:H:127:GLY:O	6:H:128:ASN:HB2	2.17	0.45
3:C:248:ILE:HD12	9:K:101:LEU:HD12	1.99	0.45
1:A:1221:LYS:CB	1:A:1221:LYS:CD	2.91	0.45
1:A:857:ARG:CA	1:A:864:ILE:HD13	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:547:VAL:O	2:B:547:VAL:HG13	2.16	0.45
2:B:788:ARG:C	2:B:789:MET:HG2	2.38	0.45
2:B:969:ARG:HH11	2:B:969:ARG:HD3	1.61	0.45
3:C:48:SER:C	3:C:49:VAL:HG23	2.37	0.45
4:E:152:LYS:CB	4:E:152:LYS:CD	2.91	0.45
9:K:39:ASP:HB2	9:K:40:HIS:H	1.55	0.45
2:B:1150:ARG:HA	2:B:1150:ARG:HD3	1.75	0.44
2:B:170:LEU:HD12	2:B:170:LEU:HA	1.75	0.44
2:B:232:SER:HA	2:B:233:PRO:HD3	1.81	0.44
4:E:191:LYS:O	4:E:192:ARG:C	2.54	0.44
9:K:105:PHE:C	9:K:107:THR:H	2.19	0.44
9:K:21:ILE:HG12	9:K:33:ILE:HG23	1.98	0.44
10:L:31:CYS:CB	10:L:34:CYS:SG	3.05	0.44
1:A:189:ARG:O	1:A:190:ALA:HB3	2.17	0.44
1:A:464:PRO:O	1:A:465:TYR:O	2.36	0.44
2:B:1079:LYS:HE3	3:C:188:HIS:CE1	2.51	0.44
2:B:213:ILE:HD11	2:B:481:GLN:OE1	2.18	0.44
2:B:644:GLU:OE1	2:B:646:LEU:HB2	2.18	0.44
4:E:79:TRP:NE1	4:E:81:GLU:HB2	2.32	0.44
4:E:80:VAL:CG1	4:E:81:GLU:N	2.79	0.44
1:A:1315:GLU:O	1:A:1318:THR:HG22	2.17	0.44
1:A:401:GLY:N	1:A:435:HIS:ND1	2.60	0.44
1:A:566:ILE:CA	1:A:566:ILE:CG2	2.91	0.44
1:A:992:ASP:CG	1:A:992:ASP:CA	2.77	0.44
2:B:787:VAL:C	2:B:787:VAL:HG12	2.36	0.44
2:B:787:VAL:CG2	2:B:787:VAL:CG1	2.84	0.44
3:C:94:LYS:CG	3:C:94:LYS:NZ	2.80	0.44
4:E:162:ARG:CG	4:E:162:ARG:NE	2.72	0.44
6:H:123:MET:HG2	6:H:124:ARG:N	2.32	0.44
9:K:47:ARG:HD2	9:K:47:ARG:C	2.38	0.44
1:A:1203:ASN:C	1:A:1205:LYS:N	2.70	0.44
1:A:507:VAL:N	1:A:508:PRO:CD	2.80	0.44
1:A:599:SER:HA	1:A:600:PRO:HD2	1.57	0.44
1:A:83:HIS:C	1:A:83:HIS:ND1	2.71	0.44
2:B:1099:VAL:O	2:B:1103:ILE:HD12	2.18	0.44
2:B:485:ARG:HG3	2:B:485:ARG:HH11	1.82	0.44
2:B:996:ARG:NH2	3:C:174:ALA:O	2.50	0.44
3:C:8:VAL:HG12	3:C:9:LYS:N	2.30	0.44
6:H:47:PHE:CG	6:H:95:TYR:CD1	3.03	0.44
6:H:63:LEU:N	6:H:63:LEU:CD1	2.76	0.44
6:H:91:ASP:O	6:H:91:ASP:OD1	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ILE:C	1:A:274:ILE:CB	2.75	0.44
1:A:399:HIS:CG	1:A:400:PRO:N	2.85	0.44
1:A:4:GLN:HG3	1:A:4:GLN:H	1.81	0.44
2:B:1020:ARG:O	2:B:1021:MET:CB	2.55	0.44
2:B:26:THR:O	2:B:28:GLU:N	2.51	0.44
2:B:724:ASP:C	2:B:726:ALA:N	2.70	0.44
3:C:80:LEU:HA	3:C:80:LEU:HD12	1.65	0.44
4:E:109:ILE:N	4:E:109:ILE:HD12	2.31	0.44
7:I:49:ILE:C	7:I:49:ILE:CG2	2.86	0.44
1:A:1172:LEU:C	1:A:1173:HIS:CD2	2.90	0.44
1:A:1205:LYS:O	1:A:1206:ASP:C	2.56	0.44
1:A:920:LEU:HD22	1:A:921:GLY:H	1.82	0.44
2:B:313:MET:HG3	2:B:313:MET:HE2	1.95	0.44
2:B:59:LEU:HD12	2:B:59:LEU:HA	1.74	0.44
4:E:24:LYS:HD2	4:E:24:LYS:NZ	2.20	0.44
6:H:115:TYR:O	6:H:116:TYR:HB2	2.16	0.44
6:H:41:ASP:O	6:H:42:ILE:HG13	2.17	0.44
6:H:63:LEU:C	6:H:90:ALA:CB	2.76	0.44
7:I:29:CYS:SG	7:I:31:THR:HB	2.58	0.44
9:K:65:HIS:CD2	9:K:66:PRO:HD2	2.53	0.44
1:A:1341:ILE:HD13	1:A:1379:GLY:C	2.38	0.44
1:A:351:THR:HG23	2:B:1103:ILE:HG12	1.95	0.44
1:A:605:MET:HE2	1:A:607:ILE:HG13	1.99	0.44
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.99	0.44
3:C:115:SER:HA	3:C:144:ILE:HD11	1.98	0.44
3:C:208:GLU:C	3:C:210:GLU:H	2.20	0.44
3:C:235:VAL:HG12	3:C:235:VAL:H	1.47	0.44
5:F:98:ALA:O	5:F:102:SER:HB3	2.18	0.44
8:J:21:TYR:CD2	8:J:50:ILE:CG2	3.01	0.44
3:C:57:VAL:CG2	8:J:60:PHE:HB3	2.48	0.44
10:L:57:LEU:O	10:L:58:LYS:C	2.55	0.44
1:A:1036:ARG:O	1:A:1037:LEU:C	2.55	0.44
1:A:679:ILE:HD11	1:A:732:LEU:CB	2.39	0.44
2:B:103:ASN:ND2	2:B:103:ASN:CB	2.69	0.44
2:B:351:TYR:O	2:B:355:ILE:HG12	2.18	0.44
2:B:400:HIS:CE1	2:B:517:THR:HG21	2.52	0.44
2:B:429:PHE:HE2	2:B:433:GLN:NE2	2.14	0.44
2:B:461:LEU:N	2:B:461:LEU:HD12	2.32	0.44
2:B:755:ILE:HD12	2:B:814:PHE:CD1	2.53	0.44
2:B:95:ILE:CG2	2:B:96:TYR:N	2.81	0.44
7:I:46:HIS:N	7:I:46:HIS:CB	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1265:ASN:O	1:A:1266:THR:O	2.36	0.44
1:A:393:ARG:NE	1:A:393:ARG:CG	2.74	0.44
1:A:903:ASN:HD21	1:A:905:ASP:H	1.66	0.44
1:A:587:HIS:CD2	1:A:966:ASN:OD1	2.65	0.44
2:B:1189:ILE:CG2	2:B:1189:ILE:C	2.86	0.44
2:B:787:VAL:O	2:B:787:VAL:HG12	2.16	0.44
2:B:916:THR:HB	2:B:935:ARG:CB	2.42	0.44
3:C:166:GLU:O	3:C:167:HIS:HB2	2.17	0.44
3:C:251:LEU:O	3:C:254:LYS:HB2	2.18	0.44
3:C:82:TYR:O	3:C:84:ARG:N	2.51	0.44
8:J:62:ARG:HB3	8:J:62:ARG:HE	0.98	0.44
9:K:54:ARG:CG	9:K:54:ARG:CA	2.84	0.44
9:K:58:PHE:CE2	9:K:74:ARG:HG2	2.52	0.44
9:K:83:PRO:C	9:K:85:ASP:N	2.69	0.44
1:A:1128:GLN:CA	1:A:1129:GLU:N	2.67	0.43
1:A:120:GLU:HG2	1:A:123:ARG:NH1	2.31	0.43
1:A:1293:SER:CB	1:A:1294:PRO:HD2	2.48	0.43
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.99	0.43
1:A:511:ILE:O	1:A:519:PRO:HA	2.18	0.43
1:A:664:THR:HG22	1:A:742:ASN:HB3	2.00	0.43
2:B:195:CYS:HA	8:J:63:TYR:OH	2.18	0.43
2:B:243:ALA:C	2:B:244:LEU:CG	2.85	0.43
2:B:382:ILE:O	2:B:386:LEU:HG	2.18	0.43
2:B:482:VAL:H	2:B:482:VAL:HG23	1.65	0.43
2:B:523:CYS:SG	2:B:524:PRO:HD2	2.58	0.43
2:B:753:ALA:HA	2:B:756:ILE:CD1	2.47	0.43
2:B:757:PRO:CD	2:B:984:HIS:HE1	2.26	0.43
7:I:95:THR:HG23	7:I:96:SER:N	2.33	0.43
10:L:31:CYS:O	10:L:32:ALA:C	2.57	0.43
1:A:113:LEU:O	1:A:164:ARG:NH2	2.48	0.43
1:A:35:ILE:HA	1:A:52:GLY:O	2.18	0.43
1:A:362:ASP:OD1	1:A:459:ARG:HD3	2.18	0.43
2:B:118:ARG:NH2	2:B:194:GLU:HG2	2.33	0.43
2:B:223:VAL:HG12	2:B:224:GLN:N	2.33	0.43
3:C:86:CYS:HG	3:C:95:CYS:CB	2.20	0.43
4:E:12:LEU:CD1	4:E:12:LEU:HG	2.20	0.43
7:I:3:THR:CG2	7:I:3:THR:C	2.86	0.43
3:C:35:ARG:HD3	9:K:41:THR:OG1	2.18	0.43
3:C:252:GLN:HA	9:K:95:ILE:CD1	2.48	0.43
1:A:1235:LYS:CE	1:A:1235:LYS:CG	2.84	0.43
1:A:162:VAL:HA	1:A:162:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:531:GLN:H	2:B:531:GLN:CD	2.20	0.43
2:B:405:ARG:HA	2:B:631:GLY:O	2.19	0.43
2:B:880:THR:H	2:B:934:LYS:HG3	1.83	0.43
3:C:112:ASN:HB2	3:C:114:TYR:CE1	2.52	0.43
3:C:181:ASP:OD2	3:C:186:LEU:HB2	2.19	0.43
3:C:186:LEU:HA	3:C:186:LEU:HD12	1.46	0.43
6:H:95:TYR:CD2	6:H:95:TYR:C	2.91	0.43
1:A:1003:LYS:CG	1:A:1003:LYS:CE	2.88	0.43
1:A:1328:TYR:CG	1:A:1329:THR:N	2.87	0.43
1:A:516:SER:O	1:A:517:ASN:C	2.55	0.43
1:A:531:ILE:HD11	1:A:578:LEU:CD1	2.48	0.43
1:A:690:VAL:O	1:A:691:LEU:C	2.52	0.43
2:B:128:LEU:O	2:B:167:ILE:N	2.48	0.43
2:B:658:ILE:O	2:B:658:ILE:HG22	2.17	0.43
2:B:69:LEU:HD12	2:B:90:ILE:O	2.19	0.43
3:C:69:LEU:O	8:J:6:ARG:NH2	2.42	0.43
4:E:79:TRP:HE1	4:E:81:GLU:HB2	1.83	0.43
9:K:18:LYS:C	9:K:19:LEU:HD23	2.37	0.43
9:K:28:PRO:O	9:K:29:ASN:CB	2.59	0.43
1:A:606:LEU:HD22	1:A:614:PHE:HE2	1.83	0.43
2:B:592:ASN:O	2:B:594:ALA:N	2.50	0.43
2:B:654:ARG:N	2:B:657:HIS:HD2	2.15	0.43
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.49	0.43
5:F:119:ARG:CG	5:F:119:ARG:HH11	2.31	0.43
6:H:11:GLN:CG	6:H:11:GLN:CA	2.86	0.43
1:A:1287:TYR:CD1	1:A:1305:VAL:HG21	2.53	0.43
1:A:412:ARG:HH11	1:A:412:ARG:HD3	1.54	0.43
1:A:543:LEU:HD11	1:A:547:LEU:HD11	1.99	0.43
1:A:523:ILE:CB	1:A:622:VAL:HG13	2.44	0.43
1:A:695:LYS:CB	1:A:695:LYS:CD	2.87	0.43
1:A:884:ASP:O	1:A:885:THR:C	2.56	0.43
2:B:99:LYS:HB3	2:B:100:PRO:CD	2.49	0.43
2:B:1065:GLN:HE21	2:B:1069:PHE:H	1.65	0.43
2:B:502:ILE:CG1	2:B:502:ILE:CA	2.88	0.43
2:B:648:HIS:HB2	2:B:649:LYS:H	1.38	0.43
2:B:658:ILE:CG2	2:B:658:ILE:O	2.65	0.43
2:B:976:ILE:N	2:B:976:ILE:HD12	2.33	0.43
3:C:115:SER:O	3:C:118:LEU:HB2	2.19	0.43
2:B:824:ILE:HD11	8:J:45:CYS:HB2	1.99	0.43
8:J:1:MET:HG3	8:J:60:PHE:HE2	1.83	0.43
9:K:58:PHE:CD2	9:K:74:ARG:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:ILE:CD1	1:A:729:ALA:HA	2.47	0.43
1:A:926:GLN:O	1:A:926:GLN:CG	2.66	0.43
1:A:752:LYS:CE	2:B:1019:SER:HB2	2.43	0.43
3:C:31:ASN:O	3:C:34:ARG:HB3	2.17	0.43
3:C:44:LEU:HB2	3:C:77:ILE:HD12	1.99	0.43
4:E:131:THR:N	4:E:131:THR:CB	2.68	0.43
6:H:104:PHE:CA	6:H:105:GLU:N	2.69	0.43
6:H:9:ILE:HA	6:H:55:LEU:O	2.18	0.43
1:A:1409:LEU:CD2	1:A:1409:LEU:CD1	2.79	0.43
1:A:7:SER:HG	2:B:1180:PHE:HZ	1.66	0.43
2:B:1073:TYR:HD2	2:B:1078:GLY:O	2.02	0.43
2:B:592:ASN:ND2	2:B:592:ASN:CB	2.78	0.43
2:B:889:THR:HG22	2:B:891:ASP:OD2	2.19	0.43
7:I:59:VAL:O	7:I:60:GLN:C	2.54	0.43
3:C:148:ARG:HH12	8:J:64:ASN:CB	2.31	0.43
10:L:49:LYS:CG	10:L:49:LYS:CA	2.86	0.43
1:A:1279:ILE:HD11	1:A:1312:ASN:N	2.33	0.43
1:A:270:LEU:O	1:A:274:ILE:N	2.35	0.43
1:A:673:GLY:N	1:A:674:PRO:HD2	2.33	0.43
2:B:121:ASN:HD22	2:B:121:ASN:N	2.17	0.43
2:B:249:ARG:C	2:B:249:ARG:CB	2.77	0.43
2:B:655:LYS:O	2:B:656:GLY:C	2.56	0.43
2:B:912:ILE:O	2:B:938:SER:CB	2.67	0.43
2:B:961:LEU:CG	2:B:961:LEU:HB3	2.19	0.43
4:E:11:ARG:HD2	4:E:11:ARG:HH11	1.55	0.43
4:E:44:ALA:CB	4:E:45:LYS:N	2.82	0.43
6:H:81:PRO:CB	6:H:82:PRO:HD3	2.49	0.43
10:L:34:CYS:HB2	10:L:51:CYS:HB3	1.94	0.43
1:A:1066:VAL:O	1:A:1067:LEU:C	2.54	0.43
1:A:407:ARG:CD	1:A:413:ILE:HD11	2.46	0.43
2:B:130:VAL:HG22	2:B:167:ILE:CD1	2.45	0.43
2:B:896:ASP:OD2	10:L:58:LYS:NZ	2.44	0.43
3:C:163:ILE:HA	3:C:163:ILE:HD13	1.32	0.43
3:C:252:GLN:HA	9:K:95:ILE:HD13	2.01	0.43
4:E:124:VAL:N	4:E:125:PRO:CD	2.82	0.43
4:E:161:LYS:NZ	4:E:193:GLY:O	2.52	0.43
6:H:89:LEU:HB3	6:H:91:ASP:OD1	2.19	0.43
1:A:567:LYS:CG	6:H:95:TYR:HA	2.48	0.43
10:L:44:ASP:O	10:L:45:ALA:CB	2.67	0.43
1:A:1169:ILE:HD12	1:A:1229:SER:HA	2.01	0.42
1:A:202:LEU:CD2	1:A:202:LEU:CB	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:THR:CG2	1:A:597:LEU:N	2.82	0.42
2:B:270:LYS:HD2	2:B:270:LYS:NZ	2.26	0.42
2:B:655:LYS:HA	2:B:658:ILE:HD12	2.01	0.42
4:E:48:ASP:C	4:E:48:ASP:OD1	2.57	0.42
6:H:28:ALA:HB3	6:H:38:LEU:HB3	2.01	0.42
6:H:91:ASP:C	6:H:91:ASP:CG	2.78	0.42
7:I:72:ASP:CA	7:I:72:ASP:CG	2.78	0.42
10:L:38:LEU:O	10:L:39:SER:CB	2.58	0.42
1:A:690:VAL:HG13	1:A:718:VAL:HG22	2.01	0.42
1:A:868:TYR:HE1	1:A:1064:VAL:HG13	1.84	0.42
2:B:273:LEU:HD13	2:B:276:ILE:CD1	2.49	0.42
2:B:404:LYS:HA	2:B:404:LYS:HD3	1.74	0.42
2:B:521:LEU:HD23	2:B:521:LEU:HA	1.65	0.42
2:B:680:THR:HG22	2:B:682:SER:N	2.22	0.42
3:C:183:TRP:CE2	3:C:207:CYS:HB3	2.54	0.42
3:C:97:VAL:CG1	3:C:98:VAL:N	2.80	0.42
3:C:6:PRO:HB2	9:K:101:LEU:HD23	2.01	0.42
9:K:33:ILE:HD13	9:K:87:LEU:HD22	2.01	0.42
10:L:61:THR:CG2	10:L:61:THR:OG1	2.53	0.42
1:A:53:LEU:HD23	1:A:54:ASN:N	2.35	0.42
1:A:768:GLN:NE2	1:A:816:HIS:HA	2.34	0.42
1:A:968:GLN:HA	1:A:973:ILE:HD12	2.00	0.42
2:B:1006:ILE:HD12	2:B:1006:ILE:N	2.35	0.42
2:B:524:PRO:HG3	2:B:748:ILE:HD13	2.02	0.42
2:B:25:ILE:CB	2:B:658:ILE:HD11	2.49	0.42
1:A:786:HIS:HA	2:B:703:ILE:O	2.19	0.42
2:B:723:VAL:CG2	2:B:723:VAL:CA	2.91	0.42
2:B:830:TYR:CE1	2:B:1000:PRO:HB3	2.55	0.42
2:B:871:THR:CA	2:B:871:THR:CG2	2.80	0.42
2:B:986:GLN:HA	2:B:986:GLN:CD	2.39	0.42
4:E:61:GLN:HG3	4:E:62:ALA:N	2.34	0.42
5:F:74:ILE:HD13	5:F:144:GLU:HG2	2.01	0.42
5:F:76:LYS:O	5:F:79:ARG:HD2	2.19	0.42
9:K:55:LYS:HB2	9:K:81:TYR:HE1	1.83	0.42
1:A:999:VAL:HG12	1:A:1000:LEU:HG	2.01	0.42
1:A:1006:ILE:HD11	4:E:163:GLU:HG2	2.00	0.42
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.19	0.42
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	2.01	0.42
1:A:705:LYS:CB	1:A:705:LYS:HA	2.24	0.42
1:A:903:ASN:ND2	1:A:904:THR:N	2.65	0.42
2:B:510:LYS:N	2:B:511:PRO:HD3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:760:ASP:N	2:B:760:ASP:OD1	2.51	0.42
4:E:115:ASN:N	4:E:115:ASN:OD1	2.52	0.42
4:E:124:VAL:HB	4:E:125:PRO:HD3	2.02	0.42
4:E:65:THR:O	4:E:69:ILE:HG13	2.17	0.42
7:I:34:TYR:CG	7:I:34:TYR:C	2.92	0.42
8:J:53:HIS:CE1	8:J:54:VAL:C	2.93	0.42
1:A:1408:ILE:HG22	1:A:1408:ILE:O	2.20	0.42
1:A:608:ILE:HG13	1:A:613:ILE:HD13	2.02	0.42
2:B:108:VAL:CG2	2:B:108:VAL:CA	2.88	0.42
2:B:817:LEU:N	2:B:818:PRO:HD3	2.34	0.42
4:E:72:PHE:HA	4:E:73:PRO:HD3	1.82	0.42
4:E:87:SER:HB2	4:E:115:ASN:OD1	2.19	0.42
7:I:10:CYS:O	7:I:11:ASN:CB	2.60	0.42
9:K:46:ILE:HG22	9:K:50:LEU:CD1	2.50	0.42
1:A:964:ILE:HD12	1:A:1037:LEU:HD11	2.02	0.42
1:A:1133:LEU:HD22	1:A:1133:LEU:HB3	1.99	0.42
1:A:1212:VAL:O	1:A:1213:GLY:C	2.54	0.42
1:A:1281:ARG:CD	1:A:1281:ARG:HB2	2.47	0.42
1:A:1293:SER:HB2	1:A:1294:PRO:HD2	2.02	0.42
1:A:582:ILE:H	1:A:582:ILE:CD1	2.23	0.42
1:A:619:LYS:NZ	1:A:619:LYS:CD	2.67	0.42
1:A:785:PRO:HB2	2:B:701:ILE:CD1	2.50	0.42
1:A:722:LEU:HD22	1:A:799:PHE:CD1	2.55	0.42
1:A:92:HIS:HD2	1:A:94:GLY:N	2.18	0.42
2:B:408:LEU:HD11	2:B:545:ILE:CD1	2.50	0.42
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	2.02	0.42
4:E:78:LEU:HD11	4:E:109:ILE:CD1	2.49	0.42
4:E:96:PHE:O	4:E:97:VAL:C	2.58	0.42
6:H:40:LEU:HD22	6:H:123:MET:HE3	2.01	0.42
7:I:107:SER:O	7:I:109:ILE:HD12	2.20	0.42
7:I:115:LYS:CD	7:I:115:LYS:NZ	2.73	0.42
8:J:2:ILE:HG22	8:J:3:VAL:HG23	2.01	0.42
1:A:547:LEU:HB3	9:K:58:PHE:CE1	2.55	0.42
1:A:427:GLN:HB2	1:A:430:TRP:NE1	2.33	0.42
1:A:674:PRO:HA	1:A:677:ARG:NH1	2.34	0.42
2:B:310:MET:O	2:B:313:MET:HB2	2.20	0.42
2:B:564:GLU:OE2	2:B:591:ARG:CD	2.68	0.42
2:B:614:SER:C	2:B:615:MET:HG3	2.40	0.42
2:B:996:ARG:CB	2:B:996:ARG:CD	2.79	0.42
3:C:262:LEU:HA	3:C:262:LEU:HD23	1.65	0.42
4:E:61:GLN:HG3	4:E:62:ALA:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:55:ILE:C	10:L:56:LEU:HG	2.40	0.42
1:A:1129:GLU:O	1:A:1133:LEU:HD12	2.19	0.42
1:A:213:HIS:CB	1:A:213:HIS:N	2.71	0.42
1:A:355:GLY:HA3	1:A:482:PHE:CE1	2.55	0.42
1:A:890:ASP:O	1:A:891:ALA:C	2.53	0.42
2:B:1081:LEU:HD12	2:B:1085:ILE:CD1	2.49	0.42
2:B:1153:GLU:HB3	2:B:1155:SER:HB3	2.02	0.42
2:B:228:LYS:O	2:B:261:ARG:NH2	2.39	0.42
3:C:56:THR:HG23	3:C:57:VAL:H	1.82	0.42
4:E:14:ARG:O	4:E:15:ALA:C	2.57	0.42
6:H:56:THR:HG21	6:H:145:ARG:HE	1.85	0.42
2:B:55:VAL:HG12	2:B:56:ASP:N	2.34	0.42
2:B:601:ARG:HH11	2:B:601:ARG:HD2	1.62	0.42
2:B:729:ILE:H	2:B:729:ILE:CD1	2.28	0.42
2:B:955:THR:O	2:B:962:LYS:HA	2.19	0.42
3:C:133:ILE:C	3:C:134:ILE:HD13	2.39	0.42
4:E:58:MET:O	4:E:59:SER:O	2.37	0.42
4:E:60:PHE:CD1	4:E:60:PHE:C	2.93	0.42
6:H:4:THR:C	6:H:5:LEU:HD23	2.39	0.42
1:A:545:GLN:O	1:A:546:VAL:C	2.55	0.42
2:B:1025:HIS:CE1	2:B:1090:THR:HG21	2.45	0.42
2:B:773:MET:O	2:B:775:LYS:N	2.53	0.42
2:B:120:ARG:NH2	2:B:956:THR:O	2.44	0.42
3:C:267:GLN:CA	3:C:268:ASP:N	2.67	0.42
3:C:66:ARG:O	3:C:67:LEU:C	2.57	0.42
4:E:100:ILE:HG23	4:E:105:PHE:HB2	2.02	0.42
4:E:157:SER:O	4:E:160:GLU:HB2	2.19	0.42
5:F:109:VAL:CG1	5:F:123:LYS:HD3	2.50	0.42
1:A:1151:GLU:HB3	7:I:42:LEU:CD1	2.50	0.42
7:I:55:THR:HB	7:I:55:THR:CG2	2.30	0.42
10:L:45:ALA:HA	10:L:45:ALA:CB	2.24	0.42
1:A:1202:MET:HE3	1:A:1208:THR:C	2.41	0.41
1:A:399:HIS:CD2	1:A:400:PRO:N	2.88	0.41
2:B:1163:CYS:HB2	2:B:1182:CYS:CB	2.49	0.41
2:B:118:ARG:NH2	2:B:194:GLU:CD	2.68	0.41
2:B:211:VAL:HG13	2:B:211:VAL:O	2.19	0.41
3:C:147:LEU:CD2	3:C:147:LEU:CB	2.76	0.41
3:C:199:LYS:CE	3:C:199:LYS:CG	2.94	0.41
3:C:31:ASN:OD1	3:C:34:ARG:HD3	2.20	0.41
4:E:30:ILE:HG22	4:E:34:GLU:HB3	2.01	0.41
4:E:43:LYS:CA	4:E:43:LYS:CG	2.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:93:MET:O	4:E:97:VAL:HG23	2.20	0.41
6:H:118:PHE:O	6:H:119:GLY:C	2.54	0.41
1:A:562:THR:CG2	6:H:98:TYR:CD2	3.03	0.41
1:A:971:PHE:O	1:A:972:HIS:C	2.56	0.41
1:A:974:ASP:HB3	6:H:136:LYS:HE2	2.02	0.41
2:B:121:ASN:HD21	2:B:965:LYS:HZ1	1.68	0.41
1:A:657:LEU:HD21	2:B:829:CYS:CB	2.50	0.41
1:A:1053:PHE:C	1:A:1053:PHE:CD2	2.94	0.41
1:A:1258:HIS:O	1:A:1259:MET:C	2.59	0.41
1:A:296:LEU:HA	1:A:296:LEU:HD12	1.71	0.41
1:A:543:LEU:O	1:A:547:LEU:HG	2.19	0.41
1:A:566:ILE:N	1:A:566:ILE:CD1	2.83	0.41
1:A:58:LEU:HB2	1:A:59:GLY:H	1.63	0.41
1:A:63:ARG:HA	1:A:74:MET:SD	2.59	0.41
1:A:700:ASN:O	7:I:115:LYS:HE3	2.20	0.41
1:A:785:PRO:HG2	2:B:703:ILE:HD12	2.02	0.41
1:A:962:ARG:O	1:A:963:ILE:C	2.53	0.41
1:A:72:GLU:CG	2:B:1175:LEU:HD12	2.49	0.41
2:B:189:LEU:O	2:B:190:TYR:C	2.58	0.41
2:B:225:VAL:HG12	2:B:226:PHE:N	2.35	0.41
2:B:458:LYS:CB	2:B:458:LYS:CD	2.91	0.41
2:B:817:LEU:HA	2:B:817:LEU:HD23	1.91	0.41
2:B:914:LYS:HD2	2:B:937:ALA:O	2.19	0.41
3:C:183:TRP:HE1	3:C:207:CYS:HB3	1.83	0.41
6:H:103:LYS:CG	6:H:105:GLU:CD	2.88	0.41
6:H:81:PRO:HB2	6:H:82:PRO:HD2	1.99	0.41
1:A:1428:VAL:HG12	1:A:1429:ILE:N	2.29	0.41
1:A:511:ILE:HG23	1:A:511:ILE:HD12	1.59	0.41
1:A:608:ILE:CG2	1:A:609:ASP:N	2.82	0.41
1:A:34:LYS:CG	1:A:83:HIS:CE1	3.03	0.41
1:A:919:ILE:HD13	1:A:983:ILE:CD1	2.49	0.41
1:A:936:LEU:HA	1:A:936:LEU:HD23	1.89	0.41
2:B:274:PRO:HG3	2:B:359:GLU:HB3	2.03	0.41
2:B:952:VAL:HG22	2:B:966:VAL:HG13	2.03	0.41
6:H:128:ASN:OD1	6:H:131:ASN:OD1	2.38	0.41
7:I:50:THR:HG23	7:I:50:THR:O	2.19	0.41
1:A:1079:MET:HG2	1:A:1359:ASP:CG	2.37	0.41
1:A:1106:ASN:O	1:A:1107:VAL:C	2.58	0.41
1:A:1194:ARG:HH11	1:A:1194:ARG:CG	2.29	0.41
1:A:896:ARG:NH2	1:A:1030:ARG:HH12	2.17	0.41
2:B:261:ARG:O	2:B:267:ARG:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:591:ARG:HH11	2:B:591:ARG:HG2	1.86	0.41
2:B:606:LYS:HA	2:B:686:ASN:O	2.21	0.41
2:B:642:ASP:HA	2:B:643:ASP:HA	1.15	0.41
2:B:643:ASP:O	2:B:644:GLU:CG	2.69	0.41
2:B:694:ASP:O	2:B:695:ALA:C	2.56	0.41
3:C:116:LYS:CE	3:C:116:LYS:CG	2.90	0.41
10:L:27:LEU:O	10:L:29:TYR:N	2.54	0.41
10:L:30:ILE:O	10:L:57:LEU:N	2.52	0.41
1:A:353:ILE:HG13	1:A:353:ILE:O	2.21	0.41
1:A:619:LYS:O	1:A:620:LYS:C	2.54	0.41
1:A:752:LYS:NZ	2:B:1019:SER:HB2	2.35	0.41
2:B:1097:HIS:C	2:B:1097:HIS:ND1	2.71	0.41
2:B:313:MET:CE	2:B:386:LEU:HD22	2.51	0.41
2:B:70:ILE:HB	2:B:429:PHE:HE1	1.85	0.41
2:B:606:LYS:CD	2:B:606:LYS:NZ	2.66	0.41
2:B:895:ASP:CB	2:B:895:ASP:C	2.74	0.41
3:C:205:LYS:H	3:C:205:LYS:HG3	1.86	0.41
3:C:248:ILE:O	3:C:248:ILE:HG22	2.20	0.41
5:F:111:LEU:CB	5:F:111:LEU:CD2	2.85	0.41
1:A:867:ILE:CD1	1:A:1000:LEU:HD21	2.48	0.41
1:A:158:PRO:O	1:A:159:THR:C	2.53	0.41
1:A:189:ARG:O	1:A:190:ALA:CB	2.69	0.41
1:A:295:LEU:CD1	1:A:295:LEU:CD2	2.86	0.41
1:A:441:PRO:O	1:A:441:PRO:HG2	2.21	0.41
1:A:566:ILE:HD13	6:H:96:VAL:C	2.41	0.41
1:A:535:THR:HG22	1:A:616:VAL:HG13	2.03	0.41
2:B:1152:MET:HE3	2:B:1152:MET:HA	2.03	0.41
2:B:412:LEU:HA	2:B:412:LEU:HD23	1.93	0.41
4:E:114:ASN:OD1	4:E:114:ASN:N	2.53	0.41
6:H:103:LYS:CD	6:H:105:GLU:OE2	2.68	0.41
6:H:55:LEU:HD22	6:H:144:ILE:HG23	2.03	0.41
6:H:77:ARG:C	6:H:78:SER:O	2.50	0.41
1:A:547:LEU:HD23	1:A:547:LEU:HA	1.95	0.41
1:A:567:LYS:CD	6:H:95:TYR:CB	2.98	0.41
1:A:70:CYS:SG	1:A:80:HIS:CE1	2.99	0.41
2:B:175:ARG:HD3	2:B:175:ARG:HH11	1.74	0.41
2:B:331:LEU:HD23	2:B:331:LEU:HA	2.01	0.41
2:B:624:LEU:C	2:B:624:LEU:HD12	2.41	0.41
2:B:648:HIS:NE2	2:B:711:GLU:HA	2.35	0.41
2:B:864:LYS:HG3	2:B:865:LYS:N	2.35	0.41
2:B:882:THR:C	2:B:882:THR:CB	2.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:76:ASP:OD2	3:C:128:ASN:N	2.43	0.41
4:E:79:TRP:CB	4:E:105:PHE:CD1	2.91	0.41
4:E:129:PRO:N	4:E:129:PRO:CG	2.74	0.41
4:E:54:GLN:CA	4:E:54:GLN:CG	2.87	0.41
5:F:128:LYS:NZ	5:F:149:GLU:O	2.50	0.41
8:J:6:ARG:HH11	8:J:6:ARG:HD2	1.57	0.41
10:L:58:LYS:O	10:L:59:ALA:O	2.38	0.41
1:A:896:ARG:NH2	1:A:1030:ARG:NH1	2.69	0.41
1:A:1096:SER:O	1:A:1099:PRO:HD2	2.21	0.41
1:A:635:ARG:HH11	1:A:635:ARG:HD3	1.65	0.41
2:B:89:GLU:N	2:B:135:ARG:O	2.54	0.41
2:B:418:LYS:CD	2:B:418:LYS:CB	2.87	0.41
2:B:900:ALA:O	2:B:901:PRO:C	2.59	0.41
3:C:147:LEU:CG	3:C:147:LEU:HB2	2.21	0.41
3:C:33:LEU:O	3:C:37:MET:HG3	2.21	0.41
1:A:566:ILE:CD1	6:H:96:VAL:HG12	2.33	0.41
2:B:892:LYS:HA	10:L:63:ARG:HH12	1.86	0.41
1:A:1204:ASP:OD1	1:A:1205:LYS:HE2	2.21	0.41
1:A:1224:LEU:HD23	1:A:1226:VAL:HG21	2.03	0.41
1:A:532:ARG:HD3	1:A:749:ALA:HB2	2.02	0.41
2:B:193:LYS:CD	2:B:193:LYS:CB	2.81	0.41
2:B:730:ARG:HD2	2:B:730:ARG:HH11	1.68	0.41
2:B:893:LEU:HD11	2:B:910:VAL:HG11	2.02	0.41
2:B:979:LYS:HE3	2:B:987:LYS:HD2	2.02	0.41
3:C:116:LYS:HZ3	3:C:116:LYS:HD3	1.84	0.41
3:C:11:ARG:O	3:C:12:GLU:CG	2.67	0.41
3:C:6:PRO:HB3	3:C:25:VAL:HG13	2.03	0.41
4:E:161:LYS:NZ	4:E:172:GLU:OE2	2.53	0.41
10:L:26:THR:CB	10:L:27:LEU:N	2.84	0.41
1:A:1049:ILE:HG22	1:A:1049:ILE:O	2.18	0.41
1:A:1209:MET:SD	1:A:1236:LEU:HD22	2.61	0.41
1:A:1284:MET:HB2	1:A:1284:MET:HE2	1.74	0.41
2:B:130:VAL:N	2:B:167:ILE:HD11	2.23	0.41
2:B:424:LEU:HD21	2:B:428:ILE:HD11	2.03	0.41
2:B:169:ARG:CG	2:B:454:THR:HG21	2.42	0.41
2:B:660:LYS:HG3	2:B:660:LYS:CE	2.44	0.41
2:B:63:ILE:CD1	2:B:92:PHE:HB2	2.50	0.41
4:E:98:ILE:CA	4:E:98:ILE:CG2	2.89	0.41
5:F:81:THR:HG22	5:F:136:ARG:HH11	1.77	0.41
6:H:32:THR:HB	6:H:33:GLN:H	1.85	0.41
1:A:1161:THR:CG2	1:A:1162:VAL:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1172:LEU:O	1:A:1173:HIS:CG	2.74	0.40
1:A:1298:TYR:C	1:A:1299:VAL:HG23	2.40	0.40
1:A:912:LEU:N	1:A:912:LEU:HD23	2.36	0.40
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	2.55	0.40
2:B:1200:ALA:O	2:B:1204:PHE:CD1	2.74	0.40
2:B:523:CYS:HA	2:B:524:PRO:HD3	1.84	0.40
3:C:136:ASP:O	3:C:137:LYS:C	2.58	0.40
4:E:167:ARG:HD3	4:E:167:ARG:HA	1.83	0.40
6:H:105:GLU:O	6:H:106:GLU:C	2.59	0.40
1:A:1225:PHE:CG	1:A:1225:PHE:CA	2.95	0.40
1:A:247:ARG:HA	1:A:248:PRO:HD3	1.94	0.40
1:A:506:ALA:HB1	1:A:508:PRO:HD2	2.02	0.40
1:A:67:CYS:HB2	1:A:70:CYS:SG	2.62	0.40
1:A:929:LEU:HA	1:A:929:LEU:HD23	1.93	0.40
2:B:1002:THR:O	2:B:1005:GLY:N	2.35	0.40
2:B:1159:ARG:NE	2:B:1161:HIS:CE1	2.89	0.40
2:B:344:LYS:CG	2:B:344:LYS:CE	2.92	0.40
2:B:419:THR:CG2	2:B:419:THR:O	2.66	0.40
2:B:510:LYS:CD	2:B:510:LYS:NZ	2.69	0.40
2:B:710:LEU:O	2:B:711:GLU:C	2.59	0.40
3:C:244:VAL:O	3:C:245:VAL:C	2.59	0.40
3:C:47:ASP:CG	3:C:47:ASP:O	2.60	0.40
4:E:65:THR:O	4:E:66:GLU:C	2.60	0.40
6:H:12:VAL:O	6:H:12:VAL:HG12	2.21	0.40
10:L:26:THR:HG22	10:L:27:LEU:N	2.28	0.40
1:A:1102:LYS:O	1:A:1106:ASN:HB2	2.21	0.40
1:A:1224:LEU:HG	1:A:1225:PHE:H	1.84	0.40
1:A:295:LEU:HG	1:A:299:HIS:CE1	2.56	0.40
2:B:1050:ILE:CG2	2:B:1051:THR:N	2.82	0.40
2:B:294:ASP:HB2	7:I:12:ASN:HA	2.04	0.40
2:B:258:LEU:HB2	2:B:385:LEU:HD21	2.02	0.40
2:B:41:LYS:CD	2:B:41:LYS:NZ	2.78	0.40
2:B:953:LEU:C	2:B:953:LEU:CD2	2.90	0.40
3:C:147:LEU:HD13	3:C:151:GLN:O	2.21	0.40
3:C:73:GLN:CG	3:C:73:GLN:OE1	2.48	0.40
3:C:8:VAL:O	3:C:9:LYS:HB2	2.20	0.40
4:E:37:LEU:HA	4:E:38:PRO:HD2	1.86	0.40
6:H:95:TYR:O	6:H:143:LEU:HA	2.22	0.40
10:L:47:ARG:CG	10:L:48:CYS:N	2.83	0.40
1:A:1204:ASP:CG	1:A:1204:ASP:O	2.60	0.40
1:A:1225:PHE:C	1:A:1226:VAL:HG23	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1406:VAL:O	1:A:1407:GLU:C	2.59	0.40
1:A:59:GLY:O	1:A:60:SER:OG	2.37	0.40
2:B:416:LEU:CD2	2:B:416:LEU:HG	2.26	0.40
2:B:89:GLU:HB3	2:B:135:ARG:O	2.22	0.40
3:C:142:VAL:CG1	3:C:143:LEU:N	2.73	0.40
3:C:255:VAL:CG1	3:C:255:VAL:O	2.68	0.40
6:H:136:LYS:CB	6:H:136:LYS:N	2.73	0.40
6:H:76:THR:CG2	6:H:76:THR:O	2.66	0.40
9:K:43:GLY:HA2	9:K:71:PHE:CE1	2.57	0.40
1:A:166:GLY:O	1:A:167:CYS:HB3	2.21	0.40
1:A:540:PHE:C	1:A:541:ILE:HD12	2.42	0.40
1:A:836:TYR:O	1:A:837:ILE:C	2.56	0.40
1:A:928:LEU:HD23	1:A:928:LEU:HA	1.79	0.40
1:A:92:HIS:HD2	1:A:94:GLY:H	1.70	0.40
1:A:351:THR:HG23	2:B:1103:ILE:HA	2.03	0.40
2:B:90:ILE:N	2:B:90:ILE:HG13	2.37	0.40
3:C:71:PRO:HB2	3:C:133:ILE:CD1	2.32	0.40

All (2) 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)
2:B:434:ARG:O	2:B:465:ASN:ND2[2_655]	2.11	0.09
2:B:1223:ASP:OD1	4:E:1:MET:CE[8_455]	2.17	0.03

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	1332/1733 (77%)	1160 (87%)	113 (8%)	59 (4%)	2	16
2	B	1071/1224 (88%)	897 (84%)	131 (12%)	43 (4%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	264/318 (83%)	218 (83%)	36 (14%)	10 (4%)	3	19
4	E	213/215 (99%)	180 (84%)	20 (9%)	13 (6%)	1	10
5	F	81/155 (52%)	71 (88%)	8 (10%)	2 (2%)	5	27
6	H	129/146 (88%)	85 (66%)	21 (16%)	23 (18%)	0	1
7	I	119/122 (98%)	108 (91%)	8 (7%)	3 (2%)	5	27
8	J	62/70 (89%)	58 (94%)	4 (6%)	0	100	100
9	K	112/120 (93%)	98 (88%)	10 (9%)	4 (4%)	3	20
10	L	44/70 (63%)	26 (59%)	11 (25%)	7 (16%)	0	1
All	All	3427/4173 (82%)	2901 (85%)	362 (11%)	164 (5%)	2	14

All (164) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	43	GLU
1	A	45	GLN
1	A	47	ARG
1	A	56	PRO
1	A	59	GLY
1	A	62	ASP
1	A	65	LEU
1	A	72	GLU
1	A	120	GLU
1	A	155	GLU
1	A	156	ASP
1	A	157	ASP
1	A	190	ALA
1	A	193	ASP
1	A	326	ARG
1	A	400	PRO
1	A	408	ASP
1	A	418	SER
1	A	567	LYS
1	A	915	SER
1	A	1080	THR
1	A	1221	LYS
1	A	1448	GLU
2	B	66	ASP
2	B	109	THR

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Mol	Chain	Res	Type
2	B	165	VAL
2	B	230	ALA
2	B	645	SER
2	B	646	LEU
2	B	733	HIS
2	B	864	LYS
2	B	879	ARG
2	B	887	HIS
2	B	957	ASN
2	B	1097	HIS
2	B	1108	ARG
2	B	1128	LEU
2	B	1167	GLY
3	C	4	GLU
3	C	9	LYS
3	C	206	ASN
3	C	231	ASN
4	E	59	SER
4	E	64	PRO
5	F	73	ALA
6	H	32	THR
6	H	52	GLN
6	H	53	ASP
6	H	78	SER
6	H	90	ALA
6	H	104	PHE
6	H	105	GLU
6	H	116	TYR
6	H	136	LYS
6	H	139	ASN
7	I	4	PHE
9	K	111	LEU
10	L	28	LYS
10	L	39	SER
10	L	45	ALA
10	L	50	ASP
1	A	32	VAL
1	A	57	ARG
1	A	60	SER
1	A	69	THR
1	A	74	MET
1	A	94	GLY

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Mol	Chain	Res	Type
1	A	286	HIS
1	A	464	PRO
1	A	465	TYR
1	A	707	GLY
1	A	1204	ASP
2	B	108	VAL
2	B	266	ALA
2	B	424	LEU
2	B	432	MET
2	B	436	VAL
2	B	451	LYS
2	B	831	SER
2	B	1223	ASP
3	C	10	ILE
3	C	209	TYR
4	E	45	LYS
4	E	56	LYS
4	E	123	LEU
4	E	126	SER
6	H	5	LEU
6	H	18	GLY
6	H	19	ARG
6	H	77	ARG
6	H	81	PRO
6	H	82	PRO
6	H	86	ASP
6	H	107	VAL
6	H	128	ASN
7	I	79	HIS
9	K	99	GLY
10	L	58	LYS
1	A	104	GLU
1	A	885	THR
1	A	1128	GLN
1	A	1200	ALA
2	B	124	TYR
2	B	137	TYR
2	B	262	GLU
2	B	891	ASP
2	B	940	PRO
2	B	1105	ALA
2	B	1155	SER

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Mol	Chain	Res	Type
2	B	1189	ILE
2	B	1221	SER
3	C	125	MET
3	C	267	GLN
4	E	48	ASP
4	E	50	MET
5	F	111	LEU
6	H	7	ASP
6	H	135	LEU
1	A	64	ASN
1	A	75	ASN
1	A	188	ASP
1	A	196	GLU
1	A	279	LEU
1	A	958	VAL
1	A	1223	ASP
2	B	711	GLU
4	E	118	PRO
9	K	100	ALA
9	K	104	ASN
10	L	46	VAL
1	A	167	CYS
1	A	599	SER
1	A	706	HIS
1	A	1280	GLU
2	B	90	ILE
2	B	452	THR
2	B	1158	PHE
2	B	1220	ARG
4	E	11	ARG
4	E	44	ALA
6	H	85	GLY
7	I	113	ASP
1	A	71	GLN
1	A	1263	ILE
2	B	19	GLU
2	B	105	SER
2	B	865	LYS
3	C	208	GLU
3	C	217	ASP
6	H	89	LEU
10	L	59	ALA

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Mol	Chain	Res	Type
1	A	51	GLY
1	A	158	PRO
1	A	38	PRO
2	B	1214	PRO
1	A	55	ASP
1	A	78	PRO
2	B	130	VAL
2	B	1078	GLY
4	E	53	PRO
4	E	127	ILE
1	A	52	GLY
1	A	1429	ILE

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	1181/1520 (78%)	984 (83%)	197 (17%)	2	10
2	B	947/1061 (89%)	795 (84%)	152 (16%)	2	10
3	C	234/274 (85%)	192 (82%)	42 (18%)	2	8
4	E	197/197 (100%)	147 (75%)	50 (25%)	0	2
5	F	73/137 (53%)	61 (84%)	12 (16%)	2	10
6	H	117/128 (91%)	72 (62%)	45 (38%)	0	0
7	I	115/116 (99%)	88 (76%)	27 (24%)	1	3
8	J	59/65 (91%)	48 (81%)	11 (19%)	1	7
9	K	99/102 (97%)	77 (78%)	22 (22%)	1	3
10	L	40/57 (70%)	18 (45%)	22 (55%)	0	0
All	All	3062/3657 (84%)	2482 (81%)	580 (19%)	1	6

All (580) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN

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Mol	Chain	Res	Type
1	A	11	LEU
1	A	15	LYS
1	A	21	LEU
1	A	22	PHE
1	A	34	LYS
1	A	36	ARG
1	A	38	PRO
1	A	39	GLU
1	A	41	MET
1	A	42	ASP
1	A	44	THR
1	A	49	LYS
1	A	54	ASN
1	A	58	LEU
1	A	60	SER
1	A	65	LEU
1	A	68	GLN
1	A	70	CYS
1	A	74	MET
1	A	84	ILE
1	A	90	VAL
1	A	93	VAL
1	A	98	LYS
1	A	106	VAL
1	A	107	CYS
1	A	110	CYS
1	A	112	LYS
1	A	114	LEU
1	A	120	GLU
1	A	123	ARG
1	A	129	LYS
1	A	133	LYS
1	A	138	ILE
1	A	143	LYS
1	A	145	LYS
1	A	147	VAL
1	A	156	ASP
1	A	159	THR
1	A	160	GLN
1	A	162	VAL
1	A	163	SER
1	A	167	CYS

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Mol	Chain	Res	Type
1	A	174	ILE
1	A	175	ARG
1	A	176	LYS
1	A	184	SER
1	A	186	LYS
1	A	191	THR
1	A	195	ASP
1	A	198	GLU
1	A	205	GLU
1	A	206	GLU
1	A	226	GLU
1	A	239	LEU
1	A	247	ARG
1	A	261	ASP
1	A	263	THR
1	A	265	LYS
1	A	268	ASP
1	A	270	LEU
1	A	275	SER
1	A	326	ARG
1	A	346	ASP
1	A	351	THR
1	A	354	SER
1	A	368	LYS
1	A	383	TYR
1	A	385	ILE
1	A	412	ARG
1	A	416	ARG
1	A	419	LYS
1	A	434	ARG
1	A	446	ARG
1	A	451	HIS
1	A	452	LYS
1	A	461	LYS
1	A	466	SER
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	493	GLN
1	A	495	GLU
1	A	498	ARG
1	A	504	LEU

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Mol	Chain	Res	Type
1	A	508	PRO
1	A	535	THR
1	A	537	ARG
1	A	543	LEU
1	A	566	ILE
1	A	571	LEU
1	A	588	LEU
1	A	590	ARG
1	A	597	LEU
1	A	599	SER
1	A	618	GLU
1	A	622	VAL
1	A	626	ASN
1	A	630	ILE
1	A	635	ARG
1	A	636	GLU
1	A	666	ILE
1	A	679	ILE
1	A	681	GLU
1	A	688	LYS
1	A	703	THR
1	A	705	LYS
1	A	708	MET
1	A	709	THR
1	A	710	LEU
1	A	720	ARG
1	A	728	LYS
1	A	741	ASN
1	A	752	LYS
1	A	764	CYS
1	A	788	SER
1	A	794	PRO
1	A	810	PRO
1	A	821	ARG
1	A	830	LYS
1	A	831	THR
1	A	843	LYS
1	A	858	ASN
1	A	885	THR
1	A	895	LYS
1	A	903	ASN
1	A	907	THR

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Mol	Chain	Res	Type
1	A	909	ASP
1	A	920	LEU
1	A	924	LYS
1	A	940	ARG
1	A	973	ILE
1	A	974	ASP
1	A	982	THR
1	A	1003	LYS
1	A	1015	VAL
1	A	1030	ARG
1	A	1064	VAL
1	A	1078	GLN
1	A	1081	LEU
1	A	1092	LYS
1	A	1093	LYS
1	A	1096	SER
1	A	1109	LYS
1	A	1120	LEU
1	A	1127	ASP
1	A	1129	GLU
1	A	1130	GLN
1	A	1133	LEU
1	A	1138	ILE
1	A	1146	VAL
1	A	1161	THR
1	A	1165	GLU
1	A	1168	GLU
1	A	1176	LEU
1	A	1187	GLN
1	A	1192	LEU
1	A	1208	THR
1	A	1217	LYS
1	A	1225	PHE
1	A	1230	GLU
1	A	1235	LYS
1	A	1236	LEU
1	A	1237	ILE
1	A	1239	ARG
1	A	1241	ARG
1	A	1257	ASP
1	A	1258	HIS
1	A	1259	MET

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Mol	Chain	Res	Type
1	A	1260	LEU
1	A	1267	MET
1	A	1269	GLU
1	A	1277	GLU
1	A	1280	GLU
1	A	1281	ARG
1	A	1291	VAL
1	A	1293	SER
1	A	1299	VAL
1	A	1309	ASP
1	A	1318	THR
1	A	1325	THR
1	A	1329	THR
1	A	1359	ASP
1	A	1366	ARG
1	A	1376	THR
1	A	1384	VAL
1	A	1405	THR
1	A	1407	GLU
1	A	1411	GLU
1	A	1418	LEU
1	A	1426	GLU
1	A	1433	MET
1	A	1438	THR
1	A	1445	ILE
1	A	1448	GLU
1	A	1449	SER
1	A	1450	LEU
2	B	18	PHE
2	B	20	ASP
2	B	21	GLU
2	B	22	SER
2	B	25	ILE
2	B	34	ILE
2	B	46	GLN
2	B	63	ILE
2	B	65	GLU
2	B	68	THR
2	B	69	LEU
2	B	70	ILE
2	B	89	GLU
2	B	92	PHE

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Mol	Chain	Res	Type
2	B	98	THR
2	B	102	VAL
2	B	106	ASP
2	B	128	LEU
2	B	130	VAL
2	B	133	LYS
2	B	134	LYS
2	B	136	THR
2	B	138	GLU
2	B	164	LYS
2	B	167	ILE
2	B	169	ARG
2	B	178	ASN
2	B	179	CYS
2	B	183	GLU
2	B	199	MET
2	B	228	LYS
2	B	239	GLU
2	B	242	SER
2	B	244	LEU
2	B	248	SER
2	B	251	ILE
2	B	252	SER
2	B	261	ARG
2	B	264	SER
2	B	269	ILE
2	B	277	LYS
2	B	283	VAL
2	B	284	ILE
2	B	305	VAL
2	B	313	MET
2	B	357	GLN
2	B	358	LYS
2	B	367	LEU
2	B	368	GLU
2	B	387	LEU
2	B	394	ASP
2	B	417	PHE
2	B	422	LYS
2	B	425	THR
2	B	434	ARG
2	B	435	THR

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Mol	Chain	Res	Type
2	B	453	ILE
2	B	463	THR
2	B	466	TRP
2	B	485	ARG
2	B	487	THR
2	B	498	THR
2	B	513	GLN
2	B	531	GLN
2	B	547	VAL
2	B	549	THR
2	B	550	ASP
2	B	566	LEU
2	B	567	GLU
2	B	572	HIS
2	B	574	SER
2	B	589	VAL
2	B	591	ARG
2	B	595	ARG
2	B	606	LYS
2	B	612	GLU
2	B	614	SER
2	B	641	GLU
2	B	648	HIS
2	B	650	GLU
2	B	652	LYS
2	B	653	VAL
2	B	680	THR
2	B	691	GLU
2	B	701	ILE
2	B	706	GLN
2	B	710	LEU
2	B	723	VAL
2	B	730	ARG
2	B	733	HIS
2	B	736	THR
2	B	790	ASP
2	B	799	PRO
2	B	806	THR
2	B	838	SER
2	B	839	MET
2	B	857	ARG
2	B	860	MET

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Mol	Chain	Res	Type
2	B	864	LYS
2	B	868	MET
2	B	871	THR
2	B	878	GLN
2	B	879	ARG
2	B	880	THR
2	B	881	ASN
2	B	882	THR
2	B	883	LEU
2	B	884	ARG
2	B	889	THR
2	B	891	ASP
2	B	895	ASP
2	B	896	ASP
2	B	908	GLU
2	B	914	LYS
2	B	933	SER
2	B	938	SER
2	B	955	THR
2	B	957	ASN
2	B	958	GLN
2	B	962	LYS
2	B	974	PRO
2	B	975	GLN
2	B	983	ARG
2	B	987	LYS
2	B	997	GLU
2	B	1000	PRO
2	B	1007	VAL
2	B	1047	PHE
2	B	1065	GLN
2	B	1077	THR
2	B	1097	HIS
2	B	1099	VAL
2	B	1101	ASP
2	B	1150	ARG
2	B	1152	MET
2	B	1155	SER
2	B	1159	ARG
2	B	1162	ILE
2	B	1163	CYS
2	B	1165	ILE

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Mol	Chain	Res	Type
2	B	1166	CYS
2	B	1174	LYS
2	B	1175	LEU
2	B	1178	ASN
2	B	1179	GLN
2	B	1183	LYS
2	B	1185	CYS
2	B	1187	ASN
2	B	1211	ASN
2	B	1220	ARG
2	B	1222	ARG
2	B	1224	PHE
3	C	3	GLU
3	C	4	GLU
3	C	14	SER
3	C	23	SER
3	C	25	VAL
3	C	26	ASP
3	C	29	MET
3	C	34	ARG
3	C	43	THR
3	C	56	THR
3	C	57	VAL
3	C	62	PHE
3	C	86	CYS
3	C	88	CYS
3	C	93	ASP
3	C	94	LYS
3	C	102	GLN
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	132	PRO
3	C	137	LYS
3	C	154	LYS
3	C	163	ILE
3	C	178	PHE
3	C	185	LYS
3	C	186	LEU
3	C	197	SER
3	C	205	LYS
3	C	209	TYR

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Mol	Chain	Res	Type
3	C	214	ASN
3	C	218	PRO
3	C	238	ILE
3	C	240	VAL
3	C	242	GLN
3	C	245	VAL
3	C	246	ARG
3	C	251	LEU
3	C	260	LEU
3	C	264	GLN
3	C	266	ASP
3	C	268	ASP
4	E	3	GLN
4	E	9	ILE
4	E	10	SER
4	E	33	GLU
4	E	37	LEU
4	E	39	LEU
4	E	43	LYS
4	E	47	CYS
4	E	49	SER
4	E	50	MET
4	E	56	LYS
4	E	57	MET
4	E	60	PHE
4	E	61	GLN
4	E	69	ILE
4	E	70	SER
4	E	74	ASP
4	E	78	LEU
4	E	81	GLU
4	E	84	ASP
4	E	90	VAL
4	E	91	LYS
4	E	92	THR
4	E	95	THR
4	E	101	GLN
4	E	102	GLU
4	E	103	LYS
4	E	107	THR
4	E	113	GLN
4	E	115	ASN

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Mol	Chain	Res	Type
4	E	116	ILE
4	E	118	PRO
4	E	121	MET
4	E	123	LEU
4	E	144	ILE
4	E	146	HIS
4	E	149	LEU
4	E	158	SER
4	E	159	ASP
4	E	161	LYS
4	E	162	ARG
4	E	167	ARG
4	E	178	ILE
4	E	179	GLN
4	E	183	PRO
4	E	192	ARG
4	E	196	VAL
4	E	200	ARG
4	E	207	ARG
4	E	212	ARG
5	F	72	LYS
5	F	77	ASP
5	F	81	THR
5	F	82	THR
5	F	90	ARG
5	F	92	ARG
5	F	97	ARG
5	F	103	MET
5	F	109	VAL
5	F	110	ASP
5	F	111	LEU
5	F	119	ARG
6	H	4	THR
6	H	5	LEU
6	H	6	PHE
6	H	7	ASP
6	H	13	SER
6	H	19	ARG
6	H	27	GLU
6	H	30	SER
6	H	34	ASP
6	H	35	GLN

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Mol	Chain	Res	Type
6	H	36	CYS
6	H	37	LYS
6	H	40	LEU
6	H	42	ILE
6	H	45	GLU
6	H	52	GLN
6	H	53	ASP
6	H	54	SER
6	H	56	THR
6	H	61	SER
6	H	63	LEU
6	H	77	ARG
6	H	78	SER
6	H	83	GLN
6	H	86	ASP
6	H	88	SER
6	H	91	ASP
6	H	92	ASP
6	H	93	TYR
6	H	95	TYR
6	H	105	GLU
6	H	106	GLU
6	H	108	SER
6	H	109	LYS
6	H	111	LEU
6	H	112	ILE
6	H	121	LEU
6	H	129	TYR
6	H	130	ARG
6	H	131	ASN
6	H	137	GLN
6	H	138	GLU
6	H	144	ILE
6	H	145	ARG
6	H	146	ARG
7	I	1	MET
7	I	2	THR
7	I	4	PHE
7	I	10	CYS
7	I	18	GLU
7	I	24	ARG
7	I	40	SER

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Mol	Chain	Res	Type
7	I	45	ARG
7	I	46	HIS
7	I	48	LEU
7	I	55	THR
7	I	59	VAL
7	I	61	ASP
7	I	70	ARG
7	I	75	CYS
7	I	76	PRO
7	I	78	CYS
7	I	81	ARG
7	I	82	GLU
7	I	84	VAL
7	I	91	ARG
7	I	95	THR
7	I	98	VAL
7	I	116	ASN
7	I	117	LYS
7	I	119	THR
7	I	120	GLN
8	J	1	MET
8	J	3	VAL
8	J	7	CYS
8	J	9	SER
8	J	20	SER
8	J	26	GLN
8	J	28	ASP
8	J	38	ARG
8	J	48	ARG
8	J	62	ARG
8	J	64	ASN
9	K	1	MET
9	K	2	ASN
9	K	11	LEU
9	K	14	GLU
9	K	18	LYS
9	K	20	LYS
9	K	31	VAL
9	K	42	LEU
9	K	47	ARG
9	K	54	ARG
9	K	55	LYS

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Mol	Chain	Res	Type
9	K	63	VAL
9	K	73	LEU
9	K	75	ILE
9	K	78	THR
9	K	93	SER
9	K	97	LYS
9	K	102	LYS
9	K	106	GLU
9	K	112	GLN
9	K	113	THR
9	K	114	LEU
10	L	27	LEU
10	L	28	LYS
10	L	31	CYS
10	L	33	GLU
10	L	36	SER
10	L	41	SER
10	L	42	ARG
10	L	44	ASP
10	L	46	VAL
10	L	47	ARG
10	L	49	LYS
10	L	50	ASP
10	L	51	CYS
10	L	53	HIS
10	L	54	ARG
10	L	60	ARG
10	L	61	THR
10	L	62	LYS
10	L	63	ARG
10	L	64	LEU
10	L	65	VAL
10	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	83	HIS
1	A	92	HIS
1	A	171	GLN
1	A	299	HIS

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Mol	Chain	Res	Type
1	A	390	GLN
1	A	399	HIS
1	A	451	HIS
1	A	479	ASN
1	A	503	GLN
1	A	515	GLN
1	A	517	ASN
1	A	587	HIS
1	A	736	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	994	GLN
1	A	1140	HIS
1	A	1173	HIS
1	A	1364	ASN
1	A	1432	GLN
2	B	115	GLN
2	B	121	ASN
2	B	215	GLN
2	B	236	HIS
2	B	300	HIS
2	B	357	GLN
2	B	366	GLN
2	B	383	ASN
2	B	433	GLN
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	531	GLN
2	B	538	ASN
2	B	590	HIS
2	B	657	HIS
2	B	706	GLN
2	B	744	HIS
2	B	862	GLN

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Mol	Chain	Res	Type
2	B	958	GLN
2	B	984	HIS
2	B	1025	HIS
2	B	1062	HIS
2	B	1065	GLN
2	B	1084	GLN
2	B	1093	GLN
2	B	1161	HIS
2	B	1179	GLN
3	C	24	ASN
3	C	73	GLN
3	C	112	ASN
3	C	167	HIS
3	C	242	GLN
3	C	252	GLN
4	E	3	GLN
4	E	5	ASN
4	E	104	ASN
4	E	147	HIS
6	H	131	ASN
7	I	12	ASN
7	I	46	HIS
7	I	83	ASN
7	I	116	ASN
9	K	65	HIS
9	K	110	ASN
10	L	53	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CTP	B	3008	11	23,30,30	2.44	3 (13%)	30,47,47	2.37	7 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CTP	B	3008	11	1/1/7/7	5/20/38/38	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	3008	CTP	C6-N1	10.78	1.49	1.35
13	B	3008	CTP	C6-C5	3.06	1.44	1.38
13	B	3008	CTP	C4-N3	2.11	1.39	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	3008	CTP	C6-N1-C2	-8.57	107.58	121.20
13	B	3008	CTP	C2-N3-C4	5.35	121.77	116.34
13	B	3008	CTP	O4'-C1'-C2'	4.26	113.14	106.93
13	B	3008	CTP	PB-O3A-PA	-3.55	120.63	132.83
13	B	3008	CTP	PB-O3B-PG	-3.43	121.06	132.83
13	B	3008	CTP	C5-C6-N1	2.66	126.63	120.68
13	B	3008	CTP	C2'-C3'-C4'	2.39	107.30	102.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	B	3008	CTP	C1'

All (5) torsion outliers are listed below:

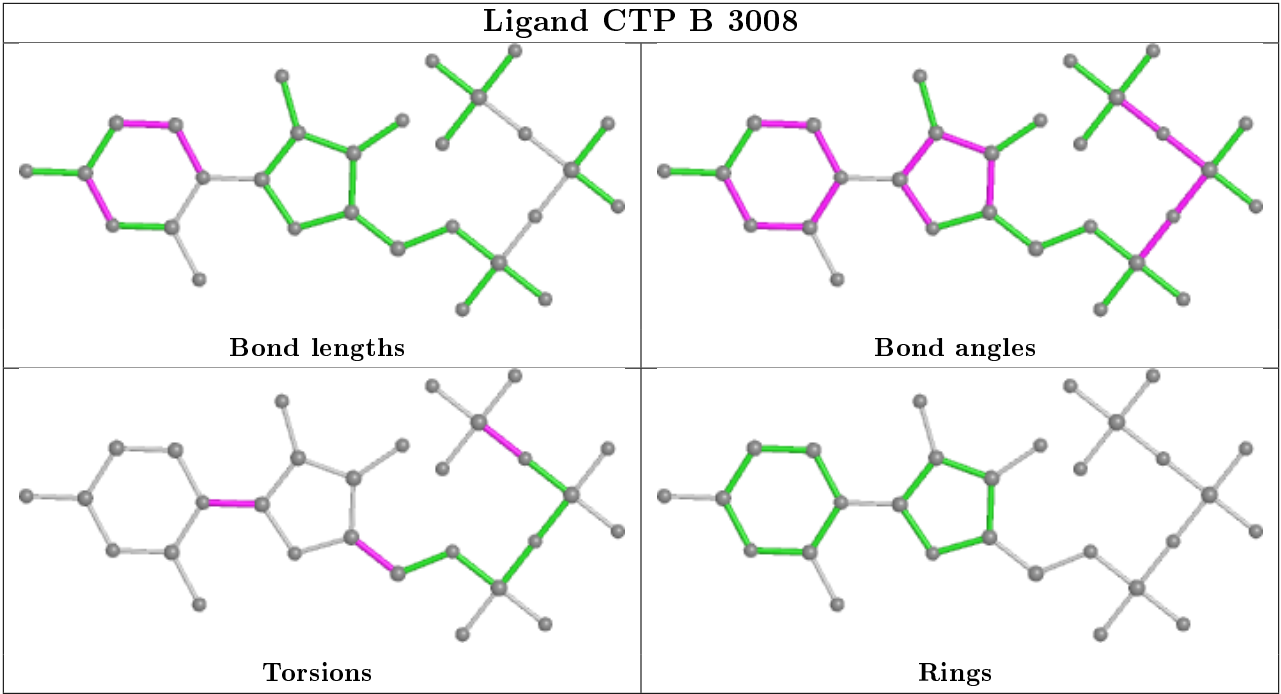
Mol	Chain	Res	Type	Atoms
13	B	3008	CTP	C2'-C1'-N1-C6
13	B	3008	CTP	C3'-C4'-C5'-O5'
13	B	3008	CTP	O4'-C4'-C5'-O5'
13	B	3008	CTP	PB-O3B-PG-O2G
13	B	3008	CTP	PB-O3B-PG-O3G

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	3008	CTP	13	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	13
1	A	13
9	K	3
4	E	2
8	J	1
6	H	1
7	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1066:VAL	C	1067:LEU	N	1.20
1	A	1106:ASN	C	1107:VAL	N	1.20
1	A	1191:TRP	C	1192:LEU	N	1.20
1	A	1328:TYR	C	1329:THR	N	1.20
1	B	224:GLN	C	225:VAL	N	1.20

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	486:TYR	C	487:THR	N	1.20
1	B	629:ASP	C	630:ALA	N	1.20
1	B	1013:ASN	C	1014:PRO	N	1.20
1	B	1074:ASN	C	1075:GLY	N	1.20
1	B	1137:CYS	C	1138:MET	N	1.20
1	B	1193:GLN	C	1194:ILE	N	1.20
1	K	97:LYS	C	98:LEU	N	1.20
1	A	645:LEU	C	646:PHE	N	1.19
1	A	983:ILE	C	984:LYS	N	1.19
1	B	31:TRP	C	32:ALA	N	1.19
1	B	1085:ILE	C	1086:PHE	N	1.19
1	E	79:TRP	C	80:VAL	N	1.19
1	H	95:TYR	C	96:VAL	N	1.19
1	J	24:LEU	C	25:LEU	N	1.19
1	A	981:LEU	C	982:THR	N	1.18
1	A	1036:ARG	C	1037:LEU	N	1.18
1	E	175:LEU	C	176:PRO	N	1.18
1	K	82:ASP	C	83:PRO	N	1.18
1	A	962:ARG	C	963:ILE	N	1.17
1	A	1367:HIS	C	1368:MET	N	1.17
1	A	1381:LEU	C	1382:THR	N	1.17
1	B	1019:SER	C	1020:ARG	N	1.17
1	I	41:PRO	C	42:LEU	N	1.17
1	A	736:ASN	C	737:LEU	N	1.16
1	B	384:ARG	C	385:LEU	N	1.16
1	B	520:GLY	C	521:LEU	N	1.16
1	B	809:MET	C	810:GLU	N	1.16
1	K	65:HIS	C	66:PRO	N	1.16
1	A	464:PRO	C	465:TYR	N	1.11

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1349/1733 (77%)	-0.23	33 (2%) 59 56	1, 24, 101, 195	0
2	B	1091/1224 (89%)	-0.16	54 (4%) 29 27	1, 25, 114, 167	0
3	C	266/318 (83%)	-0.34	3 (1%) 80 81	1, 29, 77, 167	0
4	E	215/215 (100%)	-0.05	5 (2%) 60 59	1, 38, 111, 135	0
5	F	83/155 (53%)	-0.29	1 (1%) 79 78	1, 22, 64, 86	0
6	H	133/146 (91%)	0.17	6 (4%) 33 32	22, 68, 127, 188	0
7	I	121/122 (99%)	-0.03	3 (2%) 57 54	1, 31, 83, 100	0
8	J	64/70 (91%)	-0.37	0 100 100	3, 22, 76, 91	0
9	K	114/120 (95%)	-0.23	0 100 100	3, 37, 73, 99	0
10	L	46/70 (65%)	0.27	1 (2%) 62 60	24, 73, 133, 137	0
All	All	3482/4173 (83%)	-0.18	106 (3%) 50 49	1, 28, 108, 195	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	PRO	9.6
2	B	882	THR	9.3
1	A	69	THR	7.0
2	B	1109	GLY	6.9
2	B	1110	PRO	6.1
2	B	871	THR	5.8
1	A	188	ASP	5.7
1	A	45	GLN	5.3
2	B	247	GLY	5.3
1	A	44	THR	5.2
2	B	137	TYR	5.0
3	C	268	ASP	5.0
1	A	191	THR	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	1450	LEU	4.9
2	B	1176	ASN	4.9
2	B	1223	ASP	4.8
2	B	1106	ARG	4.6
2	B	870	ILE	4.5
1	A	157	ASP	4.4
2	B	1104	HIS	4.3
2	B	136	THR	4.3
2	B	1105	ALA	4.0
2	B	1101	ASP	3.8
2	B	887	HIS	3.8
4	E	50	MET	3.7
1	A	190	ALA	3.7
2	B	436	VAL	3.7
3	C	267	GLN	3.6
4	E	51	GLY	3.6
2	B	866	TYR	3.6
1	A	65	LEU	3.4
2	B	959	ASP	3.4
1	A	1448	GLU	3.4
2	B	70	ILE	3.4
2	B	89	GLU	3.4
2	B	733	HIS	3.4
7	I	79	HIS	3.4
2	B	868	MET	3.4
1	A	43	GLU	3.3
2	B	1224	PHE	3.3
2	B	1177	HIS	3.3
2	B	135	ARG	3.3
1	A	1449	SER	3.3
6	H	85	GLY	3.2
2	B	881	ASN	3.2
1	A	192	GLY	3.2
2	B	246	LYS	3.2
1	A	68	GLN	3.1
6	H	131	ASN	3.0
1	A	3	GLY	3.0
4	E	52	ARG	3.0
1	A	193	ASP	2.8
2	B	1189	ILE	2.8
2	B	433	GLN	2.8
1	A	1446	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	68	THR	2.7
2	B	935	ARG	2.7
2	B	432	MET	2.7
7	I	74	GLU	2.7
2	B	1108	ARG	2.7
2	B	69	LEU	2.6
7	I	76	PRO	2.6
1	A	1092	LYS	2.6
4	E	123	LEU	2.6
2	B	869	SER	2.6
2	B	1102	LYS	2.5
4	E	1	MET	2.5
2	B	90	ILE	2.5
1	A	8	SER	2.5
6	H	136	LYS	2.5
2	B	1179	GLN	2.5
10	L	50	ASP	2.5
2	B	133	LYS	2.5
2	B	883	LEU	2.5
1	A	54	ASN	2.4
1	A	1222	ASN	2.4
5	F	110	ASP	2.4
6	H	132	LEU	2.4
2	B	429	PHE	2.3
2	B	1180	PHE	2.3
1	A	47	ARG	2.3
1	A	33	ALA	2.3
2	B	888	GLY	2.3
2	B	103	ASN	2.2
1	A	189	ARG	2.2
2	B	428	ILE	2.2
1	A	62	ASP	2.2
2	B	1174	LYS	2.2
2	B	1178	ASN	2.2
1	A	41	MET	2.2
6	H	127	GLY	2.2
2	B	467	GLY	2.1
2	B	231	PRO	2.1
1	A	6	TYR	2.1
2	B	131	ASP	2.1
2	B	937	ALA	2.1
2	B	1173	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	126	GLY	2.1
6	H	35	GLN	2.0
1	A	4	GLN	2.0
1	A	42	ASP	2.0
2	B	91	SER	2.0
2	B	1175	LEU	2.0
1	A	39	GLU	2.0
1	A	46	THR	2.0
1	A	1273	LEU	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.

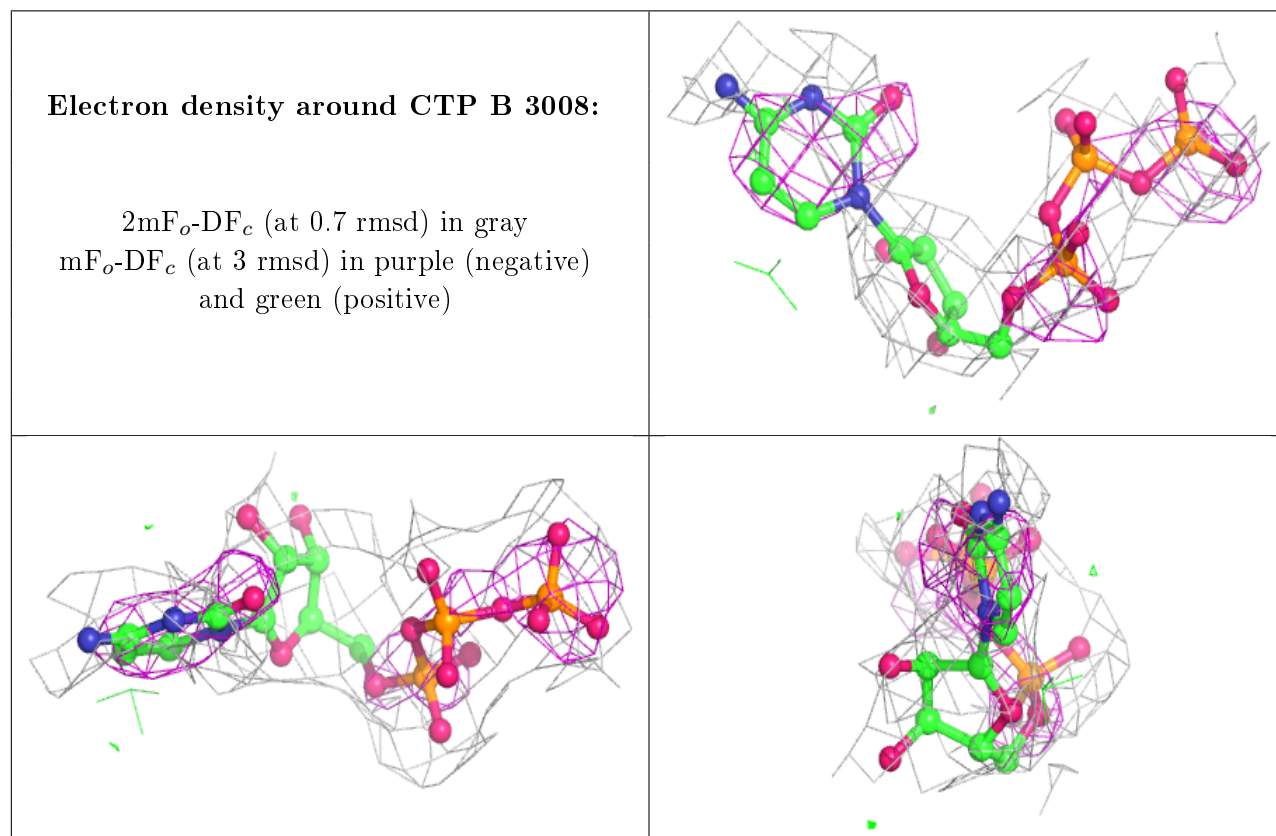
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	CTP	B	3008	29/29	0.82	0.27	26,36,73,77	0
12	ZN	L	3005	1/1	0.89	0.08	84,84,84,84	0
12	ZN	I	3004	1/1	0.89	0.17	49,49,49,49	0
12	ZN	A	3006	1/1	0.92	0.07	48,48,48,48	0
12	ZN	C	3002	1/1	0.94	0.09	35,35,35,35	0
11	MN	A	3010	1/1	0.94	0.07	29,29,29,29	0
12	ZN	I	3003	1/1	0.97	0.06	45,45,45,45	0
11	MN	A	3009	1/1	0.97	0.12	15,15,15,15	0
12	ZN	B	3007	1/1	0.97	0.08	37,37,37,37	0
12	ZN	A	3008	1/1	0.98	0.06	87,87,87,87	0
12	ZN	J	3001	1/1	0.99	0.05	31,31,31,31	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.