



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 03:56 am BST

PDB ID : 1TWA
Title : RNA polymerase II complexed with ATP
Authors : Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2004-06-30
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

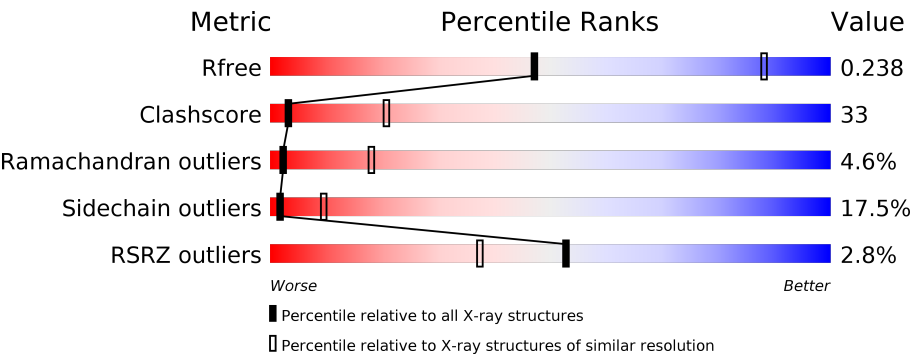
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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><div></div><div></div><div></div><div></div><div></div></div><div>16%35%20%8%22%</div></div>
2	B	1224	<div><div>4%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>18%40%23%8%11%</div></div>
3	C	318	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>13%38%25%8%16%</div></div>
4	E	215	<div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>18%41%30%11%</div></div>
5	F	155	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>11%21%16%5%46%</div></div>
6	H	146	<div><div>4%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>10%29%27%25%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	C	3002	-	-	X	-
12	ZN	J	3001	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 27757 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	1352	Total	C	N	O	S	0	0	0
			10635	6711	1842	2024	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).

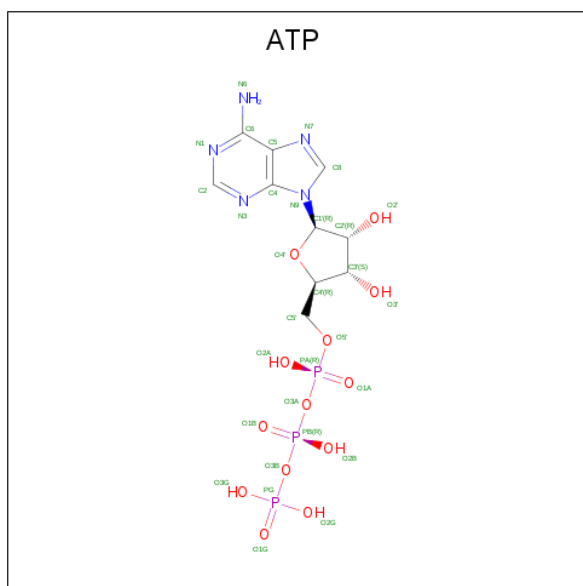
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	J	1	Total	Zn	0	0
			1	1		
12	B	1	Total	Zn	0	0
			1	1		

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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 ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

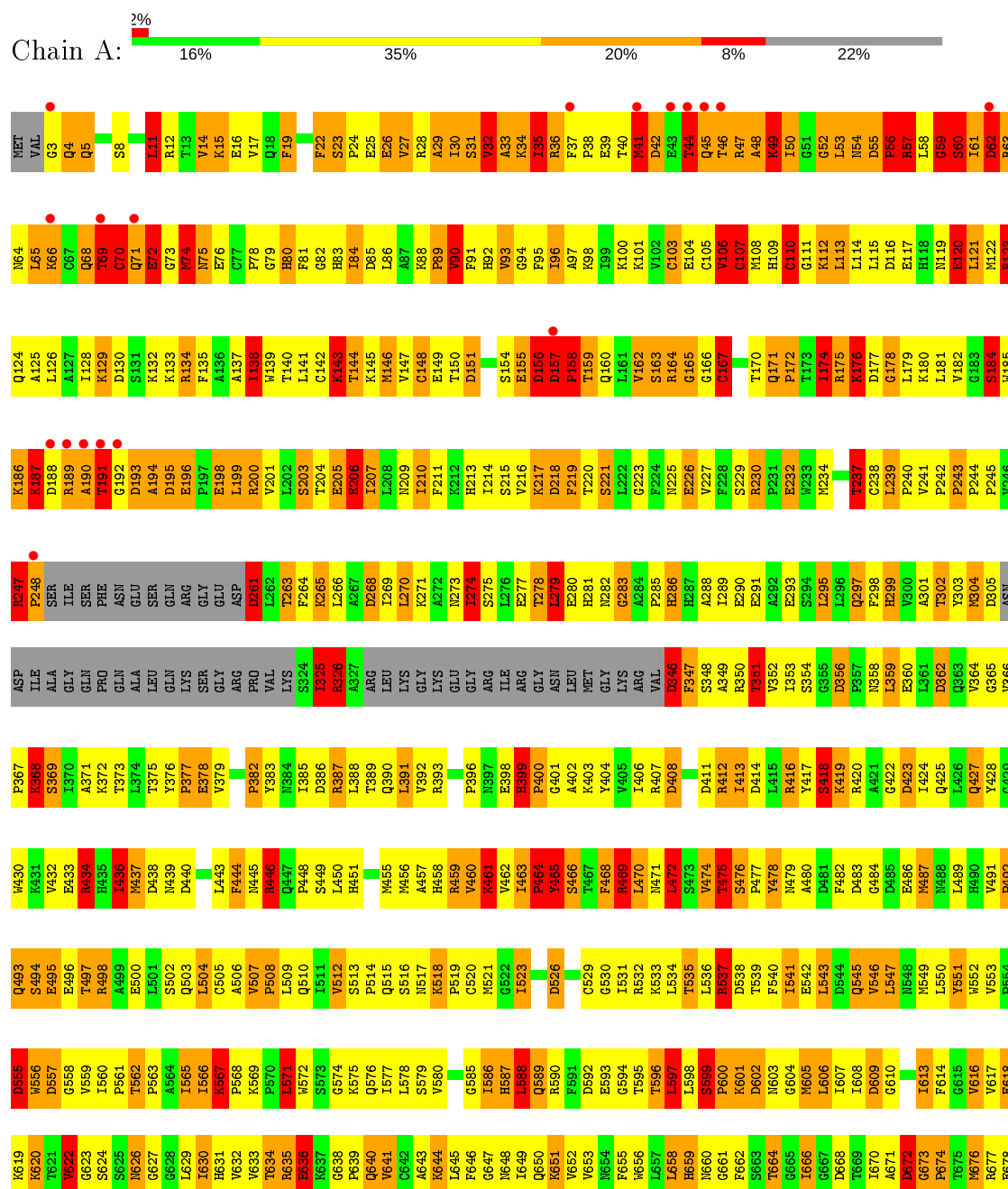


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

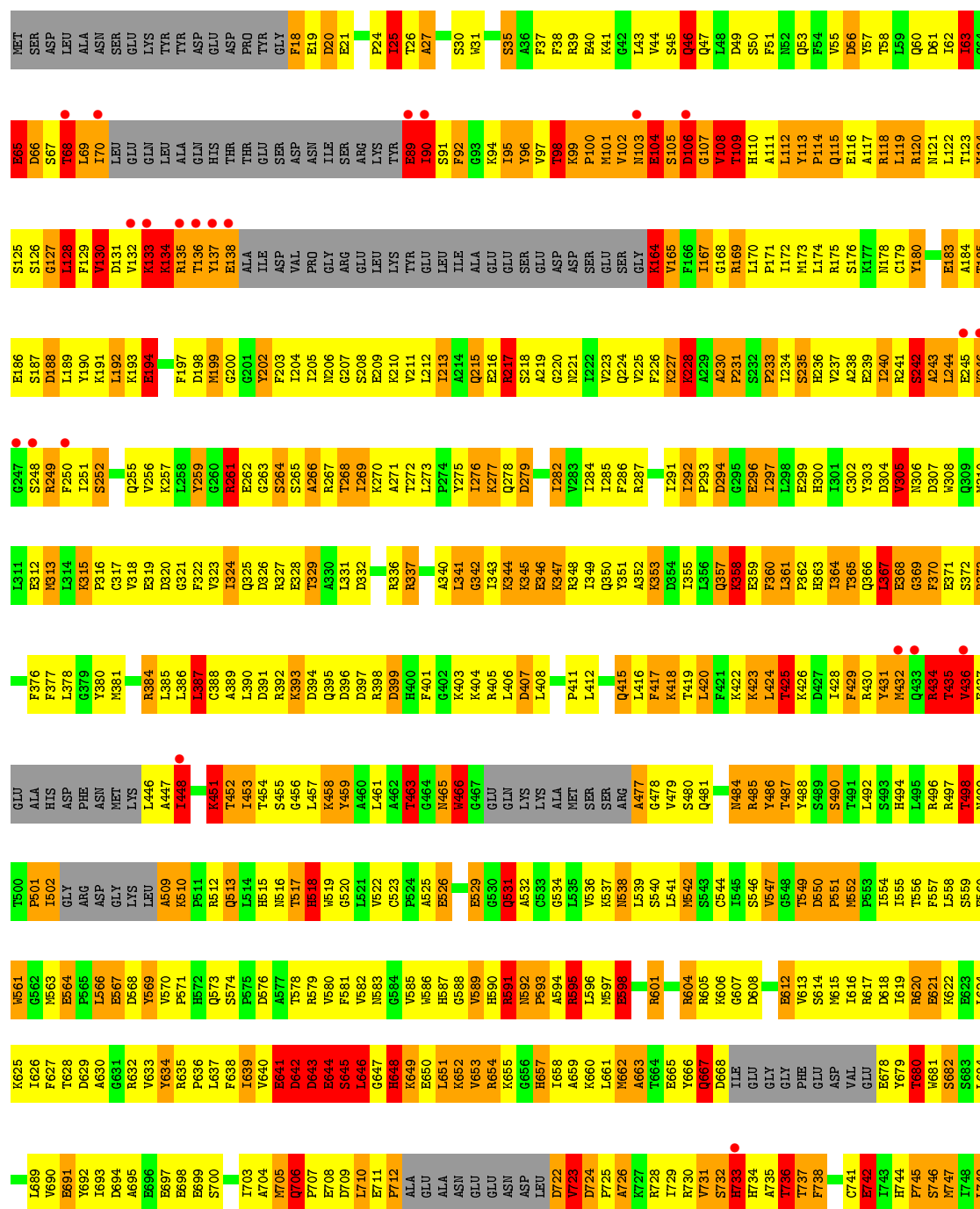
3 Residue-property plots

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

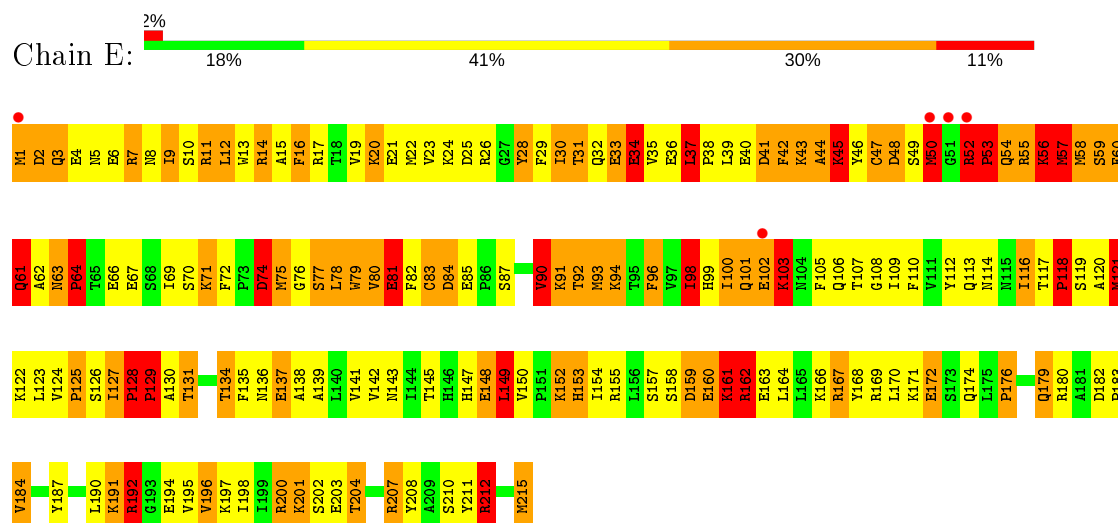


THR	GLY	G1439	T1376	E1315	A1254	R1194	L1134	A1068	Y999	V937	D874	G807	V743	E681
SER	SER	A1440	T1377	E1316	E1255	L1195	R1135	G1073	L1000	K988	A875	L808	K744	E681
PRO	ASN	F1441	G1378	E1317	E1256	L1196	A1136	E1074	R1001	D939	E879	T809	K745	I683
ASP	ASP	D1442	G1379	E1318	E1257	L1197	S1137	P1075	G1002	R940	E879	T809	M746	I683
TYR	ALA	V1443	G1380	E1319	H1258	R1198	E1138	P1076	K1003	K941	K880	Q811	M747	A684
SER	MET	M1444	L1381	E1320	H1259	R1199	E1139	A1076	N1004	F942	Q881	F813	M748	E685
PRO	ALA	M1445	L1382	E1321	L1260	A1200	H1440	T1077	E1005	L943	Q882	F813	M749	A686
THR	GLY	D1446	S1383	I1322	K1261	A1201	T1141	Q1078	I1006	E944	L883	F814	G750	K687
SER	GLY	E1447	T1385	E1323	K1262	M1202	T1142	M1079	F946	E945	D884	H816	S751	K688
PRO	PHE	S1448	T1386	E1324	E1263	N1203	L1143	T1080	T885	K752	K752	H816	S751	K688
THR	THR	S1449	T1387	E1325	E1264	D1204	K1144	L1081	F947	T885	K752	H816	S751	K689
TYR	ALA	L1450	HIS	R1326	M1265	K1205	S1145	ASN	R1012	D948	R821	E822	S754	V693
SER	TYR	L1451	GLY	T1327	T1266	D1206	T1146	THR	D1013	V949	S889	E822	S754	V694
PRO	GLY	L1452	PHE	K1267	L1267	L1207	T1147	PHE	A1014	G950	D890	E822	S754	V694
THR	GLY	T1453	ASN	L1268	L1268	T1208	T1148	HIS	V1015	G950	D890	E822	S754	V694
SER	GLY	T1454	ASN	M1269	E1269	M1209	A1149	PHE	T1016	N953	A891	I825	A759	K695
PRO	ASP	PRO	ASP	S1331	E1270	M1210	E1150	ALA	L1017	N954	A892	D826	A759	E696
SER	TYR	TYR	TYR	F1332	I1271	Q1211	S1151	GLY	F1018	P955	F893	V829	A763	Q698
GLY	GLY	GLY	THR	L1333	L1272	V1212	I1152	VAL	C1019	L956	K895	V829	A763	A699
SER	GLU	GLY	GLY	D1334	L1273	G1213	I1153	ALA	C1020	P957	K896	K830	C764	M700
PRO	ALA	ILE	ALA	I1335	L1274	E1214	Y1154	SER	G1020	P958	K897	E833	C764	L701
THR	THR	THR	THR	M1336	G1275	I1215	D1155	K1092	R1023	N959	R898	T834	G766	L702
SER	GLU	GLU	GLU	V1276	G1276	I1216	P1156	K1093	S1024	N960	V899	G835	Q767	T703
PRO	ILE	ILE	ARG	E1277	E1277	Q1217	D1157	V1094	R1025	R961	D900	Y836	Q768	A704
SER	GLU	GLU	GLU	M1278	M1278	Q1218	P1158	T1095	L1026	R962	L901	I837	S769	K705
TYR	GLY	GLY	GLY	I1279	I1279	T1219	R1159	S1096	A1027	I963	L902	Q838	V770	E706
SER	ALA	GLY	GLY	E1280	E1280	F1220	S1160	G1097	R1030	R964	R903	K772	E771	G707
PRO	GLN	GLN	GLN	K1281	K1281	K1221	T1161	V1098	T904	Q985	R840	K773	G772	M708
THR	GLY	ASP	ASP	V1282	V1282	N1223	I1162	P1099	E1034	A967	H906	T710	L710	T709
SER	GLU	GLY	GLY	G1344	G1344	D1223	I1163	R1100	Y1035	A967	H906	T710	L710	T709
PRO	ALA	GLY	GLY	R1345	M1284	L1224	P1164	L1101	Y1035	A967	H906	T710	L710	T709
SER	PRO	GLY	GLY	A1346	M1285	F1225	E1165	K1102	R1036	Q969	L908	L846	A776	E712
TYR	THR	THR	THR	K1347	K1286	V1226	E1166	E1103	L1037	T970	D909	E846	F777	S713
SER	PRO	PRO	PRO	Y1348	D1288	W1228	E1167	L1104	P1038	F971	P910	D847	F779	F714
THR	GLY	GLY	GLY	K1350	R1289	S1229	E1169	L1105	K1039	H972	S911	I848	V780	E715
SER	PHE	ASN	ASN	K1290	E1290	E1230	I1170	H1106	F1042	D974	L912	M849	D781	V718
PRO	GLY	GLU	GLU	V1291	V1291	D1231	Q1171	A1108	D1043	H975	E914	V850	D782	V719
SER	VAL	SER	SER	P1292	P1292	M1232	L1172	K1109	W1044	T976	S915	E851	T783	E720
TYR	SER	GLY	GLY	S1293	S1293	D1233	H1173	M1110	V1045	K977	G916	D853	L784	F721
SER	SER	LEU	LEU	P1294	P1294	E1234	PHE	M1111	S1047	P978	S917	N854	P785	L722
PRO	PRO	VAL	VAL	E1297	E1297	K1235	SER	K1112	R1048	S979	E918	T855	H787	N723
THR	PHE	ASN	ASN	L1297	L1297	L1236	L1176	L1116	N1049	D980	I919	T856	S788	E724
SER	PRO	ALA	ALA	V1299	V1299	I1237	LEU	T1117	E1050	L981	L920	R857	R726	A725
PRO	ASP	ASP	ASP	K1300	K1300	I1238	ASP	T1117	A1051	T982	G921	K858	D727	K728
SER	PRO	LEU	LEU	E1301	E1301	C1240	GLU	V1119	Q1052	D983	D922	S859	D790	D791
TYR	THR	VAL	VAL	P1302	P1302	R1241	ALA	Y1118	K984	L923	L923	L860	Y792	A729
SER	SER	VAL	VAL	E1303	E1303	V1242	GLU	E1121	R1055	D985	K924	G861	S793	G730
PRO	PRO	LYS	THR	V1304	V1304	V1243	GLN	P1122	S1056	N966	L925	N862	P794	R731
THR	THR	ASP	ASP	W1305	W1305	ARG	SER	G1123	V1057	V937	Q926	E795	E795	L732
SER	PRO	LEU	LEU	L1306	L1306	PRO	PHE	G1123	V1058	L988	V927	I864	S796	A733
PRO	SER	MET	MET	E1307	E1307	LYS	ASP	A1126	E1059	G989	L929	Q865	K797	E734
SER	PRO	PRO	PRO	M1308	M1308	LYS	ASP	D1127	G1061	V990	L929	F866	V735	V735
TYR	THR	THR	THR	T1308	T1308	SER	Q1187	D1127	K991	K991	D930	I867	V800	N736
SER	SER	SER	SER	D1309	D1309	LEU	Q1188	Q1128	E1062	E931	D930	Y868	E801	L737
PRO	PRO	PRO	PRO	G1310	G1310	ASP	S1189	Q1129	N1063	L993	E932	G869	N802	K738
THR	ALA	LEU	LEU	V1311	V1311	ALA	P1190	Q1130	V1064	Q994	Y933	E870	S803	D739
SER	THR	VAL	VAL	M1312	M1312	GLU	W1191	Q1131	V1065	E995	K934	D871	Y804	L740
PRO	SER	ASP	ASP	L1313	L1313	THR	W1192	K1132	G1065	L996	K934	D871	Y804	L740
SER	PRO	SER	SER	S1314	S1314	GLU	L1193	L1133	L1067	L998	L936	M873	R806	N742

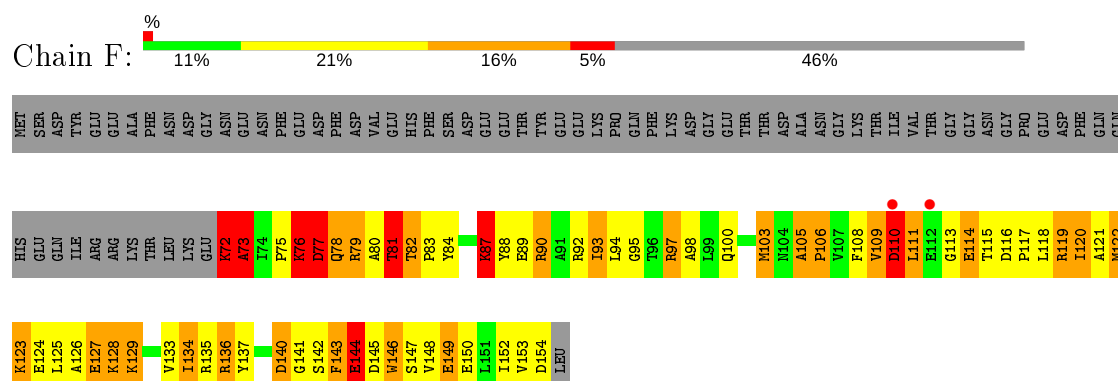




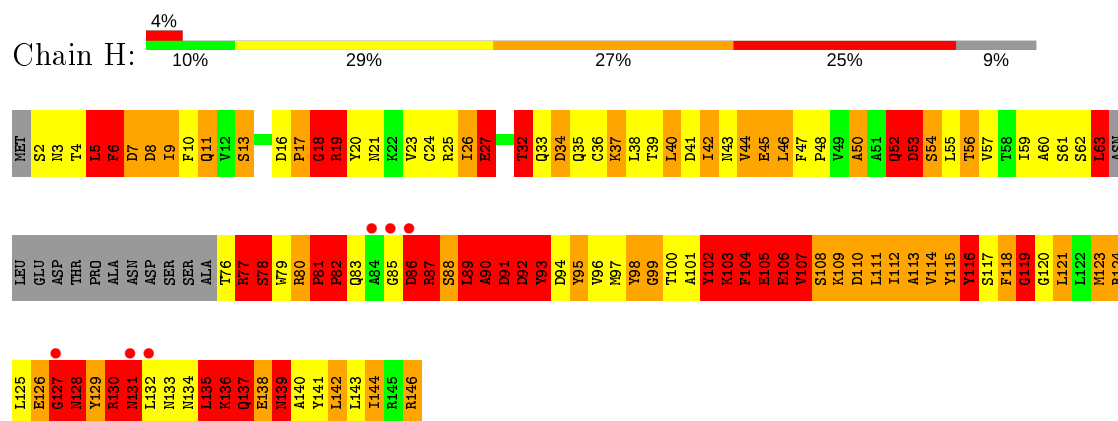
- Molecule 4: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide



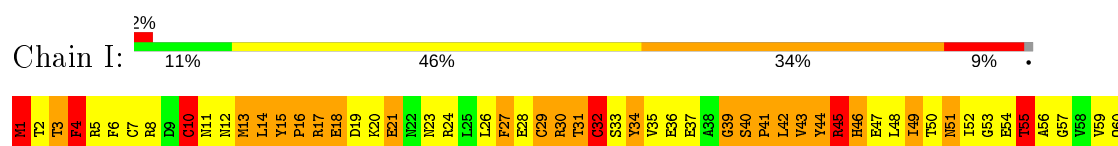
- Molecule 5: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

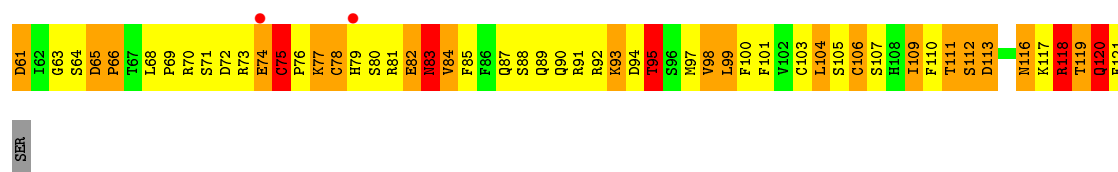


- Molecule 6: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



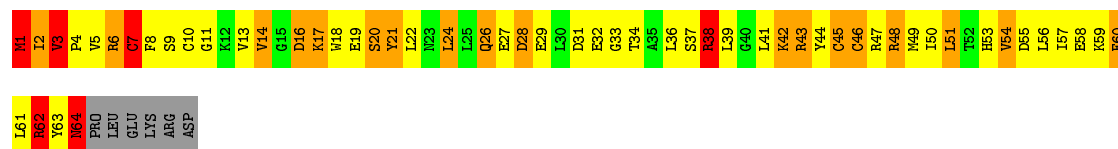
- Molecule 7: DNA-directed RNA polymerase II 14.2 kDa polypeptide





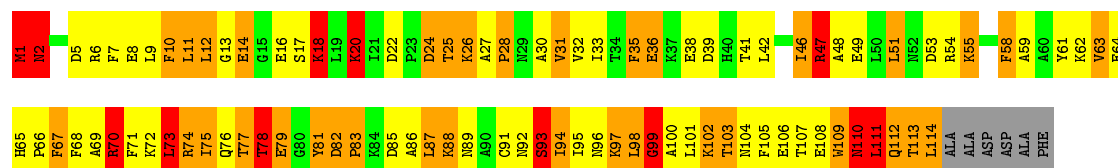
- Molecule 8: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide

Chain J: 11% 46% 26% 9% 9%



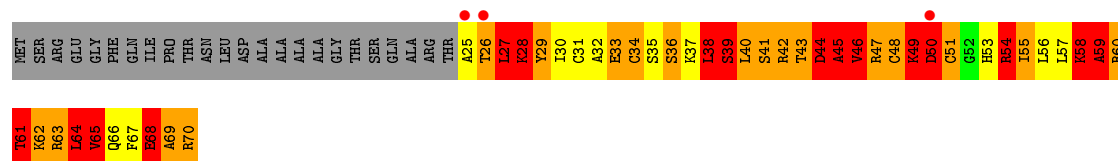
- Molecule 9: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K: 18% 38% 29% 10% 5%



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

Chain L: 4% 16% 26% 23% 34%



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.00 Å 223.00 Å 374.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 39.69 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.20) 97.5 (39.69-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.12 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.246 0.195 , 0.238	Depositor DCC
R_{free} test set	2779 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27757	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	3.53	1385/10822 (12.8%)	2.62	715/14641 (4.9%)
2	B	3.54	1164/8860 (13.1%)	2.56	552/11945 (4.6%)
3	C	3.57	288/2133 (13.5%)	2.62	126/2891 (4.4%)
4	E	3.50	210/1796 (11.7%)	2.40	107/2416 (4.4%)
5	F	3.12	78/682 (11.4%)	2.30	35/922 (3.8%)
6	H	3.37	138/1086 (12.7%)	2.46	68/1470 (4.6%)
7	I	3.73	145/1009 (14.4%)	2.69	86/1357 (6.3%)
8	J	3.41	75/533 (14.1%)	3.10	53/715 (7.4%)
9	K	3.36	117/937 (12.5%)	2.65	61/1265 (4.8%)
10	L	3.99	58/366 (15.8%)	2.90	43/485 (8.9%)
All	All	3.52	3658/28224 (13.0%)	2.59	1846/38107 (4.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	41
2	B	0	40
3	C	0	13
4	E	1	6
5	F	0	2
6	H	0	12
7	I	0	6
8	J	0	1
9	K	0	1
10	L	0	2
All	All	1	124

All (3658) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	552	MET	CG-SD	26.10	2.49	1.81
1	A	728	LYS	CD-CE	24.04	2.11	1.51
2	B	598	GLU	CG-CD	23.97	1.88	1.51
1	A	771	GLU	CD-OE2	23.53	1.51	1.25
3	C	165	LYS	CE-NZ	23.14	2.06	1.49
10	L	68	GLU	CG-CD	22.61	1.85	1.51
2	B	529	GLU	CD-OE2	22.21	1.50	1.25
2	B	194	GLU	CD-OE1	21.94	1.49	1.25
4	E	162	ARG	CG-CD	21.90	2.06	1.51
1	A	1119	TYR	CE2-CZ	-21.18	1.11	1.38
1	A	1277	GLU	CD-OE2	21.13	1.48	1.25
2	B	945	GLU	CD-OE1	19.90	1.47	1.25
1	A	1005	GLU	CD-OE1	19.84	1.47	1.25
1	A	752	LYS	CE-NZ	19.73	1.98	1.49
4	E	162	ARG	NE-CZ	19.27	1.58	1.33
1	A	801	GLU	CD-OE1	19.09	1.46	1.25
2	B	641	GLU	CG-CD	18.34	1.79	1.51
2	B	346	GLU	CG-CD	18.29	1.79	1.51
1	A	795	GLU	CG-CD	18.18	1.79	1.51
2	B	650	GLU	CD-OE2	18.05	1.45	1.25
1	A	1232	ASN	CB-CG	18.04	1.92	1.51
2	B	1041	GLU	CD-OE2	17.97	1.45	1.25
2	B	986	GLN	CG-CD	17.96	1.92	1.51
1	A	801	GLU	CD-OE2	17.86	1.45	1.25
3	C	154	LYS	CD-CE	17.73	1.95	1.51
7	I	37	GLU	CD-OE1	17.61	1.45	1.25
1	A	1280	GLU	CD-OE2	17.58	1.45	1.25
1	A	496	GLU	CD-OE1	17.47	1.44	1.25
2	B	477	ALA	CA-CB	17.45	1.89	1.52
1	A	1135	ARG	CZ-NH2	17.38	1.55	1.33
2	B	1150	ARG	CZ-NH2	17.09	1.55	1.33
7	I	55	THR	CB-CG2	17.08	2.08	1.52
2	B	598	GLU	CD-OE2	17.07	1.44	1.25
7	I	17	ARG	CG-CD	17.07	1.94	1.51
1	A	681	GLU	CD-OE1	17.06	1.44	1.25
1	A	466	SER	CB-OG	-16.98	1.20	1.42
1	A	752	LYS	CD-CE	16.90	1.93	1.51
2	B	564	GLU	CD-OE1	16.90	1.44	1.25
2	B	509	ALA	CA-CB	16.88	1.87	1.52
4	E	152	LYS	CD-CE	16.82	1.93	1.51
1	A	1225	PHE	CD1-CE1	16.80	1.72	1.39
2	B	211	VAL	CB-CG1	-16.69	1.17	1.52
3	C	209	TYR	CE2-CZ	16.67	1.60	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	82	GLU	CD-OE1	16.62	1.44	1.25
1	A	620	LYS	CD-CE	16.58	1.92	1.51
1	A	734	GLU	CD-OE2	16.52	1.43	1.25
9	K	61	TYR	CE1-CZ	-16.43	1.17	1.38
1	A	1264	GLU	CD-OE1	-16.39	1.07	1.25
1	A	610	GLY	C-O	16.37	1.49	1.23
4	E	211	TYR	CE1-CZ	-16.32	1.17	1.38
3	C	166	GLU	CD-OE2	16.26	1.43	1.25
3	C	23	SER	CB-OG	16.16	1.63	1.42
1	A	1015	VAL	CB-CG2	-16.16	1.19	1.52
1	A	934	LYS	CD-CE	16.15	1.91	1.51
4	E	50	MET	SD-CE	16.13	2.68	1.77
2	B	529	GLU	CD-OE1	16.05	1.43	1.25
1	A	1234	GLU	CD-OE1	15.96	1.43	1.25
4	E	66	GLU	CD-OE2	15.92	1.43	1.25
1	A	516	SER	CB-OG	15.82	1.62	1.42
2	B	1041	GLU	CD-OE1	15.81	1.43	1.25
1	A	217	LYS	CD-CE	15.76	1.90	1.51
1	A	1280	GLU	CG-CD	15.67	1.75	1.51
1	A	734	GLU	CD-OE1	15.58	1.42	1.25
2	B	723	VAL	CB-CG1	15.40	1.85	1.52
2	B	502	ILE	CA-CB	15.38	1.90	1.54
1	A	1349	TYR	CG-CD2	-15.32	1.19	1.39
2	B	328	GLU	CD-OE2	15.27	1.42	1.25
1	A	1230	GLU	CD-OE1	15.14	1.42	1.25
1	A	995	GLU	CD-OE2	15.10	1.42	1.25
2	B	833	TYR	CE1-CZ	-15.02	1.19	1.38
1	A	16	GLU	CD-OE1	15.00	1.42	1.25
1	A	787	PHE	CG-CD1	-14.98	1.16	1.38
2	B	1154	ALA	CA-CB	14.97	1.83	1.52
4	E	137	GLU	CD-OE1	14.90	1.42	1.25
7	I	28	GLU	CD-OE2	14.85	1.42	1.25
2	B	1019	SER	CB-OG	-14.84	1.23	1.42
1	A	117	GLU	CD-OE1	14.82	1.42	1.25
2	B	459	TYR	CG-CD2	14.79	1.58	1.39
4	E	162	ARG	CB-CG	14.71	1.92	1.52
1	A	938	LYS	CD-CE	14.68	1.88	1.51
4	E	57	MET	SD-CE	14.68	2.60	1.77
1	A	226	GLU	CD-OE2	14.67	1.41	1.25
2	B	371	GLU	CD-OE1	14.64	1.41	1.25
1	A	498	ARG	NE-CZ	-14.63	1.14	1.33
2	B	1150	ARG	CZ-NH1	14.62	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1264	GLU	CD-OE2	-14.62	1.09	1.25
1	A	931	GLU	CD-OE2	14.57	1.41	1.25
1	A	681	GLU	CD-OE2	14.51	1.41	1.25
2	B	531	GLN	CG-CD	14.50	1.84	1.51
1	A	895	LYS	CD-CE	14.36	1.87	1.51
7	I	28	GLU	CD-OE1	14.32	1.41	1.25
1	A	346	ASP	CB-CG	14.28	1.81	1.51
4	E	20	LYS	CE-NZ	14.25	1.84	1.49
10	L	68	GLU	CD-OE1	14.22	1.41	1.25
1	A	555	ASP	CB-CG	14.20	1.81	1.51
1	A	464	PRO	C-O	-14.18	0.94	1.23
1	A	487	MET	SD-CE	-14.17	0.98	1.77
1	A	1214	GLU	CD-OE1	14.13	1.41	1.25
1	A	1372	VAL	CB-CG1	-14.10	1.23	1.52
1	A	423	ASP	CB-CG	14.06	1.81	1.51
1	A	618	GLU	CD-OE2	14.05	1.41	1.25
2	B	39	ARG	NE-CZ	14.03	1.51	1.33
2	B	895	ASP	CB-CG	14.02	1.81	1.51
2	B	620	ARG	CZ-NH2	14.01	1.51	1.33
2	B	239	GLU	CG-CD	13.97	1.73	1.51
10	L	45	ALA	CA-CB	13.97	1.81	1.52
2	B	838	SER	CB-OG	-13.93	1.24	1.42
4	E	201	LYS	CG-CD	13.88	1.99	1.52
3	C	50	GLU	CG-CD	13.86	1.72	1.51
7	I	84	VAL	CB-CG2	-13.84	1.23	1.52
1	A	1411	GLU	CG-CD	13.81	1.72	1.51
1	A	1196	GLU	CD-OE1	13.77	1.40	1.25
2	B	758	PHE	CE2-CZ	-13.71	1.11	1.37
10	L	26	THR	CA-CB	13.71	1.89	1.53
2	B	811	TYR	CE2-CZ	-13.69	1.20	1.38
2	B	31	TRP	CZ3-CH2	-13.68	1.18	1.40
2	B	27	ALA	CA-CB	-13.63	1.23	1.52
1	A	496	GLU	CG-CD	13.62	1.72	1.51
1	A	601	LYS	CD-CE	13.62	1.85	1.51
8	J	44	TYR	CE1-CZ	-13.62	1.20	1.38
2	B	764	SER	CB-OG	-13.60	1.24	1.42
2	B	962	LYS	CD-CE	13.59	1.85	1.51
1	A	1135	ARG	CG-CD	13.56	1.85	1.51
4	E	34	GLU	CD-OE2	13.51	1.40	1.25
2	B	239	GLU	CD-OE2	13.50	1.40	1.25
1	A	677	ARG	NE-CZ	13.48	1.50	1.33
1	A	695	LYS	CD-CE	13.47	1.84	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	GLU	CD-OE2	13.46	1.40	1.25
7	I	84	VAL	CB-CG1	-13.43	1.24	1.52
2	B	885	MET	SD-CE	13.34	2.52	1.77
7	I	83	ASN	CB-CG	-13.32	1.20	1.51
2	B	692	TYR	CG-CD2	-13.29	1.21	1.39
7	I	45	ARG	CG-CD	13.26	1.85	1.51
2	B	1083	ALA	CA-CB	-13.26	1.24	1.52
2	B	641	GLU	CD-OE1	13.22	1.40	1.25
1	A	291	GLU	CG-CD	13.21	1.71	1.51
1	A	205	GLU	CD-OE1	13.19	1.40	1.25
1	A	941	LYS	CD-CE	13.15	1.84	1.51
2	B	216	GLU	CD-OE2	13.13	1.40	1.25
6	H	139	ASN	CB-CG	13.11	1.81	1.51
1	A	446	ARG	CZ-NH1	13.04	1.50	1.33
1	A	1103	GLU	CD-OE2	12.97	1.40	1.25
1	A	705	LYS	CB-CG	12.96	1.87	1.52
6	H	104	PHE	CA-C	12.93	1.86	1.52
2	B	347	LYS	CG-CD	12.92	1.96	1.52
6	H	19	ARG	CG-CD	12.90	1.84	1.51
2	B	479	VAL	CB-CG1	-12.88	1.25	1.52
7	I	98	VAL	CB-CG2	-12.85	1.25	1.52
2	B	164	LYS	CD-CE	12.82	1.83	1.51
2	B	621	GLU	CD-OE2	12.82	1.39	1.25
3	C	89	GLU	C-O	12.78	1.47	1.23
2	B	1097	HIS	CA-CB	12.76	1.82	1.53
6	H	20	TYR	CD2-CE2	-12.75	1.20	1.39
2	B	1101	ASP	CB-CG	12.75	1.78	1.51
1	A	593	GLU	C-O	12.74	1.47	1.23
2	B	305	VAL	CB-CG1	12.72	1.79	1.52
2	B	497	ARG	CZ-NH1	12.69	1.49	1.33
2	B	434	ARG	CG-CD	12.68	1.83	1.51
3	C	102	GLN	CB-CG	12.66	1.86	1.52
1	A	1362	TYR	CG-CD2	-12.64	1.22	1.39
1	A	620	LYS	CE-NZ	12.64	1.80	1.49
2	B	183	GLU	CG-CD	12.64	1.71	1.51
2	B	665	GLU	CD-OE2	12.62	1.39	1.25
1	A	1145	SER	C-O	-12.59	0.99	1.23
2	B	959	ASP	CB-CG	12.54	1.78	1.51
3	C	209	TYR	CD2-CE2	12.51	1.58	1.39
3	C	192	TRP	CE3-CZ3	-12.49	1.17	1.38
7	I	34	TYR	CG-CD2	-12.49	1.23	1.39
1	A	157	ASP	CB-CG	12.47	1.77	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	GLU	CD-OE1	12.44	1.39	1.25
1	A	1446	ASP	CB-CG	12.41	1.77	1.51
1	A	1144	LYS	CD-CE	12.40	1.82	1.51
1	A	833	GLU	CG-CD	12.35	1.70	1.51
2	B	996	ARG	CZ-NH1	12.34	1.49	1.33
10	L	65	VAL	CB-CG2	12.34	1.78	1.52
1	A	1277	GLU	CG-CD	12.33	1.70	1.51
1	A	1304	TRP	CE2-CZ2	-12.32	1.18	1.39
4	E	161	LYS	CD-CE	12.29	1.81	1.51
1	A	206	GLU	CD-OE2	12.28	1.39	1.25
1	A	518	LYS	CD-CE	12.28	1.81	1.51
1	A	879	GLU	CD-OE1	12.26	1.39	1.25
3	C	97	VAL	C-O	-12.26	1.00	1.23
3	C	82	TYR	CG-CD2	-12.26	1.23	1.39
9	K	32	VAL	CB-CG2	-12.26	1.27	1.52
1	A	1303	GLU	CD-OE1	12.23	1.39	1.25
2	B	987	LYS	CE-NZ	12.23	1.79	1.49
1	A	1285	MET	SD-CE	12.21	2.46	1.77
1	A	728	LYS	CG-CD	12.17	1.93	1.52
2	B	653	VAL	CB-CG2	-12.16	1.27	1.52
2	B	963	PHE	CE1-CZ	12.16	1.60	1.37
2	B	595	ARG	CG-CD	12.16	1.82	1.51
1	A	1003	LYS	CD-CE	12.14	1.81	1.51
7	I	29	CYS	C-O	12.13	1.46	1.23
4	E	28	TYR	CE1-CZ	-12.12	1.22	1.38
2	B	612	GLU	CG-CD	12.10	1.70	1.51
1	A	420	ARG	CZ-NH2	-12.10	1.17	1.33
2	B	245	GLU	CG-CD	12.09	1.70	1.51
2	B	312	GLU	CD-OE1	12.07	1.39	1.25
7	I	82	GLU	CG-CD	12.07	1.70	1.51
1	A	1132	LYS	CD-CE	12.04	1.81	1.51
1	A	304	MET	SD-CE	11.98	2.44	1.77
1	A	148	CYS	CB-SG	-11.98	1.61	1.82
2	B	773	MET	CG-SD	-11.97	1.50	1.81
2	B	18	PHE	CB-CG	11.97	1.71	1.51
9	K	35	PHE	CE1-CZ	-11.96	1.14	1.37
1	A	751	SER	CB-OG	11.90	1.57	1.42
2	B	529	GLU	CG-CD	11.89	1.69	1.51
2	B	183	GLU	CD-OE1	11.88	1.38	1.25
3	C	177	GLU	CD-OE2	11.88	1.38	1.25
1	A	1415	SER	CB-OG	-11.87	1.26	1.42
2	B	620	ARG	CG-CD	11.87	1.81	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	62	LYS	CD-CE	11.86	1.80	1.51
1	A	1259	MET	CG-SD	11.85	2.12	1.81
2	B	169	ARG	NE-CZ	11.85	1.48	1.33
3	C	3	GLU	CD-OE2	11.83	1.38	1.25
1	A	434	ARG	CD-NE	-11.82	1.26	1.46
2	B	101	MET	SD-CE	11.81	2.44	1.77
5	F	129	LYS	CE-NZ	11.76	1.78	1.49
2	B	870	ILE	CA-CB	11.75	1.81	1.54
3	C	180	TYR	CD2-CE2	11.75	1.56	1.39
1	A	843	LYS	CD-CE	11.74	1.80	1.51
2	B	137	TYR	CB-CG	11.73	1.69	1.51
1	A	787	PHE	CE2-CZ	-11.72	1.15	1.37
7	I	1	MET	CG-SD	11.70	2.11	1.81
2	B	975	GLN	CD-NE2	11.67	1.62	1.32
1	A	677	ARG	CZ-NH2	11.67	1.48	1.33
2	B	706	GLN	CB-CG	11.65	1.84	1.52
5	F	146	TRP	CB-CG	-11.64	1.29	1.50
1	A	681	GLU	CG-CD	11.64	1.69	1.51
2	B	962	LYS	CG-CD	11.62	1.92	1.52
2	B	531	GLN	CB-CG	11.61	1.83	1.52
3	C	208	GLU	CD-OE2	11.61	1.38	1.25
1	A	821	ARG	CD-NE	-11.60	1.26	1.46
3	C	199	LYS	CD-CE	11.60	1.80	1.51
4	E	41	ASP	CB-CG	11.60	1.76	1.51
2	B	1102	LYS	CB-CG	11.60	1.83	1.52
1	A	677	ARG	CZ-NH1	11.58	1.48	1.33
1	A	37	PHE	CG-CD2	11.56	1.56	1.38
1	A	1411	GLU	CD-OE1	11.52	1.38	1.25
4	E	35	VAL	CB-CG1	-11.51	1.28	1.52
2	B	344	LYS	CB-CG	11.51	1.83	1.52
2	B	96	TYR	CG-CD1	11.50	1.54	1.39
6	H	129	TYR	CE1-CZ	11.49	1.53	1.38
1	A	652	VAL	CB-CG1	-11.47	1.28	1.52
8	J	29	GLU	CD-OE1	11.45	1.38	1.25
2	B	1155	SER	CA-CB	11.45	1.70	1.52
1	A	1235	LYS	CD-CE	11.44	1.79	1.51
1	A	850	VAL	CB-CG1	-11.44	1.28	1.52
3	C	12	GLU	CD-OE2	11.43	1.38	1.25
2	B	415	GLN	CB-CG	11.41	1.83	1.52
1	A	115	LEU	C-O	11.40	1.45	1.23
2	B	1132	GLU	CG-CD	11.40	1.69	1.51
4	E	98	ILE	CA-CB	11.40	1.81	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	162	ARG	CZ-NH1	11.39	1.47	1.33
3	C	209	TYR	CG-CD2	11.37	1.53	1.39
6	H	20	TYR	CD1-CE1	-11.36	1.22	1.39
1	A	274	ILE	CA-CB	11.35	1.80	1.54
2	B	96	TYR	CE2-CZ	11.32	1.53	1.38
1	A	724	GLU	CG-CD	11.31	1.69	1.51
1	A	597	LEU	CG-CD1	11.30	1.93	1.51
2	B	137	TYR	CG-CD1	11.29	1.53	1.39
1	A	49	LYS	CD-CE	11.28	1.79	1.51
2	B	567	GLU	CD-OE2	11.28	1.38	1.25
1	A	1214	GLU	CG-CD	11.27	1.68	1.51
10	L	68	GLU	CD-OE2	11.27	1.38	1.25
2	B	459	TYR	CE2-CZ	11.27	1.53	1.38
2	B	736	THR	CB-CG2	11.26	1.89	1.52
2	B	995	ARG	NE-CZ	-11.26	1.18	1.33
1	A	1425	SER	CB-OG	11.26	1.56	1.42
2	B	552	MET	SD-CE	11.25	2.40	1.77
2	B	227	LYS	CD-CE	11.25	1.79	1.51
1	A	1109	LYS	CB-CG	11.23	1.82	1.52
1	A	264	PHE	CB-CG	11.22	1.70	1.51
2	B	399	ASP	CB-CG	11.21	1.75	1.51
9	K	1	MET	SD-CE	11.20	2.40	1.77
4	E	131	THR	CB-CG2	11.19	1.89	1.52
1	A	1223	ASP	CB-CG	11.18	1.75	1.51
7	I	54	GLU	CD-OE1	11.18	1.38	1.25
1	A	839	ARG	NE-CZ	11.18	1.47	1.33
3	C	157	CYS	CB-SG	-11.14	1.63	1.82
1	A	941	LYS	CE-NZ	11.14	1.76	1.49
1	A	1149	ALA	C-O	11.14	1.44	1.23
1	A	1074	GLU	CD-OE2	11.13	1.37	1.25
3	C	15	LYS	CG-CD	11.12	1.90	1.52
3	C	192	TRP	CB-CG	11.12	1.70	1.50
3	C	125	MET	SD-CE	11.11	2.40	1.77
3	C	180	TYR	CG-CD1	-11.07	1.24	1.39
8	J	48	ARG	CZ-NH2	-11.05	1.18	1.33
1	A	1191	TRP	CG-CD1	11.02	1.52	1.36
2	B	1097	HIS	CA-C	11.01	1.81	1.52
1	A	44	THR	CA-CB	11.00	1.81	1.53
4	E	179	GLN	CD-OE1	10.98	1.48	1.24
2	B	370	PHE	CD1-CE1	10.98	1.61	1.39
1	A	37	PHE	CD1-CE1	10.96	1.61	1.39
1	A	1171	GLN	CG-CD	10.94	1.76	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	90	VAL	CB-CG1	10.94	1.75	1.52
1	A	750	GLY	C-O	-10.93	1.06	1.23
9	K	91	CYS	CB-SG	-10.91	1.63	1.82
1	A	676	MET	CG-SD	10.90	2.09	1.81
2	B	96	TYR	CE1-CZ	10.89	1.52	1.38
9	K	17	SER	C-O	-10.89	1.02	1.23
1	A	1222	ASN	CB-CG	10.88	1.76	1.51
1	A	1187	GLN	CB-CG	10.86	1.81	1.52
2	B	115	GLN	CG-CD	10.85	1.76	1.51
1	A	1035	TYR	CG-CD1	-10.84	1.25	1.39
6	H	52	GLN	CG-CD	10.83	1.75	1.51
7	I	78	CYS	CB-SG	10.83	2.00	1.82
3	C	104	PHE	CD2-CE2	10.83	1.60	1.39
1	A	387	ARG	CG-CD	10.83	1.79	1.51
9	K	63	VAL	CB-CG1	-10.82	1.30	1.52
1	A	836	TYR	CG-CD2	10.80	1.53	1.39
5	F	129	LYS	CD-CE	10.80	1.78	1.51
2	B	65	GLU	CG-CD	10.79	1.68	1.51
6	H	77	ARG	CB-CG	10.79	1.81	1.52
1	A	720	ARG	CG-CD	10.78	1.78	1.51
9	K	111	LEU	C-O	10.74	1.43	1.23
1	A	572	TRP	CZ3-CH2	-10.73	1.22	1.40
7	I	34	TYR	CE1-CZ	-10.71	1.24	1.38
1	A	572	TRP	CG-CD1	-10.71	1.21	1.36
1	A	1301	GLU	CD-OE1	10.66	1.37	1.25
2	B	1086	PHE	CG-CD1	-10.63	1.22	1.38
1	A	52	GLY	C-O	-10.62	1.06	1.23
1	A	616	VAL	CB-CG1	-10.62	1.30	1.52
3	C	23	SER	CA-CB	10.59	1.68	1.52
2	B	198	ASP	CB-CG	-10.56	1.29	1.51
2	B	347	LYS	CD-CE	10.56	1.77	1.51
2	B	848	ARG	NE-CZ	-10.55	1.19	1.33
1	A	987	VAL	CB-CG1	-10.55	1.30	1.52
2	B	812	LEU	C-O	-10.54	1.03	1.23
9	K	108	GLU	CD-OE2	10.53	1.37	1.25
6	H	20	TYR	CE2-CZ	-10.52	1.24	1.38
2	B	130	VAL	CB-CG2	-10.52	1.30	1.52
2	B	666	TYR	CE1-CZ	10.51	1.52	1.38
2	B	706	GLN	CG-CD	10.49	1.75	1.51
2	B	875	GLU	CG-CD	10.49	1.67	1.51
4	E	33	GLU	CD-OE1	10.49	1.37	1.25
2	B	138	GLU	CD-OE2	-10.47	1.14	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	72	PHE	CG-CD1	10.46	1.54	1.38
1	A	673	GLY	C-O	-10.46	1.06	1.23
1	A	1001	ARG	C-O	10.45	1.43	1.23
2	B	328	GLU	CD-OE1	10.45	1.37	1.25
6	H	9	ILE	CA-CB	10.44	1.78	1.54
1	A	205	GLU	CG-CD	10.44	1.67	1.51
1	A	932	GLU	CD-OE2	10.44	1.37	1.25
2	B	226	PHE	CD1-CE1	10.42	1.60	1.39
1	A	1261	LYS	CD-CE	10.39	1.77	1.51
2	B	436	VAL	CA-CB	10.39	1.76	1.54
1	A	31	SER	C-O	10.39	1.43	1.23
6	H	98	TYR	CE1-CZ	-10.39	1.25	1.38
1	A	733	ALA	C-O	-10.38	1.03	1.23
2	B	319	GLU	CG-CD	10.37	1.67	1.51
6	H	131	ASN	CB-CG	10.36	1.74	1.51
3	C	261	ALA	C-O	-10.36	1.03	1.23
1	A	1365	TYR	CD2-CE2	10.34	1.54	1.39
1	A	836	TYR	CE1-CZ	10.34	1.51	1.38
6	H	107	VAL	CA-CB	10.34	1.76	1.54
9	K	79	GLU	CG-CD	10.32	1.67	1.51
4	E	72	PHE	CE2-CZ	10.32	1.56	1.37
2	B	246	LYS	CA-C	10.31	1.79	1.52
3	C	209	TYR	CD1-CE1	10.30	1.54	1.39
2	B	1050	ILE	C-O	-10.30	1.03	1.23
1	A	662	PHE	CG-CD2	-10.29	1.23	1.38
1	A	880	LYS	C-O	-10.28	1.03	1.23
2	B	239	GLU	CD-OE1	10.28	1.36	1.25
2	B	797	TYR	CE1-CZ	-10.28	1.25	1.38
2	B	359	GLU	CD-OE1	10.26	1.36	1.25
2	B	999	MET	SD-CE	-10.26	1.20	1.77
7	I	72	ASP	CB-CG	10.25	1.73	1.51
3	C	106	GLU	CD-OE1	10.25	1.36	1.25
1	A	836	TYR	CE2-CZ	10.24	1.51	1.38
7	I	110	PHE	CD1-CE1	10.21	1.59	1.39
1	A	933	TYR	CE2-CZ	-10.21	1.25	1.38
2	B	564	GLU	CD-OE2	10.20	1.36	1.25
2	B	459	TYR	CD2-CE2	10.19	1.54	1.39
2	B	1137	CYS	CB-SG	-10.19	1.65	1.82
3	C	228	PHE	CG-CD1	-10.18	1.23	1.38
2	B	525	ALA	C-O	10.17	1.42	1.23
3	C	28	ALA	C-O	10.17	1.42	1.23
7	I	34	TYR	CE2-CZ	-10.17	1.25	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	724	GLU	CD-OE2	10.16	1.36	1.25
1	A	868	TYR	CE2-CZ	-10.16	1.25	1.38
1	A	1109	LYS	CG-CD	10.16	1.86	1.52
1	A	1110	ASN	CB-CG	10.15	1.74	1.51
1	A	1298	TYR	CG-CD2	-10.15	1.25	1.39
1	A	566	ILE	CB-CG2	10.14	1.84	1.52
2	B	217	ARG	CZ-NH1	-10.12	1.19	1.33
2	B	1153	GLU	CD-OE2	10.12	1.36	1.25
2	B	785	TYR	CG-CD1	-10.11	1.26	1.39
4	E	46	TYR	CD2-CE2	10.11	1.54	1.39
1	A	1119	TYR	CG-CD1	-10.11	1.26	1.39
1	A	507	VAL	CB-CG2	-10.10	1.31	1.52
1	A	1303	GLU	CD-OE2	10.10	1.36	1.25
1	A	1283	VAL	CB-CG2	-10.08	1.31	1.52
2	B	296	GLU	CD-OE2	10.05	1.36	1.25
4	E	187	TYR	CG-CD1	-10.05	1.26	1.39
2	B	668	ASP	CB-CG	10.03	1.72	1.51
3	C	78	GLU	CD-OE2	10.03	1.36	1.25
2	B	963	PHE	CB-CG	-10.03	1.34	1.51
2	B	728	ARG	CZ-NH1	-10.02	1.20	1.33
8	J	1	MET	CG-SD	-10.02	1.55	1.81
2	B	640	VAL	CB-CG1	-10.01	1.31	1.52
10	L	54	ARG	CG-CD	10.01	1.76	1.51
1	A	552	TRP	CG-CD1	-10.00	1.22	1.36
9	K	61	TYR	CE2-CZ	-10.00	1.25	1.38
1	A	840	ARG	CG-CD	9.99	1.76	1.51
6	H	126	GLU	CD-OE1	9.99	1.36	1.25
6	H	45	GLU	CD-OE1	9.98	1.36	1.25
2	B	531	GLN	CD-NE2	9.97	1.57	1.32
3	C	179	GLU	CD-OE1	-9.97	1.14	1.25
2	B	303	TYR	CG-CD2	-9.96	1.26	1.39
2	B	646	LEU	CG-CD2	9.96	1.88	1.51
2	B	1091	TYR	CD2-CE2	9.96	1.54	1.39
2	B	484	ASN	CB-CG	-9.95	1.28	1.51
1	A	81	PHE	CE2-CZ	-9.94	1.18	1.37
1	A	1187	GLN	CG-CD	9.93	1.73	1.51
2	B	118	ARG	CG-CD	9.93	1.76	1.51
1	A	1204	ASP	CB-CG	9.92	1.72	1.51
1	A	1230	GLU	CD-OE2	9.92	1.36	1.25
10	L	63	ARG	NE-CZ	9.92	1.46	1.33
1	A	1044	TRP	CB-CG	-9.91	1.32	1.50
2	B	1156	ASP	CB-CG	9.91	1.72	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1052	VAL	CB-CG2	-9.90	1.32	1.52
1	A	893	PHE	CG-CD1	-9.89	1.24	1.38
7	I	75	CYS	CB-SG	-9.89	1.65	1.82
3	C	66	ARG	NE-CZ	-9.89	1.20	1.33
1	A	1149	ALA	CA-CB	-9.89	1.31	1.52
1	A	708	MET	SD-CE	9.89	2.33	1.77
2	B	567	GLU	CB-CG	9.88	1.71	1.52
2	B	96	TYR	CG-CD2	9.87	1.51	1.39
3	C	172	PRO	CA-C	-9.86	1.33	1.52
1	A	482	PHE	CE1-CZ	-9.86	1.18	1.37
3	C	114	TYR	CE2-CZ	-9.85	1.25	1.38
9	K	61	TYR	CG-CD2	-9.84	1.26	1.39
3	C	116	LYS	CD-CE	9.84	1.75	1.51
1	A	100	LYS	CE-NZ	-9.83	1.24	1.49
1	A	549	MET	SD-CE	-9.83	1.22	1.77
3	C	209	TYR	CG-CD1	9.83	1.51	1.39
10	L	48	CYS	CA-C	9.83	1.78	1.52
4	E	45	LYS	CD-CE	9.82	1.75	1.51
2	B	346	GLU	CD-OE1	9.82	1.36	1.25
1	A	379	VAL	CB-CG1	-9.81	1.32	1.52
2	B	797	TYR	CD2-CE2	9.81	1.54	1.39
4	E	74	ASP	CB-CG	-9.80	1.31	1.51
7	I	120	GLN	CB-CG	9.80	1.79	1.52
2	B	57	TYR	CE1-CZ	-9.80	1.25	1.38
1	A	742	ASN	CB-CG	-9.80	1.28	1.51
4	E	106	GLN	CG-CD	9.78	1.73	1.51
5	F	72	LYS	CD-CE	9.78	1.75	1.51
4	E	191	LYS	CD-CE	9.77	1.75	1.51
2	B	1204	PHE	CE1-CZ	-9.77	1.18	1.37
2	B	660	LYS	CD-CE	-9.77	1.26	1.51
1	A	14	VAL	C-O	-9.76	1.04	1.23
1	A	61	ILE	CA-CB	9.76	1.77	1.54
1	A	69	THR	CA-C	9.76	1.78	1.52
1	A	846	GLU	CG-CD	9.76	1.66	1.51
1	A	932	GLU	CD-OE1	9.76	1.36	1.25
3	C	179	GLU	CD-OE2	-9.76	1.15	1.25
2	B	652	LYS	CE-NZ	9.75	1.73	1.49
3	C	163	ILE	CA-CB	-9.74	1.32	1.54
2	B	200	GLY	C-O	-9.73	1.08	1.23
3	C	87	PHE	CD2-CE2	9.73	1.58	1.39
2	B	951	GLN	CG-CD	9.73	1.73	1.51
1	A	1438	THR	CB-CG2	-9.73	1.20	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	ARG	CG-CD	9.72	1.76	1.51
10	L	50	ASP	CB-CG	9.71	1.72	1.51
1	A	37	PHE	CD2-CE2	9.71	1.58	1.39
1	A	990	VAL	CA-CB	-9.70	1.34	1.54
9	K	64	GLU	CD-OE2	-9.69	1.15	1.25
3	C	180	TYR	CD1-CE1	9.69	1.53	1.39
9	K	20	LYS	CG-CD	9.69	1.85	1.52
2	B	556	THR	C-O	9.69	1.41	1.23
3	C	3	GLU	CD-OE1	9.69	1.36	1.25
2	B	581	PHE	CE2-CZ	-9.69	1.19	1.37
3	C	154	LYS	CG-CD	9.69	1.85	1.52
9	K	26	LYS	CB-CG	9.68	1.78	1.52
1	A	368	LYS	CD-CE	9.68	1.75	1.51
1	A	899	VAL	CB-CG1	-9.68	1.32	1.52
1	A	603	ASN	CB-CG	-9.67	1.28	1.51
1	A	874	ASP	CG-OD2	9.67	1.47	1.25
2	B	705	MET	SD-CE	-9.67	1.23	1.77
3	C	169	LYS	CD-CE	9.67	1.75	1.51
1	A	1102	LYS	CD-CE	9.66	1.75	1.51
1	A	1419	ASP	CG-OD1	9.66	1.47	1.25
2	B	641	GLU	CD-OE2	9.66	1.36	1.25
1	A	995	GLU	CD-OE1	9.65	1.36	1.25
1	A	433	GLU	CD-OE1	9.65	1.36	1.25
1	A	830	LYS	CG-CD	9.65	1.85	1.52
2	B	694	ASP	CB-CG	9.65	1.72	1.51
2	B	194	GLU	CD-OE2	9.65	1.36	1.25
1	A	227	VAL	C-O	9.64	1.41	1.23
4	E	54	GLN	CB-CG	9.63	1.78	1.52
2	B	1061	GLU	CB-CG	9.63	1.70	1.52
1	A	1362	TYR	CE1-CZ	-9.62	1.26	1.38
7	I	30	ARG	CG-CD	9.62	1.76	1.51
1	A	656	TRP	CE3-CZ3	9.62	1.54	1.38
3	C	106	GLU	CD-OE2	9.60	1.36	1.25
3	C	9	LYS	CD-CE	9.59	1.75	1.51
2	B	999	MET	CG-SD	9.59	2.06	1.81
1	A	347	PHE	N-CA	9.59	1.65	1.46
2	B	1018	PRO	CA-C	-9.59	1.33	1.52
2	B	1057	LYS	CD-CE	9.58	1.75	1.51
2	B	1036	ALA	CA-CB	9.58	1.72	1.52
1	A	1337	GLU	CD-OE1	9.57	1.36	1.25
2	B	797	TYR	CD1-CE1	9.57	1.53	1.39
6	H	3	ASN	CB-CG	9.57	1.73	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	40	GLU	CD-OE1	9.57	1.36	1.25
4	E	103	LYS	CD-CE	9.57	1.75	1.51
8	J	32	GLU	CD-OE1	9.56	1.36	1.25
2	B	643	ASP	CB-CG	9.55	1.71	1.51
1	A	155	GLU	CG-CD	9.55	1.66	1.51
6	H	102	TYR	CG-CD2	-9.54	1.26	1.39
1	A	1301	GLU	CD-OE2	9.54	1.36	1.25
1	A	1005	GLU	CD-OE2	9.54	1.36	1.25
4	E	148	GLU	CD-OE2	9.54	1.36	1.25
2	B	31	TRP	CD2-CE2	-9.53	1.29	1.41
1	A	352	VAL	CB-CG2	9.53	1.72	1.52
1	A	398	GLU	CD-OE2	9.53	1.36	1.25
9	K	68	PHE	CG-CD1	-9.53	1.24	1.38
1	A	537	ARG	CZ-NH2	9.52	1.45	1.33
1	A	368	LYS	CG-CD	9.51	1.84	1.52
1	A	1050	GLU	CD-OE1	9.51	1.36	1.25
3	C	50	GLU	CD-OE2	9.51	1.36	1.25
1	A	362	ASP	CB-CG	-9.51	1.31	1.51
5	F	103	MET	SD-CE	9.51	2.31	1.77
1	A	896	ARG	CZ-NH1	9.50	1.45	1.33
1	A	585	GLY	C-O	9.49	1.38	1.23
2	B	1135	ARG	NE-CZ	-9.49	1.20	1.33
9	K	105	PHE	CE2-CZ	9.48	1.55	1.37
2	B	662	MET	SD-CE	9.48	2.31	1.77
3	C	50	GLU	CB-CG	9.48	1.70	1.52
1	A	542	GLU	CD-OE1	9.48	1.36	1.25
1	A	1112	LYS	CD-CE	9.48	1.75	1.51
1	A	1232	ASN	CG-OD1	9.47	1.44	1.24
1	A	209	ASN	CG-ND2	9.46	1.56	1.32
1	A	1162	VAL	CB-CG1	9.46	1.72	1.52
2	B	319	GLU	CB-CG	9.46	1.70	1.52
1	A	219	PHE	CD2-CE2	-9.46	1.20	1.39
1	A	1298	TYR	CE2-CZ	-9.46	1.26	1.38
1	A	945	GLU	CD-OE1	9.45	1.36	1.25
1	A	1359	ASP	CB-CG	9.45	1.71	1.51
2	B	1219	ASP	CB-CG	9.45	1.71	1.51
1	A	37	PHE	CE1-CZ	9.44	1.55	1.37
1	A	836	TYR	CZ-OH	9.44	1.53	1.37
1	A	858	ASN	CB-CG	-9.44	1.29	1.51
1	A	1239	ARG	CG-CD	9.43	1.75	1.51
2	B	883	LEU	CA-CB	9.43	1.75	1.53
1	A	882	SER	CB-OG	-9.43	1.29	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	66	GLU	CG-CD	9.42	1.66	1.51
1	A	1227	ILE	C-O	-9.42	1.05	1.23
2	B	785	TYR	CE2-CZ	-9.42	1.26	1.38
3	C	260	LEU	CG-CD2	9.41	1.86	1.51
2	B	958	GLN	CG-CD	9.41	1.72	1.51
10	L	61	THR	CB-CG2	9.41	1.83	1.52
1	A	590	ARG	CZ-NH2	-9.41	1.20	1.33
1	A	1281	ARG	NE-CZ	9.39	1.45	1.33
9	K	102	LYS	CD-CE	9.39	1.74	1.51
2	B	1163	CYS	CA-CB	9.39	1.74	1.53
9	K	99	GLY	C-O	9.38	1.38	1.23
2	B	31	TRP	CG-CD1	-9.37	1.23	1.36
6	H	104	PHE	CE2-CZ	9.37	1.55	1.37
2	B	644	GLU	CD-OE1	9.37	1.35	1.25
2	B	542	MET	SD-CE	-9.36	1.25	1.77
5	F	84	TYR	CE2-CZ	9.36	1.50	1.38
1	A	1062	GLU	CD-OE1	-9.36	1.15	1.25
6	H	19	ARG	CB-CG	9.36	1.77	1.52
1	A	1291	VAL	CB-CG1	-9.35	1.33	1.52
1	A	135	PHE	CE2-CZ	-9.35	1.19	1.37
1	A	209	ASN	CG-OD1	9.35	1.44	1.24
1	A	689	LYS	CD-CE	9.34	1.74	1.51
1	A	1130	GLN	CG-CD	9.34	1.72	1.51
4	E	191	LYS	CE-NZ	9.34	1.72	1.49
1	A	671	ALA	CA-CB	-9.33	1.32	1.52
2	B	346	GLU	CD-OE2	9.33	1.35	1.25
1	A	787	PHE	CD1-CE1	9.33	1.57	1.39
2	B	50	SER	CB-OG	-9.33	1.30	1.42
3	C	196	ASP	CB-CG	9.33	1.71	1.51
2	B	60	GLN	C-O	-9.32	1.05	1.23
2	B	723	VAL	CA-CB	9.31	1.74	1.54
3	C	191	TYR	CD1-CE1	9.31	1.53	1.39
1	A	705	LYS	CA-CB	9.31	1.74	1.53
1	A	1196	GLU	CD-OE2	9.30	1.35	1.25
2	B	1007	VAL	CB-CG1	-9.30	1.33	1.52
1	A	1349	TYR	C-O	-9.30	1.05	1.23
2	B	775	LYS	CB-CG	9.29	1.77	1.52
2	B	1087	PHE	CD2-CE2	-9.29	1.20	1.39
2	B	418	LYS	CD-CE	9.29	1.74	1.51
2	B	1069	PHE	CB-CG	-9.29	1.35	1.51
2	B	723	VAL	CB-CG2	9.29	1.72	1.52
1	A	1056	SER	CA-CB	-9.28	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	154	LYS	CB-CG	9.28	1.77	1.52
3	C	191	TYR	CE1-CZ	-9.28	1.26	1.38
4	E	150	VAL	CB-CG1	9.28	1.72	1.52
4	E	192	ARG	NE-CZ	9.27	1.45	1.33
2	B	908	GLU	CB-CG	9.27	1.69	1.52
3	C	86	CYS	CB-SG	9.27	1.98	1.82
1	A	843	LYS	C-O	-9.26	1.05	1.23
4	E	14	ARG	CZ-NH2	-9.25	1.21	1.33
1	A	264	PHE	CE2-CZ	9.25	1.54	1.37
2	B	57	TYR	CE2-CZ	-9.24	1.26	1.38
2	B	246	LYS	N-CA	9.24	1.64	1.46
4	E	112	TYR	CD1-CE1	9.24	1.53	1.39
1	A	162	VAL	CB-CG2	9.22	1.72	1.52
1	A	885	THR	N-CA	-9.22	1.27	1.46
1	A	931	GLU	CD-OE1	9.22	1.35	1.25
1	A	1243	VAL	CA-CB	9.22	1.74	1.54
2	B	118	ARG	CZ-NH1	-9.21	1.21	1.33
2	B	103	ASN	CB-CG	9.21	1.72	1.51
2	B	275	TYR	CE2-CZ	-9.21	1.26	1.38
9	K	86	ALA	CA-CB	-9.21	1.33	1.52
1	A	1322	ILE	CB-CG2	-9.20	1.24	1.52
2	B	785	TYR	CE1-CZ	-9.20	1.26	1.38
3	C	35	ARG	CZ-NH2	-9.20	1.21	1.33
2	B	662	MET	CG-SD	-9.20	1.57	1.81
1	A	1225	PHE	CG-CD2	9.19	1.52	1.38
1	A	1280	GLU	C-O	-9.19	1.05	1.23
1	A	461	LYS	CD-CE	9.18	1.74	1.51
1	A	1342	GLU	CD-OE1	9.18	1.35	1.25
2	B	1224	PHE	CG-CD2	9.17	1.52	1.38
6	H	95	TYR	CD1-CE1	9.17	1.53	1.39
1	A	460	VAL	CB-CG2	-9.16	1.33	1.52
9	K	16	GLU	CG-CD	9.16	1.65	1.51
1	A	46	THR	CA-CB	9.15	1.77	1.53
1	A	1422	ARG	NE-CZ	9.14	1.45	1.33
2	B	547	VAL	CB-CG1	-9.14	1.33	1.52
1	A	468	PHE	CD2-CE2	-9.14	1.21	1.39
2	B	792	MET	SD-CE	9.13	2.29	1.77
1	A	1419	ASP	CB-CG	9.13	1.71	1.51
1	A	829	VAL	CB-CG2	9.12	1.72	1.52
7	I	47	GLU	CG-CD	9.12	1.65	1.51
2	B	855	PHE	CG-CD2	-9.12	1.25	1.38
3	C	122	SER	CB-OG	9.12	1.54	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	93	SER	CA-CB	9.12	1.66	1.52
1	A	948	VAL	CB-CG1	-9.12	1.33	1.52
2	B	1206	GLU	CD-OE1	9.12	1.35	1.25
5	F	88	TYR	CD2-CE2	-9.12	1.25	1.39
5	F	105	ALA	CA-CB	-9.12	1.33	1.52
2	B	235	SER	CB-OG	-9.11	1.30	1.42
8	J	21	TYR	CE2-CZ	-9.12	1.26	1.38
2	B	344	LYS	CD-CE	9.11	1.74	1.51
6	H	93	TYR	CG-CD1	9.11	1.50	1.39
1	A	656	TRP	CG-CD2	-9.11	1.28	1.43
1	A	221	SER	CB-OG	-9.11	1.30	1.42
2	B	184	ALA	C-O	-9.11	1.06	1.23
6	H	141	TYR	CE1-CZ	-9.11	1.26	1.38
3	C	75	MET	SD-CE	9.09	2.28	1.77
10	L	28	LYS	CA-C	9.09	1.76	1.52
1	A	1109	LYS	CD-CE	9.08	1.74	1.51
1	A	1290	LYS	CE-NZ	9.08	1.71	1.49
2	B	531	GLN	CD-OE1	9.08	1.44	1.24
8	J	47	ARG	NE-CZ	-9.08	1.21	1.33
1	A	474	VAL	CB-CG2	-9.08	1.33	1.52
4	E	162	ARG	CD-NE	9.08	1.61	1.46
1	A	71	GLN	CG-CD	9.07	1.72	1.51
2	B	434	ARG	CB-CG	9.07	1.77	1.52
2	B	227	LYS	CE-NZ	9.07	1.71	1.49
1	A	419	LYS	C-O	-9.06	1.06	1.23
1	A	174	ILE	CA-CB	9.06	1.75	1.54
1	A	653	VAL	CB-CG2	-9.06	1.33	1.52
1	A	933	TYR	CG-CD1	-9.05	1.27	1.39
1	A	347	PHE	CG-CD2	9.05	1.52	1.38
2	B	853	SER	CB-OG	9.04	1.54	1.42
2	B	250	PHE	CG-CD2	9.04	1.52	1.38
2	B	191	LYS	CD-CE	9.04	1.73	1.51
2	B	1069	PHE	CG-CD2	-9.04	1.25	1.38
4	E	200	ARG	CB-CG	-9.03	1.28	1.52
1	A	497	THR	CB-CG2	-9.03	1.22	1.52
2	B	108	VAL	CA-CB	9.02	1.73	1.54
1	A	1234	GLU	CG-CD	9.02	1.65	1.51
1	A	940	ARG	CZ-NH1	-9.02	1.21	1.33
1	A	1212	VAL	CB-CG1	-9.02	1.33	1.52
7	I	100	PHE	CE1-CZ	-9.01	1.20	1.37
1	A	437	MET	SD-CE	9.01	2.28	1.77
1	A	1123	GLY	CA-C	9.00	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	GLU	CD-OE1	9.00	1.35	1.25
1	A	931	GLU	CG-CD	8.99	1.65	1.51
1	A	734	GLU	CG-CD	8.99	1.65	1.51
1	A	962	ARG	CG-CD	8.99	1.74	1.51
2	B	1192	TYR	CE1-CZ	-8.98	1.26	1.38
2	B	1217	TYR	CG-CD1	-8.98	1.27	1.39
1	A	229	SER	CB-OG	8.98	1.53	1.42
1	A	180	LYS	CD-CE	8.97	1.73	1.51
1	A	95	PHE	CD1-CE1	8.97	1.57	1.39
1	A	792	TYR	CE1-CZ	-8.97	1.26	1.38
8	J	58	GLU	CD-OE1	-8.97	1.15	1.25
2	B	175	ARG	C-O	-8.97	1.06	1.23
1	A	1160	SER	CB-OG	8.96	1.53	1.42
1	A	1214	GLU	C-O	8.96	1.40	1.23
2	B	230	ALA	CA-CB	8.95	1.71	1.52
1	A	66	LYS	CB-CG	8.94	1.76	1.52
1	A	74	MET	CB-CG	8.95	1.79	1.51
1	A	945	GLU	CD-OE2	8.94	1.35	1.25
8	J	60	PHE	CE1-CZ	-8.94	1.20	1.37
1	A	198	GLU	CD-OE2	8.94	1.35	1.25
7	I	59	VAL	CB-CG1	-8.94	1.34	1.52
1	A	719	VAL	CB-CG1	-8.93	1.34	1.52
2	B	663	ALA	CA-CB	8.93	1.71	1.52
2	B	1080	LYS	CD-CE	8.93	1.73	1.51
6	H	105	GLU	CG-CD	8.92	1.65	1.51
1	A	1259	MET	SD-CE	8.92	2.27	1.77
7	I	70	ARG	NE-CZ	-8.91	1.21	1.33
2	B	202	TYR	CE1-CZ	-8.91	1.26	1.38
6	H	129	TYR	CE2-CZ	8.91	1.50	1.38
1	A	190	ALA	CA-CB	8.91	1.71	1.52
2	B	875	GLU	CD-OE2	8.91	1.35	1.25
1	A	1045	VAL	CA-CB	-8.90	1.36	1.54
3	C	49	VAL	C-O	-8.90	1.06	1.23
2	B	651	LEU	CG-CD2	-8.89	1.19	1.51
1	A	815	PHE	CG-CD2	-8.89	1.25	1.38
2	B	650	GLU	CD-OE1	8.89	1.35	1.25
2	B	697	GLU	CD-OE2	8.89	1.35	1.25
3	C	255	VAL	CA-CB	-8.89	1.36	1.54
2	B	370	PHE	CE2-CZ	8.89	1.54	1.37
1	A	288	ALA	CA-CB	8.88	1.71	1.52
2	B	1067	ARG	CZ-NH2	-8.89	1.21	1.33
1	A	729	ALA	CA-CB	-8.88	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	895	LYS	CG-CD	8.88	1.82	1.52
2	B	1077	THR	C-O	-8.88	1.06	1.23
2	B	1021	MET	CG-SD	-8.87	1.58	1.81
2	B	970	THR	CA-CB	-8.87	1.30	1.53
1	A	546	VAL	CB-CG2	-8.87	1.34	1.52
2	B	39	ARG	CZ-NH2	8.86	1.44	1.33
2	B	227	LYS	CG-CD	8.86	1.82	1.52
2	B	238	ALA	CA-CB	8.86	1.71	1.52
3	C	50	GLU	CD-OE1	8.86	1.35	1.25
2	B	1164	GLY	C-O	8.85	1.37	1.23
6	H	23	VAL	CA-CB	-8.85	1.36	1.54
6	H	37	LYS	C-O	8.85	1.40	1.23
1	A	1225	PHE	CE1-CZ	8.85	1.54	1.37
6	H	77	ARG	NE-CZ	8.84	1.44	1.33
1	A	1235	LYS	CE-NZ	8.84	1.71	1.49
10	L	34	CYS	CB-SG	-8.84	1.67	1.82
1	A	830	LYS	CD-CE	8.83	1.73	1.51
7	I	74	GLU	CG-CD	8.83	1.65	1.51
1	A	264	PHE	CG-CD2	8.83	1.51	1.38
2	B	250	PHE	CE1-CZ	8.83	1.54	1.37
7	I	8	ARG	CZ-NH1	8.83	1.44	1.33
6	H	127	GLY	CA-C	8.82	1.66	1.51
9	K	2	ASN	C-O	8.81	1.40	1.23
1	A	1141	THR	C-O	8.81	1.40	1.23
6	H	104	PHE	CG-CD1	8.80	1.51	1.38
6	H	95	TYR	CD2-CE2	8.79	1.52	1.39
2	B	312	GLU	CD-OE2	8.79	1.35	1.25
3	C	127	ARG	N-CA	8.77	1.63	1.46
9	K	81	TYR	CD2-CE2	-8.77	1.26	1.39
6	H	136	LYS	CA-C	8.76	1.75	1.52
2	B	874	PHE	CD2-CE2	-8.76	1.21	1.39
1	A	551	TYR	CE1-CZ	-8.76	1.27	1.38
2	B	690	VAL	CB-CG1	-8.75	1.34	1.52
4	E	212	ARG	CZ-NH1	-8.74	1.21	1.33
3	C	84	ARG	NE-CZ	8.74	1.44	1.33
1	A	792	TYR	CE2-CZ	-8.73	1.27	1.38
2	B	1061	GLU	CD-OE1	8.73	1.35	1.25
1	A	5	GLN	CB-CG	8.73	1.76	1.52
2	B	592	ASN	CG-OD1	8.73	1.43	1.24
2	B	1224	PHE	CE1-CZ	8.73	1.53	1.37
9	K	54	ARG	CG-CD	8.73	1.73	1.51
7	I	27	PHE	CE1-CZ	-8.72	1.20	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	106	ASP	CB-CG	8.72	1.70	1.51
2	B	808	ALA	CA-CB	-8.72	1.34	1.52
2	B	1102	LYS	N-CA	8.71	1.63	1.46
3	C	191	TYR	CG-CD2	-8.71	1.27	1.39
2	B	1183	LYS	CA-CB	8.70	1.73	1.53
8	J	47	ARG	CZ-NH1	-8.68	1.21	1.33
1	A	1061	GLY	CA-C	8.68	1.65	1.51
1	A	635	ARG	CZ-NH2	8.68	1.44	1.33
1	A	91	PHE	CG-CD1	-8.67	1.25	1.38
1	A	129	LYS	C-O	8.67	1.39	1.23
10	L	27	LEU	CA-CB	8.67	1.73	1.53
2	B	370	PHE	CD2-CE2	8.66	1.56	1.39
2	B	852	ARG	CZ-NH1	-8.65	1.21	1.33
6	H	91	ASP	CA-C	8.65	1.75	1.52
1	A	567	LYS	CD-CE	8.65	1.72	1.51
2	B	711	GLU	CG-CD	8.64	1.65	1.51
2	B	747	MET	SD-CE	-8.64	1.29	1.77
10	L	47	ARG	CG-CD	8.64	1.73	1.51
1	A	1384	VAL	CB-CG2	8.64	1.71	1.52
8	J	38	ARG	CB-CG	8.64	1.75	1.52
2	B	1155	SER	CB-OG	8.63	1.53	1.42
2	B	1155	SER	N-CA	8.63	1.63	1.46
7	I	20	LYS	CD-CE	8.63	1.72	1.51
6	H	41	ASP	CB-CG	8.62	1.69	1.51
3	C	15	LYS	CB-CG	8.62	1.75	1.52
4	E	44	ALA	CA-CB	8.62	1.70	1.52
1	A	1290	LYS	CD-CE	8.62	1.72	1.51
2	B	875	GLU	CD-OE1	8.62	1.35	1.25
1	A	1112	LYS	CE-NZ	8.61	1.70	1.49
3	C	138	GLU	CD-OE2	8.60	1.35	1.25
3	C	78	GLU	C-O	-8.59	1.07	1.23
2	B	315	LYS	CE-NZ	8.58	1.70	1.49
3	C	102	GLN	C-O	8.58	1.39	1.23
6	H	45	GLU	CD-OE2	8.57	1.35	1.25
3	C	26	ASP	CG-OD1	8.57	1.45	1.25
1	A	1381	LEU	C-O	-8.57	1.07	1.23
2	B	465	ASN	CB-CG	8.57	1.70	1.51
3	C	20	PHE	CB-CG	-8.56	1.36	1.51
4	E	200	ARG	NE-CZ	-8.56	1.22	1.33
1	A	191	THR	CA-CB	8.56	1.75	1.53
2	B	1027	ILE	N-CA	-8.56	1.29	1.46
3	C	203	GLN	CG-CD	-8.56	1.31	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1060	ARG	CZ-NH2	-8.56	1.22	1.33
4	E	210	SER	CB-OG	8.56	1.53	1.42
6	H	107	VAL	CB-CG1	8.56	1.70	1.52
1	A	537	ARG	CZ-NH1	8.55	1.44	1.33
7	I	93	LYS	CD-CE	8.55	1.72	1.51
1	A	1303	GLU	CG-CD	8.55	1.64	1.51
1	A	1215	ARG	CB-CG	8.54	1.75	1.52
2	B	488	TYR	CG-CD2	-8.54	1.28	1.39
1	A	295	LEU	CG-CD2	8.54	1.83	1.51
2	B	592	ASN	CB-CG	8.54	1.70	1.51
1	A	648	ASN	CB-CG	-8.53	1.31	1.51
2	B	459	TYR	CD1-CE1	8.54	1.52	1.39
4	E	102	GLU	CD-OE1	8.53	1.35	1.25
2	B	769	TYR	CB-CG	8.52	1.64	1.51
6	H	123	MET	CG-SD	8.52	2.03	1.81
8	J	26	GLN	CB-CG	8.52	1.75	1.52
1	A	163	SER	CA-CB	8.52	1.65	1.52
3	C	267	GLN	CA-C	8.51	1.75	1.52
1	A	155	GLU	CD-OE2	8.51	1.35	1.25
1	A	1302	PRO	C-O	8.51	1.40	1.23
2	B	968	VAL	CB-CG2	-8.50	1.34	1.52
1	A	19	PHE	CD1-CE1	-8.49	1.22	1.39
2	B	995	ARG	CD-NE	-8.49	1.32	1.46
1	A	1337	GLU	CD-OE2	8.48	1.34	1.25
2	B	797	TYR	CG-CD2	-8.48	1.28	1.39
2	B	742	GLU	CD-OE2	-8.48	1.16	1.25
1	A	264	PHE	CG-CD1	8.48	1.51	1.38
1	A	643	ALA	CA-CB	-8.47	1.34	1.52
1	A	1152	ILE	CA-CB	-8.47	1.35	1.54
4	E	152	LYS	CG-CD	8.46	1.81	1.52
1	A	478	TYR	CD1-CE1	-8.46	1.26	1.39
1	A	376	TYR	CG-CD1	-8.46	1.28	1.39
8	J	62	ARG	CG-CD	-8.46	1.30	1.51
3	C	155	LEU	C-O	8.46	1.39	1.23
1	A	826	ASP	CG-OD2	8.45	1.44	1.25
3	C	30	ALA	CA-CB	-8.45	1.34	1.52
2	B	485	ARG	CG-CD	-8.45	1.30	1.51
6	H	129	TYR	CG-CD2	8.45	1.50	1.39
3	C	16	ASP	C-O	-8.43	1.07	1.23
1	A	601	LYS	CE-NZ	8.43	1.70	1.49
1	A	961	ARG	CZ-NH2	8.42	1.44	1.33
2	B	358	LYS	CB-CG	8.42	1.75	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	155	ARG	CD-NE	8.42	1.60	1.46
1	A	1191	TRP	CZ3-CH2	-8.42	1.26	1.40
2	B	458	LYS	C-O	-8.41	1.07	1.23
2	B	798	TYR	CD2-CE2	8.41	1.51	1.39
2	B	875	GLU	CB-CG	8.41	1.68	1.52
1	A	1214	GLU	CB-CG	8.40	1.68	1.52
3	C	160	LYS	CE-NZ	8.40	1.70	1.49
1	A	1074	GLU	CG-CD	8.40	1.64	1.51
1	A	965	GLN	CG-CD	8.39	1.70	1.51
1	A	999	VAL	CB-CG1	-8.39	1.35	1.52
2	B	781	PHE	CE2-CZ	8.39	1.53	1.37
4	E	52	ARG	CB-CG	8.38	1.75	1.52
5	F	93	ILE	C-O	-8.37	1.07	1.23
1	A	15	LYS	C-O	-8.37	1.07	1.23
1	A	213	HIS	CA-CB	8.37	1.72	1.53
2	B	184	ALA	CA-CB	-8.36	1.34	1.52
1	A	1441	PHE	CG-CD1	-8.35	1.26	1.38
1	A	1417	GLU	CD-OE1	8.35	1.34	1.25
2	B	959	ASP	CA-CB	8.35	1.72	1.53
2	B	1221	SER	CA-CB	8.35	1.65	1.52
4	E	102	GLU	CG-CD	8.35	1.64	1.51
4	E	85	GLU	CD-OE2	8.35	1.34	1.25
8	J	21	TYR	CB-CG	8.35	1.64	1.51
1	A	1012	ARG	C-O	8.33	1.39	1.23
4	E	30	ILE	C-O	-8.33	1.07	1.23
1	A	1226	VAL	CA-CB	-8.33	1.37	1.54
2	B	265	SER	CA-CB	8.32	1.65	1.52
1	A	1111	MET	CG-SD	8.31	2.02	1.81
3	C	94	LYS	CB-CG	8.31	1.75	1.52
2	B	186	GLU	CD-OE2	8.31	1.34	1.25
8	J	3	VAL	CA-CB	-8.31	1.37	1.54
2	B	120	ARG	CZ-NH2	8.30	1.43	1.33
2	B	746	SER	CB-OG	-8.30	1.31	1.42
1	A	469	ARG	NE-CZ	-8.30	1.22	1.33
9	K	26	LYS	CG-CD	8.30	1.80	1.52
1	A	264	PHE	CE1-CZ	8.29	1.53	1.37
9	K	7	PHE	CB-CG	-8.29	1.37	1.51
7	I	50	THR	CA-C	-8.29	1.31	1.52
1	A	1298	TYR	CG-CD1	-8.29	1.28	1.39
7	I	45	ARG	CZ-NH2	-8.28	1.22	1.33
8	J	63	TYR	CE2-CZ	-8.28	1.27	1.38
2	B	851	PHE	CB-CG	8.28	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1057	LYS	CG-CD	8.28	1.80	1.52
1	A	1119	TYR	CG-CD2	-8.27	1.28	1.39
3	C	205	LYS	CB-CG	8.27	1.74	1.52
2	B	190	TYR	CD2-CE2	8.27	1.51	1.39
7	I	36	GLU	CG-CD	8.27	1.64	1.51
9	K	64	GLU	C-O	-8.26	1.07	1.23
9	K	94	ILE	CA-CB	8.26	1.73	1.54
8	J	45	CYS	CB-SG	8.26	1.96	1.82
4	E	83	CYS	CB-SG	8.26	1.96	1.82
4	E	50	MET	CG-SD	8.25	2.02	1.81
1	A	781	ASP	C-O	8.25	1.39	1.23
2	B	231	PRO	CA-C	8.25	1.69	1.52
1	A	1136	SER	CB-OG	8.25	1.52	1.42
2	B	113	TYR	CD2-CE2	-8.24	1.26	1.39
2	B	381	MET	SD-CE	-8.23	1.31	1.77
2	B	915	THR	CA-CB	8.23	1.74	1.53
3	C	215	GLU	CD-OE1	8.22	1.34	1.25
1	A	16	GLU	CG-CD	8.22	1.64	1.51
1	A	390	GLN	C-O	8.22	1.39	1.23
1	A	1289	ARG	CZ-NH2	-8.22	1.22	1.33
2	B	370	PHE	CG-CD1	8.22	1.51	1.38
1	A	572	TRP	CB-CG	-8.22	1.35	1.50
1	A	788	SER	CA-CB	8.21	1.65	1.52
1	A	558	GLY	C-O	-8.21	1.10	1.23
2	B	202	TYR	CE2-CZ	-8.21	1.27	1.38
7	I	15	TYR	CD1-CE1	8.21	1.51	1.39
2	B	1129	ARG	NE-CZ	8.21	1.43	1.33
10	L	26	THR	CB-CG2	8.21	1.79	1.52
1	A	572	TRP	CD2-CE2	-8.20	1.31	1.41
2	B	124	TYR	CD2-CE2	8.20	1.51	1.39
5	F	148	VAL	C-O	8.20	1.39	1.23
1	A	175	ARG	CB-CG	8.19	1.74	1.52
1	A	863	VAL	CB-CG2	8.19	1.70	1.52
4	E	20	LYS	CD-CE	8.19	1.71	1.51
4	E	184	VAL	CB-CG1	-8.19	1.35	1.52
7	I	54	GLU	CD-OE2	8.19	1.34	1.25
2	B	137	TYR	CE1-CZ	8.18	1.49	1.38
1	A	464	PRO	CA-C	-8.18	1.36	1.52
1	A	961	ARG	NE-CZ	8.18	1.43	1.33
4	E	196	VAL	CB-CG1	-8.18	1.35	1.52
1	A	305	ASP	N-CA	8.18	1.62	1.46
1	A	776	ALA	C-O	-8.17	1.07	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	607	GLY	C-O	-8.17	1.10	1.23
2	B	320	ASP	CB-CG	8.17	1.69	1.51
1	A	1417	GLU	CG-CD	8.17	1.64	1.51
4	E	1	MET	SD-CE	8.17	2.23	1.77
7	I	92	ARG	C-O	8.16	1.38	1.23
1	A	175	ARG	CG-CD	8.16	1.72	1.51
5	F	87	LYS	CE-NZ	8.15	1.69	1.49
9	K	26	LYS	CD-CE	8.14	1.71	1.51
1	A	123	ARG	CB-CG	8.14	1.74	1.52
4	E	28	TYR	CE2-CZ	-8.14	1.27	1.38
2	B	353	LYS	CD-CE	8.13	1.71	1.51
3	C	193	TYR	CG-CD2	8.14	1.49	1.39
1	A	206	GLU	CD-OE1	8.13	1.34	1.25
7	I	82	GLU	CD-OE2	8.13	1.34	1.25
7	I	111	THR	C-O	-8.13	1.07	1.23
1	A	1108	ALA	N-CA	-8.13	1.30	1.46
1	A	1347	ALA	C-O	-8.13	1.07	1.23
2	B	703	ILE	C-O	8.12	1.38	1.23
2	B	1106	ARG	CA-C	8.12	1.74	1.52
1	A	1005	GLU	CG-CD	8.12	1.64	1.51
1	A	958	VAL	CB-CG1	-8.11	1.35	1.52
2	B	699	GLU	N-CA	-8.11	1.30	1.46
1	A	193	ASP	CB-CG	8.10	1.68	1.51
1	A	303	TYR	CG-CD2	-8.10	1.28	1.39
7	I	28	GLU	C-O	-8.10	1.07	1.23
1	A	217	LYS	CG-CD	8.09	1.79	1.52
2	B	89	GLU	C-O	8.09	1.38	1.23
1	A	1353	TYR	CE2-CZ	-8.09	1.28	1.38
2	B	18	PHE	CG-CD2	8.09	1.50	1.38
1	A	225	ASN	C-O	8.08	1.38	1.23
1	A	1302	PRO	CB-CG	8.08	1.90	1.50
2	B	488	TYR	C-O	8.08	1.38	1.23
2	B	846	ILE	C-O	8.08	1.38	1.23
1	A	478	TYR	CG-CD1	-8.07	1.28	1.39
1	A	1138	ILE	C-O	8.07	1.38	1.23
1	A	593	GLU	CD-OE1	8.07	1.34	1.25
1	A	25	GLU	CG-CD	8.07	1.64	1.51
1	A	875	ALA	CA-CB	-8.07	1.35	1.52
1	A	940	ARG	CD-NE	-8.07	1.32	1.46
4	E	93	MET	SD-CE	8.07	2.23	1.77
6	H	19	ARG	NE-CZ	8.07	1.43	1.33
1	A	515	GLN	CG-CD	8.06	1.69	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	724	GLU	CD-OE1	8.06	1.34	1.25
1	A	1326	ARG	C-O	-8.06	1.08	1.23
2	B	250	PHE	CB-CG	8.05	1.65	1.51
10	L	29	TYR	CG-CD2	-8.05	1.28	1.39
1	A	644	LYS	CE-NZ	8.04	1.69	1.49
2	B	815	ARG	CZ-NH2	8.04	1.43	1.33
1	A	459	ARG	CD-NE	-8.04	1.32	1.46
1	A	464	PRO	C-N	-8.04	1.15	1.34
2	B	351	TYR	CE2-CZ	-8.03	1.28	1.38
1	A	849	MET	SD-CE	-8.03	1.32	1.77
3	C	137	LYS	CD-CE	8.03	1.71	1.51
2	B	833	TYR	CG-CD2	-8.03	1.28	1.39
1	A	979	SER	CB-OG	8.03	1.52	1.42
2	B	1091	TYR	CB-CG	-8.03	1.39	1.51
1	A	1299	VAL	C-O	8.02	1.38	1.23
9	K	111	LEU	CG-CD1	8.02	1.81	1.51
2	B	336	ARG	CB-CG	-8.02	1.30	1.52
2	B	594	ALA	CA-CB	-8.02	1.35	1.52
2	B	327	ARG	CB-CG	-8.02	1.30	1.52
3	C	215	GLU	CG-CD	8.02	1.64	1.51
3	C	231	ASN	CB-CG	8.02	1.69	1.51
1	A	199	LEU	CG-CD1	8.01	1.81	1.51
6	H	126	GLU	CG-CD	8.01	1.64	1.51
2	B	263	GLY	C-O	8.01	1.36	1.23
7	I	103	CYS	C-O	-8.01	1.08	1.23
3	C	70	ILE	N-CA	8.01	1.62	1.46
2	B	115	GLN	CB-CG	8.01	1.74	1.52
2	B	401	PHE	CG-CD2	-8.01	1.26	1.38
2	B	1140	ALA	CA-CB	-8.00	1.35	1.52
1	A	1293	SER	CB-OG	-8.00	1.31	1.42
3	C	191	TYR	CB-CG	8.00	1.63	1.51
1	A	149	GLU	CD-OE2	8.00	1.34	1.25
2	B	1224	PHE	CD2-CE2	7.99	1.55	1.39
1	A	1093	LYS	CB-CG	7.99	1.74	1.52
2	B	968	VAL	CB-CG1	7.99	1.69	1.52
2	B	1004	GLU	C-O	7.99	1.38	1.23
4	E	43	LYS	CB-CG	7.98	1.74	1.52
4	E	155	ARG	NE-CZ	7.98	1.43	1.33
4	E	142	VAL	C-O	7.98	1.38	1.23
3	C	244	VAL	CB-CG1	-7.97	1.36	1.52
2	B	1064	TYR	CZ-OH	7.97	1.51	1.37
6	H	13	SER	CA-CB	7.97	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	448	ILE	CA-CB	7.97	1.73	1.54
1	A	782	ARG	C-O	-7.97	1.08	1.23
2	B	70	ILE	CA-CB	7.97	1.73	1.54
4	E	152	LYS	CB-CG	7.96	1.74	1.52
4	E	7	ARG	NE-CZ	7.95	1.43	1.33
10	L	25	ALA	CA-CB	7.95	1.69	1.52
1	A	135	PHE	CG-CD1	-7.95	1.26	1.38
1	A	1129	GLU	CD-OE1	7.95	1.34	1.25
2	B	732	SER	CA-CB	7.95	1.64	1.52
4	E	121	MET	CG-SD	7.95	2.01	1.81
8	J	13	VAL	CB-CG2	-7.95	1.36	1.52
1	A	420	ARG	CB-CG	-7.95	1.31	1.52
1	A	198	GLU	C-O	-7.95	1.08	1.23
5	F	153	VAL	CB-CG2	-7.95	1.36	1.52
2	B	733	HIS	N-CA	7.95	1.62	1.46
8	J	42	LYS	CD-CE	7.94	1.71	1.51
1	A	521	MET	SD-CE	-7.94	1.33	1.77
4	E	34	GLU	CD-OE1	7.93	1.34	1.25
1	A	1120	LEU	C-O	-7.93	1.08	1.23
1	A	730	GLY	CA-C	-7.93	1.39	1.51
1	A	1105	LEU	CA-C	-7.93	1.32	1.52
3	C	252	GLN	CG-CD	7.93	1.69	1.51
2	B	89	GLU	CA-C	7.92	1.73	1.52
2	B	138	GLU	N-CA	7.92	1.62	1.46
4	E	207	ARG	NE-CZ	7.92	1.43	1.33
1	A	422	GLY	C-O	-7.92	1.10	1.23
1	A	1132	LYS	CE-NZ	7.92	1.68	1.49
1	A	656	TRP	CD2-CE3	-7.92	1.28	1.40
2	B	172	ILE	C-O	7.91	1.38	1.23
2	B	1224	PHE	CG-CD1	7.91	1.50	1.38
2	B	488	TYR	CE1-CZ	-7.91	1.28	1.38
4	E	52	ARG	C-O	7.91	1.38	1.23
1	A	1288	ASP	N-CA	7.91	1.62	1.46
2	B	323	VAL	CB-CG1	7.91	1.69	1.52
1	A	1385	THR	CA-C	7.90	1.73	1.52
1	A	1232	ASN	C-O	7.90	1.38	1.23
5	F	106	PRO	CG-CD	-7.89	1.24	1.50
7	I	23	ASN	CB-CG	7.89	1.69	1.51
3	C	168	ALA	C-O	-7.89	1.08	1.23
3	C	225	ALA	CA-CB	-7.89	1.35	1.52
2	B	529	GLU	CB-CG	7.88	1.67	1.52
1	A	69	THR	CA-CB	7.88	1.73	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	121	ALA	C-O	-7.88	1.08	1.23
8	J	54	VAL	CB-CG2	-7.88	1.36	1.52
1	A	290	GLU	CD-OE2	7.87	1.34	1.25
1	A	144	THR	CB-CG2	7.87	1.78	1.52
3	C	81	GLU	C-O	7.86	1.38	1.23
1	A	1339	LEU	CA-CB	-7.86	1.35	1.53
3	C	197	SER	CB-OG	7.86	1.52	1.42
2	B	108	VAL	CB-CG2	7.86	1.69	1.52
5	F	108	PHE	CE2-CZ	7.86	1.52	1.37
2	B	766	ARG	CZ-NH2	7.86	1.43	1.33
2	B	249	ARG	NE-CZ	7.85	1.43	1.33
2	B	634	TYR	CG-CD2	-7.84	1.28	1.39
4	E	129	PRO	CG-CD	7.84	1.76	1.50
1	A	618	GLU	CD-OE1	7.84	1.34	1.25
1	A	1129	GLU	CG-CD	7.84	1.63	1.51
2	B	712	PRO	CG-CD	7.84	1.76	1.50
4	E	42	PHE	CE1-CZ	-7.84	1.22	1.37
7	I	6	PHE	CD1-CE1	7.83	1.54	1.39
3	C	26	ASP	CB-CG	7.83	1.68	1.51
1	A	1268	LEU	N-CA	-7.83	1.30	1.46
2	B	479	VAL	C-O	-7.83	1.08	1.23
1	A	1011	GLN	CD-OE1	-7.83	1.06	1.24
2	B	707	PRO	N-CD	-7.83	1.36	1.47
2	B	104	GLU	CA-C	7.83	1.73	1.52
1	A	111	GLY	C-O	7.82	1.36	1.23
2	B	401	PHE	CB-CG	-7.82	1.38	1.51
2	B	123	THR	CA-CB	-7.82	1.33	1.53
7	I	15	TYR	CD2-CE2	7.82	1.51	1.39
7	I	74	GLU	CD-OE2	7.82	1.34	1.25
1	A	688	LYS	CD-CE	7.82	1.70	1.51
1	A	291	GLU	C-O	-7.81	1.08	1.23
3	C	219	PHE	CE1-CZ	-7.81	1.22	1.37
1	A	1104	ILE	CB-CG2	-7.81	1.28	1.52
2	B	245	GLU	CB-CG	7.81	1.67	1.52
1	A	795	GLU	CD-OE2	7.81	1.34	1.25
1	A	171	GLN	CD-NE2	7.80	1.52	1.32
2	B	352	ALA	CA-CB	-7.80	1.36	1.52
2	B	859	TYR	CE1-CZ	7.80	1.48	1.38
3	C	252	GLN	CD-OE1	7.80	1.41	1.24
1	A	1080	THR	CA-CB	7.80	1.73	1.53
1	A	1284	MET	CA-C	-7.79	1.32	1.52
10	L	62	LYS	CE-NZ	7.79	1.68	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	43	VAL	CB-CG1	-7.79	1.36	1.52
9	K	48	ALA	CA-CB	-7.78	1.36	1.52
1	A	580	VAL	C-O	7.78	1.38	1.23
1	A	366	VAL	C-N	-7.78	1.19	1.34
2	B	855	PHE	CG-CD1	-7.77	1.27	1.38
2	B	780	VAL	CB-CG2	-7.77	1.36	1.52
2	B	1092	TYR	CE2-CZ	-7.77	1.28	1.38
6	H	136	LYS	CA-CB	7.76	1.71	1.53
1	A	1221	LYS	CB-CG	7.76	1.73	1.52
3	C	15	LYS	CD-CE	7.75	1.70	1.51
1	A	326	ARG	CG-CD	7.75	1.71	1.51
2	B	635	ARG	CZ-NH2	-7.75	1.23	1.33
2	B	25	ILE	C-O	-7.75	1.08	1.23
9	K	89	ASN	CB-CG	7.75	1.68	1.51
1	A	468	PHE	CE2-CZ	-7.75	1.22	1.37
1	A	291	GLU	CD-OE1	7.74	1.34	1.25
1	A	1103	GLU	CB-CG	-7.74	1.37	1.52
7	I	44	TYR	CG-CD1	-7.74	1.29	1.39
2	B	582	VAL	CB-CG1	-7.74	1.36	1.52
9	K	20	LYS	CB-CG	7.73	1.73	1.52
9	K	110	ASN	CB-CG	7.73	1.68	1.51
8	J	1	MET	SD-CE	7.72	2.21	1.77
9	K	54	ARG	NE-CZ	7.72	1.43	1.33
10	L	42	ARG	NE-CZ	7.72	1.43	1.33
1	A	407	ARG	CZ-NH1	7.72	1.43	1.33
1	A	990	VAL	CB-CG1	-7.72	1.36	1.52
2	B	608	ASP	C-O	-7.72	1.08	1.23
4	E	112	TYR	CG-CD1	-7.72	1.29	1.39
1	A	762	SER	CB-OG	-7.72	1.32	1.42
1	A	346	ASP	CA-CB	7.71	1.71	1.53
2	B	308	TRP	CG-CD1	-7.71	1.25	1.36
1	A	978	PRO	CB-CG	7.71	1.88	1.50
7	I	90	GLN	C-O	-7.71	1.08	1.23
2	B	785	TYR	CD1-CE1	-7.71	1.27	1.39
6	H	104	PHE	C-O	7.71	1.38	1.23
1	A	110	CYS	CB-SG	7.71	1.95	1.82
3	C	35	ARG	CG-CD	7.70	1.71	1.51
2	B	735	ALA	N-CA	7.70	1.61	1.46
1	A	205	GLU	CD-OE2	7.69	1.34	1.25
2	B	975	GLN	CB-CG	-7.69	1.31	1.52
7	I	1	MET	CB-CG	7.69	1.75	1.51
1	A	1280	GLU	CB-CG	7.68	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	212	LEU	C-O	-7.68	1.08	1.23
1	A	469	ARG	CD-NE	-7.68	1.33	1.46
1	A	670	ILE	CA-CB	-7.68	1.37	1.54
2	B	681	TRP	CG-CD1	-7.68	1.25	1.36
2	B	763	GLN	CB-CG	-7.68	1.31	1.52
5	F	127	GLU	CD-OE1	7.68	1.34	1.25
1	A	298	PHE	CG-CD2	7.68	1.50	1.38
1	A	510	GLN	CB-CG	7.67	1.73	1.52
3	C	170	TRP	CZ3-CH2	-7.67	1.27	1.40
8	J	7	CYS	CB-SG	-7.67	1.69	1.82
9	K	61	TYR	CZ-OH	-7.67	1.24	1.37
1	A	4	GLN	CB-CG	7.67	1.73	1.52
2	B	820	GLY	N-CA	-7.66	1.34	1.46
5	F	88	TYR	CG-CD1	-7.66	1.29	1.39
2	B	1069	PHE	CE2-CZ	-7.65	1.22	1.37
4	E	192	ARG	CZ-NH2	7.65	1.43	1.33
3	C	84	ARG	C-O	-7.65	1.08	1.23
1	A	1131	ALA	CA-CB	-7.65	1.36	1.52
1	A	655	PHE	CG-CD2	-7.64	1.27	1.38
3	C	113	VAL	C-O	-7.64	1.08	1.23
1	A	647	GLY	C-O	-7.64	1.11	1.23
3	C	195	GLN	CG-CD	7.64	1.68	1.51
9	K	5	ASP	CG-OD2	7.64	1.43	1.25
2	B	394	ASP	CB-CG	7.63	1.67	1.51
7	I	56	ALA	C-O	-7.63	1.08	1.23
1	A	839	ARG	CZ-NH1	7.63	1.43	1.33
2	B	700	SER	C-O	-7.63	1.08	1.23
1	A	1316	VAL	CB-CG2	-7.62	1.36	1.52
4	E	67	GLU	CD-OE1	7.62	1.34	1.25
4	E	1	MET	CG-SD	7.62	2.00	1.81
2	B	105	SER	CB-OG	7.62	1.52	1.42
3	C	253	LYS	C-O	7.62	1.37	1.23
1	A	836	TYR	CG-CD1	7.61	1.49	1.39
2	B	380	TYR	CE1-CZ	-7.61	1.28	1.38
1	A	1035	TYR	CE2-CZ	-7.61	1.28	1.38
1	A	1039	LYS	CE-NZ	7.61	1.68	1.49
6	H	105	GLU	CD-OE2	7.60	1.34	1.25
3	C	34	ARG	CD-NE	-7.60	1.33	1.46
1	A	123	ARG	NE-CZ	7.60	1.43	1.33
1	A	1439	GLY	C-O	-7.60	1.11	1.23
1	A	186	LYS	CD-CE	7.60	1.70	1.51
2	B	250	PHE	CG-CD1	7.60	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	111	THR	CA-CB	-7.60	1.33	1.53
1	A	777	PHE	CD2-CE2	7.59	1.54	1.39
2	B	97	VAL	CB-CG1	-7.59	1.36	1.52
1	A	1278	ASN	CG-OD1	7.59	1.40	1.24
2	B	169	ARG	CZ-NH2	7.59	1.43	1.33
6	H	139	ASN	C-O	7.58	1.37	1.23
1	A	196	GLU	CG-CD	7.58	1.63	1.51
3	C	220	ASP	CB-CG	7.58	1.67	1.51
6	H	2	SER	CA-CB	7.57	1.64	1.52
3	C	12	GLU	CD-OE1	7.57	1.33	1.25
1	A	1132	LYS	CG-CD	7.57	1.78	1.52
1	A	303	TYR	CD2-CE2	-7.57	1.28	1.39
1	A	229	SER	CA-CB	-7.56	1.41	1.52
2	B	37	PHE	CE2-CZ	-7.56	1.23	1.37
8	J	22	LEU	CA-C	7.56	1.72	1.52
2	B	118	ARG	CD-NE	-7.56	1.33	1.46
2	B	758	PHE	CG-CD2	-7.55	1.27	1.38
2	B	1143	ALA	CA-CB	-7.55	1.36	1.52
3	C	55	THR	CB-OG1	-7.55	1.28	1.43
9	K	10	PHE	CB-CG	7.55	1.64	1.51
10	L	46	VAL	CB-CG2	7.54	1.68	1.52
1	A	1331	SER	C-O	7.53	1.37	1.23
1	A	1038	THR	C-O	-7.53	1.09	1.23
1	A	186	LYS	CB-CG	7.53	1.72	1.52
2	B	1191	ILE	CA-CB	-7.53	1.37	1.54
6	H	116	TYR	CG-CD1	7.53	1.49	1.39
1	A	1111	MET	SD-CE	-7.53	1.35	1.77
2	B	1221	SER	N-CA	7.53	1.61	1.46
2	B	583	ASN	CG-OD1	-7.52	1.07	1.24
5	F	87	LYS	CD-CE	7.52	1.70	1.51
3	C	67	LEU	C-O	7.52	1.37	1.23
2	B	394	ASP	CG-OD2	7.51	1.42	1.25
2	B	904	ARG	CB-CG	-7.51	1.32	1.52
10	L	66	GLN	C-O	-7.51	1.09	1.23
2	B	319	GLU	CD-OE1	7.51	1.33	1.25
3	C	159	ALA	C-O	-7.50	1.09	1.23
10	L	29	TYR	CE1-CZ	-7.50	1.28	1.38
3	C	88	CYS	CB-SG	-7.50	1.69	1.82
6	H	93	TYR	CE2-CZ	7.48	1.48	1.38
2	B	908	GLU	CA-CB	7.48	1.70	1.53
2	B	1073	TYR	CG-CD2	-7.48	1.29	1.39
9	K	54	ARG	CZ-NH2	7.48	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	169	ARG	CZ-NH1	7.48	1.42	1.33
2	B	958	GLN	CB-CG	7.48	1.72	1.52
2	B	478	GLY	N-CA	7.47	1.57	1.46
2	B	782	LEU	CG-CD1	-7.47	1.24	1.51
2	B	1002	THR	CA-C	7.47	1.72	1.52
2	B	337	ARG	CD-NE	-7.47	1.33	1.46
2	B	646	LEU	CG-CD1	7.47	1.79	1.51
5	F	76	LYS	CE-NZ	7.47	1.67	1.49
10	L	29	TYR	CD2-CE2	-7.47	1.28	1.39
4	E	191	LYS	C-O	-7.47	1.09	1.23
1	A	1206	ASP	CB-CG	7.47	1.67	1.51
1	A	1365	TYR	CD1-CE1	7.46	1.50	1.39
2	B	786	ASN	CG-OD1	-7.46	1.07	1.24
2	B	371	GLU	CG-CD	7.46	1.63	1.51
3	C	49	VAL	CB-CG1	7.46	1.68	1.52
1	A	367	PRO	N-CA	-7.46	1.34	1.47
7	I	36	GLU	CA-CB	-7.46	1.37	1.53
1	A	1304	TRP	CE3-CZ3	-7.46	1.25	1.38
1	A	940	ARG	CG-CD	7.46	1.70	1.51
1	A	196	GLU	CD-OE2	7.45	1.33	1.25
6	H	103	LYS	CA-C	-7.45	1.33	1.52
1	A	478	TYR	CE1-CZ	-7.45	1.28	1.38
2	B	241	ARG	NE-CZ	7.45	1.42	1.33
2	B	448	ILE	N-CA	7.45	1.61	1.46
1	A	446	ARG	CZ-NH2	7.44	1.42	1.33
1	A	1280	GLU	CD-OE1	7.44	1.33	1.25
2	B	595	ARG	CD-NE	7.43	1.59	1.46
6	H	121	LEU	C-O	7.43	1.37	1.23
6	H	127	GLY	N-CA	7.43	1.57	1.46
2	B	1156	ASP	CA-CB	7.43	1.70	1.53
1	A	12	ARG	CZ-NH1	7.43	1.42	1.33
2	B	661	LEU	C-O	-7.43	1.09	1.23
3	C	265	MET	SD-CE	7.42	2.19	1.77
1	A	1332	PHE	CB-CG	-7.42	1.38	1.51
1	A	1239	ARG	N-CA	-7.42	1.31	1.46
2	B	605	ARG	NE-CZ	-7.41	1.23	1.33
1	A	1307	GLU	CD-OE2	-7.41	1.17	1.25
1	A	1023	ARG	CZ-NH2	-7.41	1.23	1.33
1	A	1112	LYS	CB-CG	7.41	1.72	1.52
2	B	325	GLN	CD-OE1	7.41	1.40	1.24
1	A	728	LYS	CE-NZ	7.40	1.67	1.49
1	A	1050	GLU	CG-CD	7.40	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	143	ASN	C-O	-7.40	1.09	1.23
1	A	995	GLU	C-O	-7.39	1.09	1.23
2	B	265	SER	CB-OG	7.39	1.51	1.42
1	A	155	GLU	CD-OE1	7.39	1.33	1.25
2	B	1070	GLU	CD-OE1	7.39	1.33	1.25
2	B	1158	PHE	C-O	-7.39	1.09	1.23
7	I	48	LEU	CG-CD2	-7.39	1.24	1.51
2	B	638	PHE	CG-CD2	-7.38	1.27	1.38
9	K	105	PHE	CD1-CE1	-7.38	1.24	1.39
1	A	1157	ASP	CB-CG	7.38	1.67	1.51
2	B	203	PHE	CG-CD2	-7.38	1.27	1.38
1	A	383	TYR	CD1-CE1	7.38	1.50	1.39
1	A	1443	VAL	C-O	-7.38	1.09	1.23
2	B	546	SER	C-O	-7.37	1.09	1.23
1	A	762	SER	C-O	-7.37	1.09	1.23
2	B	328	GLU	CB-CG	7.37	1.66	1.52
1	A	1080	THR	CA-C	7.37	1.72	1.52
1	A	1003	LYS	CB-CG	7.36	1.72	1.52
1	A	1277	GLU	CD-OE1	7.36	1.33	1.25
1	A	23	SER	C-O	7.35	1.37	1.23
2	B	772	ALA	CA-CB	-7.35	1.37	1.52
1	A	985	ASP	CG-OD2	7.35	1.42	1.25
4	E	91	LYS	CB-CG	7.35	1.72	1.52
1	A	911	SER	C-O	7.34	1.37	1.23
2	B	798	TYR	CE1-CZ	7.34	1.48	1.38
2	B	526	GLU	CD-OE2	7.34	1.33	1.25
1	A	1228	TRP	CG-CD1	-7.33	1.26	1.36
1	A	589	GLN	CG-CD	7.33	1.68	1.51
1	A	1073	GLY	C-O	-7.33	1.11	1.23
1	A	1385	THR	CB-CG2	7.33	1.76	1.52
1	A	942	PHE	CD2-CE2	-7.32	1.24	1.39
7	I	18	GLU	CD-OE2	7.32	1.33	1.25
2	B	124	TYR	CE2-CZ	-7.32	1.29	1.38
6	H	139	ASN	CA-CB	7.32	1.72	1.53
2	B	308	TRP	CE2-CZ2	-7.32	1.27	1.39
2	B	1073	TYR	CB-CG	7.31	1.62	1.51
4	E	172	GLU	CD-OE2	7.31	1.33	1.25
1	A	211	PHE	CB-CG	7.31	1.63	1.51
2	B	299	GLU	CD-OE1	7.31	1.33	1.25
9	K	16	GLU	CD-OE2	7.31	1.33	1.25
2	B	250	PHE	CD2-CE2	7.30	1.53	1.39
2	B	337	ARG	CZ-NH1	-7.30	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1102	LYS	CG-CD	7.30	1.77	1.52
1	A	738	LYS	C-O	-7.30	1.09	1.23
2	B	1224	PHE	CD1-CE1	7.30	1.53	1.39
7	I	70	ARG	CZ-NH2	-7.30	1.23	1.33
1	A	806	ARG	CZ-NH2	7.30	1.42	1.33
1	A	1155	ASP	CB-CG	-7.30	1.36	1.51
9	K	92	ASN	N-CA	7.30	1.60	1.46
9	K	6	ARG	CB-CG	-7.29	1.32	1.52
2	B	865	LYS	CA-CB	7.29	1.70	1.53
2	B	899	ILE	CA-CB	-7.29	1.38	1.54
6	H	131	ASN	CA-CB	7.29	1.72	1.53
1	A	836	TYR	CA-C	7.29	1.71	1.52
2	B	337	ARG	NE-CZ	-7.29	1.23	1.33
1	A	944	ARG	CZ-NH2	-7.28	1.23	1.33
2	B	388	CYS	CB-SG	-7.28	1.69	1.82
2	B	738	PHE	N-CA	-7.28	1.31	1.46
2	B	974	PRO	C-O	-7.28	1.08	1.23
2	B	1033	LYS	CB-CG	-7.27	1.32	1.52
1	A	915	SER	CA-CB	7.27	1.63	1.52
1	A	939	ASP	CB-CG	7.27	1.67	1.51
3	C	56	THR	CB-CG2	-7.27	1.28	1.52
5	F	122	MET	SD-CE	-7.26	1.37	1.77
7	I	101	PHE	CD1-CE1	7.26	1.53	1.39
2	B	1192	TYR	CD2-CE2	7.26	1.50	1.39
1	A	709	THR	CB-CG2	-7.26	1.28	1.52
1	A	1345	ARG	NE-CZ	-7.25	1.23	1.33
2	B	826	ALA	C-O	-7.25	1.09	1.23
2	B	1097	HIS	CD2-NE2	7.25	1.57	1.42
4	E	28	TYR	CB-CG	7.25	1.62	1.51
4	E	103	LYS	CE-NZ	7.25	1.67	1.49
2	B	19	GLU	N-CA	7.24	1.60	1.46
5	F	142	SER	CB-OG	-7.24	1.32	1.42
2	B	124	TYR	CE1-CZ	-7.24	1.29	1.38
2	B	1069	PHE	CE1-CZ	-7.24	1.23	1.37
2	B	38	PHE	CE1-CZ	-7.24	1.23	1.37
2	B	1100	ASP	CB-CG	7.24	1.67	1.51
3	C	7	GLN	CB-CG	7.23	1.72	1.52
1	A	446	ARG	NE-CZ	-7.23	1.23	1.33
1	A	815	PHE	CE2-CZ	-7.23	1.23	1.37
2	B	957	ASN	CA-C	7.23	1.71	1.52
8	J	7	CYS	CA-CB	7.22	1.69	1.53
2	B	271	ALA	C-O	-7.22	1.09	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	392	VAL	CA-CB	-7.22	1.39	1.54
1	A	967	ALA	CA-CB	-7.22	1.37	1.52
7	I	91	ARG	CA-C	-7.22	1.34	1.52
2	B	542	MET	CA-CB	7.21	1.69	1.53
7	I	6	PHE	CD2-CE2	7.21	1.53	1.39
10	L	63	ARG	CD-NE	7.21	1.58	1.46
1	A	1151	GLU	CG-CD	7.20	1.62	1.51
2	B	183	GLU	CB-CG	7.20	1.65	1.52
5	F	146	TRP	CG-CD1	-7.20	1.26	1.36
1	A	1064	VAL	C-N	-7.20	1.20	1.33
3	C	68	GLY	N-CA	7.20	1.56	1.46
2	B	1189	ILE	CG1-CD1	7.20	2.00	1.50
7	I	93	LYS	CG-CD	7.20	1.76	1.52
2	B	259	TYR	C-O	-7.20	1.09	1.23
1	A	184	SER	CB-OG	-7.19	1.32	1.42
3	C	201	TRP	CZ3-CH2	-7.19	1.28	1.40
1	A	1236	LEU	CG-CD2	7.19	1.78	1.51
1	A	804	TYR	CE2-CZ	7.19	1.47	1.38
2	B	1091	TYR	CG-CD2	-7.19	1.29	1.39
1	A	393	ARG	CG-CD	7.18	1.70	1.51
1	A	870	GLU	CD-OE2	7.18	1.33	1.25
1	A	1359	ASP	N-CA	7.18	1.60	1.46
7	I	118	ARG	NE-CZ	7.18	1.42	1.33
4	E	99	HIS	N-CA	7.18	1.60	1.46
6	H	20	TYR	CE1-CZ	-7.18	1.29	1.38
3	C	181	ASP	C-O	-7.18	1.09	1.23
1	A	787	PHE	N-CA	-7.17	1.32	1.46
2	B	1192	TYR	CD1-CE1	7.17	1.50	1.39
4	E	72	PHE	CD1-CE1	-7.17	1.25	1.39
1	A	1118	VAL	CB-CG2	-7.17	1.37	1.52
1	A	130	ASP	CB-CG	7.17	1.66	1.51
1	A	135	PHE	CD2-CE2	-7.17	1.25	1.39
8	J	58	GLU	CG-CD	7.17	1.62	1.51
1	A	459	ARG	CG-CD	7.16	1.69	1.51
1	A	980	ASP	C-O	7.16	1.36	1.23
1	A	1338	VAL	CB-CG2	-7.16	1.37	1.52
1	A	1225	PHE	CE2-CZ	7.16	1.50	1.37
6	H	90	ALA	CA-CB	-7.15	1.37	1.52
1	A	1225	PHE	CD2-CE2	7.15	1.53	1.39
1	A	1318	THR	C-O	-7.15	1.09	1.23
1	A	44	THR	N-CA	7.15	1.60	1.46
1	A	482	PHE	CG-CD2	-7.15	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	180	ARG	CG-CD	7.15	1.69	1.51
1	A	237	THR	CB-CG2	7.15	1.75	1.52
1	A	469	ARG	CG-CD	7.15	1.69	1.51
3	C	207	CYS	CA-C	7.15	1.71	1.52
1	A	571	LEU	CG-CD2	7.14	1.78	1.51
1	A	661	GLY	CA-C	7.13	1.63	1.51
2	B	949	VAL	CA-CB	-7.13	1.39	1.54
8	J	27	GLU	CD-OE1	7.13	1.33	1.25
2	B	646	LEU	CB-CG	7.12	1.73	1.52
6	H	79	TRP	CA-CB	-7.12	1.38	1.53
8	J	8	PHE	CD2-CE2	7.12	1.53	1.39
2	B	612	GLU	CD-OE2	-7.12	1.17	1.25
1	A	1027	ALA	C-O	7.11	1.36	1.23
2	B	1127	GLY	CA-C	7.11	1.63	1.51
9	K	74	ARG	NE-CZ	-7.11	1.23	1.33
10	L	70	ARG	NE-CZ	7.11	1.42	1.33
3	C	34	ARG	CG-CD	7.11	1.69	1.51
2	B	882	THR	CB-CG2	7.11	1.75	1.52
1	A	171	GLN	CD-OE1	7.10	1.39	1.24
1	A	699	ALA	C-O	-7.10	1.09	1.23
1	A	767	GLN	CD-OE1	-7.10	1.08	1.24
9	K	88	LYS	CG-CD	7.10	1.76	1.52
1	A	593	GLU	CB-CG	7.10	1.65	1.52
1	A	957	PRO	CA-CB	-7.09	1.39	1.53
2	B	766	ARG	CZ-NH1	7.09	1.42	1.33
2	B	769	TYR	CD2-CE2	-7.09	1.28	1.39
1	A	1057	VAL	CB-CG1	-7.09	1.38	1.52
2	B	706	GLN	CD-NE2	7.09	1.50	1.32
2	B	35	SER	CA-CB	-7.09	1.42	1.52
2	B	1097	HIS	CB-CG	-7.09	1.37	1.50
1	A	1057	VAL	CB-CG2	-7.08	1.38	1.52
2	B	124	TYR	CA-CB	-7.08	1.38	1.53
2	B	791	THR	N-CA	-7.08	1.32	1.46
2	B	945	GLU	C-O	7.08	1.36	1.23
7	I	45	ARG	CD-NE	7.08	1.58	1.46
3	C	163	ILE	CB-CG2	7.08	1.74	1.52
4	E	31	THR	CA-CB	7.07	1.71	1.53
1	A	1212	VAL	CA-CB	-7.07	1.40	1.54
2	B	1168	LEU	CA-C	-7.07	1.34	1.52
2	B	1096	ARG	C-O	-7.06	1.09	1.23
7	I	28	GLU	CG-CD	7.06	1.62	1.51
2	B	567	GLU	CG-CD	7.06	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	3	THR	CA-C	-7.06	1.34	1.52
1	A	969	GLN	CD-OE1	7.06	1.39	1.24
2	B	305	VAL	CB-CG2	7.06	1.67	1.52
1	A	1209	MET	N-CA	-7.05	1.32	1.46
2	B	459	TYR	CG-CD1	7.05	1.48	1.39
9	K	55	LYS	CD-CE	7.05	1.68	1.51
2	B	510	LYS	CB-CG	-7.05	1.33	1.52
1	A	1202	MET	SD-CE	7.05	2.17	1.77
2	B	935	ARG	NE-CZ	7.05	1.42	1.33
2	B	173	MET	C-O	-7.04	1.09	1.23
1	A	1025	ARG	NE-CZ	-7.04	1.23	1.33
2	B	203	PHE	CE1-CZ	-7.04	1.24	1.37
4	E	66	GLU	CA-CB	7.04	1.69	1.53
2	B	215	GLN	N-CA	-7.04	1.32	1.46
2	B	733	HIS	CA-C	7.04	1.71	1.52
1	A	146	MET	CG-SD	7.04	1.99	1.81
1	A	1003	LYS	CG-CD	7.04	1.76	1.52
1	A	1281	ARG	CG-CD	7.04	1.69	1.51
1	A	1355	VAL	C-O	-7.04	1.09	1.23
2	B	626	ILE	C-O	-7.04	1.09	1.23
2	B	1106	ARG	NE-CZ	7.04	1.42	1.33
3	C	193	TYR	CB-CG	7.04	1.62	1.51
1	A	684	ALA	CA-CB	7.04	1.67	1.52
6	H	13	SER	CB-OG	7.03	1.51	1.42
1	A	416	ARG	CZ-NH2	-7.03	1.24	1.33
1	A	973	ILE	CB-CG2	7.03	1.74	1.52
1	A	1350	LYS	CG-CD	7.03	1.76	1.52
2	B	937	ALA	CA-CB	7.03	1.67	1.52
8	J	3	VAL	CB-CG1	-7.03	1.38	1.52
1	A	1349	TYR	CD2-CE2	7.03	1.49	1.39
2	B	694	ASP	CG-OD2	7.02	1.41	1.25
2	B	722	ASP	CB-CG	7.02	1.66	1.51
2	B	1070	GLU	C-O	-7.02	1.10	1.23
2	B	1085	ILE	CB-CG2	-7.02	1.31	1.52
2	B	1101	ASP	CA-C	7.02	1.71	1.52
1	A	1445	ILE	CB-CG2	7.02	1.74	1.52
3	C	134	ILE	CA-CB	-7.02	1.38	1.54
1	A	808	LEU	N-CA	-7.02	1.32	1.46
1	A	1064	VAL	CB-CG1	-7.02	1.38	1.52
2	B	1020	ARG	CZ-NH1	7.02	1.42	1.33
1	A	982	THR	CB-OG1	-7.01	1.29	1.43
1	A	977	LYS	CB-CG	7.01	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	784	ASN	N-CA	-7.01	1.32	1.46
1	A	1298	TYR	CD1-CE1	7.01	1.49	1.39
2	B	1075	GLY	C-O	7.01	1.34	1.23
1	A	895	LYS	N-CA	7.01	1.60	1.46
1	A	974	ASP	N-CA	7.01	1.60	1.46
1	A	1211	GLN	CB-CG	7.01	1.71	1.52
1	A	1294	PRO	CB-CG	7.01	1.84	1.50
2	B	425	THR	CB-CG2	7.01	1.75	1.52
3	C	47	ASP	C-O	-7.00	1.10	1.23
1	A	427	GLN	CG-CD	7.00	1.67	1.51
3	C	9	LYS	CG-CD	7.00	1.76	1.52
3	C	241	ASP	CA-CB	7.00	1.69	1.53
2	B	1102	LYS	CA-CB	7.00	1.69	1.53
2	B	384	ARG	CG-CD	6.99	1.69	1.51
1	A	1042	PHE	CG-CD2	-6.99	1.28	1.38
9	K	54	ARG	CD-NE	6.99	1.58	1.46
1	A	383	TYR	CE1-CZ	6.99	1.47	1.38
2	B	380	TYR	CE2-CZ	-6.99	1.29	1.38
2	B	57	TYR	CB-CG	6.99	1.62	1.51
2	B	965	LYS	CD-CE	6.98	1.68	1.51
8	J	44	TYR	CG-CD2	-6.98	1.30	1.39
1	A	1308	THR	CB-CG2	-6.98	1.29	1.52
7	I	60	GLN	CG-CD	6.98	1.67	1.51
1	A	125	ALA	CA-CB	-6.98	1.37	1.52
1	A	1362	TYR	CD1-CE1	6.98	1.49	1.39
2	B	1134	GLU	CD-OE1	6.98	1.33	1.25
3	C	146	LYS	CB-CG	6.98	1.71	1.52
1	A	1103	GLU	C-O	6.98	1.36	1.23
1	A	1426	GLU	CD-OE2	6.98	1.33	1.25
1	A	1383	SER	CA-CB	-6.97	1.42	1.52
2	B	127	GLY	C-O	-6.97	1.12	1.23
3	C	18	VAL	CB-CG2	-6.97	1.38	1.52
4	E	154	ILE	CB-CG2	-6.97	1.31	1.52
8	J	31	ASP	C-O	6.97	1.36	1.23
2	B	579	ARG	NE-CZ	-6.97	1.24	1.33
1	A	1333	ILE	CB-CG2	-6.97	1.31	1.52
8	J	48	ARG	CZ-NH1	-6.96	1.24	1.33
2	B	1063	GLY	CA-C	-6.96	1.40	1.51
2	B	1210	MET	CG-SD	-6.96	1.63	1.81
10	L	43	THR	CB-CG2	6.96	1.75	1.52
4	E	131	THR	CA-CB	6.96	1.71	1.53
2	B	459	TYR	CE1-CZ	6.96	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	95	GLY	C-O	-6.96	1.12	1.23
2	B	625	LYS	CD-CE	6.95	1.68	1.51
2	B	916	THR	CA-C	6.95	1.71	1.52
7	I	47	GLU	CD-OE2	6.95	1.33	1.25
9	K	25	THR	CB-CG2	6.95	1.75	1.52
2	B	961	LEU	CG-CD1	6.95	1.77	1.51
7	I	83	ASN	CG-OD1	6.94	1.39	1.24
9	K	58	PHE	CB-CG	6.94	1.63	1.51
6	H	50	ALA	N-CA	6.94	1.60	1.46
6	H	136	LYS	N-CA	6.94	1.60	1.46
1	A	1289	ARG	NE-CZ	-6.93	1.24	1.33
6	H	48	PRO	C-O	6.93	1.37	1.23
2	B	136	THR	C-O	6.93	1.36	1.23
2	B	649	LYS	CB-CG	-6.93	1.33	1.52
1	A	578	LEU	N-CA	6.92	1.60	1.46
2	B	828	ALA	C-O	-6.92	1.10	1.23
2	B	226	PHE	CE2-CZ	6.92	1.50	1.37
1	A	1350	LYS	CE-NZ	6.92	1.66	1.49
1	A	1299	VAL	CB-CG1	-6.92	1.38	1.52
1	A	188	ASP	N-CA	6.91	1.60	1.46
1	A	843	LYS	CG-CD	6.91	1.75	1.52
2	B	380	TYR	CG-CD2	-6.91	1.30	1.39
2	B	1132	GLU	CB-CG	6.91	1.65	1.52
2	B	612	GLU	CB-CG	-6.91	1.39	1.52
2	B	1186	ASP	CA-CB	6.91	1.69	1.53
5	F	114	GLU	CD-OE1	6.91	1.33	1.25
1	A	369	SER	CA-CB	-6.91	1.42	1.52
1	A	898	ARG	NE-CZ	6.91	1.42	1.33
1	A	1287	TYR	CG-CD1	6.91	1.48	1.39
1	A	626	ASN	CG-ND2	6.90	1.50	1.32
1	A	941	LYS	CG-CD	6.90	1.75	1.52
2	B	788	ARG	CD-NE	-6.90	1.34	1.46
1	A	750	GLY	CA-C	-6.90	1.40	1.51
1	A	901	LEU	C-O	6.90	1.36	1.23
4	E	61	GLN	CB-CG	6.90	1.71	1.52
1	A	383	TYR	CD2-CE2	6.90	1.49	1.39
1	A	852	TYR	CG-CD1	-6.90	1.30	1.39
2	B	811	TYR	CG-CD1	-6.90	1.30	1.39
2	B	1140	ALA	C-O	6.90	1.36	1.23
2	B	176	SER	CA-CB	6.90	1.63	1.52
1	A	1308	THR	N-CA	-6.89	1.32	1.46
2	B	1158	PHE	CE1-CZ	6.89	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	806	ARG	CB-CG	6.89	1.71	1.52
2	B	605	ARG	CZ-NH1	-6.89	1.24	1.33
9	K	81	TYR	CE1-CZ	-6.89	1.29	1.38
10	L	27	LEU	CB-CG	6.89	1.72	1.52
1	A	866	PHE	CE2-CZ	-6.89	1.24	1.37
3	C	236	GLY	N-CA	-6.89	1.35	1.46
1	A	117	GLU	CD-OE2	6.88	1.33	1.25
4	E	195	VAL	CA-CB	-6.88	1.40	1.54
1	A	1225	PHE	CG-CD1	6.88	1.49	1.38
2	B	451	LYS	CD-CE	6.88	1.68	1.51
2	B	114	PRO	CG-CD	-6.88	1.27	1.50
6	H	111	LEU	CA-C	6.88	1.70	1.52
2	B	137	TYR	CG-CD2	6.88	1.48	1.39
2	B	523	CYS	CA-C	-6.87	1.35	1.52
1	A	1358	SER	CB-OG	6.87	1.51	1.42
2	B	228	LYS	CB-CG	6.86	1.71	1.52
1	A	469	ARG	CB-CG	6.86	1.71	1.52
3	C	78	GLU	CG-CD	6.86	1.62	1.51
1	A	1362	TYR	CE2-CZ	6.86	1.47	1.38
2	B	39	ARG	C-O	-6.86	1.10	1.23
4	E	162	ARG	CA-CB	6.86	1.69	1.53
3	C	254	LYS	CD-CE	-6.85	1.34	1.51
2	B	1091	TYR	CE2-CZ	-6.85	1.29	1.38
3	C	20	PHE	CD1-CE1	6.85	1.52	1.39
1	A	191	THR	CA-C	6.84	1.70	1.52
1	A	1291	VAL	CA-CB	-6.84	1.40	1.54
2	B	593	PRO	CB-CG	6.84	1.84	1.50
4	E	7	ARG	CD-NE	6.84	1.58	1.46
2	B	365	THR	C-O	6.84	1.36	1.23
2	B	844	SER	CB-OG	-6.84	1.33	1.42
2	B	306	ASN	CB-CG	6.83	1.66	1.51
2	B	364	ILE	CA-CB	-6.83	1.39	1.54
4	E	204	THR	CB-CG2	-6.83	1.29	1.52
1	A	1191	TRP	CB-CG	-6.83	1.38	1.50
2	B	357	GLN	C-O	-6.83	1.10	1.23
2	B	1087	PHE	CG-CD1	-6.83	1.28	1.38
1	A	364	VAL	CB-CG1	-6.82	1.38	1.52
2	B	975	GLN	C-O	-6.82	1.10	1.23
2	B	986	GLN	CB-CG	6.82	1.71	1.52
1	A	8	SER	CA-CB	6.82	1.63	1.52
1	A	662	PHE	CE1-CZ	-6.82	1.24	1.37
2	B	825	VAL	CA-CB	-6.82	1.40	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1185	CYS	CA-CB	6.81	1.69	1.53
1	A	1020	CYS	C-O	6.81	1.36	1.23
1	A	268	ASP	CB-CG	6.81	1.66	1.51
2	B	983	ARG	CZ-NH1	-6.81	1.24	1.33
1	A	123	ARG	CZ-NH2	6.81	1.42	1.33
1	A	1420	ASP	CG-OD2	6.81	1.41	1.25
1	A	1217	LYS	C-O	6.81	1.36	1.23
2	B	709	ASP	CA-C	-6.81	1.35	1.52
1	A	350	ARG	CG-CD	-6.80	1.34	1.51
2	B	1224	PHE	CB-CG	6.80	1.62	1.51
7	I	6	PHE	CB-CG	-6.80	1.39	1.51
2	B	1137	CYS	C-O	-6.80	1.10	1.23
1	A	1282	VAL	CA-CB	-6.79	1.40	1.54
1	A	1030	ARG	CB-CG	-6.79	1.34	1.52
1	A	1188	GLN	C-O	6.79	1.36	1.23
2	B	406	LEU	CG-CD2	-6.79	1.26	1.51
4	E	47	CYS	CA-C	6.79	1.70	1.52
10	L	41	SER	N-CA	6.79	1.59	1.46
2	B	250	PHE	CD1-CE1	6.79	1.52	1.39
1	A	1228	TRP	CD2-CE2	-6.79	1.33	1.41
7	I	30	ARG	CA-CB	-6.79	1.39	1.53
2	B	1154	ALA	CA-C	6.79	1.70	1.52
2	B	18	PHE	CG-CD1	6.78	1.49	1.38
2	B	619	ILE	CA-CB	-6.78	1.39	1.54
3	C	26	ASP	C-O	6.78	1.36	1.23
6	H	129	TYR	CG-CD1	6.78	1.48	1.39
1	A	1092	LYS	CB-CG	6.78	1.70	1.52
4	E	149	LEU	CG-CD1	-6.78	1.26	1.51
1	A	1287	TYR	C-O	6.78	1.36	1.23
1	A	378	GLU	CG-CD	-6.78	1.41	1.51
2	B	895	ASP	CA-CB	6.77	1.68	1.53
4	E	190	LEU	C-O	6.77	1.36	1.23
7	I	42	LEU	C-O	-6.77	1.10	1.23
1	A	677	ARG	CD-NE	6.77	1.57	1.46
2	B	742	GLU	CD-OE1	-6.77	1.18	1.25
2	B	351	TYR	CG-CD2	-6.76	1.30	1.39
2	B	368	GLU	CA-CB	6.76	1.68	1.53
2	B	1204	PHE	CE2-CZ	-6.76	1.24	1.37
2	B	816	GLU	CD-OE1	6.76	1.33	1.25
3	C	198	ALA	CA-CB	-6.76	1.38	1.52
7	I	44	TYR	N-CA	6.75	1.59	1.46
1	A	450	LEU	N-CA	-6.75	1.32	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	204	ILE	CA-CB	-6.75	1.39	1.54
1	A	1426	GLU	CG-CD	6.75	1.62	1.51
9	K	8	GLU	C-O	6.75	1.36	1.23
1	A	933	TYR	CG-CD2	-6.75	1.30	1.39
2	B	348	ARG	CZ-NH1	-6.75	1.24	1.33
2	B	1149	GLU	C-O	-6.75	1.10	1.23
8	J	33	GLY	N-CA	6.75	1.56	1.46
1	A	53	LEU	N-CA	6.74	1.59	1.46
3	C	201	TRP	CE3-CZ3	-6.74	1.26	1.38
6	H	132	LEU	CA-CB	6.74	1.69	1.53
1	A	434	ARG	C-O	-6.74	1.10	1.23
3	C	5	GLY	CA-C	6.74	1.62	1.51
1	A	412	ARG	NE-CZ	-6.74	1.24	1.33
2	B	41	LYS	CE-NZ	6.73	1.65	1.49
1	A	879	GLU	CG-CD	6.73	1.62	1.51
5	F	100	GLN	CD-OE1	6.73	1.38	1.24
1	A	449	SER	C-O	-6.73	1.10	1.23
4	E	71	LYS	CG-CD	6.73	1.75	1.52
1	A	992	ASP	CB-CG	6.73	1.65	1.51
1	A	772	GLY	C-O	-6.72	1.12	1.23
1	A	1211	GLN	CG-CD	6.72	1.66	1.51
3	C	138	GLU	CD-OE1	6.72	1.33	1.25
1	A	896	ARG	N-CA	-6.72	1.32	1.46
9	K	81	TYR	C-O	-6.72	1.10	1.23
1	A	26	GLU	CG-CD	6.71	1.62	1.51
1	A	24	PRO	CA-C	6.71	1.66	1.52
1	A	177	ASP	CG-OD2	6.71	1.40	1.25
1	A	502	SER	CB-OG	6.71	1.50	1.42
1	A	1218	GLN	CD-OE1	6.71	1.38	1.24
2	B	1181	GLU	CD-OE2	-6.71	1.18	1.25
4	E	42	PHE	C-O	6.71	1.36	1.23
2	B	1132	GLU	CD-OE1	6.70	1.33	1.25
7	I	4	PHE	CE2-CZ	6.70	1.50	1.37
1	A	476	SER	C-O	-6.70	1.10	1.23
2	B	191	LYS	CB-CG	6.70	1.70	1.52
3	C	139	GLY	CA-C	6.70	1.62	1.51
2	B	434	ARG	NE-CZ	6.70	1.41	1.33
2	B	595	ARG	NE-CZ	6.70	1.41	1.33
2	B	843	GLN	CG-CD	-6.70	1.35	1.51
7	I	4	PHE	CG-CD2	6.70	1.48	1.38
1	A	940	ARG	CZ-NH2	-6.69	1.24	1.33
1	A	1080	THR	N-CA	6.69	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1118	VAL	N-CA	-6.69	1.32	1.46
1	A	1126	ALA	CA-CB	-6.69	1.38	1.52
1	A	641	VAL	C-O	-6.69	1.10	1.23
1	A	1153	TYR	CG-CD1	-6.69	1.30	1.39
1	A	1118	VAL	C-O	-6.69	1.10	1.23
4	E	56	LYS	N-CA	-6.69	1.32	1.46
1	A	795	GLU	CD-OE1	6.69	1.33	1.25
2	B	18	PHE	CE1-CZ	6.68	1.50	1.37
2	B	116	GLU	CG-CD	6.68	1.61	1.51
4	E	28	TYR	CG-CD1	-6.68	1.30	1.39
4	E	40	GLU	CB-CG	6.68	1.64	1.52
6	H	85	GLY	CA-C	6.68	1.62	1.51
2	B	1149	GLU	CD-OE1	6.68	1.32	1.25
2	B	980	PHE	CG-CD1	-6.68	1.28	1.38
1	A	962	ARG	C-O	-6.67	1.10	1.23
2	B	257	LYS	N-CA	-6.67	1.33	1.46
2	B	99	LYS	CD-CE	6.67	1.68	1.51
1	A	672	ASP	CB-CG	-6.67	1.37	1.51
1	A	918	GLU	CD-OE1	-6.67	1.18	1.25
2	B	165	VAL	CA-CB	6.66	1.68	1.54
2	B	303	TYR	CE1-CZ	-6.66	1.29	1.38
2	B	874	PHE	CD1-CE1	-6.66	1.25	1.39
3	C	218	PRO	CG-CD	6.66	1.72	1.50
9	K	58	PHE	CD2-CE2	-6.66	1.25	1.39
1	A	462	VAL	CA-CB	-6.66	1.40	1.54
3	C	199	LYS	CG-CD	6.66	1.75	1.52
1	A	1243	VAL	CB-CG2	6.66	1.66	1.52
1	A	177	ASP	CB-CG	6.66	1.65	1.51
1	A	1349	TYR	CB-CG	-6.65	1.41	1.51
1	A	947	PHE	CE1-CZ	-6.65	1.24	1.37
3	C	35	ARG	CB-CG	6.65	1.70	1.52
3	C	186	LEU	CA-C	6.65	1.70	1.52
1	A	468	PHE	CG-CD1	-6.65	1.28	1.38
1	A	498	ARG	CZ-NH2	-6.65	1.24	1.33
2	B	893	LEU	CG-CD2	-6.65	1.27	1.51
7	I	103	CYS	CB-SG	6.65	1.93	1.82
2	B	129	PHE	CD1-CE1	-6.65	1.25	1.39
1	A	770	VAL	CB-CG1	-6.65	1.38	1.52
2	B	866	TYR	N-CA	6.65	1.59	1.46
1	A	1349	TYR	CE1-CZ	-6.65	1.29	1.38
2	B	249	ARG	CG-CD	6.65	1.68	1.51
2	B	40	GLU	CD-OE1	6.64	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	231	PRO	CB-CG	6.64	1.83	1.50
2	B	393	LYS	CD-CE	6.64	1.67	1.51
1	A	1228	TRP	CB-CG	6.64	1.62	1.50
2	B	800	GLN	CG-CD	6.64	1.66	1.51
2	B	916	THR	CB-CG2	6.64	1.74	1.52
2	B	1101	ASP	CA-CB	6.64	1.68	1.53
1	A	744	LYS	CD-CE	6.63	1.67	1.51
2	B	63	ILE	CA-C	6.63	1.70	1.52
4	E	108	GLY	C-O	-6.63	1.13	1.23
1	A	74	MET	CG-SD	6.63	1.98	1.81
2	B	883	LEU	CB-CG	6.63	1.71	1.52
2	B	987	LYS	CA-CB	-6.63	1.39	1.53
2	B	1082	MET	CA-C	-6.63	1.35	1.52
2	B	705	MET	CG-SD	6.62	1.98	1.81
1	A	205	GLU	CB-CG	6.62	1.64	1.52
1	A	496	GLU	CD-OE2	6.62	1.32	1.25
2	B	1087	PHE	CD1-CE1	-6.62	1.26	1.39
7	I	83	ASN	C-O	6.62	1.35	1.23
1	A	32	VAL	C-O	6.62	1.35	1.23
1	A	795	GLU	C-O	-6.61	1.10	1.23
2	B	481	GLN	C-O	6.61	1.35	1.23
1	A	301	ALA	C-O	-6.61	1.10	1.23
1	A	483	ASP	CG-OD1	6.61	1.40	1.25
1	A	1154	TYR	CG-CD2	-6.61	1.30	1.39
2	B	1103	ILE	N-CA	6.61	1.59	1.46
7	I	63	GLY	C-O	-6.61	1.13	1.23
10	L	59	ALA	N-CA	6.61	1.59	1.46
2	B	1083	ALA	N-CA	6.61	1.59	1.46
3	C	57	VAL	CA-CB	-6.61	1.40	1.54
2	B	307	ASP	CB-CG	-6.61	1.37	1.51
3	C	82	TYR	CZ-OH	6.61	1.49	1.37
1	A	61	ILE	CB-CG2	6.61	1.73	1.52
2	B	787	VAL	N-CA	-6.61	1.33	1.46
1	A	417	TYR	CG-CD2	6.60	1.47	1.39
1	A	1062	GLU	CD-OE2	6.60	1.32	1.25
2	B	466	TRP	CA-C	6.60	1.70	1.52
4	E	203	GLU	CD-OE1	-6.60	1.18	1.25
2	B	224	GLN	N-CA	-6.60	1.33	1.46
2	B	519	TRP	CB-CG	6.59	1.62	1.50
2	B	557	PHE	N-CA	-6.59	1.33	1.46
2	B	223	VAL	C-O	-6.59	1.10	1.23
3	C	148	ARG	N-CA	-6.59	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	703	THR	CB-CG2	6.58	1.74	1.52
2	B	106	ASP	CA-C	6.58	1.70	1.52
1	A	143	LYS	CE-NZ	6.58	1.65	1.49
1	A	1262	LYS	CB-CG	6.58	1.70	1.52
2	B	972	LYS	C-O	-6.58	1.10	1.23
3	C	61	GLU	N-CA	6.58	1.59	1.46
1	A	580	VAL	CB-CG2	-6.58	1.39	1.52
2	B	113	TYR	CD1-CE1	-6.58	1.29	1.39
6	H	43	ASN	CB-CG	6.57	1.66	1.51
1	A	966	ASN	N-CA	-6.57	1.33	1.46
1	A	129	LYS	CB-CG	6.57	1.70	1.52
1	A	580	VAL	CA-CB	-6.57	1.41	1.54
1	A	25	GLU	CD-OE2	6.57	1.32	1.25
1	A	303	TYR	CD1-CE1	-6.57	1.29	1.39
1	A	873	MET	C-O	-6.57	1.10	1.23
1	A	960	ILE	CB-CG2	-6.57	1.32	1.52
9	K	9	LEU	C-O	6.57	1.35	1.23
1	A	463	ILE	CB-CG2	-6.56	1.32	1.52
1	A	1195	LEU	C-N	-6.56	1.19	1.34
2	B	643	ASP	CA-CB	6.56	1.68	1.53
6	H	56	THR	CA-CB	6.56	1.70	1.53
9	K	20	LYS	CD-CE	6.56	1.67	1.51
2	B	1190	ASP	C-O	-6.56	1.10	1.23
6	H	6	PHE	CA-C	-6.56	1.35	1.52
1	A	810	PRO	CG-CD	6.56	1.72	1.50
2	B	1178	ASN	CB-CG	-6.56	1.35	1.51
9	K	36	GLU	CA-CB	-6.56	1.39	1.53
1	A	193	ASP	N-CA	6.56	1.59	1.46
1	A	440	ASP	CB-CG	-6.56	1.38	1.51
3	C	158	VAL	C-O	-6.56	1.10	1.23
2	B	197	PHE	CG-CD2	6.56	1.48	1.38
1	A	479	ASN	C-O	-6.55	1.10	1.23
10	L	44	ASP	C-O	6.55	1.35	1.23
1	A	182	VAL	CB-CG1	6.55	1.66	1.52
2	B	618	ASP	CB-CG	-6.55	1.38	1.51
2	B	1097	HIS	ND1-CE1	6.54	1.51	1.34
5	F	108	PHE	CG-CD1	6.54	1.48	1.38
1	A	1292	PRO	C-O	6.54	1.36	1.23
3	C	177	GLU	CG-CD	6.54	1.61	1.51
4	E	207	ARG	CG-CD	6.54	1.68	1.51
1	A	1119	TYR	C-O	6.53	1.35	1.23
2	B	105	SER	CA-CB	6.53	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1078	GLN	CG-CD	6.53	1.66	1.51
1	A	1116	LEU	C-O	-6.53	1.10	1.23
2	B	1189	ILE	CB-CG2	6.52	1.73	1.52
1	A	1335	ILE	CB-CG2	-6.52	1.32	1.52
1	A	1434	ALA	CA-CB	-6.52	1.38	1.52
6	H	116	TYR	N-CA	6.52	1.59	1.46
1	A	1030	ARG	CZ-NH2	-6.52	1.24	1.33
2	B	245	GLU	CA-C	6.52	1.69	1.52
8	J	63	TYR	CB-CG	6.51	1.61	1.51
2	B	1181	GLU	N-CA	6.51	1.59	1.46
2	B	807	ARG	CG-CD	6.51	1.68	1.51
2	B	935	ARG	CG-CD	6.51	1.68	1.51
5	F	90	ARG	NE-CZ	-6.51	1.24	1.33
2	B	353	LYS	CG-CD	6.51	1.74	1.52
6	H	115	TYR	CG-CD2	-6.51	1.30	1.39
1	A	286	HIS	CB-CG	6.51	1.61	1.50
2	B	792	MET	CA-CB	-6.51	1.39	1.53
5	F	97	ARG	CB-CG	-6.51	1.34	1.52
1	A	539	THR	CB-CG2	-6.50	1.30	1.52
4	E	67	GLU	CB-CG	6.50	1.64	1.52
1	A	840	ARG	NE-CZ	6.50	1.41	1.33
1	A	1450	LEU	N-CA	6.50	1.59	1.46
1	A	465	TYR	CG-CD1	-6.50	1.30	1.39
1	A	962	ARG	NE-CZ	-6.50	1.24	1.33
2	B	581	PHE	CG-CD1	-6.50	1.29	1.38
7	I	101	PHE	CB-CG	-6.50	1.40	1.51
1	A	731	ARG	C-O	-6.49	1.11	1.23
2	B	349	ILE	CB-CG2	-6.49	1.32	1.52
4	E	195	VAL	CB-CG1	-6.49	1.39	1.52
2	B	604	ARG	NE-CZ	-6.49	1.24	1.33
2	B	1215	ARG	CG-CD	6.49	1.68	1.51
1	A	913	LEU	CA-CB	6.49	1.68	1.53
2	B	174	LEU	CA-C	-6.49	1.36	1.52
2	B	785	TYR	CG-CD2	-6.49	1.30	1.39
2	B	618	ASP	CG-OD1	6.49	1.40	1.25
2	B	742	GLU	N-CA	-6.49	1.33	1.46
8	J	2	ILE	C-O	-6.49	1.11	1.23
1	A	950	GLY	C-O	-6.48	1.13	1.23
2	B	581	PHE	C-O	6.48	1.35	1.23
2	B	561	TRP	CE3-CZ3	6.48	1.49	1.38
1	A	1272	THR	CB-CG2	6.47	1.73	1.52
2	B	370	PHE	N-CA	6.47	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	11	GLN	CB-CG	6.47	1.70	1.52
10	L	26	THR	N-CA	6.47	1.59	1.46
1	A	1282	VAL	CB-CG1	6.47	1.66	1.52
2	B	798	TYR	CD1-CE1	6.47	1.49	1.39
2	B	994	TYR	CD1-CE1	-6.47	1.29	1.39
3	C	143	LEU	C-O	-6.47	1.11	1.23
7	I	29	CYS	CB-SG	6.47	1.93	1.82
2	B	218	SER	C-O	-6.47	1.11	1.23
4	E	103	LYS	N-CA	6.47	1.59	1.46
1	A	563	PRO	CA-C	-6.46	1.40	1.52
2	B	858	SER	CA-CB	-6.46	1.43	1.52
1	A	193	ASP	CA-CB	6.46	1.68	1.53
1	A	350	ARG	CZ-NH2	-6.46	1.24	1.33
1	A	1012	ARG	CG-CD	6.46	1.68	1.51
1	A	833	GLU	CD-OE1	6.45	1.32	1.25
2	B	737	THR	C-O	-6.45	1.11	1.23
1	A	1194	ARG	CD-NE	-6.45	1.35	1.46
3	C	174	ALA	CA-CB	-6.45	1.39	1.52
3	C	180	TYR	CB-CG	-6.45	1.42	1.51
1	A	404	TYR	CG-CD1	-6.45	1.30	1.39
2	B	1094	ARG	NE-CZ	-6.45	1.24	1.33
2	B	1153	GLU	CG-CD	6.45	1.61	1.51
2	B	176	SER	C-O	-6.45	1.11	1.23
7	I	75	CYS	CA-C	-6.45	1.36	1.52
3	C	57	VAL	CB-CG2	-6.44	1.39	1.52
2	B	190	TYR	CE2-CZ	-6.44	1.30	1.38
1	A	326	ARG	CA-C	6.44	1.69	1.52
1	A	1275	GLY	C-O	6.44	1.33	1.23
2	B	39	ARG	CZ-NH1	6.44	1.41	1.33
2	B	809	MET	CG-SD	6.44	1.97	1.81
1	A	484	GLY	C-O	-6.44	1.13	1.23
2	B	981	ALA	CA-CB	-6.44	1.39	1.52
4	E	122	LYS	CA-CB	6.44	1.68	1.53
5	F	123	LYS	CE-NZ	6.44	1.65	1.49
2	B	638	PHE	CE1-CZ	-6.43	1.25	1.37
3	C	210	GLU	CD-OE1	6.43	1.32	1.25
2	B	266	ALA	C-O	6.43	1.35	1.23
3	C	181	ASP	CA-C	-6.43	1.36	1.52
7	I	5	ARG	NE-CZ	6.43	1.41	1.33
1	A	929	LEU	N-CA	-6.43	1.33	1.46
2	B	1071	VAL	C-O	6.43	1.35	1.23
1	A	813	PHE	CD2-CE2	6.42	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	118	ARG	CD-NE	6.42	1.57	1.46
1	A	710	LEU	CG-CD2	6.42	1.75	1.51
1	A	85	ASP	C-O	6.42	1.35	1.23
1	A	396	PRO	CA-C	-6.42	1.40	1.52
1	A	1075	PRO	C-O	-6.42	1.10	1.23
3	C	3	GLU	CG-CD	6.42	1.61	1.51
2	B	51	PHE	CB-CG	-6.42	1.40	1.51
1	A	299	HIS	C-O	-6.41	1.11	1.23
9	K	103	THR	C-O	6.41	1.35	1.23
1	A	174	ILE	C-O	-6.41	1.11	1.23
6	H	102	TYR	CE1-CZ	-6.41	1.30	1.38
1	A	373	THR	CB-CG2	-6.41	1.31	1.52
2	B	1008	PRO	CA-CB	-6.41	1.40	1.53
3	C	252	GLN	CB-CG	6.41	1.69	1.52
1	A	530	GLY	N-CA	-6.41	1.36	1.46
1	A	666	ILE	CA-CB	-6.41	1.40	1.54
1	A	902	LEU	CG-CD2	-6.41	1.28	1.51
2	B	749	LEU	C-O	6.41	1.35	1.23
1	A	639	PRO	CG-CD	-6.40	1.29	1.50
7	I	48	LEU	C-O	-6.40	1.11	1.23
9	K	97	LYS	C-O	-6.40	1.11	1.23
2	B	319	GLU	CD-OE2	6.40	1.32	1.25
7	I	8	ARG	CZ-NH2	6.40	1.41	1.33
7	I	73	ARG	CB-CG	-6.40	1.35	1.52
2	B	237	VAL	CB-CG2	-6.39	1.39	1.52
2	B	1017	ILE	CG1-CD1	-6.39	1.06	1.50
1	A	572	TRP	CE2-CZ2	-6.39	1.28	1.39
1	A	697	ALA	CA-CB	-6.39	1.39	1.52
1	A	1157	ASP	C-O	6.39	1.35	1.23
4	E	17	ARG	NE-CZ	6.39	1.41	1.33
4	E	7	ARG	CG-CD	6.39	1.68	1.51
7	I	14	LEU	C-O	-6.39	1.11	1.23
2	B	60	GLN	CB-CG	-6.39	1.35	1.52
2	B	660	LYS	N-CA	-6.39	1.33	1.46
1	A	745	GLN	CD-OE1	6.38	1.38	1.24
2	B	369	GLY	CA-C	6.38	1.62	1.51
5	F	72	LYS	CG-CD	6.38	1.74	1.52
7	I	61	ASP	C-O	-6.38	1.11	1.23
1	A	523	ILE	N-CA	-6.38	1.33	1.46
6	H	115	TYR	CB-CG	-6.38	1.42	1.51
5	F	137	TYR	CD2-CE2	-6.38	1.29	1.39
1	A	779	PHE	CB-CG	-6.38	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	903	ASN	CB-CG	-6.38	1.36	1.51
1	A	1154	TYR	CD1-CE1	6.38	1.49	1.39
1	A	247	ARG	C-O	6.37	1.35	1.23
1	A	705	LYS	CE-NZ	6.37	1.65	1.49
1	A	806	ARG	CZ-NH1	6.37	1.41	1.33
2	B	242	SER	C-O	-6.37	1.11	1.23
1	A	198	GLU	CG-CD	6.37	1.61	1.51
2	B	40	GLU	CB-CG	6.37	1.64	1.52
2	B	1022	THR	CB-OG1	-6.37	1.30	1.43
2	B	726	ALA	CA-CB	6.36	1.65	1.52
2	B	1069	PHE	C-O	6.36	1.35	1.23
1	A	420	ARG	CZ-NH1	-6.36	1.24	1.33
1	A	624	SER	CA-CB	6.36	1.62	1.52
1	A	685	GLU	CD-OE1	6.36	1.32	1.25
2	B	279	ASP	CB-CG	6.36	1.65	1.51
9	K	67	PHE	C-O	-6.36	1.11	1.23
1	A	1195	LEU	N-CA	6.36	1.59	1.46
2	B	351	TYR	CG-CD1	-6.36	1.30	1.39
2	B	1032	SER	CB-OG	6.36	1.50	1.42
9	K	2	ASN	CB-CG	6.36	1.65	1.51
1	A	144	THR	C-O	-6.35	1.11	1.23
1	A	180	LYS	C-O	-6.35	1.11	1.23
1	A	1045	VAL	CB-CG1	-6.35	1.39	1.52
4	E	23	VAL	C-O	6.35	1.35	1.23
7	I	85	PHE	CG-CD2	-6.35	1.29	1.38
1	A	958	VAL	CB-CG2	6.35	1.66	1.52
4	E	110	PHE	CG-CD2	-6.35	1.29	1.38
2	B	245	GLU	CD-OE2	6.35	1.32	1.25
1	A	1303	GLU	C-O	-6.35	1.11	1.23
2	B	614	SER	CB-OG	-6.34	1.34	1.42
1	A	714	PHE	CD2-CE2	-6.34	1.26	1.39
2	B	1214	PRO	C-O	6.34	1.35	1.23
2	B	225	VAL	CB-CG2	-6.34	1.39	1.52
3	C	195	GLN	CD-OE1	6.34	1.38	1.24
5	F	136	ARG	CZ-NH1	-6.34	1.24	1.33
2	B	90	ILE	N-CA	6.34	1.59	1.46
2	B	730	ARG	CZ-NH1	-6.34	1.24	1.33
9	K	79	GLU	CD-OE2	6.34	1.32	1.25
1	A	739	ASP	CB-CG	6.34	1.65	1.51
9	K	109	TRP	CG-CD1	6.34	1.45	1.36
2	B	589	VAL	CA-CB	-6.33	1.41	1.54
1	A	149	GLU	CA-CB	-6.33	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	23	VAL	CB-CG1	6.33	1.66	1.52
2	B	19	GLU	CG-CD	6.33	1.61	1.51
2	B	840	ILE	CA-CB	-6.33	1.40	1.54
1	A	714	PHE	CD1-CE1	-6.33	1.26	1.39
2	B	798	TYR	CG-CD2	6.33	1.47	1.39
3	C	3	GLU	N-CA	6.32	1.58	1.46
6	H	116	TYR	CE1-CZ	6.32	1.46	1.38
1	A	175	ARG	CD-NE	6.32	1.57	1.46
1	A	1355	VAL	CB-CG2	-6.32	1.39	1.52
1	A	491	VAL	CA-CB	-6.32	1.41	1.54
2	B	735	ALA	CA-CB	-6.32	1.39	1.52
3	C	68	GLY	C-O	6.32	1.33	1.23
1	A	423	ASP	CG-OD1	6.32	1.39	1.25
1	A	678	GLU	CD-OE2	6.32	1.32	1.25
2	B	904	ARG	C-O	-6.32	1.11	1.23
1	A	579	SER	C-O	6.31	1.35	1.23
1	A	746	MET	CG-SD	-6.31	1.64	1.81
1	A	1361	SER	CB-OG	6.31	1.50	1.42
2	B	1211	ASN	CG-OD1	-6.31	1.10	1.24
5	F	119	ARG	CZ-NH1	6.31	1.41	1.33
1	A	1056	SER	C-O	-6.31	1.11	1.23
1	A	815	PHE	CG-CD1	-6.31	1.29	1.38
2	B	361	LEU	C-N	-6.30	1.22	1.34
2	B	836	GLU	CD-OE1	6.30	1.32	1.25
2	B	486	TYR	CG-CD1	6.30	1.47	1.39
1	A	1210	GLY	C-O	6.30	1.33	1.23
2	B	209	GLU	CA-CB	-6.30	1.40	1.53
2	B	325	GLN	CB-CG	-6.30	1.35	1.52
2	B	973	ILE	C-O	6.30	1.35	1.23
3	C	201	TRP	CD2-CE2	-6.30	1.33	1.41
4	E	212	ARG	CG-CD	6.30	1.67	1.51
1	A	17	VAL	CA-CB	-6.30	1.41	1.54
1	A	106	VAL	CB-CG2	-6.30	1.39	1.52
8	J	56	LEU	N-CA	-6.30	1.33	1.46
10	L	47	ARG	NE-CZ	6.30	1.41	1.33
3	C	4	GLU	CD-OE1	6.29	1.32	1.25
3	C	47	ASP	CG-OD2	6.29	1.39	1.25
1	A	139	TRP	CG-CD2	-6.29	1.32	1.43
1	A	1155	ASP	CA-CB	-6.29	1.40	1.53
2	B	803	LEU	CA-CB	-6.29	1.39	1.53
2	B	983	ARG	CD-NE	-6.29	1.35	1.46
1	A	427	GLN	CB-CG	6.29	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	979	LYS	CB-CG	-6.29	1.35	1.52
2	B	242	SER	CB-OG	6.29	1.50	1.42
1	A	1379	GLY	N-CA	-6.29	1.36	1.46
2	B	520	GLY	C-O	-6.29	1.13	1.23
1	A	722	LEU	C-O	-6.29	1.11	1.23
2	B	126	SER	CA-CB	-6.29	1.43	1.52
2	B	598	GLU	N-CA	6.29	1.58	1.46
8	J	21	TYR	CD2-CE2	6.29	1.48	1.39
1	A	1325	THR	CB-CG2	-6.28	1.31	1.52
2	B	359	GLU	CG-CD	-6.28	1.42	1.51
4	E	67	GLU	CG-CD	6.28	1.61	1.51
10	L	64	LEU	CG-CD1	6.28	1.75	1.51
7	I	84	VAL	CA-CB	-6.28	1.41	1.54
9	K	39	ASP	CB-CG	6.28	1.65	1.51
7	I	35	VAL	CB-CG2	-6.28	1.39	1.52
1	A	1288	ASP	CG-OD1	6.28	1.39	1.25
2	B	561	TRP	CZ3-CH2	6.28	1.50	1.40
6	H	85	GLY	C-O	6.28	1.33	1.23
1	A	273	ASN	CB-CG	6.27	1.65	1.51
1	A	121	LEU	CG-CD1	6.27	1.75	1.51
2	B	1060	ARG	CB-CG	-6.27	1.35	1.52
4	E	54	GLN	CA-CB	6.27	1.67	1.53
2	B	814	PHE	CB-CG	-6.27	1.40	1.51
7	I	107	SER	CB-OG	-6.27	1.34	1.42
1	A	843	LYS	CA-CB	6.27	1.67	1.53
2	B	573	GLN	C-O	-6.26	1.11	1.23
4	E	37	LEU	CG-CD1	6.26	1.75	1.51
8	J	54	VAL	N-CA	-6.26	1.33	1.46
1	A	1198	ASP	N-CA	6.26	1.58	1.46
1	A	438	ASP	CA-CB	-6.25	1.40	1.53
1	A	1300	LYS	CD-CE	6.25	1.66	1.51
2	B	1019	SER	CA-CB	-6.25	1.43	1.52
3	C	228	PHE	N-CA	-6.25	1.33	1.46
3	C	119	VAL	CB-CG1	-6.25	1.39	1.52
7	I	51	ASN	C-O	-6.25	1.11	1.23
1	A	25	GLU	CD-OE1	6.25	1.32	1.25
1	A	196	GLU	CD-OE1	6.25	1.32	1.25
1	A	696	GLU	CD-OE2	-6.25	1.18	1.25
2	B	255	GLN	N-CA	-6.25	1.33	1.46
2	B	604	ARG	CD-NE	-6.25	1.35	1.46
2	B	814	PHE	CE2-CZ	-6.25	1.25	1.37
9	K	13	GLY	C-O	6.25	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	26	LYS	CE-NZ	6.25	1.64	1.49
1	A	37	PHE	CB-CG	6.24	1.61	1.51
3	C	178	PHE	CG-CD2	-6.24	1.29	1.38
4	E	150	VAL	CA-CB	-6.24	1.41	1.54
1	A	603	ASN	N-CA	-6.24	1.33	1.46
1	A	1205	LYS	C-O	6.24	1.35	1.23
2	B	866	TYR	CD1-CE1	6.24	1.48	1.39
9	K	61	TYR	CD2-CE2	6.23	1.48	1.39
1	A	1049	ILE	CA-CB	-6.23	1.40	1.54
9	K	10	PHE	CE2-CZ	-6.23	1.25	1.37
2	B	579	ARG	CG-CD	6.23	1.67	1.51
2	B	745	PRO	N-CD	-6.23	1.39	1.47
4	E	164	LEU	CA-CB	-6.23	1.39	1.53
1	A	137	ALA	C-O	6.23	1.35	1.23
1	A	203	SER	CA-CB	6.23	1.62	1.52
1	A	553	VAL	CB-CG1	-6.23	1.39	1.52
5	F	144	GLU	CD-OE1	6.23	1.32	1.25
3	C	10	ILE	CG1-CD1	-6.23	1.07	1.50
7	I	20	LYS	CE-NZ	6.23	1.64	1.49
3	C	10	ILE	CA-CB	-6.22	1.40	1.54
6	H	118	PHE	CE2-CZ	6.22	1.49	1.37
1	A	774	ARG	CD-NE	-6.22	1.35	1.46
2	B	30	SER	CB-OG	-6.22	1.34	1.42
2	B	55	VAL	C-O	6.22	1.35	1.23
2	B	659	ALA	CA-CB	6.22	1.65	1.52
4	E	19	VAL	CB-CG2	-6.22	1.39	1.52
1	A	400	PRO	C-O	-6.22	1.10	1.23
2	B	221	ASN	C-O	6.22	1.35	1.23
1	A	1191	TRP	CG-CD2	-6.21	1.33	1.43
2	B	751	VAL	CB-CG1	-6.21	1.39	1.52
2	B	859	TYR	CG-CD1	-6.21	1.31	1.39
6	H	110	ASP	CB-CG	6.21	1.64	1.51
7	I	74	GLU	CB-CG	6.21	1.64	1.52
1	A	920	LEU	CG-CD2	-6.21	1.28	1.51
2	B	1073	TYR	CZ-OH	6.21	1.48	1.37
1	A	432	VAL	C-O	-6.21	1.11	1.23
2	B	557	PHE	C-O	6.21	1.35	1.23
2	B	871	THR	CA-CB	6.21	1.69	1.53
3	C	184	ASN	N-CA	6.21	1.58	1.46
1	A	106	VAL	CB-CG1	6.21	1.65	1.52
3	C	123	ASN	CB-CG	6.21	1.65	1.51
4	E	114	ASN	CG-OD1	6.21	1.37	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1	MET	CA-CB	-6.21	1.40	1.53
1	A	189	ARG	N-CA	6.20	1.58	1.46
1	A	897	TYR	CG-CD2	-6.20	1.31	1.39
1	A	969	GLN	CD-NE2	6.20	1.48	1.32
8	J	43	ARG	CZ-NH1	-6.20	1.25	1.33
2	B	213	ILE	N-CA	-6.20	1.33	1.46
1	A	1415	SER	C-O	-6.20	1.11	1.23
3	C	20	PHE	CE2-CZ	6.20	1.49	1.37
2	B	792	MET	CG-SD	6.20	1.97	1.81
1	A	188	ASP	CB-CG	6.19	1.64	1.51
1	A	1411	GLU	CD-OE2	6.19	1.32	1.25
2	B	436	VAL	CA-C	6.19	1.69	1.52
1	A	1426	GLU	C-O	6.18	1.35	1.23
2	B	324	ILE	C-O	-6.18	1.11	1.23
2	B	711	GLU	CA-CB	-6.18	1.40	1.53
5	F	150	GLU	CB-CG	-6.18	1.40	1.52
3	C	119	VAL	CA-CB	6.18	1.67	1.54
1	A	811	GLN	N-CA	-6.18	1.33	1.46
1	A	1287	TYR	CD1-CE1	6.18	1.48	1.39
1	A	1428	VAL	C-O	-6.18	1.11	1.23
1	A	1286	LYS	CB-CG	6.17	1.69	1.52
3	C	228	PHE	CG-CD2	-6.17	1.29	1.38
1	A	775	ILE	CA-CB	-6.17	1.40	1.54
6	H	63	LEU	C-O	6.17	1.35	1.23
8	J	62	ARG	C-O	-6.17	1.11	1.23
9	K	83	PRO	CA-CB	-6.17	1.41	1.53
1	A	72	GLU	CD-OE1	6.17	1.32	1.25
3	C	160	LYS	CG-CD	6.17	1.73	1.52
1	A	956	LEU	C-O	-6.16	1.11	1.23
2	B	190	TYR	CA-CB	-6.16	1.40	1.53
2	B	859	TYR	CD1-CE1	6.16	1.48	1.39
9	K	93	SER	C-O	6.16	1.35	1.23
6	H	85	GLY	N-CA	6.16	1.55	1.46
1	A	81	PHE	CB-CG	6.16	1.61	1.51
2	B	30	SER	C-O	-6.16	1.11	1.23
2	B	226	PHE	CG-CD2	6.16	1.48	1.38
7	I	8	ARG	CB-CG	6.16	1.69	1.52
2	B	209	GLU	CD-OE1	-6.16	1.18	1.25
1	A	800	VAL	CA-CB	-6.16	1.41	1.54
2	B	371	GLU	C-O	-6.16	1.11	1.23
2	B	691	GLU	CD-OE1	6.16	1.32	1.25
7	I	51	ASN	CB-CG	6.16	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	203	PHE	CD2-CE2	-6.15	1.26	1.39
2	B	797	TYR	CE2-CZ	-6.15	1.30	1.38
1	A	1344	GLY	C-O	-6.15	1.13	1.23
2	B	666	TYR	CG-CD2	6.15	1.47	1.39
4	E	79	TRP	CB-CG	6.15	1.61	1.50
2	B	788	ARG	CZ-NH1	-6.15	1.25	1.33
1	A	911	SER	CB-OG	6.15	1.50	1.42
2	B	313	MET	SD-CE	-6.15	1.43	1.77
2	B	1188	LYS	CG-CD	6.15	1.73	1.52
1	A	1298	TYR	CE1-CZ	-6.15	1.30	1.38
1	A	1314	SER	C-O	6.15	1.35	1.23
2	B	219	ALA	CA-CB	6.15	1.65	1.52
2	B	1193	GLN	C-O	-6.15	1.11	1.23
1	A	1225	PHE	CA-CB	6.14	1.67	1.53
2	B	198	ASP	C-O	-6.14	1.11	1.23
1	A	213	HIS	CB-CG	6.14	1.61	1.50
1	A	371	ALA	CA-CB	-6.14	1.39	1.52
3	C	179	GLU	C-O	-6.14	1.11	1.23
8	J	22	LEU	N-CA	-6.14	1.34	1.46
1	A	185	TRP	CG-CD2	-6.14	1.33	1.43
2	B	978	ASP	CG-OD2	6.14	1.39	1.25
2	B	627	PHE	CE2-CZ	-6.14	1.25	1.37
2	B	1219	ASP	N-CA	6.14	1.58	1.46
6	H	130	ARG	NE-CZ	-6.14	1.25	1.33
1	A	1286	LYS	C-O	-6.14	1.11	1.23
2	B	490	SER	CA-CB	6.13	1.62	1.52
1	A	110	CYS	CA-CB	6.13	1.67	1.53
2	B	304	ASP	N-CA	6.13	1.58	1.46
2	B	622	LYS	CE-NZ	6.13	1.64	1.49
4	E	208	TYR	CZ-OH	6.13	1.48	1.37
1	A	379	VAL	CB-CG2	6.13	1.65	1.52
2	B	261	ARG	NE-CZ	6.13	1.41	1.33
2	B	397	ASP	CG-OD1	6.13	1.39	1.25
4	E	163	GLU	CA-CB	6.13	1.67	1.53
6	H	19	ARG	CZ-NH2	6.13	1.41	1.33
2	B	479	VAL	CA-CB	-6.12	1.41	1.54
9	K	30	ALA	CA-CB	-6.12	1.39	1.52
1	A	219	PHE	C-O	-6.12	1.11	1.23
1	A	1277	GLU	CA-CB	6.12	1.67	1.53
2	B	781	PHE	CB-CG	-6.12	1.41	1.51
2	B	862	GLN	CG-CD	6.12	1.65	1.51
4	E	33	GLU	CD-OE2	6.12	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1007	VAL	CB-CG2	-6.12	1.40	1.52
6	H	98	TYR	CD1-CE1	6.12	1.48	1.39
9	K	79	GLU	CD-OE1	6.12	1.32	1.25
1	A	646	PHE	CD1-CE1	-6.12	1.27	1.39
2	B	708	GLU	N-CA	-6.12	1.34	1.46
1	A	416	ARG	C-O	-6.12	1.11	1.23
1	A	1448	GLU	CA-C	6.12	1.68	1.52
2	B	18	PHE	CA-CB	6.12	1.67	1.53
2	B	367	LEU	CA-CB	6.12	1.67	1.53
6	H	115	TYR	CZ-OH	6.12	1.48	1.37
1	A	70	CYS	CB-SG	6.11	1.92	1.82
7	I	17	ARG	CA-C	-6.11	1.37	1.52
8	J	59	LYS	CE-NZ	-6.11	1.33	1.49
6	H	80	ARG	NE-CZ	6.11	1.41	1.33
1	A	685	GLU	CG-CD	6.11	1.61	1.51
2	B	752	ALA	CA-CB	6.11	1.65	1.52
1	A	512	VAL	CB-CG1	-6.11	1.40	1.52
1	A	1191	TRP	C-O	6.11	1.34	1.23
2	B	224	GLN	CB-CG	6.11	1.69	1.52
2	B	1041	GLU	N-CA	6.11	1.58	1.46
1	A	983	ILE	CB-CG2	-6.10	1.33	1.52
3	C	204	SER	C-O	6.10	1.34	1.23
2	B	996	ARG	CG-CD	6.10	1.67	1.51
8	J	18	TRP	CE2-CZ2	-6.10	1.29	1.39
3	C	64	ALA	CA-CB	-6.10	1.39	1.52
1	A	920	LEU	CA-CB	-6.09	1.39	1.53
2	B	112	LEU	C-O	-6.09	1.11	1.23
3	C	79	GLN	CD-OE1	6.09	1.37	1.24
1	A	211	PHE	CE1-CZ	6.09	1.49	1.37
1	A	382	PRO	CG-CD	-6.09	1.30	1.50
4	E	135	PHE	C-O	-6.09	1.11	1.23
5	F	143	PHE	CB-CG	-6.09	1.41	1.51
2	B	89	GLU	CG-CD	6.09	1.61	1.51
2	B	870	ILE	N-CA	6.09	1.58	1.46
3	C	43	THR	N-CA	-6.08	1.34	1.46
1	A	622	VAL	CA-CB	-6.08	1.42	1.54
2	B	790	ASP	CA-CB	6.08	1.67	1.53
2	B	1192	TYR	CB-CG	-6.08	1.42	1.51
1	A	151	ASP	C-O	-6.08	1.11	1.23
1	A	782	ARG	CB-CG	-6.08	1.36	1.52
1	A	1227	ILE	N-CA	-6.08	1.34	1.46
1	A	1263	ILE	CG1-CD1	6.08	1.92	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	233	PRO	CA-C	6.08	1.65	1.52
1	A	34	LYS	C-O	-6.08	1.11	1.23
1	A	596	THR	CB-CG2	6.08	1.72	1.52
2	B	220	GLY	C-O	-6.08	1.14	1.23
2	B	984	HIS	C-O	-6.08	1.11	1.23
2	B	1224	PHE	N-CA	6.08	1.58	1.46
7	I	39	GLY	C-O	-6.08	1.14	1.23
7	I	120	GLN	CG-CD	6.08	1.65	1.51
1	A	1268	LEU	CA-CB	-6.07	1.39	1.53
2	B	1108	ARG	CA-C	6.07	1.68	1.52
3	C	117	ASP	C-O	6.07	1.34	1.23
1	A	375	THR	C-O	-6.07	1.11	1.23
3	C	223	ALA	CA-CB	-6.07	1.39	1.52
4	E	208	TYR	CE1-CZ	-6.07	1.30	1.38
1	A	1200	ALA	C-O	6.07	1.34	1.23
1	A	1274	ARG	CZ-NH2	6.07	1.41	1.33
2	B	348	ARG	NE-CZ	-6.07	1.25	1.33
5	F	150	GLU	CD-OE2	6.07	1.32	1.25
1	A	1359	ASP	CG-OD1	6.07	1.39	1.25
2	B	593	PRO	CG-CD	6.07	1.70	1.50
1	A	1214	GLU	CD-OE2	6.06	1.32	1.25
4	E	157	SER	CA-CB	6.06	1.62	1.52
1	A	57	ARG	CG-CD	6.06	1.67	1.51
1	A	285	PRO	CB-CG	-6.06	1.19	1.50
2	B	586	TRP	CZ3-CH2	-6.06	1.30	1.40
6	H	87	ARG	CB-CG	6.06	1.69	1.52
9	K	81	TYR	CD1-CE1	-6.06	1.30	1.39
9	K	10	PHE	CD1-CE1	-6.06	1.27	1.39
2	B	1055	ILE	CA-CB	6.06	1.68	1.54
3	C	11	ARG	C-O	6.05	1.34	1.23
3	C	162	GLY	C-O	6.05	1.33	1.23
1	A	529	CYS	CB-SG	-6.05	1.72	1.82
3	C	134	ILE	CB-CG2	-6.05	1.34	1.52
5	F	134	ILE	CB-CG2	-6.05	1.34	1.52
1	A	404	TYR	CE1-CZ	-6.04	1.30	1.38
1	A	958	VAL	CA-CB	-6.04	1.42	1.54
1	A	107	CYS	CA-CB	6.04	1.67	1.53
8	J	24	LEU	C-O	-6.04	1.11	1.23
2	B	430	ARG	NE-CZ	6.04	1.40	1.33
2	B	582	VAL	CA-C	-6.04	1.37	1.52
2	B	618	ASP	C-O	6.04	1.34	1.23
1	A	139	TRP	CG-CD1	6.04	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	LYS	CG-CD	6.03	1.73	1.52
2	B	106	ASP	CG-OD2	6.03	1.39	1.25
2	B	1008	PRO	CG-CD	-6.03	1.30	1.50
1	A	465	TYR	CZ-OH	6.03	1.48	1.37
2	B	197	PHE	CG-CD1	-6.02	1.29	1.38
2	B	832	GLY	C-O	-6.02	1.14	1.23
7	I	45	ARG	NE-CZ	-6.02	1.25	1.33
1	A	860	LEU	C-O	-6.02	1.11	1.23
1	A	188	ASP	CA-CB	6.02	1.67	1.53
1	A	976	THR	CA-CB	6.02	1.69	1.53
2	B	192	LEU	CG-CD2	6.02	1.74	1.51
3	C	100	THR	C-O	6.02	1.34	1.23
6	H	111	LEU	N-CA	6.02	1.58	1.46
1	A	1256	GLU	CG-CD	6.02	1.60	1.51
9	K	7	PHE	CE2-CZ	6.02	1.48	1.37
2	B	316	PRO	C-O	6.01	1.35	1.23
4	E	166	LYS	C-O	6.01	1.34	1.23
1	A	444	PHE	CE1-CZ	-6.01	1.25	1.37
2	B	958	GLN	N-CA	6.01	1.58	1.46
2	B	1021	MET	CB-CG	6.01	1.70	1.51
2	B	1070	GLU	CD-OE2	6.01	1.32	1.25
3	C	148	ARG	CZ-NH1	6.01	1.40	1.33
3	C	97	VAL	CA-CB	-6.01	1.42	1.54
8	J	49	MET	SD-CE	-6.01	1.44	1.77
3	C	74	SER	CB-OG	6.01	1.50	1.42
1	A	487	MET	CG-SD	6.00	1.96	1.81
2	B	561	TRP	C-N	-6.00	1.22	1.33
2	B	1165	ILE	CA-CB	6.00	1.68	1.54
1	A	1256	GLU	CD-OE2	6.00	1.32	1.25
10	L	60	ARG	CG-CD	6.00	1.67	1.51
2	B	138	GLU	CD-OE1	-6.00	1.19	1.25
10	L	47	ARG	CZ-NH2	6.00	1.40	1.33
1	A	1135	ARG	NE-CZ	6.00	1.40	1.33
9	K	1	MET	N-CA	6.00	1.58	1.46
2	B	1216	LEU	C-O	5.99	1.34	1.23
2	B	308	TRP	CD2-CE2	-5.99	1.34	1.41
1	A	123	ARG	CD-NE	5.99	1.56	1.46
1	A	589	GLN	CD-OE1	5.99	1.37	1.24
1	A	803	SER	C-O	-5.99	1.11	1.23
2	B	188	ASP	C-O	5.99	1.34	1.23
1	A	15	LYS	CD-CE	5.99	1.66	1.51
1	A	789	LYS	CG-CD	-5.99	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1088	GLY	C-O	-5.98	1.14	1.23
2	B	632	ARG	C-N	-5.98	1.20	1.34
2	B	1212	ILE	N-CA	5.98	1.58	1.46
7	I	49	ILE	CB-CG2	5.98	1.71	1.52
1	A	240	PRO	C-O	5.98	1.35	1.23
6	H	6	PHE	CA-CB	-5.98	1.40	1.53
9	K	108	GLU	CG-CD	5.98	1.60	1.51
1	A	1277	GLU	N-CA	5.98	1.58	1.46
1	A	66	LYS	CA-CB	5.97	1.67	1.53
1	A	181	LEU	C-O	5.97	1.34	1.23
1	A	622	VAL	CB-CG1	-5.97	1.40	1.52
1	A	636	GLU	CB-CG	5.97	1.63	1.52
1	A	1433	MET	SD-CE	-5.97	1.44	1.77
2	B	574	SER	CB-OG	-5.97	1.34	1.42
9	K	35	PHE	CG-CD2	-5.97	1.29	1.38
1	A	686	ALA	C-N	-5.97	1.20	1.34
2	B	983	ARG	CZ-NH2	-5.97	1.25	1.33
3	C	107	SER	CB-OG	-5.97	1.34	1.42
5	F	110	ASP	C-O	5.97	1.34	1.23
5	F	149	GLU	CD-OE2	5.97	1.32	1.25
1	A	1038	THR	CA-C	-5.97	1.37	1.52
2	B	534	GLY	N-CA	-5.97	1.37	1.46
1	A	678	GLU	CG-CD	5.97	1.60	1.51
2	B	709	ASP	C-O	-5.97	1.12	1.23
5	F	137	TYR	CE1-CZ	-5.96	1.30	1.38
1	A	191	THR	N-CA	5.96	1.58	1.46
2	B	278	GLN	CB-CG	-5.96	1.36	1.52
2	B	321	GLY	C-O	-5.96	1.14	1.23
1	A	960	ILE	CA-CB	5.96	1.68	1.54
2	B	815	ARG	CD-NE	-5.96	1.36	1.46
6	H	129	TYR	CZ-OH	5.96	1.48	1.37
7	I	24	ARG	CG-CD	5.96	1.66	1.51
1	A	297	GLN	C-O	-5.96	1.12	1.23
2	B	209	GLU	C-O	-5.96	1.12	1.23
7	I	66	PRO	CA-C	-5.96	1.41	1.52
8	J	48	ARG	CG-CD	-5.96	1.37	1.51
1	A	917	SER	C-O	-5.96	1.12	1.23
1	A	419	LYS	CE-NZ	-5.95	1.34	1.49
1	A	673	GLY	CA-C	-5.95	1.42	1.51
4	E	79	TRP	CG-CD1	5.95	1.45	1.36
7	I	87	GLN	CB-CG	5.95	1.68	1.52
2	B	612	GLU	CA-CB	-5.95	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1020	ARG	CG-CD	-5.95	1.37	1.51
6	H	20	TYR	CG-CD2	-5.95	1.31	1.39
1	A	401	GLY	N-CA	-5.95	1.37	1.46
4	E	57	MET	CG-SD	5.95	1.96	1.81
1	A	45	GLN	CA-C	5.94	1.68	1.52
1	A	113	LEU	C-O	5.94	1.34	1.23
4	E	121	MET	SD-CE	5.94	2.11	1.77
1	A	838	GLN	CD-OE1	5.94	1.37	1.24
1	A	1027	ALA	N-CA	-5.94	1.34	1.46
1	A	90	VAL	CA-CB	-5.94	1.42	1.54
2	B	336	ARG	CZ-NH1	5.94	1.40	1.33
1	A	271	LYS	CD-CE	5.93	1.66	1.51
1	A	367	PRO	CA-CB	-5.93	1.41	1.53
1	A	486	GLU	CD-OE2	-5.93	1.19	1.25
1	A	509	LEU	C-O	-5.93	1.12	1.23
1	A	1117	THR	N-CA	5.93	1.58	1.46
1	A	1237	ILE	N-CA	-5.93	1.34	1.46
1	A	1446	ASP	CA-CB	5.93	1.67	1.53
1	A	687	LYS	CE-NZ	5.93	1.63	1.49
2	B	596	LEU	CG-CD1	-5.93	1.29	1.51
1	A	1242	VAL	CB-CG1	5.93	1.65	1.52
2	B	337	ARG	CZ-NH2	-5.93	1.25	1.33
1	A	121	LEU	CB-CG	5.93	1.69	1.52
1	A	1238	ILE	C-O	-5.93	1.12	1.23
1	A	695	LYS	CE-NZ	5.93	1.63	1.49
1	A	1338	VAL	CA-CB	-5.93	1.42	1.54
3	C	209	TYR	CE1-CZ	5.93	1.46	1.38
4	E	74	ASP	CG-OD2	-5.93	1.11	1.25
5	F	80	ALA	CA-CB	5.93	1.64	1.52
1	A	764	CYS	CA-CB	-5.92	1.41	1.53
3	C	139	GLY	N-CA	5.92	1.54	1.46
6	H	80	ARG	CZ-NH2	5.92	1.40	1.33
2	B	846	ILE	CB-CG2	5.92	1.71	1.52
1	A	1224	LEU	CA-CB	-5.92	1.40	1.53
4	E	54	GLN	CG-CD	5.92	1.64	1.51
10	L	26	THR	C-O	5.92	1.34	1.23
1	A	1333	ILE	CA-CB	-5.92	1.41	1.54
9	K	36	GLU	CD-OE2	5.92	1.32	1.25
8	J	63	TYR	CE1-CZ	-5.92	1.30	1.38
1	A	1222	ASN	CA-CB	5.91	1.68	1.53
1	A	852	TYR	CZ-OH	-5.91	1.27	1.37
8	J	41	LEU	CG-CD2	-5.91	1.29	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	718	VAL	CA-CB	-5.91	1.42	1.54
1	A	655	PHE	CG-CD1	-5.91	1.29	1.38
2	B	455	SER	CA-CB	5.91	1.61	1.52
1	A	1366	ARG	CD-NE	-5.90	1.36	1.46
3	C	212	PRO	C-O	-5.90	1.11	1.23
9	K	35	PHE	CD2-CE2	-5.90	1.27	1.39
1	A	220	THR	N-CA	5.90	1.58	1.46
1	A	998	LEU	C-O	-5.90	1.12	1.23
2	B	351	TYR	C-O	5.90	1.34	1.23
1	A	135	PHE	CD1-CE1	-5.89	1.27	1.39
2	B	191	LYS	CG-CD	5.89	1.72	1.52
2	B	194	GLU	CB-CG	5.89	1.63	1.52
2	B	267	ARG	CG-CD	5.89	1.66	1.51
5	F	137	TYR	CA-CB	-5.89	1.41	1.53
2	B	793	ALA	N-CA	-5.89	1.34	1.46
2	B	1004	GLU	CG-CD	5.89	1.60	1.51
2	B	1215	ARG	CZ-NH2	-5.89	1.25	1.33
3	C	104	PHE	CE1-CZ	5.89	1.48	1.37
4	E	211	TYR	CD1-CE1	-5.89	1.30	1.39
8	J	3	VAL	CB-CG2	-5.89	1.40	1.52
2	B	880	THR	CB-CG2	5.89	1.71	1.52
3	C	203	GLN	CB-CG	5.89	1.68	1.52
1	A	491	VAL	C-O	-5.89	1.12	1.23
3	C	113	VAL	CA-CB	-5.89	1.42	1.54
1	A	433	GLU	CG-CD	5.88	1.60	1.51
1	A	516	SER	CA-CB	-5.88	1.44	1.52
1	A	659	HIS	CA-CB	-5.88	1.41	1.53
1	A	1291	VAL	CB-CG2	5.88	1.65	1.52
8	J	5	VAL	CA-CB	5.88	1.67	1.54
1	A	133	LYS	CD-CE	5.88	1.66	1.51
1	A	925	LEU	C-O	-5.88	1.12	1.23
2	B	355	ILE	C-O	-5.88	1.12	1.23
2	B	411	PRO	C-O	5.88	1.35	1.23
1	A	188	ASP	CA-C	5.88	1.68	1.52
1	A	1239	ARG	CZ-NH2	-5.88	1.25	1.33
2	B	679	TYR	CE1-CZ	-5.88	1.30	1.38
1	A	975	HIS	CA-CB	5.88	1.66	1.53
1	A	1137	ALA	C-O	5.88	1.34	1.23
2	B	277	LYS	CD-CE	5.88	1.66	1.51
1	A	624	SER	N-CA	5.87	1.58	1.46
2	B	704	ALA	C-O	-5.87	1.12	1.23
4	E	136	ASN	C-O	-5.87	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	822	ASN	C-O	-5.87	1.12	1.23
3	C	104	PHE	CB-CG	-5.87	1.41	1.51
1	A	713	SER	N-CA	-5.87	1.34	1.46
1	A	927	VAL	CB-CG1	-5.87	1.40	1.52
5	F	123	LYS	CB-CG	5.87	1.68	1.52
7	I	19	ASP	C-O	5.87	1.34	1.23
3	C	21	ILE	CA-CB	-5.86	1.41	1.54
4	E	13	TRP	CB-CG	5.86	1.60	1.50
10	L	68	GLU	CB-CG	5.86	1.63	1.52
1	A	847	ASP	CG-OD1	5.86	1.38	1.25
2	B	570	VAL	CB-CG1	-5.86	1.40	1.52
3	C	42	PRO	CA-CB	-5.86	1.41	1.53
3	C	126	GLY	C-O	5.86	1.33	1.23
4	E	85	GLU	CD-OE1	5.86	1.32	1.25
9	K	78	THR	CA-CB	-5.86	1.38	1.53
1	A	917	SER	CA-CB	-5.86	1.44	1.52
1	A	390	GLN	CB-CG	5.86	1.68	1.52
1	A	747	VAL	CB-CG1	-5.86	1.40	1.52
2	B	620	ARG	NE-CZ	-5.86	1.25	1.33
4	E	41	ASP	CG-OD1	5.86	1.38	1.25
4	E	75	MET	C-O	5.86	1.34	1.23
1	A	1320	PRO	CA-C	-5.85	1.41	1.52
2	B	46	GLN	CG-CD	-5.85	1.37	1.51
2	B	586	TRP	CE2-CZ2	-5.85	1.29	1.39
2	B	323	VAL	CB-CG2	5.85	1.65	1.52
2	B	1150	ARG	CG-CD	-5.85	1.37	1.51
5	F	110	ASP	CG-OD1	5.85	1.38	1.25
1	A	280	GLU	CD-OE2	-5.85	1.19	1.25
1	A	518	LYS	CE-NZ	-5.85	1.34	1.49
10	L	47	ARG	CB-CG	5.85	1.68	1.52
1	A	510	GLN	CD-NE2	-5.85	1.18	1.32
1	A	1068	ALA	CA-CB	-5.85	1.40	1.52
6	H	9	ILE	C-O	5.85	1.34	1.23
9	K	54	ARG	CZ-NH1	5.85	1.40	1.33
1	A	41	MET	SD-CE	5.85	2.10	1.77
2	B	296	GLU	CD-OE1	5.84	1.32	1.25
3	C	25	VAL	N-CA	5.84	1.58	1.46
6	H	45	GLU	CG-CD	5.84	1.60	1.51
4	E	138	ALA	C-O	-5.84	1.12	1.23
5	F	109	VAL	CB-CG1	-5.84	1.40	1.52
1	A	277	GLU	CG-CD	5.84	1.60	1.51
1	A	517	ASN	CG-OD1	-5.84	1.11	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	208	SER	C-O	5.84	1.34	1.23
4	E	21	GLU	CG-CD	5.84	1.60	1.51
3	C	249	ASP	CA-CB	5.84	1.66	1.53
2	B	1094	ARG	CZ-NH1	-5.84	1.25	1.33
7	I	118	ARG	CA-C	5.84	1.68	1.52
3	C	174	ALA	C-O	-5.83	1.12	1.23
1	A	495	GLU	CD-OE1	-5.83	1.19	1.25
2	B	582	VAL	C-O	-5.83	1.12	1.23
2	B	916	THR	N-CA	5.83	1.58	1.46
2	B	1129	ARG	CZ-NH1	5.83	1.40	1.33
10	L	54	ARG	CB-CG	5.83	1.68	1.52
3	C	185	LYS	CB-CG	5.83	1.68	1.52
6	H	82	PRO	CA-C	5.83	1.64	1.52
2	B	787	VAL	CB-CG1	5.83	1.65	1.52
1	A	1326	ARG	CD-NE	-5.83	1.36	1.46
2	B	370	PHE	CB-CG	5.83	1.61	1.51
2	B	1188	LYS	CD-CE	5.83	1.65	1.51
10	L	37	LYS	C-O	-5.83	1.12	1.23
1	A	1311	VAL	N-CA	-5.82	1.34	1.46
8	J	6	ARG	CZ-NH1	-5.82	1.25	1.33
10	L	50	ASP	CA-CB	5.82	1.66	1.53
1	A	148	CYS	CA-CB	5.82	1.66	1.53
1	A	1287	TYR	CD2-CE2	5.82	1.48	1.39
5	F	135	ARG	CG-CD	5.82	1.66	1.51
9	K	66	PRO	CB-CG	-5.82	1.20	1.50
4	E	3	GLN	CB-CG	5.82	1.68	1.52
2	B	340	ALA	CA-CB	-5.82	1.40	1.52
2	B	57	TYR	CA-CB	5.81	1.66	1.53
4	E	74	ASP	C-O	5.81	1.34	1.23
1	A	1366	ARG	CG-CD	-5.81	1.37	1.51
2	B	855	PHE	CE1-CZ	5.81	1.48	1.37
2	B	1102	LYS	CD-CE	5.81	1.65	1.51
2	B	241	ARG	CD-NE	5.81	1.56	1.46
2	B	519	TRP	CE2-CZ2	-5.81	1.29	1.39
2	B	636	PRO	N-CA	-5.81	1.37	1.47
1	A	400	PRO	CB-CG	-5.81	1.21	1.50
1	A	892	ALA	CA-CB	-5.81	1.40	1.52
3	C	205	LYS	CG-CD	5.81	1.72	1.52
1	A	1119	TYR	CD2-CE2	-5.81	1.30	1.39
1	A	1095	THR	CA-C	-5.80	1.37	1.52
2	B	296	GLU	CG-CD	5.80	1.60	1.51
2	B	380	TYR	CD2-CE2	-5.80	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	174	GLN	CD-NE2	-5.80	1.18	1.32
1	A	934	LYS	CG-CD	5.80	1.72	1.52
2	B	39	ARG	CG-CD	5.80	1.66	1.51
4	E	112	TYR	CZ-OH	5.80	1.47	1.37
2	B	754	SER	CA-CB	-5.80	1.44	1.52
3	C	179	GLU	CG-CD	-5.80	1.43	1.51
7	I	95	THR	CB-CG2	-5.80	1.33	1.52
1	A	1424	VAL	CA-CB	-5.80	1.42	1.54
5	F	79	ARG	NE-CZ	-5.80	1.25	1.33
1	A	1438	THR	CA-CB	-5.80	1.38	1.53
2	B	1219	ASP	CA-CB	5.80	1.66	1.53
1	A	1023	ARG	CA-CB	-5.80	1.41	1.53
5	F	135	ARG	CD-NE	5.80	1.56	1.46
2	B	262	GLU	CB-CG	5.79	1.63	1.52
3	C	235	VAL	CB-CG1	-5.79	1.40	1.52
7	I	1	MET	CA-CB	5.79	1.66	1.53
1	A	1420	ASP	CG-OD1	5.79	1.38	1.25
1	A	767	GLN	CB-CG	-5.79	1.36	1.52
2	B	376	PHE	CE2-CZ	-5.79	1.26	1.37
9	K	108	GLU	CD-OE1	5.79	1.32	1.25
1	A	356	ASP	CA-C	-5.79	1.38	1.52
1	A	773	LYS	CB-CG	-5.79	1.36	1.52
2	B	842	ASN	CG-ND2	-5.79	1.18	1.32
1	A	1239	ARG	CD-NE	5.79	1.56	1.46
2	B	729	ILE	C-O	-5.79	1.12	1.23
2	B	747	MET	CG-SD	5.79	1.96	1.81
4	E	46	TYR	C-O	5.79	1.34	1.23
6	H	19	ARG	N-CA	5.79	1.57	1.46
1	A	201	VAL	CB-CG2	-5.78	1.40	1.52
1	A	1420	ASP	CB-CG	5.78	1.63	1.51
2	B	586	TRP	CB-CG	-5.78	1.39	1.50
2	B	1205	GLN	CA-CB	-5.78	1.41	1.53
1	A	489	LEU	CA-CB	-5.78	1.40	1.53
1	A	797	LYS	CA-C	-5.78	1.38	1.52
3	C	114	TYR	CD2-CE2	-5.78	1.30	1.39
3	C	232	VAL	CA-CB	-5.78	1.42	1.54
6	H	116	TYR	CZ-OH	5.78	1.47	1.37
1	A	1203	ASN	C-O	5.77	1.34	1.23
1	A	1385	THR	C-O	5.77	1.34	1.23
2	B	1012	ILE	CB-CG1	-5.77	1.37	1.54
7	I	119	THR	N-CA	5.77	1.57	1.46
1	A	1366	ARG	CA-CB	-5.77	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	754	SER	CB-OG	5.77	1.49	1.42
1	A	1228	TRP	CA-C	-5.77	1.38	1.52
2	B	774	GLY	CA-C	5.77	1.61	1.51
6	H	121	LEU	CG-CD1	-5.77	1.30	1.51
2	B	951	GLN	CB-CG	5.76	1.68	1.52
4	E	204	THR	CA-CB	-5.76	1.38	1.53
2	B	259	TYR	CG-CD1	-5.76	1.31	1.39
2	B	730	ARG	C-O	-5.76	1.12	1.23
1	A	1441	PHE	CB-CG	-5.76	1.41	1.51
1	A	25	GLU	CB-CG	5.76	1.63	1.52
1	A	976	THR	CB-CG2	5.76	1.71	1.52
1	A	1444	MET	SD-CE	5.76	2.10	1.77
1	A	198	GLU	CA-C	-5.76	1.38	1.52
1	A	1159	ARG	NE-CZ	5.76	1.40	1.33
2	B	44	VAL	CB-CG1	-5.76	1.40	1.52
1	A	606	LEU	N-CA	-5.75	1.34	1.46
1	A	896	ARG	NE-CZ	-5.75	1.25	1.33
1	A	1264	GLU	CG-CD	-5.75	1.43	1.51
3	C	111	THR	CB-CG2	5.75	1.71	1.52
9	K	77	THR	CB-OG1	5.75	1.54	1.43
2	B	759	PRO	C-O	5.75	1.34	1.23
2	B	1064	TYR	CG-CD1	-5.75	1.31	1.39
5	F	98	ALA	CA-CB	-5.75	1.40	1.52
5	F	109	VAL	CA-CB	-5.75	1.42	1.54
7	I	34	TYR	CD2-CE2	5.75	1.48	1.39
1	A	821	ARG	NE-CZ	-5.75	1.25	1.33
3	C	18	VAL	CA-C	-5.75	1.38	1.52
1	A	494	SER	CB-OG	5.75	1.49	1.42
1	A	705	LYS	CD-CE	5.75	1.65	1.51
2	B	57	TYR	CG-CD1	-5.75	1.31	1.39
2	B	887	HIS	CA-CB	5.74	1.66	1.53
1	A	1374	VAL	CB-CG1	-5.74	1.40	1.52
1	A	1447	GLU	CB-CG	5.74	1.63	1.52
1	A	1163	ILE	C-O	5.74	1.34	1.23
1	A	714	PHE	CG-CD1	-5.74	1.30	1.38
1	A	1443	VAL	CB-CG1	-5.74	1.40	1.52
2	B	1103	ILE	C-O	5.74	1.34	1.23
3	C	36	VAL	CB-CG2	-5.73	1.40	1.52
2	B	651	LEU	CG-CD1	-5.73	1.30	1.51
5	F	116	ASP	C-O	-5.73	1.12	1.23
2	B	710	LEU	CG-CD1	-5.73	1.30	1.51
2	B	937	ALA	N-CA	5.73	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1215	ARG	C-O	-5.73	1.12	1.23
8	J	58	GLU	CB-CG	5.73	1.63	1.52
1	A	1127	ASP	CB-CG	5.73	1.63	1.51
2	B	962	LYS	CE-NZ	5.73	1.63	1.49
4	E	155	ARG	CZ-NH1	5.73	1.40	1.33
2	B	695	ALA	N-CA	-5.73	1.34	1.46
4	E	63	ASN	CG-OD1	5.72	1.36	1.24
1	A	1270	ASN	C-O	5.72	1.34	1.23
2	B	940	PRO	C-O	-5.72	1.11	1.23
3	C	268	ASP	CA-C	5.72	1.67	1.52
4	E	66	GLU	CB-CG	5.72	1.63	1.52
4	E	109	ILE	CB-CG2	-5.72	1.35	1.52
10	L	28	LYS	CE-NZ	5.72	1.63	1.49
2	B	775	LYS	CE-NZ	5.72	1.63	1.49
3	C	173	ALA	C-O	-5.72	1.12	1.23
8	J	14	VAL	CB-CG1	-5.72	1.40	1.52
1	A	478	TYR	CD2-CE2	-5.71	1.30	1.39
2	B	1180	PHE	CE1-CZ	5.71	1.48	1.37
3	C	106	GLU	CG-CD	5.71	1.60	1.51
1	A	1146	VAL	CB-CG1	-5.71	1.40	1.52
5	F	145	ASP	C-O	5.71	1.34	1.23
2	B	235	SER	CA-CB	-5.71	1.44	1.52
1	A	1220	PHE	CE1-CZ	5.71	1.48	1.37
1	A	104	GLU	C-O	5.71	1.34	1.23
1	A	1062	GLU	CA-CB	-5.71	1.41	1.53
2	B	38	PHE	CG-CD1	-5.71	1.30	1.38
2	B	581	PHE	CG-CD2	-5.71	1.30	1.38
4	E	26	ARG	CG-CD	-5.71	1.37	1.51
1	A	944	ARG	CA-CB	-5.70	1.41	1.53
1	A	408	ASP	C-O	5.70	1.34	1.23
2	B	405	ARG	CZ-NH2	-5.70	1.25	1.33
3	C	92	CYS	CA-CB	5.70	1.66	1.53
1	A	587	HIS	CA-CB	5.70	1.66	1.53
1	A	1191	TRP	CE2-CZ2	-5.70	1.30	1.39
2	B	502	ILE	CB-CG2	5.70	1.70	1.52
2	B	111	ALA	CA-CB	5.70	1.64	1.52
4	E	94	LYS	CG-CD	5.70	1.71	1.52
1	A	917	SER	CB-OG	-5.69	1.34	1.42
2	B	465	ASN	CG-OD1	5.69	1.36	1.24
1	A	813	PHE	N-CA	-5.69	1.34	1.46
1	A	439	ASN	CG-ND2	-5.69	1.18	1.32
2	B	1109	GLY	CA-C	5.69	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	697	GLU	C-O	-5.68	1.12	1.23
1	A	552	TRP	CD2-CE2	-5.68	1.34	1.41
1	A	685	GLU	CD-OE2	5.68	1.31	1.25
2	B	951	GLN	N-CA	-5.68	1.34	1.46
8	J	13	VAL	C-O	-5.68	1.12	1.23
1	A	792	TYR	CD2-CE2	-5.68	1.30	1.39
2	B	65	GLU	CD-OE2	5.68	1.31	1.25
2	B	1142	GLY	CA-C	-5.68	1.42	1.51
9	K	72	LYS	C-O	-5.68	1.12	1.23
3	C	66	ARG	CZ-NH1	-5.68	1.25	1.33
1	A	589	GLN	CD-NE2	5.68	1.47	1.32
1	A	1220	PHE	CD2-CE2	5.68	1.50	1.39
3	C	229	TYR	CG-CD2	5.68	1.46	1.39
8	J	39	LEU	CA-C	-5.68	1.38	1.52
1	A	1221	LYS	CG-CD	5.67	1.71	1.52
2	B	485	ARG	CZ-NH1	-5.67	1.25	1.33
3	C	70	ILE	C-N	-5.67	1.23	1.34
1	A	881	GLN	N-CA	-5.67	1.35	1.46
1	A	1256	GLU	N-CA	5.67	1.57	1.46
6	H	99	GLY	C-O	5.67	1.32	1.23
2	B	1198	TYR	CD2-CE2	5.67	1.47	1.39
6	H	81	PRO	CA-C	5.67	1.64	1.52
10	L	49	LYS	CG-CD	5.67	1.71	1.52
1	A	1144	LYS	N-CA	-5.67	1.35	1.46
3	C	19	ASP	CB-CG	-5.67	1.39	1.51
6	H	117	SER	CB-OG	5.67	1.49	1.42
1	A	1450	LEU	CG-CD2	5.67	1.72	1.51
1	A	459	ARG	C-O	-5.66	1.12	1.23
1	A	1045	VAL	CB-CG2	-5.66	1.41	1.52
2	B	1073	TYR	CE2-CZ	5.66	1.46	1.38
2	B	1144	ALA	CA-CB	-5.66	1.40	1.52
2	B	1221	SER	CA-C	5.66	1.67	1.52
3	C	13	ALA	CA-C	-5.66	1.38	1.52
7	I	65	ASP	N-CA	5.66	1.57	1.46
1	A	671	ALA	C-O	-5.66	1.12	1.23
7	I	3	THR	CB-CG2	5.66	1.71	1.52
1	A	1226	VAL	CB-CG1	-5.66	1.41	1.52
2	B	969	ARG	CZ-NH1	5.66	1.40	1.33
4	E	26	ARG	CB-CG	-5.66	1.37	1.52
10	L	40	LEU	CB-CG	5.66	1.69	1.52
3	C	132	PRO	N-CD	-5.66	1.40	1.47
7	I	75	CYS	C-O	-5.66	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	73	LEU	C-O	5.66	1.34	1.23
1	A	551	TYR	CG-CD2	-5.65	1.31	1.39
10	L	58	LYS	CE-NZ	5.65	1.63	1.49
1	A	1035	TYR	CA-CB	5.65	1.66	1.53
3	C	145	CYS	N-CA	-5.65	1.35	1.46
3	C	186	LEU	C-O	5.65	1.34	1.23
6	H	78	SER	CB-OG	-5.65	1.34	1.42
1	A	56	PRO	C-O	5.65	1.34	1.23
3	C	15	LYS	C-O	-5.65	1.12	1.23
4	E	64	PRO	CG-CD	5.65	1.69	1.50
1	A	81	PHE	CE1-CZ	-5.65	1.26	1.37
1	A	909	ASP	CG-OD1	5.65	1.38	1.25
2	B	39	ARG	N-CA	5.65	1.57	1.46
2	B	178	ASN	CG-OD1	5.65	1.36	1.24
8	J	21	TYR	CA-CB	5.65	1.66	1.53
6	H	98	TYR	CD2-CE2	5.65	1.47	1.39
1	A	143	LYS	CG-CD	5.64	1.71	1.52
1	A	171	GLN	C-O	-5.64	1.12	1.23
2	B	557	PHE	CG-CD2	5.64	1.47	1.38
2	B	604	ARG	CB-CG	5.64	1.67	1.52
2	B	916	THR	CA-CB	5.64	1.68	1.53
2	B	1087	PHE	C-O	-5.64	1.12	1.23
1	A	1228	TRP	CZ3-CH2	-5.64	1.31	1.40
2	B	90	ILE	C-O	5.64	1.34	1.23
4	E	192	ARG	CD-NE	5.64	1.56	1.46
2	B	518	HIS	CA-CB	-5.64	1.41	1.53
9	K	55	LYS	C-O	5.64	1.34	1.23
1	A	1052	GLN	CD-OE1	5.64	1.36	1.24
9	K	61	TYR	C-O	-5.64	1.12	1.23
1	A	248	PRO	N-CD	5.63	1.55	1.47
1	A	953	ASN	CG-OD1	5.63	1.36	1.24
1	A	1081	LEU	N-CA	5.63	1.57	1.46
2	B	1128	LEU	N-CA	5.63	1.57	1.46
6	H	81	PRO	CG-CD	5.63	1.69	1.50
2	B	1176	ASN	CB-CG	5.63	1.64	1.51
1	A	387	ARG	CZ-NH2	-5.63	1.25	1.33
2	B	1186	ASP	CB-CG	5.63	1.63	1.51
4	E	153	HIS	CA-CB	-5.63	1.41	1.53
9	K	18	LYS	C-O	-5.63	1.12	1.23
6	H	131	ASN	N-CA	5.63	1.57	1.46
3	C	214	ASN	CB-CG	5.63	1.64	1.51
5	F	124	GLU	CD-OE1	-5.63	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	PRO	CG-CD	-5.63	1.32	1.50
2	B	1106	ARG	N-CA	5.62	1.57	1.46
2	B	364	ILE	N-CA	-5.62	1.35	1.46
2	B	559	SER	CB-OG	-5.62	1.34	1.42
2	B	734	HIS	C-N	5.62	1.47	1.34
2	B	1109	GLY	C-O	5.62	1.32	1.23
7	I	6	PHE	C-O	-5.62	1.12	1.23
2	B	844	SER	CA-CB	-5.62	1.44	1.52
3	C	148	ARG	CD-NE	5.62	1.56	1.46
6	H	119	GLY	C-O	5.62	1.32	1.23
3	C	90	ASP	N-CA	5.62	1.57	1.46
2	B	190	TYR	CE1-CZ	5.61	1.45	1.38
2	B	698	GLU	C-O	5.61	1.34	1.23
3	C	43	THR	C-O	5.61	1.34	1.23
6	H	118	PHE	CD2-CE2	5.61	1.50	1.39
1	A	91	PHE	CE2-CZ	-5.61	1.26	1.37
1	A	1301	GLU	CG-CD	5.61	1.60	1.51
3	C	79	GLN	CG-CD	5.61	1.64	1.51
3	C	210	GLU	CD-OE2	5.61	1.31	1.25
1	A	1153	TYR	CB-CG	-5.61	1.43	1.51
2	B	269	ILE	CB-CG2	-5.61	1.35	1.52
2	B	595	ARG	C-O	-5.61	1.12	1.23
3	C	29	MET	SD-CE	5.61	2.09	1.77
1	A	1336	MET	CB-CG	-5.61	1.33	1.51
2	B	1183	LYS	CA-C	5.61	1.67	1.52
2	B	982	SER	C-O	-5.60	1.12	1.23
4	E	4	GLU	CD-OE1	-5.60	1.19	1.25
1	A	515	GLN	C-O	5.60	1.33	1.23
1	A	1154	TYR	CE2-CZ	5.60	1.45	1.38
3	C	192	TRP	CD2-CE2	-5.60	1.34	1.41
4	E	93	MET	CG-SD	5.60	1.95	1.81
1	A	27	VAL	CA-CB	-5.60	1.43	1.54
1	A	65	LEU	CA-CB	5.60	1.66	1.53
1	A	777	PHE	CD1-CE1	5.60	1.50	1.39
2	B	268	THR	N-CA	-5.60	1.35	1.46
2	B	345	LYS	C-O	-5.60	1.12	1.23
2	B	811	TYR	CZ-OH	-5.60	1.28	1.37
2	B	1019	SER	C-N	-5.60	1.21	1.34
2	B	1128	LEU	CA-C	5.60	1.67	1.52
7	I	36	GLU	CB-CG	-5.60	1.41	1.52
2	B	55	VAL	N-CA	-5.60	1.35	1.46
7	I	99	LEU	C-O	-5.60	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	ASN	CA-C	-5.59	1.38	1.52
2	B	372	SER	C-O	5.59	1.33	1.23
8	J	37	SER	CA-CB	-5.59	1.44	1.52
1	A	144	THR	CA-CB	5.59	1.67	1.53
1	A	434	ARG	CG-CD	5.59	1.66	1.51
1	A	1121	GLU	CG-CD	5.59	1.60	1.51
1	A	1255	GLU	CG-CD	5.59	1.60	1.51
6	H	21	ASN	C-O	-5.59	1.12	1.23
2	B	770	GLN	CG-CD	-5.59	1.38	1.51
1	A	514	PRO	CA-CB	-5.59	1.42	1.53
1	A	614	PHE	CE1-CZ	5.59	1.48	1.37
1	A	668	ASP	N-CA	-5.59	1.35	1.46
1	A	1164	PRO	CA-C	5.59	1.64	1.52
1	A	1237	ILE	CA-CB	-5.59	1.42	1.54
1	A	1414	ALA	N-CA	-5.59	1.35	1.46
2	B	250	PHE	CE2-CZ	5.59	1.48	1.37
2	B	1130	PHE	CD1-CE1	-5.59	1.28	1.39
4	E	81	GLU	CG-CD	-5.59	1.43	1.51
6	H	63	LEU	CA-C	5.59	1.67	1.52
7	I	105	SER	N-CA	5.58	1.57	1.46
1	A	192	GLY	C-O	5.58	1.32	1.23
3	C	190	ASP	C-O	-5.58	1.12	1.23
2	B	24	PRO	CA-CB	-5.58	1.42	1.53
2	B	882	THR	N-CA	5.58	1.57	1.46
6	H	2	SER	N-CA	5.58	1.57	1.46
1	A	402	ALA	CA-CB	-5.58	1.40	1.52
1	A	681	GLU	CB-CG	5.58	1.62	1.52
5	F	127	GLU	CG-CD	5.58	1.60	1.51
1	A	162	VAL	C-O	-5.58	1.12	1.23
2	B	103	ASN	CA-CB	5.58	1.67	1.53
2	B	946	ASN	C-O	-5.58	1.12	1.23
9	K	30	ALA	CA-C	-5.58	1.38	1.52
2	B	538	ASN	CA-CB	-5.57	1.38	1.53
6	H	2	SER	CA-C	5.57	1.67	1.52
7	I	50	THR	C-O	-5.57	1.12	1.23
2	B	1002	THR	CB-OG1	-5.57	1.32	1.43
2	B	604	ARG	N-CA	5.57	1.57	1.46
4	E	62	ALA	CA-CB	-5.57	1.40	1.52
2	B	933	SER	CA-C	5.57	1.67	1.52
1	A	425	GLN	C-O	5.57	1.33	1.23
1	A	520	CYS	CB-SG	-5.57	1.72	1.81
1	A	1203	ASN	CA-C	5.57	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	211	TYR	CG-CD2	-5.57	1.31	1.39
10	L	67	PHE	C-O	-5.57	1.12	1.23
1	A	959	ASN	CA-CB	-5.57	1.38	1.53
1	A	1285	MET	CG-SD	5.57	1.95	1.81
1	A	167	CYS	N-CA	5.56	1.57	1.46
1	A	81	PHE	CG-CD1	-5.56	1.30	1.38
1	A	852	TYR	CE1-CZ	-5.56	1.31	1.38
2	B	404	LYS	CE-NZ	-5.56	1.35	1.49
1	A	30	ILE	CB-CG2	5.56	1.70	1.52
1	A	1411	GLU	CB-CG	5.56	1.62	1.52
10	L	56	LEU	C-O	-5.56	1.12	1.23
1	A	808	LEU	C-O	-5.56	1.12	1.23
1	A	1349	TYR	CZ-OH	-5.56	1.28	1.37
2	B	344	LYS	CG-CD	5.56	1.71	1.52
5	F	127	GLU	CD-OE2	5.56	1.31	1.25
1	A	811	GLN	CB-CG	-5.56	1.37	1.52
1	A	1055	ARG	CG-CD	5.55	1.65	1.51
4	E	184	VAL	CB-CG2	5.55	1.64	1.52
1	A	708	MET	CB-CG	-5.55	1.33	1.51
1	A	737	LEU	C-O	5.55	1.33	1.23
1	A	191	THR	CB-CG2	5.55	1.70	1.52
1	A	724	GLU	CB-CG	5.55	1.62	1.52
3	C	180	TYR	CE2-CZ	-5.55	1.31	1.38
1	A	639	PRO	CA-C	5.55	1.64	1.52
2	B	945	GLU	CG-CD	5.55	1.60	1.51
1	A	15	LYS	CE-NZ	5.54	1.62	1.49
1	A	892	ALA	C-O	-5.54	1.12	1.23
2	B	227	LYS	C-O	-5.54	1.12	1.23
2	B	551	PRO	N-CD	-5.54	1.40	1.47
2	B	560	GLU	CB-CG	5.54	1.62	1.52
2	B	866	TYR	CE2-CZ	5.54	1.45	1.38
5	F	154	ASP	CB-CG	5.54	1.63	1.51
1	A	178	GLY	C-O	-5.54	1.14	1.23
1	A	1424	VAL	CB-CG1	-5.54	1.41	1.52
2	B	769	TYR	CE1-CZ	-5.54	1.31	1.38
7	I	120	GLN	CA-C	5.54	1.67	1.52
1	A	1426	GLU	CB-CG	5.54	1.62	1.52
1	A	507	VAL	CB-CG1	5.54	1.64	1.52
1	A	714	PHE	CE2-CZ	-5.54	1.26	1.37
1	A	1447	GLU	CA-C	5.54	1.67	1.52
4	E	187	TYR	CZ-OH	5.54	1.47	1.37
1	A	198	GLU	CB-CG	5.54	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	248	PRO	CB-CG	5.54	1.77	1.50
1	A	1017	LEU	CG-CD1	-5.54	1.31	1.51
2	B	778	MET	CB-CG	-5.54	1.33	1.51
4	E	139	ALA	CA-CB	5.53	1.64	1.52
2	B	96	TYR	CD2-CE2	5.53	1.47	1.39
1	A	455	MET	N-CA	5.53	1.57	1.46
4	E	102	GLU	N-CA	-5.53	1.35	1.46
2	B	65	GLU	CB-CG	5.53	1.62	1.52
1	A	505	CYS	C-O	-5.52	1.12	1.23
1	A	904	THR	CB-OG1	5.52	1.54	1.43
2	B	100	PRO	CB-CG	-5.52	1.22	1.50
9	K	46	ILE	C-N	-5.52	1.21	1.34
2	B	911	ILE	CA-CB	5.52	1.67	1.54
1	A	681	GLU	C-O	5.52	1.33	1.23
4	E	67	GLU	CD-OE2	5.52	1.31	1.25
5	F	121	ALA	C-N	-5.52	1.21	1.34
8	J	8	PHE	C-O	-5.52	1.12	1.23
1	A	688	LYS	CG-CD	5.52	1.71	1.52
1	A	12	ARG	C-O	-5.51	1.12	1.23
1	A	1064	VAL	CA-C	-5.51	1.38	1.52
1	A	1077	THR	CB-CG2	5.51	1.70	1.52
2	B	183	GLU	CD-OE2	5.51	1.31	1.25
1	A	1273	LEU	C-O	5.51	1.33	1.23
1	A	389	THR	CB-CG2	5.51	1.70	1.52
1	A	787	PHE	CB-CG	-5.51	1.42	1.51
2	B	1180	PHE	C-O	5.51	1.33	1.23
4	E	162	ARG	CZ-NH2	5.51	1.40	1.33
6	H	57	VAL	CB-CG2	5.51	1.64	1.52
1	A	1159	ARG	CB-CG	5.51	1.67	1.52
1	A	1156	PRO	C-O	5.51	1.34	1.23
1	A	1264	GLU	CA-C	-5.50	1.38	1.52
2	B	678	GLU	CD-OE1	5.50	1.31	1.25
3	C	49	VAL	CB-CG2	-5.50	1.41	1.52
1	A	744	LYS	CG-CD	5.50	1.71	1.52
1	A	912	LEU	CA-C	-5.50	1.38	1.52
2	B	1012	ILE	CA-CB	-5.50	1.42	1.54
9	K	2	ASN	CA-C	5.50	1.67	1.52
10	L	57	LEU	CG-CD1	5.50	1.72	1.51
2	B	678	GLU	CG-CD	5.50	1.60	1.51
2	B	738	PHE	CG-CD2	-5.50	1.30	1.38
2	B	643	ASP	C-O	-5.50	1.12	1.23
1	A	924	LYS	CG-CD	5.49	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	772	ALA	CA-C	5.49	1.67	1.52
4	E	57	MET	CA-CB	5.49	1.66	1.53
2	B	203	PHE	CD1-CE1	-5.49	1.28	1.39
3	C	142	VAL	CB-CG1	5.49	1.64	1.52
5	F	144	GLU	N-CA	-5.49	1.35	1.46
1	A	644	LYS	C-O	-5.49	1.12	1.23
10	L	29	TYR	CE2-CZ	-5.49	1.31	1.38
1	A	918	GLU	CA-C	-5.49	1.38	1.52
1	A	921	GLY	C-N	-5.49	1.21	1.34
2	B	367	LEU	CG-CD2	5.49	1.72	1.51
6	H	91	ASP	C-O	5.49	1.33	1.23
1	A	640	GLN	CD-OE1	5.49	1.36	1.24
2	B	70	ILE	CB-CG2	5.49	1.69	1.52
10	L	28	LYS	CD-CE	5.49	1.65	1.51
1	A	1309	ASP	CA-C	-5.49	1.38	1.52
2	B	226	PHE	CE1-CZ	5.49	1.47	1.37
2	B	237	VAL	CB-CG1	-5.49	1.41	1.52
2	B	385	LEU	CG-CD2	5.49	1.72	1.51
1	A	1284	MET	CG-SD	-5.48	1.66	1.81
1	A	1422	ARG	CZ-NH1	5.48	1.40	1.33
7	I	79	HIS	C-O	5.48	1.33	1.23
2	B	18	PHE	C-O	5.48	1.33	1.23
2	B	1154	ALA	N-CA	5.48	1.57	1.46
4	E	58	MET	CB-CG	-5.48	1.33	1.51
2	B	1160	VAL	CB-CG1	-5.48	1.41	1.52
1	A	358	ASN	C-O	-5.48	1.12	1.23
1	A	593	GLU	CG-CD	5.48	1.60	1.51
1	A	1328	TYR	CD1-CE1	-5.48	1.31	1.39
9	K	96	ASN	CB-CG	5.48	1.63	1.51
1	A	1303	GLU	N-CA	-5.48	1.35	1.46
2	B	243	ALA	CA-CB	5.48	1.64	1.52
2	B	256	VAL	CB-CG1	-5.48	1.41	1.52
1	A	712	GLU	CB-CG	5.47	1.62	1.52
2	B	20	ASP	CB-CG	5.47	1.63	1.51
2	B	1129	ARG	CZ-NH2	5.47	1.40	1.33
6	H	115	TYR	CA-CB	-5.47	1.42	1.53
1	A	1225	PHE	CB-CG	5.47	1.60	1.51
1	A	738	LYS	CE-NZ	5.47	1.62	1.49
1	A	766	GLY	C-O	-5.47	1.14	1.23
2	B	585	VAL	CB-CG2	-5.47	1.41	1.52
2	B	587	HIS	C-O	-5.47	1.12	1.23
3	C	85	ASP	CB-CG	5.47	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	GLU	N-CA	-5.47	1.35	1.46
1	A	28	ARG	CZ-NH1	5.47	1.40	1.33
1	A	1162	VAL	CB-CG2	5.46	1.64	1.52
2	B	613	VAL	CB-CG1	-5.46	1.41	1.52
1	A	594	GLY	C-O	-5.46	1.15	1.23
2	B	255	GLN	CA-CB	-5.46	1.42	1.53
2	B	377	PHE	CD1-CE1	-5.46	1.28	1.39
2	B	1211	ASN	CB-CG	-5.46	1.38	1.51
4	E	134	THR	C-O	-5.46	1.12	1.23
6	H	88	SER	CA-CB	5.46	1.61	1.52
7	I	57	GLY	C-O	-5.46	1.15	1.23
1	A	437	MET	C-O	-5.46	1.12	1.23
3	C	82	TYR	CE2-CZ	5.46	1.45	1.38
3	C	146	LYS	CG-CD	5.46	1.71	1.52
1	A	279	LEU	CA-C	-5.46	1.38	1.52
2	B	841	MET	CG-SD	-5.46	1.67	1.81
2	B	691	GLU	CB-CG	-5.46	1.41	1.52
2	B	358	LYS	CE-NZ	5.45	1.62	1.49
3	C	152	GLU	CD-OE1	5.45	1.31	1.25
5	F	141	GLY	C-O	-5.45	1.15	1.23
2	B	613	VAL	CA-C	-5.45	1.38	1.52
1	A	623	GLY	CA-C	-5.45	1.43	1.51
1	A	940	ARG	CA-CB	-5.45	1.42	1.53
2	B	1098	MET	C-O	-5.45	1.12	1.23
3	C	87	PHE	CB-CG	-5.45	1.42	1.51
6	H	115	TYR	C-O	-5.45	1.12	1.23
3	C	233	GLU	CD-OE1	5.45	1.31	1.25
6	H	109	LYS	CB-CG	5.45	1.67	1.52
4	E	16	PHE	CE2-CZ	-5.45	1.27	1.37
1	A	446	ARG	CG-CD	-5.44	1.38	1.51
2	B	99	LYS	C-O	5.44	1.33	1.23
2	B	647	GLY	C-O	-5.44	1.15	1.23
2	B	970	THR	C-O	-5.44	1.13	1.23
1	A	98	LYS	CD-CE	5.44	1.64	1.51
3	C	83	SER	CA-CB	-5.44	1.44	1.52
1	A	414	ASP	C-O	-5.44	1.13	1.23
1	A	536	LEU	CA-C	5.44	1.67	1.52
1	A	837	ILE	N-CA	-5.44	1.35	1.46
1	A	1154	TYR	CG-CD1	-5.44	1.32	1.39
2	B	1173	ALA	CA-CB	-5.44	1.41	1.52
1	A	1450	LEU	CA-CB	5.43	1.66	1.53
2	B	217	ARG	CZ-NH2	5.43	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	370	PHE	CA-CB	5.43	1.66	1.53
9	K	46	ILE	CA-CB	-5.43	1.42	1.54
3	C	82	TYR	CB-CG	-5.43	1.43	1.51
1	A	656	TRP	CZ3-CH2	-5.43	1.31	1.40
1	A	1448	GLU	N-CA	5.43	1.57	1.46
2	B	736	THR	CB-OG1	-5.43	1.32	1.43
1	A	367	PRO	CA-C	-5.43	1.42	1.52
2	B	731	VAL	CB-CG2	5.43	1.64	1.52
9	K	107	THR	C-O	5.43	1.33	1.23
1	A	386	ASP	CG-OD1	5.42	1.37	1.25
1	A	1190	PRO	N-CD	5.42	1.55	1.47
5	F	77	ASP	CG-OD1	5.42	1.37	1.25
7	I	24	ARG	C-O	5.42	1.33	1.23
1	A	49	LYS	N-CA	5.42	1.57	1.46
1	A	103	CYS	CB-SG	5.42	1.91	1.82
1	A	740	LEU	N-CA	-5.42	1.35	1.46
2	B	211	VAL	N-CA	-5.42	1.35	1.46
2	B	398	ARG	NE-CZ	-5.42	1.26	1.33
2	B	987	LYS	C-O	-5.42	1.13	1.23
2	B	933	SER	C-O	5.42	1.33	1.23
2	B	370	PHE	CG-CD2	5.42	1.46	1.38
4	E	11	ARG	CB-CG	5.42	1.67	1.52
1	A	302	THR	CA-CB	5.42	1.67	1.53
2	B	275	TYR	CD1-CE1	-5.42	1.31	1.39
3	C	84	ARG	N-CA	-5.42	1.35	1.46
4	E	74	ASP	CG-OD1	-5.42	1.12	1.25
1	A	1269	GLU	C-O	-5.41	1.13	1.23
3	C	115	SER	CB-OG	-5.41	1.35	1.42
5	F	76	LYS	CG-CD	5.41	1.70	1.52
5	F	147	SER	CB-OG	5.41	1.49	1.42
7	I	85	PHE	C-O	-5.41	1.13	1.23
3	C	194	GLU	CB-CG	5.41	1.62	1.52
1	A	351	THR	CB-CG2	-5.41	1.34	1.52
3	C	65	HIS	N-CA	-5.41	1.35	1.46
1	A	104	GLU	CG-CD	5.41	1.60	1.51
1	A	867	ILE	CB-CG1	-5.41	1.39	1.54
1	A	1324	PRO	N-CD	-5.41	1.40	1.47
2	B	30	SER	N-CA	5.41	1.57	1.46
2	B	351	TYR	CE1-CZ	-5.41	1.31	1.38
9	K	91	CYS	CA-C	5.41	1.67	1.52
1	A	514	PRO	CA-C	-5.41	1.42	1.52
2	B	608	ASP	CG-OD2	5.41	1.37	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	935	ARG	CB-CG	5.41	1.67	1.52
8	J	19	GLU	CD-OE1	-5.41	1.19	1.25
1	A	264	PHE	CA-CB	5.41	1.65	1.53
1	A	486	GLU	CG-CD	5.41	1.60	1.51
1	A	821	ARG	CZ-NH1	-5.41	1.26	1.33
1	A	1297	GLU	N-CA	-5.41	1.35	1.46
2	B	1106	ARG	CB-CG	5.41	1.67	1.52
6	H	32	THR	CA-CB	5.41	1.67	1.53
7	I	7	CYS	CB-SG	-5.41	1.73	1.81
8	J	44	TYR	CD1-CE1	5.41	1.47	1.39
2	B	308	TRP	CA-C	-5.40	1.39	1.52
9	K	66	PRO	N-CD	-5.40	1.40	1.47
1	A	599	SER	CA-C	-5.40	1.39	1.52
1	A	1210	GLY	CA-C	5.40	1.60	1.51
2	B	509	ALA	CA-C	5.40	1.67	1.52
3	C	256	ALA	CA-CB	-5.40	1.41	1.52
1	A	577	ILE	CA-CB	-5.40	1.42	1.54
1	A	645	LEU	C-O	-5.40	1.13	1.23
7	I	72	ASP	CG-OD1	5.40	1.37	1.25
2	B	310	MET	SD-CE	-5.40	1.47	1.77
4	E	160	GLU	CD-OE2	5.40	1.31	1.25
3	C	159	ALA	N-CA	-5.40	1.35	1.46
2	B	905	VAL	CB-CG1	-5.39	1.41	1.52
1	A	230	ARG	CZ-NH1	5.39	1.40	1.33
1	A	387	ARG	CB-CG	5.39	1.67	1.52
1	A	741	ASN	C-O	-5.39	1.13	1.23
5	F	128	LYS	CD-CE	5.39	1.64	1.51
1	A	419	LYS	CB-CG	5.39	1.67	1.52
3	C	252	GLN	C-O	-5.39	1.13	1.23
2	B	866	TYR	CG-CD2	5.39	1.46	1.39
2	B	174	LEU	C-O	-5.39	1.13	1.23
2	B	342	GLY	CA-C	-5.39	1.43	1.51
2	B	373	ARG	CZ-NH1	5.39	1.40	1.33
4	E	191	LYS	CB-CG	5.39	1.67	1.52
4	E	74	ASP	CA-C	5.38	1.67	1.52
5	F	78	GLN	C-O	-5.38	1.13	1.23
7	I	118	ARG	CG-CD	5.38	1.65	1.51
2	B	692	TYR	CE1-CZ	-5.38	1.31	1.38
1	A	650	GLN	CD-NE2	-5.38	1.19	1.32
1	A	1224	LEU	C-O	-5.38	1.13	1.23
4	E	9	ILE	CA-CB	5.38	1.67	1.54
9	K	31	VAL	CA-CB	5.38	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	272	THR	CA-C	-5.38	1.39	1.52
2	B	496	ARG	CB-CG	-5.38	1.38	1.52
1	A	614	PHE	CG-CD1	-5.38	1.30	1.38
1	A	1093	LYS	CG-CD	5.38	1.70	1.52
2	B	1220	ARG	NE-CZ	5.38	1.40	1.33
1	A	105	CYS	N-CA	5.38	1.57	1.46
1	A	172	PRO	CG-CD	5.38	1.68	1.50
1	A	734	GLU	CA-C	-5.38	1.39	1.52
1	A	1161	THR	C-O	5.38	1.33	1.23
10	L	46	VAL	C-O	-5.37	1.13	1.23
2	B	935	ARG	CD-NE	5.37	1.55	1.46
1	A	1147	THR	C-O	-5.37	1.13	1.23
2	B	700	SER	CA-CB	-5.37	1.45	1.52
4	E	194	GLU	CD-OE2	-5.37	1.19	1.25
1	A	301	ALA	N-CA	5.36	1.57	1.46
1	A	576	GLN	CA-C	-5.36	1.39	1.52
1	A	1169	ILE	CA-CB	5.36	1.67	1.54
2	B	262	GLU	CD-OE2	5.36	1.31	1.25
2	B	882	THR	CA-C	5.36	1.66	1.52
7	I	66	PRO	C-O	5.36	1.33	1.23
1	A	638	GLY	N-CA	-5.36	1.38	1.46
1	A	1136	SER	N-CA	-5.36	1.35	1.46
5	F	94	LEU	C-N	-5.36	1.23	1.33
5	F	106	PRO	CA-CB	-5.36	1.42	1.53
1	A	1048	ASN	CG-ND2	5.36	1.46	1.32
2	B	285	ILE	CA-CB	-5.36	1.42	1.54
2	B	397	ASP	CG-OD2	5.36	1.37	1.25
2	B	641	GLU	CB-CG	5.36	1.62	1.52
4	E	59	SER	CB-OG	5.36	1.49	1.42
2	B	557	PHE	CG-CD1	5.36	1.46	1.38
2	B	568	ASP	C-O	-5.36	1.13	1.23
2	B	857	ARG	CA-CB	-5.36	1.42	1.53
2	B	870	ILE	CB-CG2	5.36	1.69	1.52
1	A	710	LEU	CG-CD1	5.35	1.71	1.51
1	A	163	SER	N-CA	5.35	1.57	1.46
2	B	1047	PHE	CD1-CE1	-5.35	1.28	1.39
1	A	109	HIS	CB-CG	5.35	1.59	1.50
1	A	360	GLU	CB-CG	5.35	1.62	1.52
1	A	720	ARG	CD-NE	5.35	1.55	1.46
1	A	793	SER	CA-CB	-5.35	1.45	1.52
2	B	318	VAL	CB-CG1	-5.35	1.41	1.52
1	A	36	ARG	CA-C	-5.35	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	40	GLU	CD-OE2	5.35	1.31	1.25
9	K	55	LYS	CB-CG	5.35	1.67	1.52
2	B	580	VAL	CA-CB	-5.34	1.43	1.54
1	A	132	LYS	CG-CD	5.34	1.70	1.52
4	E	79	TRP	C-O	-5.34	1.13	1.23
1	A	943	LEU	C-O	-5.34	1.13	1.23
2	B	208	SER	CB-OG	-5.34	1.35	1.42
2	B	366	GLN	C-O	-5.34	1.13	1.23
2	B	643	ASP	CA-C	-5.34	1.39	1.52
3	C	205	LYS	N-CA	5.34	1.57	1.46
1	A	424	ILE	CB-CG2	-5.34	1.36	1.52
2	B	130	VAL	CA-C	5.34	1.66	1.52
7	I	89	GLN	CG-CD	-5.34	1.38	1.51
1	A	22	PHE	CB-CG	-5.34	1.42	1.51
2	B	769	TYR	N-CA	-5.34	1.35	1.46
3	C	267	GLN	C-O	5.33	1.33	1.23
7	I	44	TYR	C-O	5.33	1.33	1.23
1	A	656	TRP	CE2-CZ2	-5.33	1.30	1.39
1	A	1002	GLY	C-O	5.33	1.32	1.23
2	B	365	THR	CB-CG2	-5.33	1.34	1.52
2	B	779	GLY	C-O	-5.33	1.15	1.23
2	B	1182	CYS	N-CA	5.33	1.57	1.46
3	C	22	LEU	C-O	-5.33	1.13	1.23
4	E	71	LYS	CE-NZ	-5.33	1.35	1.49
5	F	72	LYS	CB-CG	5.33	1.67	1.52
1	A	508	PRO	CA-CB	5.33	1.64	1.53
2	B	466	TRP	C-N	5.33	1.42	1.33
2	B	598	GLU	CB-CG	5.33	1.62	1.52
7	I	93	LYS	C-O	5.33	1.33	1.23
1	A	510	GLN	C-O	5.33	1.33	1.23
6	H	137	GLN	CG-CD	5.33	1.63	1.51
7	I	44	TYR	CE1-CZ	-5.33	1.31	1.38
10	L	39	SER	CA-CB	5.33	1.60	1.52
1	A	517	ASN	CB-CG	5.33	1.63	1.51
2	B	320	ASP	CG-OD1	5.33	1.37	1.25
1	A	1443	VAL	CB-CG2	5.33	1.64	1.52
2	B	456	GLY	N-CA	5.33	1.54	1.46
3	C	89	GLU	CD-OE1	5.33	1.31	1.25
5	F	136	ARG	NE-CZ	-5.33	1.26	1.33
9	K	85	ASP	CB-CG	5.33	1.62	1.51
1	A	209	ASN	C-O	5.32	1.33	1.23
1	A	772	GLY	CA-C	-5.32	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1102	LYS	CB-CG	5.32	1.67	1.52
1	A	1315	GLU	CB-CG	5.32	1.62	1.52
2	B	240	ILE	C-O	-5.32	1.13	1.23
3	C	4	GLU	CA-C	-5.32	1.39	1.52
1	A	1311	VAL	CB-CG2	-5.32	1.41	1.52
4	E	148	GLU	CD-OE1	-5.32	1.19	1.25
1	A	651	LYS	CE-NZ	-5.32	1.35	1.49
1	A	804	TYR	N-CA	-5.32	1.35	1.46
8	J	18	TRP	CZ3-CH2	5.32	1.48	1.40
1	A	973	ILE	C-O	5.32	1.33	1.23
2	B	973	ILE	N-CA	-5.32	1.35	1.46
3	C	135	GLN	CG-CD	5.32	1.63	1.51
3	C	211	ASP	CG-OD2	5.32	1.37	1.25
9	K	69	ALA	N-CA	5.32	1.56	1.46
2	B	512	ARG	CG-CD	-5.32	1.38	1.51
2	B	1070	GLU	CG-CD	5.32	1.59	1.51
4	E	92	THR	N-CA	5.32	1.56	1.46
2	B	1132	GLU	C-O	5.31	1.33	1.23
1	A	805	LEU	CG-CD1	-5.31	1.32	1.51
1	A	689	LYS	C-O	-5.31	1.13	1.23
2	B	38	PHE	CD2-CE2	-5.31	1.28	1.39
9	K	113	THR	CA-CB	5.31	1.67	1.53
4	E	79	TRP	CA-C	-5.31	1.39	1.52
1	A	881	GLN	CD-NE2	5.31	1.46	1.32
1	A	1003	LYS	C-O	5.31	1.33	1.23
1	A	1426	GLU	CD-OE1	5.31	1.31	1.25
2	B	203	PHE	CA-CB	-5.31	1.42	1.53
1	A	883	LEU	N-CA	-5.30	1.35	1.46
1	A	1262	LYS	CA-CB	5.30	1.65	1.53
2	B	509	ALA	N-CA	-5.30	1.35	1.46
2	B	582	VAL	CB-CG2	5.30	1.64	1.52
2	B	810	GLU	CG-CD	5.30	1.59	1.51
2	B	1018	PRO	N-CA	-5.30	1.38	1.47
1	A	351	THR	C-O	-5.30	1.13	1.23
2	B	389	ALA	CA-CB	-5.30	1.41	1.52
2	B	458	LYS	CG-CD	5.30	1.70	1.52
2	B	1204	PHE	CB-CG	5.30	1.60	1.51
3	C	145	CYS	CA-CB	-5.30	1.42	1.53
6	H	142	LEU	CA-CB	-5.30	1.41	1.53
7	I	15	TYR	CG-CD2	-5.30	1.32	1.39
2	B	1041	GLU	CG-CD	5.30	1.59	1.51
1	A	1450	LEU	CA-C	5.30	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	605	ARG	CG-CD	5.30	1.65	1.51
1	A	902	LEU	N-CA	-5.30	1.35	1.46
4	E	114	ASN	CB-CG	-5.29	1.38	1.51
1	A	360	GLU	CG-CD	5.29	1.59	1.51
1	A	1023	ARG	CZ-NH1	-5.29	1.26	1.33
1	A	1193	LEU	CG-CD1	-5.29	1.32	1.51
2	B	865	LYS	CA-C	5.29	1.66	1.52
1	A	1222	ASN	CA-C	5.29	1.66	1.52
2	B	1039	GLY	CA-C	-5.29	1.43	1.51
1	A	604	GLY	CA-C	-5.29	1.43	1.51
2	B	137	TYR	CD1-CE1	5.29	1.47	1.39
1	A	966	ASN	CA-C	-5.29	1.39	1.52
1	A	1145	SER	CA-C	5.29	1.66	1.52
6	H	104	PHE	CA-CB	5.29	1.65	1.53
9	K	114	LEU	CA-C	5.29	1.66	1.52
1	A	53	LEU	CA-CB	5.29	1.66	1.53
1	A	1093	LYS	N-CA	5.29	1.56	1.46
3	C	95	CYS	C-O	-5.29	1.13	1.23
7	I	69	PRO	N-CD	-5.29	1.40	1.47
1	A	822	GLU	C-O	-5.28	1.13	1.23
2	B	1094	ARG	CA-CB	-5.28	1.42	1.53
3	C	82	TYR	N-CA	5.28	1.56	1.46
9	K	28	PRO	C-O	-5.28	1.12	1.23
1	A	946	VAL	CB-CG1	-5.28	1.41	1.52
1	A	993	LEU	CA-C	-5.28	1.39	1.52
2	B	209	GLU	CD-OE2	-5.28	1.19	1.25
2	B	1012	ILE	C-O	-5.27	1.13	1.23
1	A	807	GLY	CA-C	5.27	1.60	1.51
2	B	135	ARG	C-O	5.27	1.33	1.23
2	B	586	TRP	C-O	-5.27	1.13	1.23
2	B	1149	GLU	CG-CD	5.27	1.59	1.51
1	A	130	ASP	CG-OD1	5.27	1.37	1.25
2	B	368	GLU	CG-CD	5.27	1.59	1.51
1	A	1154	TYR	CD2-CE2	-5.27	1.31	1.39
1	A	1336	MET	C-O	-5.27	1.13	1.23
1	A	1353	TYR	CG-CD2	-5.27	1.32	1.39
7	I	44	TYR	CD1-CE1	5.26	1.47	1.39
1	A	35	ILE	CA-C	5.26	1.66	1.52
2	B	869	SER	CA-C	5.26	1.66	1.52
4	E	66	GLU	CD-OE1	5.26	1.31	1.25
1	A	187	LYS	CA-C	5.26	1.66	1.52
1	A	1176	LEU	CA-CB	5.26	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	523	CYS	C-O	-5.26	1.13	1.23
1	A	660	ASN	CG-ND2	-5.26	1.19	1.32
2	B	538	ASN	CB-CG	-5.26	1.39	1.51
2	B	682	SER	CA-CB	-5.26	1.45	1.52
1	A	154	SER	CB-OG	-5.26	1.35	1.42
1	A	502	SER	C-O	-5.26	1.13	1.23
1	A	864	ILE	C-O	5.26	1.33	1.23
1	A	905	ASP	CA-CB	-5.26	1.42	1.53
2	B	322	PHE	CD2-CE2	-5.26	1.28	1.39
2	B	655	LYS	CG-CD	5.26	1.70	1.52
2	B	800	GLN	CA-CB	-5.26	1.42	1.53
3	C	136	ASP	CG-OD1	-5.26	1.13	1.25
6	H	81	PRO	CA-CB	5.26	1.64	1.53
2	B	783	THR	C-O	-5.25	1.13	1.23
3	C	118	LEU	C-O	5.25	1.33	1.23
1	A	1078	GLN	CD-NE2	5.25	1.46	1.32
1	A	1309	ASP	CA-CB	-5.25	1.42	1.53
2	B	297	ILE	CG1-CD1	-5.25	1.14	1.50
2	B	870	ILE	CG1-CD1	5.25	1.86	1.50
3	C	264	GLN	CB-CG	5.25	1.66	1.52
2	B	265	SER	CA-C	5.25	1.66	1.52
2	B	490	SER	CB-OG	5.25	1.49	1.42
2	B	1135	ARG	C-O	-5.25	1.13	1.23
8	J	63	TYR	CG-CD1	-5.25	1.32	1.39
9	K	68	PHE	CB-CG	-5.25	1.42	1.51
2	B	267	ARG	C-O	-5.25	1.13	1.23
3	C	248	ILE	CA-CB	-5.25	1.42	1.54
8	J	18	TRP	CE3-CZ3	-5.25	1.29	1.38
2	B	234	ILE	N-CA	-5.25	1.35	1.46
2	B	479	VAL	CA-C	-5.25	1.39	1.52
2	B	833	TYR	CE2-CZ	-5.25	1.31	1.38
1	A	959	ASN	C-O	-5.25	1.13	1.23
1	A	167	CYS	CB-SG	-5.24	1.73	1.81
1	A	632	VAL	CB-CG1	-5.24	1.41	1.52
1	A	744	LYS	CA-C	-5.24	1.39	1.52
2	B	100	PRO	CA-C	5.24	1.63	1.52
2	B	554	ILE	CG1-CD1	-5.24	1.14	1.50
2	B	1030	LEU	CA-CB	-5.24	1.41	1.53
2	B	896	ASP	CA-C	-5.24	1.39	1.52
2	B	1177	HIS	N-CA	5.24	1.56	1.46
6	H	105	GLU	CD-OE1	5.24	1.31	1.25
7	I	97	MET	CA-CB	-5.24	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	955	PRO	CA-CB	-5.24	1.43	1.53
1	A	1308	THR	C-N	5.24	1.46	1.34
1	A	29	ALA	CA-CB	5.24	1.63	1.52
1	A	662	PHE	CA-C	-5.24	1.39	1.52
2	B	657	HIS	C-O	-5.24	1.13	1.23
4	E	31	THR	CB-CG2	5.24	1.69	1.52
1	A	792	TYR	CA-C	-5.23	1.39	1.52
2	B	1180	PHE	CD1-CE1	-5.23	1.28	1.39
2	B	1090	THR	CA-CB	-5.23	1.39	1.53
1	A	433	GLU	CA-CB	-5.23	1.42	1.53
1	A	1287	TYR	CB-CG	-5.23	1.43	1.51
6	H	87	ARG	CG-CD	5.23	1.65	1.51
2	B	401	PHE	CE2-CZ	5.23	1.47	1.37
2	B	540	SER	CB-OG	-5.23	1.35	1.42
1	A	348	SER	C-O	-5.22	1.13	1.23
8	J	21	TYR	CG-CD2	-5.22	1.32	1.39
1	A	965	GLN	CD-NE2	5.22	1.45	1.32
1	A	1263	ILE	CB-CG2	-5.22	1.36	1.52
1	A	1336	MET	CA-CB	-5.22	1.42	1.53
1	A	751	SER	C-O	-5.22	1.13	1.23
2	B	360	PHE	CD2-CE2	5.22	1.49	1.39
2	B	991	GLY	C-O	-5.22	1.15	1.23
4	E	72	PHE	CB-CG	5.22	1.60	1.51
6	H	27	GLU	CA-C	5.22	1.66	1.52
9	K	14	GLU	CA-C	5.22	1.66	1.52
2	B	299	GLU	C-O	-5.21	1.13	1.23
2	B	325	GLN	CA-CB	-5.21	1.42	1.53
2	B	378	LEU	CG-CD2	-5.21	1.32	1.51
2	B	595	ARG	CZ-NH2	-5.21	1.26	1.33
2	B	822	ASN	CA-C	-5.21	1.39	1.52
1	A	540	PHE	CG-CD1	-5.21	1.30	1.38
3	C	86	CYS	CA-CB	5.21	1.65	1.53
1	A	269	ILE	C-O	-5.21	1.13	1.23
1	A	411	ASP	CG-OD1	5.21	1.37	1.25
1	A	919	ILE	N-CA	5.21	1.56	1.46
1	A	1236	LEU	N-CA	5.21	1.56	1.46
2	B	1146	PHE	C-O	-5.21	1.13	1.23
1	A	448	PRO	CG-CD	-5.21	1.33	1.50
1	A	839	ARG	CZ-NH2	5.21	1.39	1.33
1	A	971	PHE	CE2-CZ	-5.21	1.27	1.37
3	C	248	ILE	CB-CG2	5.21	1.69	1.52
9	K	55	LYS	CG-CD	5.21	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1025	HIS	CA-CB	5.21	1.65	1.53
2	B	303	TYR	C-O	5.21	1.33	1.23
1	A	614	PHE	CB-CG	-5.20	1.42	1.51
1	A	1261	LYS	CG-CD	5.20	1.70	1.52
4	E	90	VAL	CA-CB	5.20	1.65	1.54
1	A	295	LEU	CG-CD1	5.20	1.71	1.51
1	A	1147	THR	CB-OG1	5.20	1.53	1.43
1	A	406	ILE	CA-CB	-5.20	1.42	1.54
1	A	1193	LEU	C-N	-5.20	1.22	1.34
2	B	57	TYR	CZ-OH	-5.20	1.29	1.37
2	B	230	ALA	CA-C	5.20	1.66	1.52
2	B	401	PHE	C-O	-5.20	1.13	1.23
7	I	94	ASP	CA-CB	5.20	1.65	1.53
2	B	25	ILE	CB-CG2	5.20	1.69	1.52
3	C	146	LYS	CE-NZ	-5.20	1.36	1.49
1	A	220	THR	CB-OG1	5.20	1.53	1.43
1	A	844	ALA	CA-C	-5.20	1.39	1.52
1	A	1345	ARG	CZ-NH2	-5.20	1.26	1.33
2	B	512	ARG	CZ-NH1	5.20	1.39	1.33
2	B	905	VAL	CB-CG2	5.20	1.63	1.52
1	A	1058	VAL	C-O	-5.19	1.13	1.23
4	E	180	ARG	CD-NE	5.19	1.55	1.46
2	B	536	VAL	CB-CG1	-5.19	1.42	1.52
2	B	1217	TYR	CD1-CE1	-5.19	1.31	1.39
3	C	31	ASN	CG-ND2	5.19	1.45	1.32
6	H	138	GLU	CD-OE2	5.19	1.31	1.25
1	A	1448	GLU	CB-CG	5.19	1.62	1.52
3	C	55	THR	C-O	5.19	1.33	1.23
1	A	619	LYS	CE-NZ	5.19	1.62	1.49
2	B	116	GLU	CB-CG	5.19	1.62	1.52
1	A	988	LEU	CG-CD2	-5.19	1.32	1.51
1	A	187	LYS	C-O	5.19	1.33	1.23
1	A	383	TYR	CG-CD2	5.18	1.45	1.39
4	E	124	VAL	CB-CG2	-5.18	1.42	1.52
6	H	56	THR	N-CA	-5.18	1.35	1.46
1	A	491	VAL	CB-CG2	-5.18	1.42	1.52
1	A	1148	ILE	C-O	-5.18	1.13	1.23
2	B	889	THR	N-CA	5.18	1.56	1.46
1	A	223	GLY	C-O	5.17	1.31	1.23
2	B	187	SER	CA-CB	-5.17	1.45	1.52
2	B	224	GLN	C-O	-5.17	1.13	1.23
2	B	418	LYS	CG-CD	5.17	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	695	ALA	CA-C	-5.17	1.39	1.52
2	B	1091	TYR	CE1-CZ	-5.17	1.31	1.38
7	I	51	ASN	CG-OD1	5.17	1.35	1.24
1	A	48	ALA	CA-CB	5.17	1.63	1.52
1	A	627	GLY	C-O	-5.17	1.15	1.23
2	B	754	SER	CB-OG	5.17	1.49	1.42
2	B	832	GLY	CA-C	-5.17	1.43	1.51
4	E	202	SER	C-O	-5.17	1.13	1.23
4	E	201	LYS	CE-NZ	5.17	1.61	1.49
1	A	1139	GLU	CA-CB	-5.17	1.42	1.53
2	B	494	HIS	C-O	-5.17	1.13	1.23
4	E	145	THR	CA-CB	-5.17	1.40	1.53
2	B	348	ARG	CB-CG	-5.17	1.38	1.52
4	E	128	PRO	CA-C	5.17	1.63	1.52
1	A	587	HIS	N-CA	-5.16	1.36	1.46
1	A	702	LEU	N-CA	-5.16	1.36	1.46
1	A	1187	GLN	C-O	5.16	1.33	1.23
2	B	986	GLN	C-O	5.16	1.33	1.23
8	J	54	VAL	CA-CB	-5.16	1.44	1.54
1	A	285	PRO	C-O	-5.16	1.12	1.23
1	A	747	VAL	CA-CB	-5.16	1.44	1.54
1	A	1064	VAL	N-CA	-5.16	1.36	1.46
2	B	815	ARG	C-O	-5.16	1.13	1.23
2	B	958	GLN	CA-CB	5.16	1.65	1.53
3	C	127	ARG	C-O	5.16	1.33	1.23
10	L	65	VAL	CA-C	-5.16	1.39	1.52
1	A	872	GLY	CA-C	-5.16	1.43	1.51
1	A	1384	VAL	CA-CB	-5.16	1.44	1.54
2	B	1067	ARG	C-N	-5.16	1.23	1.33
1	A	411	ASP	CA-C	-5.16	1.39	1.52
2	B	1100	ASP	CA-CB	5.16	1.65	1.53
8	J	62	ARG	CB-CG	5.16	1.66	1.52
2	B	755	ILE	C-O	5.15	1.33	1.23
1	A	165	GLY	N-CA	5.15	1.53	1.46
2	B	107	GLY	CA-C	5.15	1.60	1.51
7	I	21	GLU	C-O	-5.15	1.13	1.23
8	J	47	ARG	CB-CG	-5.15	1.38	1.52
1	A	1362	TYR	CB-CG	-5.15	1.44	1.51
1	A	1365	TYR	CE1-CZ	5.15	1.45	1.38
1	A	1012	ARG	NE-CZ	5.15	1.39	1.33
2	B	350	GLN	C-O	-5.15	1.13	1.23
3	C	249	ASP	CA-C	5.15	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	304	ASP	CG-OD1	5.15	1.37	1.25
3	C	48	SER	CB-OG	5.15	1.49	1.42
9	K	114	LEU	CB-CG	5.15	1.67	1.52
2	B	220	GLY	N-CA	-5.14	1.38	1.46
3	C	67	LEU	C-N	5.14	1.42	1.33
4	E	136	ASN	CG-ND2	5.14	1.45	1.32
1	A	886	ILE	CA-CB	5.14	1.66	1.54
2	B	226	PHE	CA-C	-5.14	1.39	1.52
2	B	692	TYR	C-O	-5.14	1.13	1.23
6	H	118	PHE	CA-CB	5.14	1.65	1.53
1	A	1363	VAL	CB-CG1	5.14	1.63	1.52
1	A	1283	VAL	CA-C	5.14	1.66	1.52
1	A	1418	LEU	C-O	-5.14	1.13	1.23
2	B	390	LEU	CB-CG	-5.14	1.37	1.52
2	B	586	TRP	CD2-CE2	-5.14	1.35	1.41
3	C	159	ALA	CA-CB	5.14	1.63	1.52
5	F	126	ALA	C-O	-5.14	1.13	1.23
1	A	1328	TYR	CD2-CE2	-5.14	1.31	1.39
8	J	14	VAL	CA-CB	-5.14	1.44	1.54
8	J	42	LYS	C-O	5.14	1.33	1.23
1	A	445	ASN	C-O	5.13	1.33	1.23
2	B	398	ARG	CB-CG	-5.13	1.38	1.52
2	B	870	ILE	CB-CG1	5.13	1.68	1.54
1	A	493	GLN	CA-CB	-5.13	1.42	1.53
2	B	45	SER	CA-C	-5.13	1.39	1.52
1	A	1419	ASP	CG-OD2	5.13	1.37	1.25
4	E	25	ASP	CB-CG	5.13	1.62	1.51
4	E	194	GLU	CD-OE1	-5.13	1.20	1.25
2	B	420	LEU	CA-C	-5.13	1.39	1.52
1	A	854	ASN	CA-CB	-5.13	1.39	1.53
1	A	1015	VAL	CB-CG1	-5.13	1.42	1.52
1	A	1127	ASP	CA-CB	5.13	1.65	1.53
2	B	769	TYR	CD1-CE1	-5.13	1.31	1.39
2	B	1073	TYR	CA-CB	5.13	1.65	1.53
1	A	923	LEU	CA-CB	5.13	1.65	1.53
1	A	63	ARG	CB-CG	5.12	1.66	1.52
1	A	387	ARG	NE-CZ	5.12	1.39	1.33
5	F	100	GLN	CG-CD	5.12	1.62	1.51
7	I	11	ASN	CB-CG	-5.12	1.39	1.51
1	A	23	SER	CA-C	5.12	1.66	1.52
1	A	652	VAL	CA-C	-5.12	1.39	1.52
2	B	828	ALA	CA-CB	-5.12	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1366	ARG	N-CA	-5.12	1.36	1.46
2	B	191	LYS	CE-NZ	5.12	1.61	1.49
1	A	195	ASP	CA-C	5.12	1.66	1.52
1	A	718	VAL	C-O	-5.12	1.13	1.23
2	B	51	PHE	CE2-CZ	5.12	1.47	1.37
2	B	387	LEU	CG-CD1	-5.12	1.32	1.51
2	B	1222	ARG	CD-NE	-5.12	1.37	1.46
3	C	75	MET	CB-CG	-5.12	1.34	1.51
5	F	118	LEU	CG-CD1	-5.12	1.32	1.51
6	H	104	PHE	CE1-CZ	5.12	1.47	1.37
8	J	22	LEU	CG-CD2	-5.12	1.32	1.51
2	B	793	ALA	CA-CB	-5.12	1.41	1.52
2	B	908	GLU	CD-OE1	-5.12	1.20	1.25
2	B	996	ARG	CA-CB	-5.12	1.42	1.53
1	A	1312	ASN	CG-OD1	5.12	1.35	1.24
2	B	644	GLU	N-CA	-5.12	1.36	1.46
7	I	52	ILE	C-N	-5.12	1.23	1.33
1	A	1269	GLU	CD-OE2	5.11	1.31	1.25
1	A	1305	VAL	CB-CG1	-5.11	1.42	1.52
2	B	315	LYS	CA-CB	-5.11	1.42	1.53
2	B	541	LEU	CA-CB	-5.11	1.42	1.53
2	B	868	MET	CB-CG	5.11	1.67	1.51
6	H	137	GLN	CB-CG	5.11	1.66	1.52
2	B	1045	SER	N-CA	-5.11	1.36	1.46
1	A	873	MET	SD-CE	-5.11	1.49	1.77
6	H	109	LYS	CD-CE	5.11	1.64	1.51
2	B	1153	GLU	CB-CG	5.11	1.61	1.52
1	A	372	LYS	CD-CE	-5.11	1.38	1.51
1	A	480	ALA	CA-CB	5.11	1.63	1.52
1	A	861	GLY	CA-C	-5.11	1.43	1.51
2	B	332	ASP	CB-CG	-5.11	1.41	1.51
2	B	850	LEU	CG-CD2	-5.11	1.32	1.51
2	B	1149	GLU	CA-C	-5.11	1.39	1.52
1	A	545	GLN	C-O	-5.11	1.13	1.23
1	A	813	PHE	CA-CB	-5.11	1.42	1.53
1	A	1277	GLU	CA-C	-5.11	1.39	1.52
2	B	569	TYR	CE2-CZ	-5.11	1.31	1.38
6	H	10	PHE	CD1-CE1	5.11	1.49	1.39
6	H	113	ALA	CA-CB	-5.11	1.41	1.52
1	A	1013	ASP	CG-OD2	5.10	1.37	1.25
1	A	124	GLN	CD-NE2	5.10	1.45	1.32
1	A	376	TYR	CD1-CE1	-5.10	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	556	TRP	CD2-CE3	-5.10	1.32	1.40
2	B	429	PHE	CE1-CZ	5.10	1.47	1.37
4	E	23	VAL	CB-CG2	5.10	1.63	1.52
2	B	92	PHE	CA-CB	5.10	1.65	1.53
2	B	287	ARG	CA-CB	-5.10	1.42	1.53
2	B	308	TRP	CE3-CZ3	-5.10	1.29	1.38
1	A	924	LYS	CA-CB	-5.10	1.42	1.53
5	F	73	ALA	N-CA	5.10	1.56	1.46
5	F	152	ILE	N-CA	-5.10	1.36	1.46
6	H	87	ARG	CD-NE	5.10	1.55	1.46
7	I	44	TYR	CE2-CZ	-5.10	1.31	1.38
8	J	61	LEU	CA-CB	-5.10	1.42	1.53
2	B	1149	GLU	C-N	-5.10	1.22	1.34
8	J	26	GLN	CG-CD	5.09	1.62	1.51
1	A	465	TYR	CG-CD2	-5.09	1.32	1.39
1	A	1358	SER	CA-CB	5.09	1.60	1.52
6	H	17	PRO	CG-CD	5.09	1.67	1.50
1	A	1168	GLU	CB-CG	5.09	1.61	1.52
9	K	109	TRP	CE3-CZ3	-5.09	1.29	1.38
1	A	941	LYS	CA-CB	5.09	1.65	1.53
2	B	180	TYR	CB-CG	5.09	1.59	1.51
2	B	513	GLN	CG-CD	-5.08	1.39	1.51
2	B	1011	ILE	CA-CB	5.08	1.66	1.54
1	A	82	GLY	C-O	-5.08	1.15	1.23
1	A	356	ASP	C-N	-5.08	1.24	1.34
1	A	838	GLN	CG-CD	5.08	1.62	1.51
3	C	174	ALA	N-CA	-5.08	1.36	1.46
2	B	233	PRO	CB-CG	5.08	1.75	1.50
2	B	732	SER	CA-C	5.08	1.66	1.52
9	K	98	LEU	C-O	5.08	1.33	1.23
1	A	889	SER	C-O	-5.08	1.13	1.23
8	J	42	LYS	CG-CD	5.08	1.69	1.52
1	A	498	ARG	CG-CD	5.08	1.64	1.51
2	B	480	SER	CB-OG	-5.08	1.35	1.42
4	E	21	GLU	CD-OE2	5.08	1.31	1.25
4	E	122	LYS	N-CA	5.08	1.56	1.46
7	I	65	ASP	C-O	5.08	1.32	1.23
1	A	526	ASP	CB-CG	5.08	1.62	1.51
1	A	1159	ARG	CD-NE	5.08	1.55	1.46
1	A	1171	GLN	CB-CG	5.08	1.66	1.52
2	B	1171	VAL	CB-CG1	-5.08	1.42	1.52
2	B	1171	VAL	C-O	5.08	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	202	PRO	N-CD	-5.08	1.40	1.47
3	C	234	SER	CB-OG	5.08	1.48	1.42
1	A	425	GLN	CD-NE2	5.07	1.45	1.32
1	A	1337	GLU	CG-CD	5.07	1.59	1.51
2	B	680	THR	CB-CG2	-5.07	1.35	1.52
3	C	137	LYS	CB-CG	5.07	1.66	1.52
8	J	44	TYR	CA-CB	-5.07	1.42	1.53
1	A	616	VAL	CB-CG2	-5.07	1.42	1.52
2	B	381	MET	CG-SD	5.07	1.94	1.81
1	A	70	CYS	N-CA	5.07	1.56	1.46
1	A	1144	LYS	CA-C	-5.07	1.39	1.52
1	A	1193	LEU	N-CA	5.07	1.56	1.46
1	A	1442	ASP	CA-C	-5.07	1.39	1.52
2	B	580	VAL	CB-CG2	-5.07	1.42	1.52
2	B	1181	GLU	CA-CB	5.07	1.65	1.53
3	C	20	PHE	C-O	-5.07	1.13	1.23
1	A	1010	ALA	CA-C	-5.07	1.39	1.52
2	B	624	LEU	CA-CB	-5.07	1.42	1.53
4	E	11	ARG	C-O	5.07	1.32	1.23
10	L	43	THR	N-CA	5.07	1.56	1.46
1	A	532	ARG	CB-CG	-5.06	1.38	1.52
1	A	1159	ARG	CG-CD	5.06	1.64	1.51
1	A	1354	ASN	C-O	-5.06	1.13	1.23
2	B	434	ARG	CD-NE	5.06	1.55	1.46
4	E	129	PRO	CB-CG	5.06	1.75	1.50
6	H	109	LYS	CA-CB	5.06	1.65	1.53
2	B	807	ARG	CB-CG	5.06	1.66	1.52
6	H	78	SER	C-O	-5.06	1.13	1.23
9	K	74	ARG	C-O	5.06	1.32	1.23
1	A	11	LEU	C-O	-5.06	1.13	1.23
2	B	109	THR	CA-CB	5.06	1.66	1.53
2	B	597	MET	SD-CE	-5.06	1.49	1.77
1	A	89	PRO	CA-C	-5.06	1.42	1.52
1	A	187	LYS	N-CA	5.06	1.56	1.46
2	B	119	LEU	C-O	5.06	1.32	1.23
2	B	699	GLU	CA-CB	-5.06	1.42	1.53
5	F	76	LYS	CD-CE	5.06	1.63	1.51
6	H	83	GLN	CA-C	5.06	1.66	1.52
6	H	118	PHE	CE1-CZ	-5.06	1.27	1.37
2	B	136	THR	CA-CB	5.06	1.66	1.53
1	A	418	SER	C-O	-5.05	1.13	1.23
1	A	696	GLU	N-CA	-5.05	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	435	THR	N-CA	5.05	1.56	1.46
2	B	802	PRO	N-CD	-5.05	1.40	1.47
1	A	436	ILE	N-CA	-5.05	1.36	1.46
1	A	1050	GLU	CB-CG	5.05	1.61	1.52
2	B	346	GLU	CB-CG	5.05	1.61	1.52
4	E	35	VAL	CB-CG2	-5.05	1.42	1.52
6	H	10	PHE	CE2-CZ	5.05	1.47	1.37
1	A	529	CYS	C-N	-5.05	1.24	1.33
1	A	767	GLN	CA-CB	-5.05	1.42	1.53
1	A	994	GLN	CD-OE1	-5.05	1.12	1.24
2	B	347	LYS	CA-CB	-5.05	1.42	1.53
7	I	68	LEU	N-CA	-5.05	1.36	1.46
1	A	1383	SER	C-O	-5.05	1.13	1.23
2	B	174	LEU	CG-CD1	5.05	1.70	1.51
3	C	229	TYR	CA-C	5.05	1.66	1.52
2	B	193	LYS	CD-CE	5.04	1.63	1.51
2	B	857	ARG	CB-CG	-5.04	1.39	1.52
4	E	79	TRP	CD2-CE3	5.04	1.48	1.40
10	L	33	GLU	CA-C	5.04	1.66	1.52
1	A	613	ILE	CB-CG2	-5.04	1.37	1.52
2	B	679	TYR	CE2-CZ	-5.04	1.31	1.38
2	B	822	ASN	CG-ND2	5.04	1.45	1.32
9	K	26	LYS	CA-C	5.04	1.66	1.52
9	K	71	PHE	CD2-CE2	-5.04	1.29	1.39
1	A	232	GLU	CD-OE1	5.04	1.31	1.25
1	A	858	ASN	C-O	-5.04	1.13	1.23
1	A	1348	LEU	C-O	-5.04	1.13	1.23
2	B	667	GLN	CD-OE1	5.04	1.35	1.24
2	B	738	PHE	CE1-CZ	-5.04	1.27	1.37
2	B	972	LYS	CA-CB	-5.04	1.42	1.53
7	I	77	LYS	CG-CD	5.04	1.69	1.52
9	K	67	PHE	CD1-CE1	5.04	1.49	1.39
2	B	813	LYS	C-O	-5.04	1.13	1.23
2	B	1178	ASN	N-CA	5.04	1.56	1.46
4	E	91	LYS	CA-CB	5.04	1.65	1.53
1	A	109	HIS	C-O	-5.04	1.13	1.23
2	B	870	ILE	C-O	5.04	1.32	1.23
3	C	54	ASN	C-O	-5.04	1.13	1.23
1	A	138	ILE	C-O	5.03	1.32	1.23
1	A	218	ASP	CG-OD2	5.03	1.36	1.25
1	A	1277	GLU	CB-CG	5.03	1.61	1.52
3	C	263	THR	CA-CB	-5.03	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	38	PHE	CG-CD2	5.03	1.46	1.38
2	B	546	SER	CB-OG	-5.03	1.35	1.42
1	A	777	PHE	CE1-CZ	5.03	1.47	1.37
2	B	395	GLN	CB-CG	-5.03	1.39	1.52
2	B	857	ARG	C-O	-5.03	1.13	1.23
1	A	359	LEU	CA-CB	-5.03	1.42	1.53
1	A	46	THR	CB-CG2	5.03	1.69	1.52
1	A	1309	ASP	CB-CG	-5.03	1.41	1.51
2	B	904	ARG	CZ-NH1	-5.03	1.26	1.33
3	C	67	LEU	CG-CD1	-5.03	1.33	1.51
9	K	74	ARG	CZ-NH1	-5.03	1.26	1.33
1	A	33	ALA	C-O	-5.03	1.13	1.23
2	B	323	VAL	N-CA	-5.03	1.36	1.46
3	C	218	PRO	CA-C	5.02	1.62	1.52
1	A	736	ASN	C-N	-5.02	1.22	1.34
3	C	20	PHE	CD2-CE2	5.02	1.49	1.39
5	F	121	ALA	CA-CB	-5.02	1.42	1.52
1	A	562	THR	CA-CB	5.02	1.66	1.53
2	B	327	ARG	NE-CZ	-5.02	1.26	1.33
1	A	93	VAL	CA-C	-5.02	1.40	1.52
1	A	1256	GLU	CA-CB	5.02	1.65	1.53
2	B	1064	TYR	CA-CB	-5.02	1.43	1.53
3	C	170	TRP	CZ2-CH2	-5.02	1.27	1.37
5	F	97	ARG	N-CA	-5.02	1.36	1.46
6	H	54	SER	CA-CB	5.01	1.60	1.52
7	I	100	PHE	CG-CD2	-5.01	1.31	1.38
6	H	86	ASP	CA-CB	5.01	1.65	1.53
1	A	98	LYS	CB-CG	-5.01	1.39	1.52
1	A	428	TYR	CG-CD2	-5.01	1.32	1.39
1	A	769	SER	N-CA	-5.01	1.36	1.46
3	C	79	GLN	N-CA	-5.01	1.36	1.46
3	C	156	THR	CB-CG2	5.01	1.68	1.52
9	K	92	ASN	CA-CB	5.01	1.66	1.53
2	B	695	ALA	CA-CB	-5.01	1.42	1.52
10	L	66	GLN	CD-OE1	5.01	1.34	1.24
3	C	125	MET	CA-C	5.00	1.66	1.52
1	A	369	SER	CB-OG	-5.00	1.35	1.42
2	B	68	THR	CA-CB	5.00	1.66	1.53
2	B	729	ILE	CA-CB	-5.00	1.43	1.54
4	E	197	LYS	N-CA	-5.00	1.36	1.46
1	A	1199	ARG	CZ-NH1	5.00	1.39	1.33
2	B	657	HIS	C-N	-5.00	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1085	ILE	CG1-CD1	-5.00	1.16	1.50
5	F	117	PRO	CG-CD	5.00	1.67	1.50
8	J	38	ARG	CG-CD	-5.00	1.39	1.51

All (1846) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	774	ARG	NE-CZ-NH1	34.28	137.44	120.30
1	A	469	ARG	NE-CZ-NH2	-32.36	104.12	120.30
1	A	1366	ARG	NE-CZ-NH1	31.49	136.04	120.30
3	C	35	ARG	NE-CZ-NH2	-28.02	106.29	120.30
3	C	34	ARG	NE-CZ-NH2	-27.97	106.32	120.30
1	A	1366	ARG	NE-CZ-NH2	-27.86	106.37	120.30
2	B	995	ARG	NE-CZ-NH2	-27.80	106.40	120.30
1	A	896	ARG	NE-CZ-NH2	-25.20	107.70	120.30
1	A	434	ARG	NE-CZ-NH1	24.37	132.49	120.30
3	C	35	ARG	NE-CZ-NH1	24.01	132.31	120.30
2	B	496	ARG	NE-CZ-NH1	23.83	132.22	120.30
2	B	1150	ARG	NE-CZ-NH1	-23.77	108.41	120.30
1	A	469	ARG	NE-CZ-NH1	23.24	131.92	120.30
1	A	962	ARG	NE-CZ-NH2	-23.09	108.75	120.30
1	A	1100	ARG	NE-CZ-NH2	-23.01	108.80	120.30
2	B	620	ARG	NE-CZ-NH1	-22.68	108.96	120.30
3	C	66	ARG	NE-CZ-NH2	22.65	131.63	120.30
1	A	821	ARG	NE-CZ-NH2	-22.36	109.12	120.30
1	A	774	ARG	NE-CZ-NH2	-22.33	109.13	120.30
2	B	807	ARG	NE-CZ-NH2	-22.09	109.25	120.30
9	K	47	ARG	NE-CZ-NH2	-21.55	109.52	120.30
2	B	604	ARG	NE-CZ-NH1	21.31	130.95	120.30
2	B	604	ARG	NE-CZ-NH2	-20.70	109.95	120.30
1	A	459	ARG	NE-CZ-NH2	-20.30	110.15	120.30
1	A	940	ARG	NE-CZ-NH1	20.15	130.37	120.30
1	A	1100	ARG	NE-CZ-NH1	20.12	130.36	120.30
2	B	106	ASP	CB-CG-OD2	19.58	135.92	118.30
8	J	43	ARG	NE-CZ-NH1	-19.55	110.53	120.30
1	A	434	ARG	NE-CZ-NH2	-19.27	110.67	120.30
1	A	446	ARG	NE-CZ-NH2	-18.62	110.99	120.30
8	J	43	ARG	NE-CZ-NH2	18.50	129.55	120.30
3	C	16	ASP	CB-CG-OD2	18.14	134.63	118.30
2	B	1043	ASP	CB-CG-OD2	17.89	134.40	118.30
6	H	77	ARG	NE-CZ-NH1	17.84	129.22	120.30
2	B	839	MET	CG-SD-CE	-17.75	71.80	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	66	ARG	NE-CZ-NH1	-17.38	111.61	120.30
1	A	1336	MET	CG-SD-CE	17.34	127.95	100.20
8	J	2	ILE	CG1-CB-CG2	-17.29	73.36	111.40
1	A	985	ASP	CB-CG-OD1	-17.20	102.82	118.30
3	C	34	ARG	NE-CZ-NH1	17.16	128.88	120.30
1	A	1241	ARG	NE-CZ-NH2	-17.01	111.79	120.30
8	J	48	ARG	NE-CZ-NH1	16.42	128.51	120.30
4	E	11	ARG	NE-CZ-NH1	-16.35	112.12	120.30
2	B	287	ARG	NE-CZ-NH2	-16.31	112.14	120.30
8	J	38	ARG	NE-CZ-NH1	16.19	128.40	120.30
9	K	114	LEU	CB-CG-CD2	16.18	138.51	111.00
1	A	801	GLU	OE1-CD-OE2	16.01	142.52	123.30
9	K	22	ASP	CB-CG-OD1	15.97	132.67	118.30
2	B	909	ASP	CB-CG-OD2	15.81	132.53	118.30
1	A	1422	ARG	NE-CZ-NH1	15.81	128.21	120.30
2	B	620	ARG	NH1-CZ-NH2	15.70	136.68	119.40
7	I	70	ARG	NE-CZ-NH2	-15.63	112.48	120.30
2	B	496	ARG	NE-CZ-NH2	-15.61	112.50	120.30
2	B	394	ASP	CB-CG-OD2	15.49	132.24	118.30
1	A	1241	ARG	NE-CZ-NH1	15.48	128.04	120.30
4	E	24	LYS	CD-CE-NZ	-15.31	76.50	111.70
2	B	605	ARG	NE-CZ-NH2	15.27	127.94	120.30
1	A	157	ASP	CB-CG-OD1	15.26	132.03	118.30
2	B	1135	ARG	NE-CZ-NH2	-15.22	112.69	120.30
1	A	459	ARG	NE-CZ-NH1	15.17	127.88	120.30
3	C	160	LYS	CD-CE-NZ	15.14	146.52	111.70
2	B	983	ARG	NE-CZ-NH1	15.14	127.87	120.30
7	I	91	ARG	NE-CZ-NH2	-14.92	112.84	120.30
2	B	106	ASP	CB-CG-OD1	-14.90	104.89	118.30
2	B	967	ARG	NE-CZ-NH1	-14.89	112.85	120.30
1	A	420	ARG	NE-CZ-NH1	14.86	127.73	120.30
7	I	91	ARG	NE-CZ-NH1	14.80	127.70	120.30
1	A	748	MET	CG-SD-CE	14.75	123.80	100.20
10	L	70	ARG	NE-CZ-NH1	14.73	127.66	120.30
2	B	326	ASP	CB-CG-OD2	14.72	131.54	118.30
2	B	790	ASP	CB-CG-OD2	-14.57	105.19	118.30
2	B	294	ASP	CB-CG-OD2	14.49	131.34	118.30
1	A	826	ASP	CB-CG-OD2	14.39	131.25	118.30
1	A	949	ASP	CB-CG-OD2	14.35	131.21	118.30
6	H	41	ASP	CB-CG-OD1	14.33	131.20	118.30
2	B	391	ASP	CB-CG-OD2	14.33	131.19	118.30
1	A	752	LYS	CD-CE-NZ	14.30	144.58	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1345	ARG	NE-CZ-NH2	-14.14	113.23	120.30
1	A	884	ASP	CB-CG-OD2	14.12	131.01	118.30
6	H	110	ASP	CB-CG-OD2	14.04	130.94	118.30
2	B	983	ARG	NE-CZ-NH2	-13.95	113.32	120.30
5	F	119	ARG	NE-CZ-NH2	-13.94	113.33	120.30
1	A	1135	ARG	NE-CZ-NH1	-13.92	113.34	120.30
10	L	68	GLU	OE1-CD-OE2	-13.88	106.64	123.30
2	B	564	GLU	OE1-CD-OE2	13.81	139.88	123.30
9	K	5	ASP	CB-CG-OD1	-13.78	105.90	118.30
2	B	904	ARG	NE-CZ-NH2	13.75	127.17	120.30
2	B	996	ARG	NE-CZ-NH2	-13.71	113.45	120.30
1	A	498	ARG	NE-CZ-NH1	-13.67	113.47	120.30
1	A	416	ARG	NE-CZ-NH2	-13.56	113.52	120.30
1	A	407	ARG	NE-CZ-NH2	-13.53	113.54	120.30
8	J	49	MET	CG-SD-CE	-13.51	78.58	100.20
8	J	7	CYS	CA-CB-SG	13.48	138.26	114.00
2	B	497	ARG	NE-CZ-NH2	-13.42	113.59	120.30
1	A	12	ARG	NE-CZ-NH2	-13.34	113.63	120.30
2	B	629	ASP	CB-CG-OD2	13.29	130.26	118.30
4	E	14	ARG	NE-CZ-NH1	13.28	126.94	120.30
2	B	995	ARG	NE-CZ-NH1	13.25	126.92	120.30
1	A	590	ARG	NE-CZ-NH2	-13.24	113.68	120.30
2	B	1129	ARG	NE-CZ-NH1	13.19	126.89	120.30
1	A	446	ARG	NH1-CZ-NH2	13.18	133.90	119.40
4	E	212	ARG	CD-NE-CZ	13.15	142.01	123.60
2	B	1010	LEU	CB-CG-CD1	-13.14	88.66	111.00
2	B	766	ARG	NE-CZ-NH1	-13.14	113.73	120.30
4	E	212	ARG	NE-CZ-NH2	-13.13	113.73	120.30
2	B	249	ARG	NE-CZ-NH1	13.06	126.83	120.30
2	B	1150	ARG	NH1-CZ-NH2	12.98	133.68	119.40
1	A	352	VAL	CG1-CB-CG2	-12.96	90.16	110.90
9	K	6	ARG	NE-CZ-NH2	-12.88	113.86	120.30
7	I	61	ASP	CB-CG-OD2	12.83	129.85	118.30
3	C	136	ASP	CB-CG-OD2	12.83	129.84	118.30
1	A	1006	ILE	CG1-CB-CG2	-12.77	83.31	111.40
2	B	188	ASP	CB-CG-OD2	12.77	129.79	118.30
8	J	48	ARG	NE-CZ-NH2	-12.77	113.92	120.30
2	B	996	ARG	NE-CZ-NH1	-12.69	113.95	120.30
5	F	92	ARG	NE-CZ-NH1	12.60	126.60	120.30
4	E	207	ARG	NE-CZ-NH1	12.56	126.58	120.30
1	A	884	ASP	CB-CG-OD1	-12.53	107.02	118.30
2	B	384	ARG	NE-CZ-NH1	12.53	126.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	204	THR	CA-CB-CG2	12.53	129.94	112.40
2	B	1019	SER	CB-CA-C	-12.51	86.34	110.10
1	A	1442	ASP	CB-CG-OD2	12.46	129.51	118.30
2	B	883	LEU	CA-CB-CG	12.45	143.94	115.30
1	A	386	ASP	CB-CG-OD2	-12.42	107.12	118.30
3	C	86	CYS	CA-CB-SG	12.37	136.27	114.00
2	B	654	ARG	NE-CZ-NH1	-12.31	114.15	120.30
1	A	962	ARG	NE-CZ-NH1	12.30	126.45	120.30
1	A	961	ARG	NE-CZ-NH2	12.21	126.41	120.30
1	A	416	ARG	NE-CZ-NH1	12.18	126.39	120.30
1	A	130	ASP	CB-CG-OD1	12.17	129.25	118.30
4	E	14	ARG	NE-CZ-NH2	-12.15	114.23	120.30
2	B	605	ARG	NE-CZ-NH1	-12.13	114.23	120.30
1	A	538	ASP	CB-CA-C	-12.13	86.15	110.40
3	C	85	ASP	CB-CG-OD2	12.04	129.13	118.30
2	B	996	ARG	NH1-CZ-NH2	12.00	132.60	119.40
1	A	782	ARG	NE-CZ-NH1	11.99	126.29	120.30
2	B	405	ARG	NE-CZ-NH1	11.97	126.29	120.30
2	B	1129	ARG	NE-CZ-NH2	-11.90	114.35	120.30
10	L	27	LEU	CA-CB-CG	11.89	142.64	115.30
2	B	620	ARG	NE-CZ-NH2	-11.88	114.36	120.30
1	A	549	MET	CG-SD-CE	11.87	119.19	100.20
3	C	220	ASP	CB-CG-OD1	11.87	128.98	118.30
1	A	961	ARG	NE-CZ-NH1	-11.84	114.38	120.30
2	B	120	ARG	NE-CZ-NH1	-11.82	114.39	120.30
2	B	552	MET	CG-SD-CE	11.78	119.05	100.20
2	B	642	ASP	CB-CG-OD1	11.78	128.90	118.30
2	B	747	MET	CG-SD-CE	-11.75	81.39	100.20
2	B	346	GLU	OE1-CD-OE2	-11.73	109.22	123.30
1	A	949	ASP	N-CA-CB	-11.64	89.64	110.60
5	F	81	THR	N-CA-CB	-11.57	88.32	110.30
1	A	346	ASP	CB-CG-OD1	11.56	128.70	118.30
1	A	42	ASP	CB-CG-OD2	11.48	128.64	118.30
8	J	1	MET	CG-SD-CE	-11.46	81.86	100.20
1	A	1036	ARG	NE-CZ-NH2	-11.46	114.57	120.30
1	A	806	ARG	NE-CZ-NH1	-11.45	114.57	120.30
1	A	909	ASP	CB-CG-OD2	-11.40	108.04	118.30
2	B	711	GLU	OE1-CD-OE2	-11.40	109.62	123.30
1	A	781	ASP	CB-CG-OD1	11.38	128.54	118.30
2	B	1096	ARG	NE-CZ-NH2	-11.34	114.63	120.30
1	A	992	ASP	CB-CG-OD2	11.33	128.50	118.30
1	A	941	LYS	CD-CE-NZ	-11.29	85.74	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1062	GLU	CB-CA-C	-11.24	87.92	110.40
2	B	394	ASP	CB-CG-OD1	-11.22	108.20	118.30
7	I	30	ARG	NE-CZ-NH1	-11.17	114.71	120.30
1	A	291	GLU	OE1-CD-OE2	-11.16	109.91	123.30
2	B	1097	HIS	CB-CG-ND1	-11.13	95.37	123.20
7	I	54	GLU	OE1-CD-OE2	11.10	136.62	123.30
1	A	857	ARG	NE-CZ-NH1	-11.08	114.76	120.30
2	B	598	GLU	OE1-CD-OE2	-11.01	110.09	123.30
1	A	609	ASP	CB-CG-OD2	11.01	128.21	118.30
9	K	1	MET	CG-SD-CE	10.97	117.75	100.20
2	B	373	ARG	NE-CZ-NH2	-10.94	114.83	120.30
5	F	92	ARG	NE-CZ-NH2	-10.92	114.84	120.30
2	B	287	ARG	NE-CZ-NH1	10.89	125.75	120.30
2	B	790	ASP	CB-CG-OD1	10.83	128.05	118.30
7	I	106	CYS	CA-CB-SG	10.78	133.41	114.00
2	B	1060	ARG	NE-CZ-NH2	-10.78	114.91	120.30
2	B	629	ASP	CB-CG-OD1	-10.75	108.62	118.30
7	I	81	ARG	NE-CZ-NH1	10.75	125.67	120.30
1	A	1366	ARG	CD-NE-CZ	10.75	138.65	123.60
2	B	1185	CYS	CA-CB-SG	10.73	133.32	114.00
1	A	438	ASP	CB-CG-OD2	10.71	127.94	118.30
1	A	350	ARG	NE-CZ-NH1	10.70	125.65	120.30
1	A	1196	GLU	OE1-CD-OE2	10.68	136.12	123.30
1	A	853	ASP	CB-CG-OD2	10.66	127.89	118.30
2	B	1050	ILE	CG1-CB-CG2	-10.66	87.94	111.40
1	A	1334	ASP	CB-CG-OD1	10.65	127.88	118.30
9	K	73	LEU	CB-CG-CD1	-10.64	92.91	111.00
1	A	944	ARG	NE-CZ-NH1	10.61	125.61	120.30
1	A	93	VAL	CB-CA-C	-10.60	91.26	111.40
2	B	434	ARG	NE-CZ-NH1	10.55	125.58	120.30
1	A	1207	LEU	CB-CG-CD1	-10.55	93.07	111.00
1	A	885	THR	CA-CB-CG2	10.53	127.15	112.40
1	A	1375	MET	CG-SD-CE	10.48	116.96	100.20
1	A	537	ARG	NE-CZ-NH2	-10.47	115.07	120.30
2	B	620	ARG	CG-CD-NE	-10.46	89.83	111.80
6	H	135	LEU	CA-CB-CG	10.46	139.36	115.30
1	A	386	ASP	CB-CG-OD1	10.45	127.71	118.30
2	B	24	PRO	N-CD-CG	-10.43	87.56	103.20
1	A	1326	ARG	NE-CZ-NH1	10.42	125.51	120.30
4	E	167	ARG	NE-CZ-NH1	-10.42	115.09	120.30
1	A	446	ARG	NE-CZ-NH1	-10.40	115.10	120.30
9	K	47	ARG	NE-CZ-NH1	10.40	125.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	43	VAL	N-CA-CB	-10.38	88.65	111.50
3	C	76	ASP	CB-CG-OD2	-10.38	108.96	118.30
1	A	486	GLU	OE1-CD-OE2	-10.36	110.86	123.30
7	I	81	ARG	NE-CZ-NH2	-10.36	115.12	120.30
3	C	11	ARG	NE-CZ-NH1	10.33	125.47	120.30
3	C	125	MET	CG-SD-CE	10.32	116.71	100.20
1	A	740	LEU	CB-CG-CD1	10.31	128.52	111.00
1	A	1442	ASP	CB-CG-OD1	-10.29	109.03	118.30
1	A	36	ARG	NE-CZ-NH1	10.29	125.44	120.30
2	B	730	ARG	NE-CZ-NH2	10.28	125.44	120.30
3	C	155	LEU	CB-CA-C	-10.25	90.72	110.20
3	C	163	ILE	CA-CB-CG2	10.25	131.39	110.90
2	B	760	ASP	CB-CG-OD2	10.22	127.50	118.30
1	A	1202	MET	CG-SD-CE	10.21	116.54	100.20
1	A	174	ILE	CG1-CB-CG2	-10.19	88.98	111.40
1	A	28	ARG	NE-CZ-NH1	10.15	125.38	120.30
4	E	201	LYS	CD-CE-NZ	-10.11	88.44	111.70
10	L	34	CYS	CA-CB-SG	-10.11	95.81	114.00
2	B	46	GLN	CA-CB-CG	-10.08	91.21	113.40
2	B	198	ASP	CB-CG-OD1	10.08	127.37	118.30
2	B	579	ARG	NE-CZ-NH1	-10.06	115.27	120.30
1	A	532	ARG	NE-CZ-NH1	10.05	125.33	120.30
2	B	95	ILE	CG1-CB-CG2	-10.04	89.32	111.40
1	A	557	ASP	CB-CG-OD2	10.03	127.33	118.30
1	A	1204	ASP	CB-CG-OD2	10.03	127.32	118.30
1	A	53	LEU	CA-CB-CG	10.02	138.35	115.30
1	A	731	ARG	NE-CZ-NH2	-9.97	115.31	120.30
2	B	1060	ARG	NE-CZ-NH1	9.96	125.28	120.30
10	L	68	GLU	CG-CD-OE1	9.95	138.21	118.30
6	H	130	ARG	NE-CZ-NH1	-9.95	115.32	120.30
1	A	518	LYS	CD-CE-NZ	-9.93	88.85	111.70
2	B	304	ASP	CB-CG-OD1	9.93	127.24	118.30
1	A	974	ASP	N-CA-CB	9.92	128.45	110.60
7	I	73	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	A	949	ASP	CB-CG-OD1	-9.91	109.38	118.30
2	B	1215	ARG	NE-CZ-NH1	9.91	125.25	120.30
2	B	384	ARG	NE-CZ-NH2	-9.89	115.35	120.30
1	A	1043	ASP	CB-CG-OD2	9.88	127.19	118.30
2	B	807	ARG	NE-CZ-NH1	9.87	125.23	120.30
8	J	1	MET	N-CA-CB	-9.86	92.84	110.60
1	A	393	ARG	NE-CZ-NH2	9.86	125.23	120.30
2	B	407	ASP	CB-CG-OD1	9.85	127.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	5	ASP	CB-CG-OD2	9.83	127.15	118.30
9	K	114	LEU	CA-CB-CG	9.81	137.87	115.30
1	A	620	LYS	CD-CE-NZ	9.80	134.23	111.70
1	A	1062	GLU	OE1-CD-OE2	9.79	135.04	123.30
9	K	39	ASP	CB-CG-OD1	9.77	127.09	118.30
1	A	728	LYS	CD-CE-NZ	9.76	134.15	111.70
2	B	353	LYS	CD-CE-NZ	9.76	134.14	111.70
2	B	1067	ARG	NE-CZ-NH1	9.75	125.18	120.30
3	C	165	LYS	CD-CE-NZ	9.75	134.12	111.70
3	C	18	VAL	CB-CA-C	-9.74	92.89	111.40
1	A	782	ARG	NE-CZ-NH2	-9.74	115.43	120.30
4	E	81	GLU	OE1-CD-OE2	9.73	134.97	123.30
8	J	62	ARG	NE-CZ-NH1	9.73	125.16	120.30
4	E	25	ASP	CB-CG-OD2	9.72	127.05	118.30
1	A	1064	VAL	N-CA-CB	-9.70	90.16	111.50
1	A	909	ASP	CB-CG-OD1	9.69	127.02	118.30
1	A	982	THR	CA-CB-CG2	9.69	125.97	112.40
1	A	1284	MET	CA-CB-CG	-9.69	96.82	113.30
2	B	303	TYR	CB-CG-CD1	9.69	126.82	121.00
2	B	728	ARG	NE-CZ-NH1	-9.68	115.46	120.30
2	B	646	LEU	CB-CG-CD2	9.66	127.42	111.00
5	F	135	ARG	NE-CZ-NH1	-9.64	115.48	120.30
2	B	337	ARG	CG-CD-NE	-9.63	91.57	111.80
1	A	163	SER	N-CA-CB	9.63	124.94	110.50
2	B	791	THR	OG1-CB-CG2	-9.61	87.89	110.00
1	A	419	LYS	CD-CE-NZ	-9.61	89.60	111.70
1	A	1228	TRP	CB-CA-C	-9.61	91.19	110.40
1	A	391	LEU	CB-CG-CD2	-9.60	94.68	111.00
6	H	80	ARG	NE-CZ-NH2	9.59	125.10	120.30
1	A	821	ARG	CG-CD-NE	-9.55	91.74	111.80
1	A	896	ARG	NH1-CZ-NH2	9.54	129.90	119.40
1	A	940	ARG	NE-CZ-NH2	-9.52	115.54	120.30
7	I	75	CYS	CA-CB-SG	9.52	131.14	114.00
7	I	113	ASP	CB-CG-OD2	9.50	126.85	118.30
1	A	771	GLU	OE1-CD-OE2	9.50	134.70	123.30
3	C	26	ASP	CB-CG-OD1	9.49	126.84	118.30
3	C	183	TRP	C-N-CA	-9.45	98.07	121.70
7	I	7	CYS	CA-CB-SG	9.45	131.01	114.00
7	I	92	ARG	NE-CZ-NH1	-9.43	115.58	120.30
2	B	652	LYS	CD-CE-NZ	9.43	133.38	111.70
1	A	1267	MET	CG-SD-CE	-9.42	85.13	100.20
1	A	555	ASP	CB-CG-OD1	9.39	126.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	367	LEU	CB-CG-CD2	9.39	126.96	111.00
1	A	1223	ASP	CB-CG-OD1	9.38	126.74	118.30
3	C	84	ARG	NE-CZ-NH2	9.38	124.99	120.30
2	B	972	LYS	CD-CE-NZ	-9.38	90.14	111.70
2	B	1009	ASP	CB-CG-OD1	9.37	126.73	118.30
3	C	172	PRO	N-CD-CG	9.34	117.21	103.20
7	I	72	ASP	CB-CG-OD1	9.34	126.70	118.30
2	B	722	ASP	CB-CG-OD1	9.31	126.68	118.30
2	B	416	LEU	CB-CA-C	-9.30	92.53	110.20
1	A	857	ARG	NE-CZ-NH2	9.29	124.94	120.30
1	A	200	ARG	NE-CZ-NH2	-9.27	115.67	120.30
1	A	466	SER	CB-CA-C	-9.26	92.51	110.10
1	A	1055	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	A	727	ASP	CB-CG-OD1	9.25	126.63	118.30
1	A	565	ILE	CG1-CB-CG2	-9.25	91.06	111.40
5	F	119	ARG	NE-CZ-NH1	9.23	124.92	120.30
2	B	705	MET	CG-SD-CE	-9.22	85.44	100.20
7	I	109	ILE	CG1-CB-CG2	-9.22	91.12	111.40
1	A	1155	ASP	CB-CG-OD1	9.21	126.59	118.30
9	K	51	LEU	CB-CG-CD1	-9.21	95.34	111.00
6	H	8	ASP	CB-CG-OD2	9.20	126.58	118.30
2	B	320	ASP	CB-CG-OD1	9.14	126.53	118.30
1	A	982	THR	N-CA-CB	-9.13	92.94	110.30
1	A	1233	ASP	CB-CG-OD2	9.13	126.52	118.30
1	A	720	ARG	NE-CZ-NH2	9.13	124.86	120.30
9	K	83	PRO	N-CD-CG	-9.11	89.54	103.20
3	C	143	LEU	CB-CG-CD2	-9.10	95.52	111.00
2	B	118	ARG	NE-CZ-NH1	9.08	124.84	120.30
2	B	57	TYR	CB-CG-CD2	9.07	126.44	121.00
2	B	642	ASP	N-CA-C	-9.07	86.52	111.00
1	A	177	ASP	CB-CG-OD2	9.05	126.44	118.30
1	A	1264	GLU	OE1-CD-OE2	-9.05	112.44	123.30
2	B	391	ASP	OD1-CG-OD2	-9.04	106.12	123.30
1	A	74	MET	CG-SD-CE	9.02	114.62	100.20
1	A	618	GLU	OE1-CD-OE2	9.00	134.10	123.30
1	A	652	VAL	CG1-CB-CG2	-8.99	96.52	110.90
2	B	1098	MET	CG-SD-CE	8.97	114.56	100.20
2	B	1028	GLU	OE1-CD-OE2	-8.97	112.54	123.30
1	A	1326	ARG	NE-CZ-NH2	8.96	124.78	120.30
1	A	414	ASP	CB-CG-OD1	8.95	126.36	118.30
2	B	552	MET	CA-CB-CG	8.94	128.50	113.30
2	B	485	ARG	NE-CZ-NH2	-8.93	115.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ILE	CG1-CB-CG2	-8.93	91.75	111.40
1	A	134	ARG	NE-CZ-NH1	8.93	124.76	120.30
1	A	230	ARG	NE-CZ-NH2	-8.91	115.84	120.30
2	B	632	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	A	1285	MET	CG-SD-CE	8.87	114.39	100.20
9	K	53	ASP	CB-CG-OD2	8.86	126.28	118.30
1	A	70	CYS	CA-CB-SG	8.86	129.94	114.00
10	L	47	ARG	NE-CZ-NH2	8.86	124.73	120.30
1	A	1269	GLU	OE1-CD-OE2	8.85	133.92	123.30
1	A	504	LEU	CA-CB-CG	8.84	135.63	115.30
1	A	1257	ASP	CB-CG-OD2	8.82	126.24	118.30
6	H	25	ARG	NE-CZ-NH1	8.82	124.71	120.30
2	B	303	TYR	CZ-CE2-CD2	8.82	127.74	119.80
1	A	1438	THR	N-CA-CB	-8.81	93.56	110.30
1	A	1326	ARG	NH1-CZ-NH2	-8.81	109.71	119.40
2	B	1043	ASP	CB-CG-OD1	-8.81	110.37	118.30
2	B	998	ASP	CB-CG-OD2	8.79	126.22	118.30
5	F	97	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	A	913	LEU	CB-CG-CD1	-8.78	96.08	111.00
1	A	472	LEU	CA-CB-CG	-8.77	95.12	115.30
1	A	28	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	A	107	CYS	CA-CB-SG	8.75	129.74	114.00
1	A	636	GLU	OE1-CD-OE2	-8.75	112.81	123.30
7	I	1	MET	CG-SD-CE	8.74	114.19	100.20
6	H	132	LEU	CA-CB-CG	8.74	135.39	115.30
2	B	1006	ILE	CG1-CB-CG2	-8.73	92.19	111.40
2	B	1219	ASP	CB-CG-OD2	8.72	126.15	118.30
1	A	1230	GLU	OE1-CD-OE2	8.72	133.77	123.30
2	B	1097	HIS	CB-CA-C	8.72	127.84	110.40
2	B	1160	VAL	CB-CA-C	-8.72	94.84	111.40
2	B	1041	GLU	OE1-CD-OE2	8.70	133.74	123.30
2	B	1127	GLY	N-CA-C	8.69	134.81	113.10
1	A	393	ARG	NE-CZ-NH1	-8.68	115.96	120.30
1	A	283	GLY	N-CA-C	-8.67	91.42	113.10
3	C	93	ASP	CB-CG-OD2	8.67	126.10	118.30
1	A	199	LEU	CA-CB-CG	8.66	135.22	115.30
1	A	567	LYS	CD-CE-NZ	8.66	131.62	111.70
2	B	591	ARG	NE-CZ-NH1	8.66	124.63	120.30
2	B	138	GLU	OE1-CD-OE2	-8.65	112.92	123.30
1	A	1284	MET	CG-SD-CE	-8.65	86.37	100.20
2	B	90	ILE	CB-CA-C	-8.64	94.33	111.60
2	B	1220	ARG	NE-CZ-NH2	8.63	124.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	13	MET	CG-SD-CE	-8.62	86.40	100.20
2	B	622	LYS	CA-CB-CG	8.62	132.37	113.40
1	A	1134	ILE	CG1-CB-CG2	-8.62	92.44	111.40
1	A	455	MET	CG-SD-CE	-8.62	86.42	100.20
3	C	194	GLU	OE1-CD-OE2	8.62	133.64	123.30
2	B	680	THR	N-CA-CB	-8.61	93.94	110.30
2	B	327	ARG	NE-CZ-NH1	-8.61	116.00	120.30
2	B	1132	GLU	OE1-CD-OE2	-8.60	112.98	123.30
1	A	464	PRO	O-C-N	-8.60	108.95	122.70
1	A	157	ASP	OD1-CG-OD2	-8.55	107.05	123.30
4	E	72	PHE	CG-CD2-CE2	-8.55	111.39	120.80
2	B	498	THR	N-CA-CB	-8.55	94.06	110.30
4	E	154	ILE	CG1-CB-CG2	-8.54	92.61	111.40
2	B	398	ARG	NE-CZ-NH1	-8.53	116.03	120.30
7	I	31	THR	N-CA-CB	-8.53	94.09	110.30
10	L	27	LEU	CB-CG-CD2	8.51	125.47	111.00
1	A	115	LEU	CB-CG-CD1	8.51	125.47	111.00
7	I	45	ARG	NE-CZ-NH1	-8.50	116.05	120.30
2	B	1182	CYS	CA-CB-SG	8.49	129.29	114.00
1	A	1307	GLU	OE1-CD-OE2	-8.48	113.12	123.30
1	A	771	GLU	CG-CD-OE1	-8.47	101.36	118.30
1	A	908	LEU	CB-CG-CD2	-8.47	96.61	111.00
2	B	963	PHE	CB-CA-C	-8.46	93.47	110.40
2	B	1077	THR	N-CA-CB	-8.46	94.23	110.30
1	A	389	THR	OG1-CB-CG2	-8.45	90.56	110.00
1	A	1062	GLU	CA-CB-CG	8.45	131.98	113.40
2	B	359	GLU	OE1-CD-OE2	8.44	133.43	123.30
4	E	84	ASP	CB-CG-OD1	8.43	125.89	118.30
1	A	239	LEU	CA-CB-CG	8.42	134.68	115.30
2	B	959	ASP	CB-CG-OD2	8.42	125.87	118.30
3	C	26	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	A	188	ASP	CB-CG-OD2	8.41	125.87	118.30
1	A	1318	THR	N-CA-CB	-8.40	94.34	110.30
1	A	600	PRO	N-CD-CG	-8.40	90.60	103.20
1	A	53	LEU	CB-CG-CD1	8.39	125.26	111.00
2	B	348	ARG	NE-CZ-NH2	-8.38	116.11	120.30
2	B	999	MET	CG-SD-CE	-8.38	86.80	100.20
2	B	137	TYR	CA-CB-CG	8.37	129.31	113.40
1	A	126	LEU	CB-CG-CD1	-8.37	96.78	111.00
2	B	852	ARG	NE-CZ-NH2	8.36	124.48	120.30
1	A	922	ASP	CB-CG-OD1	8.35	125.82	118.30
7	I	5	ARG	NE-CZ-NH1	8.35	124.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	25	ASP	OD1-CG-OD2	-8.34	107.45	123.30
1	A	547	LEU	CB-CG-CD2	-8.31	96.86	111.00
6	H	127	GLY	N-CA-C	8.31	133.88	113.10
8	J	63	TYR	CB-CG-CD1	8.31	125.99	121.00
1	A	1012	ARG	CG-CD-NE	-8.30	94.38	111.80
2	B	165	VAL	CB-CA-C	-8.29	95.64	111.40
2	B	408	LEU	CB-CG-CD2	-8.29	96.90	111.00
1	A	706	HIS	N-CA-CB	8.29	125.53	110.60
1	A	399	HIS	C-N-CD	-8.28	102.37	120.60
1	A	243	PRO	N-CD-CG	-8.28	90.78	103.20
1	A	65	LEU	CA-CB-CG	8.26	134.30	115.30
1	A	1376	THR	N-CA-CB	-8.25	94.62	110.30
8	J	45	CYS	CA-CB-SG	8.25	128.85	114.00
1	A	761	MET	CG-SD-CE	8.25	113.39	100.20
4	E	182	ASP	CB-CG-OD1	8.24	125.72	118.30
4	E	163	GLU	OE1-CD-OE2	-8.24	113.41	123.30
2	B	630	ALA	CB-CA-C	-8.24	97.74	110.10
1	A	164	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	A	537	ARG	CB-CG-CD	8.22	132.98	111.60
3	C	260	LEU	CB-CG-CD2	8.22	124.97	111.00
1	A	1404	GLU	C-N-CA	-8.21	101.17	121.70
2	B	49	ASP	CB-CG-OD2	8.20	125.68	118.30
3	C	117	ASP	CB-CG-OD1	8.20	125.68	118.30
5	F	90	ARG	NE-CZ-NH1	-8.20	116.20	120.30
1	A	1415	SER	CB-CA-C	-8.18	94.57	110.10
2	B	764	SER	N-CA-CB	-8.18	98.24	110.50
1	A	683	ILE	CG1-CB-CG2	-8.17	93.42	111.40
2	B	568	ASP	CB-CG-OD2	8.17	125.65	118.30
2	B	895	ASP	CB-CG-OD2	8.17	125.65	118.30
1	A	1385	THR	N-CA-CB	-8.17	94.78	110.30
2	B	326	ASP	CB-CG-OD1	-8.16	110.95	118.30
2	B	101	MET	CG-SD-CE	8.16	113.25	100.20
3	C	53	THR	OG1-CB-CG2	-8.16	91.24	110.00
2	B	1004	GLU	OE1-CD-OE2	-8.15	113.52	123.30
1	A	364	VAL	CG1-CB-CG2	-8.14	97.87	110.90
4	E	211	TYR	CB-CG-CD1	8.13	125.88	121.00
2	B	547	VAL	CG1-CB-CG2	8.12	123.88	110.90
1	A	709	THR	OG1-CB-CG2	-8.11	91.35	110.00
2	B	513	GLN	CA-CB-CG	8.10	131.23	113.40
2	B	89	GLU	OE1-CD-OE2	-8.10	113.58	123.30
1	A	483	ASP	CB-CG-OD1	-8.10	111.01	118.30
2	B	100	PRO	N-CD-CG	-8.09	91.06	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	56	ASP	CB-CG-OD2	8.08	125.58	118.30
8	J	2	ILE	CB-CA-C	-8.08	95.44	111.60
4	E	16	PHE	CB-CG-CD1	8.07	126.45	120.80
1	A	557	ASP	C-N-CA	-8.07	105.35	122.30
2	B	940	PRO	N-CD-CG	-8.07	91.10	103.20
2	B	598	GLU	CG-CD-OE2	8.06	134.43	118.30
3	C	29	MET	CG-SD-CE	8.06	113.09	100.20
1	A	146	MET	N-CA-CB	-8.05	96.11	110.60
1	A	450	LEU	CB-CG-CD1	-8.05	97.32	111.00
2	B	598	GLU	N-CA-CB	8.04	125.08	110.60
1	A	149	GLU	OE1-CD-OE2	8.03	132.94	123.30
2	B	848	ARG	NE-CZ-NH1	-8.03	116.28	120.30
1	A	709	THR	N-CA-CB	-8.03	95.05	110.30
2	B	1096	ARG	NE-CZ-NH1	8.02	124.31	120.30
3	C	85	ASP	CB-CG-OD1	-8.02	111.08	118.30
1	A	1012	ARG	NE-CZ-NH1	8.01	124.31	120.30
2	B	559	SER	CA-CB-OG	-8.01	89.57	111.20
1	A	1271	ILE	CG1-CB-CG2	-8.01	93.78	111.40
1	A	895	LYS	CD-CE-NZ	-8.01	93.28	111.70
1	A	1226	VAL	CB-CA-C	-8.01	96.19	111.40
9	K	10	PHE	CB-CG-CD2	8.01	126.40	120.80
1	A	898	ARG	NE-CZ-NH1	8.00	124.30	120.30
4	E	25	ASP	CB-CG-OD1	7.99	125.49	118.30
2	B	1033	LYS	CD-CE-NZ	-7.99	93.32	111.70
2	B	911	ILE	CG1-CB-CG2	-7.99	93.83	111.40
2	B	1026	LEU	CB-CG-CD1	-7.98	97.43	111.00
1	A	731	ARG	NH1-CZ-NH2	7.98	128.18	119.40
1	A	740	LEU	CB-CG-CD2	-7.98	97.44	111.00
2	B	601	ARG	NE-CZ-NH1	-7.98	116.31	120.30
1	A	177	ASP	CB-CG-OD1	-7.97	111.13	118.30
1	A	787	PHE	CB-CG-CD2	7.97	126.38	120.80
1	A	1385	THR	N-CA-C	7.96	132.48	111.00
1	A	1103	GLU	CB-CA-C	7.94	126.28	110.40
6	H	114	VAL	CG1-CB-CG2	-7.94	98.20	110.90
8	J	3	VAL	CG1-CB-CG2	7.93	123.59	110.90
1	A	630	ILE	CG1-CB-CG2	-7.93	93.95	111.40
1	A	592	ASP	CB-CG-OD1	7.93	125.43	118.30
1	A	659	HIS	CB-CG-ND1	-7.93	103.38	123.20
2	B	174	LEU	CB-CG-CD2	7.92	124.47	111.00
9	K	24	ASP	CB-CG-OD2	7.92	125.43	118.30
1	A	728	LYS	N-CA-CB	7.92	124.85	110.60
9	K	70	ARG	NE-CZ-NH2	7.90	124.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	708	MET	N-CA-CB	-7.89	96.40	110.60
2	B	1129	ARG	CG-CD-NE	-7.88	95.25	111.80
1	A	1356	ILE	CG1-CB-CG2	-7.88	94.06	111.40
1	A	57	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	A	1239	ARG	CB-CA-C	7.86	126.13	110.40
1	A	532	ARG	NE-CZ-NH2	-7.86	116.37	120.30
8	J	22	LEU	N-CA-CB	-7.86	94.68	110.40
1	A	1119	TYR	CG-CD2-CE2	7.86	127.58	121.30
1	A	1151	GLU	OE1-CD-OE2	-7.86	113.87	123.30
2	B	257	LYS	CD-CE-NZ	-7.85	93.64	111.70
2	B	1135	ARG	NH1-CZ-NH2	7.85	128.04	119.40
2	B	387	LEU	CB-CG-CD1	-7.84	97.67	111.00
6	H	102	TYR	CD1-CE1-CZ	-7.82	112.77	119.80
10	L	58	LYS	CA-C-N	7.81	134.39	117.20
1	A	982	THR	OG1-CB-CG2	-7.81	92.04	110.00
1	A	1055	ARG	CG-CD-NE	-7.80	95.41	111.80
2	B	118	ARG	CD-NE-CZ	7.80	134.52	123.60
7	I	55	THR	CA-CB-CG2	7.79	123.30	112.40
1	A	372	LYS	CD-CE-NZ	-7.78	93.81	111.70
7	I	61	ASP	CB-CG-OD1	-7.77	111.30	118.30
1	A	1418	LEU	CB-CG-CD1	7.77	124.21	111.00
1	A	468	PHE	CB-CG-CD1	-7.76	115.36	120.80
3	C	217	ASP	CB-CG-OD2	7.76	125.29	118.30
2	B	712	PRO	N-CD-CG	-7.76	91.56	103.20
2	B	1099	VAL	CB-CA-C	-7.76	96.66	111.40
7	I	4	PHE	CB-CG-CD1	-7.75	115.37	120.80
1	A	962	ARG	O-C-N	-7.75	110.30	122.70
5	F	150	GLU	N-CA-CB	-7.75	96.65	110.60
7	I	98	VAL	CA-CB-CG2	-7.75	99.27	110.90
3	C	191	TYR	CZ-CE2-CD2	7.74	126.77	119.80
2	B	1166	CYS	CA-CB-SG	7.74	127.93	114.00
2	B	268	THR	N-CA-CB	-7.74	95.60	110.30
1	A	885	THR	OG1-CB-CG2	-7.73	92.22	110.00
2	B	120	ARG	NE-CZ-NH2	7.72	124.16	120.30
2	B	368	GLU	C-N-CA	-7.72	106.09	122.30
6	H	46	LEU	CB-CG-CD2	7.72	124.12	111.00
1	A	1349	TYR	CG-CD1-CE1	7.71	127.47	121.30
2	B	412	LEU	CB-CG-CD2	7.71	124.11	111.00
3	C	11	ARG	CB-CA-C	-7.71	94.98	110.40
3	C	116	LYS	CD-CE-NZ	-7.70	93.99	111.70
7	I	54	GLU	CG-CD-OE2	-7.70	102.91	118.30
1	A	960	ILE	CG1-CB-CG2	-7.68	94.50	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	722	ASP	OD1-CG-OD2	-7.68	108.71	123.30
1	A	412	ARG	NE-CZ-NH1	-7.67	116.46	120.30
2	B	1166	CYS	N-CA-CB	-7.67	96.80	110.60
2	B	38	PHE	CB-CG-CD2	7.66	126.16	120.80
3	C	57	VAL	CG1-CB-CG2	7.66	123.16	110.90
1	A	1017	LEU	CB-CG-CD2	-7.65	98.00	111.00
2	B	635	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	A	1365	TYR	CB-CG-CD2	-7.65	116.41	121.00
1	A	1081	LEU	CB-CG-CD2	7.64	124.00	111.00
9	K	14	GLU	CB-CA-C	7.64	125.69	110.40
1	A	557	ASP	O-C-N	-7.64	110.21	123.20
9	K	24	ASP	CB-CG-OD1	-7.63	111.43	118.30
1	A	598	LEU	CA-CB-CG	7.62	132.83	115.30
1	A	605	MET	CG-SD-CE	-7.62	88.01	100.20
2	B	329	THR	OG1-CB-CG2	-7.62	92.48	110.00
2	B	452	THR	OG1-CB-CG2	-7.62	92.48	110.00
2	B	589	VAL	CB-CA-C	7.62	125.87	111.40
1	A	495	GLU	N-CA-CB	-7.61	96.89	110.60
1	A	1281	ARG	CB-CA-C	-7.61	95.17	110.40
2	B	284	ILE	CG1-CB-CG2	-7.61	94.65	111.40
4	E	50	MET	CG-SD-CE	7.61	112.38	100.20
5	F	72	LYS	N-CA-C	7.61	131.54	111.00
1	A	526	ASP	CB-CG-OD1	7.60	125.14	118.30
1	A	843	LYS	CB-CG-CD	7.60	131.36	111.60
1	A	720	ARG	CG-CD-NE	7.59	127.74	111.80
1	A	731	ARG	NE-CZ-NH1	-7.59	116.50	120.30
9	K	82	ASP	CB-CG-OD2	7.59	125.13	118.30
8	J	61	LEU	CB-CG-CD2	7.59	123.90	111.00
2	B	38	PHE	CB-CG-CD1	-7.58	115.49	120.80
6	H	89	LEU	CA-CB-CG	7.57	132.71	115.30
1	A	613	ILE	CG1-CB-CG2	-7.57	94.75	111.40
1	A	672	ASP	CB-CG-OD1	7.56	125.11	118.30
4	E	208	TYR	CG-CD1-CE1	7.55	127.34	121.30
2	B	241	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	414	ASP	OD1-CG-OD2	-7.55	108.96	123.30
2	B	217	ARG	CB-CG-CD	7.55	131.22	111.60
1	A	50	ILE	CB-CA-C	-7.54	96.51	111.60
1	A	634	THR	CA-CB-CG2	-7.54	101.85	112.40
2	B	807	ARG	CG-CD-NE	-7.53	95.99	111.80
1	A	1301	GLU	OE1-CD-OE2	7.52	132.32	123.30
10	L	63	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	A	883	LEU	N-CA-C	-7.51	90.72	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	852	ARG	NH1-CZ-NH2	-7.51	111.14	119.40
5	F	72	LYS	C-N-CA	7.51	140.48	121.70
1	A	1005	GLU	CG-CD-OE1	7.51	133.31	118.30
4	E	66	GLU	N-CA-CB	7.50	124.11	110.60
8	J	3	VAL	CB-CA-C	-7.50	97.15	111.40
1	A	360	GLU	OE1-CD-OE2	-7.49	114.31	123.30
1	A	826	ASP	CB-CG-OD1	-7.49	111.56	118.30
1	A	85	ASP	CB-CG-OD1	-7.48	111.57	118.30
2	B	385	LEU	CB-CG-CD1	-7.48	98.29	111.00
1	A	938	LYS	CB-CA-C	-7.47	95.45	110.40
1	A	234	MET	CG-SD-CE	7.47	112.15	100.20
2	B	390	LEU	CB-CG-CD1	-7.47	98.31	111.00
1	A	1281	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	261	ASP	CB-CG-OD2	7.46	125.01	118.30
1	A	596	THR	CA-CB-CG2	-7.45	101.97	112.40
10	L	54	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	A	793	SER	N-CA-CB	-7.43	99.35	110.50
1	A	1157	ASP	CB-CG-OD2	7.43	124.98	118.30
4	E	11	ARG	NH1-CZ-NH2	7.42	127.57	119.40
2	B	170	LEU	CB-CG-CD1	-7.42	98.39	111.00
2	B	650	GLU	OE1-CD-OE2	7.41	132.19	123.30
1	A	32	VAL	CG1-CB-CG2	-7.41	99.04	110.90
4	E	1	MET	CG-SD-CE	7.41	112.05	100.20
1	A	649	ILE	CA-CB-CG1	7.41	125.07	111.00
6	H	102	TYR	CG-CD1-CE1	7.40	127.22	121.30
2	B	331	LEU	CB-CG-CD1	7.40	123.58	111.00
2	B	852	ARG	N-CA-CB	-7.40	97.28	110.60
1	A	821	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	1136	SER	CB-CA-C	7.38	124.11	110.10
2	B	125	SER	CB-CA-C	7.37	124.10	110.10
2	B	728	ARG	NE-CZ-NH2	7.37	123.98	120.30
1	A	588	LEU	CB-CG-CD1	-7.36	98.49	111.00
1	A	1280	GLU	CG-CD-OE2	7.36	133.01	118.30
1	A	1241	ARG	CG-CD-NE	-7.36	96.35	111.80
1	A	1259	MET	CG-SD-CE	7.35	111.96	100.20
2	B	945	GLU	CG-CD-OE2	-7.35	103.60	118.30
1	A	63	ARG	NE-CZ-NH1	7.34	123.97	120.30
2	B	894	ASP	CB-CG-OD1	7.34	124.91	118.30
1	A	1005	GLU	CG-CD-OE2	-7.34	103.62	118.30
1	A	266	LEU	CA-CB-CG	7.33	132.17	115.30
1	A	709	THR	CA-CB-CG2	7.32	122.65	112.40
1	A	1176	LEU	CA-CB-CG	7.32	132.13	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	45	ARG	CA-CB-CG	7.31	129.49	113.40
1	A	1198	ASP	CB-CG-OD1	7.31	124.88	118.30
5	F	82	THR	CB-CA-C	-7.30	91.89	111.60
2	B	641	GLU	OE1-CD-OE2	-7.30	114.54	123.30
6	H	19	ARG	NE-CZ-NH2	-7.29	116.66	120.30
2	B	691	GLU	CA-CB-CG	7.29	129.43	113.40
2	B	217	ARG	CG-CD-NE	-7.28	96.51	111.80
2	B	496	ARG	CD-NE-CZ	7.28	133.79	123.60
7	I	113	ASP	OD1-CG-OD2	-7.28	109.47	123.30
2	B	479	VAL	CG1-CB-CG2	-7.27	99.27	110.90
2	B	1136	ASP	CB-CG-OD2	7.26	124.83	118.30
1	A	839	ARG	NE-CZ-NH1	7.25	123.93	120.30
7	I	13	MET	N-CA-CB	-7.25	97.54	110.60
9	K	6	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	A	170	THR	OG1-CB-CG2	-7.25	93.32	110.00
1	A	603	ASN	N-CA-CB	-7.25	97.55	110.60
3	C	268	ASP	CB-CG-OD2	7.25	124.82	118.30
2	B	964	VAL	CA-CB-CG2	-7.24	100.04	110.90
7	I	84	VAL	N-CA-CB	-7.24	95.58	111.50
7	I	30	ARG	CG-CD-NE	-7.23	96.62	111.80
9	K	36	GLU	OE1-CD-OE2	7.23	131.97	123.30
2	B	1222	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	A	59	GLY	N-CA-C	7.22	131.15	113.10
3	C	252	GLN	CB-CA-C	7.22	124.84	110.40
1	A	61	ILE	N-CA-C	-7.21	91.53	111.00
1	A	1176	LEU	N-CA-C	-7.21	91.54	111.00
4	E	48	ASP	CB-CG-OD2	7.19	124.77	118.30
1	A	711	ARG	NE-CZ-NH1	7.19	123.89	120.30
7	I	73	ARG	NE-CZ-NH2	-7.19	116.71	120.30
3	C	38	ILE	CG1-CB-CG2	-7.18	95.60	111.40
2	B	1094	ARG	NE-CZ-NH2	7.17	123.89	120.30
7	I	31	THR	C-N-CA	7.17	139.62	121.70
1	A	610	GLY	O-C-N	7.17	134.17	122.70
10	L	47	ARG	NE-CZ-NH1	-7.16	116.72	120.30
2	B	978	ASP	CB-CG-OD2	7.16	124.74	118.30
2	B	245	GLU	CA-CB-CG	7.16	129.15	113.40
7	I	111	THR	OG1-CB-CG2	-7.15	93.55	110.00
3	C	81	GLU	N-CA-C	-7.14	91.72	111.00
1	A	325	ILE	CG1-CB-CG2	-7.14	95.69	111.40
1	A	424	ILE	CG1-CB-CG2	-7.13	95.72	111.40
1	A	203	SER	N-CA-CB	7.12	121.18	110.50
2	B	348	ARG	NE-CZ-NH1	7.12	123.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	273	LEU	CB-CG-CD1	7.11	123.09	111.00
6	H	86	ASP	CB-CA-C	7.11	124.62	110.40
1	A	146	MET	CG-SD-CE	7.11	111.57	100.20
2	B	709	ASP	CB-CG-OD2	7.11	124.70	118.30
1	A	1365	TYR	CG-CD1-CE1	-7.11	115.61	121.30
6	H	107	VAL	N-CA-C	-7.10	91.82	111.00
1	A	833	GLU	CG-CD-OE1	7.10	132.50	118.30
8	J	17	LYS	CD-CE-NZ	-7.09	95.38	111.70
1	A	414	ASP	CB-CG-OD2	7.08	124.67	118.30
2	B	272	THR	OG1-CB-CG2	-7.08	93.72	110.00
2	B	1085	ILE	CG1-CB-CG2	-7.08	95.83	111.40
2	B	642	ASP	CB-CA-C	7.08	124.55	110.40
8	J	59	LYS	CD-CE-NZ	-7.08	95.43	111.70
6	H	44	VAL	CG1-CB-CG2	7.07	122.22	110.90
1	A	940	ARG	CG-CD-NE	-7.07	96.95	111.80
2	B	1212	ILE	CA-CB-CG1	-7.07	97.57	111.00
5	F	103	MET	CG-SD-CE	7.07	111.51	100.20
1	A	1323	ASP	CB-CG-OD2	7.07	124.66	118.30
3	C	180	TYR	CD1-CE1-CZ	7.06	126.16	119.80
3	C	196	ASP	CB-CG-OD1	7.06	124.65	118.30
4	E	17	ARG	NE-CZ-NH2	7.04	123.82	120.30
8	J	48	ARG	CA-CB-CG	7.04	128.88	113.40
9	K	87	LEU	CB-CG-CD2	7.03	122.96	111.00
2	B	1009	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	A	596	THR	CB-CA-C	-7.03	92.63	111.60
1	A	900	ASP	CB-CG-OD2	-7.03	111.97	118.30
4	E	22	MET	CG-SD-CE	7.03	111.44	100.20
1	A	1280	GLU	O-C-N	-7.02	111.47	122.70
8	J	1	MET	CA-CB-CG	7.02	125.23	113.30
2	B	722	ASP	CB-CG-OD2	7.02	124.61	118.30
2	B	817	LEU	CB-CG-CD2	-7.01	99.08	111.00
7	I	44	TYR	CB-CG-CD2	7.01	125.20	121.00
2	B	303	TYR	CB-CG-CD2	-7.00	116.80	121.00
3	C	193	TYR	CD1-CE1-CZ	7.00	126.10	119.80
2	B	512	ARG	NE-CZ-NH1	-6.99	116.80	120.30
1	A	117	GLU	OE1-CD-OE2	6.99	131.69	123.30
2	B	488	TYR	CB-CG-CD1	6.99	125.19	121.00
2	B	983	ARG	CA-CB-CG	6.99	128.77	113.40
1	A	944	ARG	NH1-CZ-NH2	-6.99	111.72	119.40
4	E	77	SER	N-CA-C	-6.99	92.14	111.00
9	K	6	ARG	N-CA-CB	-6.99	98.03	110.60
10	L	40	LEU	CA-CB-CG	6.98	131.36	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	41	ASP	OD1-CG-OD2	-6.98	110.05	123.30
4	E	103	LYS	N-CA-CB	6.97	123.14	110.60
1	A	492	PRO	O-C-N	6.96	133.84	122.70
2	B	639	ILE	CA-CB-CG1	6.96	124.22	111.00
6	H	126	GLU	OE1-CD-OE2	-6.96	114.95	123.30
1	A	486	GLU	CG-CD-OE1	6.95	132.20	118.30
8	J	48	ARG	CD-NE-CZ	6.95	133.33	123.60
3	C	89	GLU	N-CA-C	-6.95	92.24	111.00
1	A	666	ILE	CG1-CB-CG2	6.95	126.68	111.40
1	A	1407	GLU	OE1-CD-OE2	-6.95	114.96	123.30
1	A	1357	ALA	CB-CA-C	-6.94	99.68	110.10
2	B	1166	CYS	O-C-N	-6.93	111.41	123.20
3	C	186	LEU	CB-CG-CD1	-6.93	99.22	111.00
1	A	764	CYS	CA-CB-SG	6.93	126.47	114.00
6	H	135	LEU	CB-CG-CD2	6.92	122.77	111.00
4	E	200	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	A	1234	GLU	CA-CB-CG	6.91	128.61	113.40
1	A	895	LYS	N-CA-CB	6.91	123.03	110.60
1	A	364	VAL	CA-CB-CG1	6.90	121.25	110.90
2	B	435	THR	OG1-CB-CG2	-6.90	94.14	110.00
1	A	856	THR	OG1-CB-CG2	-6.89	94.15	110.00
2	B	434	ARG	CG-CD-NE	6.89	126.28	111.80
2	B	1223	ASP	CB-CG-OD1	-6.89	112.10	118.30
1	A	179	LEU	CB-CG-CD1	6.89	122.71	111.00
1	A	726	ARG	NE-CZ-NH1	-6.88	116.86	120.30
2	B	336	ARG	CB-CA-C	-6.88	96.64	110.40
1	A	1274	ARG	CG-CD-NE	-6.87	97.38	111.80
1	A	1111	MET	N-CA-CB	-6.87	98.24	110.60
2	B	942	ARG	CG-CD-NE	-6.87	97.38	111.80
10	L	57	LEU	N-CA-C	6.86	129.53	111.00
1	A	655	PHE	CB-CG-CD1	6.86	125.60	120.80
7	I	70	ARG	NH1-CZ-NH2	6.86	126.94	119.40
1	A	151	ASP	CB-CG-OD2	6.85	124.47	118.30
2	B	898	LEU	CB-CG-CD2	6.85	122.65	111.00
2	B	188	ASP	CB-CG-OD1	-6.85	112.14	118.30
1	A	1155	ASP	OD1-CG-OD2	-6.85	110.29	123.30
2	B	217	ARG	NE-CZ-NH2	6.84	123.72	120.30
1	A	1274	ARG	CB-CA-C	-6.84	96.72	110.40
1	A	839	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	436	ILE	CG1-CB-CG2	-6.84	96.36	111.40
1	A	1280	GLU	CA-C-N	6.84	132.24	117.20
1	A	205	GLU	CB-CA-C	6.83	124.07	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	7	CYS	N-CA-CB	6.83	122.90	110.60
1	A	193	ASP	CB-CG-OD1	6.83	124.45	118.30
2	B	595	ARG	N-CA-CB	6.83	122.90	110.60
8	J	29	GLU	OE1-CD-OE2	6.83	131.50	123.30
2	B	133	LYS	CD-CE-NZ	-6.83	95.99	111.70
1	A	465	TYR	O-C-N	-6.82	111.78	122.70
9	K	78	THR	CA-CB-CG2	-6.82	102.85	112.40
2	B	997	GLU	CA-CB-CG	-6.82	98.39	113.40
2	B	405	ARG	NE-CZ-NH2	-6.82	116.89	120.30
9	K	93	SER	N-CA-CB	6.82	120.72	110.50
1	A	359	LEU	CB-CG-CD1	-6.81	99.42	111.00
1	A	475	THR	N-CA-CB	-6.81	97.36	110.30
2	B	328	GLU	OE1-CD-OE2	6.81	131.47	123.30
9	K	39	ASP	OD1-CG-OD2	-6.81	110.36	123.30
2	B	567	GLU	O-C-N	-6.81	111.81	122.70
1	A	487	MET	CG-SD-CE	-6.81	89.31	100.20
1	A	1143	LEU	CB-CG-CD2	-6.80	99.43	111.00
5	F	154	ASP	CB-CG-OD1	6.80	124.42	118.30
7	I	1	MET	CA-CB-CG	6.80	124.86	113.30
4	E	197	LYS	N-CA-C	-6.80	92.65	111.00
10	L	40	LEU	CB-CA-C	6.80	123.11	110.20
7	I	118	ARG	CA-CB-CG	6.79	128.35	113.40
1	A	470	LEU	CB-CA-C	-6.79	97.30	110.20
9	K	73	LEU	CB-CG-CD2	6.79	122.54	111.00
1	A	512	VAL	CA-CB-CG1	6.78	121.07	110.90
1	A	1274	ARG	NE-CZ-NH1	-6.78	116.91	120.30
7	I	5	ARG	NH1-CZ-NH2	-6.78	111.95	119.40
4	E	162	ARG	CB-CG-CD	6.77	129.21	111.60
1	A	498	ARG	CD-NE-CZ	-6.77	114.12	123.60
1	A	776	ALA	CB-CA-C	-6.77	99.94	110.10
1	A	907	THR	CB-CA-C	-6.77	93.33	111.60
2	B	959	ASP	OD1-CG-OD2	-6.77	110.44	123.30
1	A	557	ASP	OD1-CG-OD2	-6.76	110.45	123.30
2	B	484	ASN	CB-CA-C	-6.76	96.87	110.40
8	J	43	ARG	CG-CD-NE	-6.76	97.59	111.80
2	B	942	ARG	NE-CZ-NH2	-6.76	116.92	120.30
2	B	563	MET	CG-SD-CE	6.75	111.01	100.20
3	C	66	ARG	CD-NE-CZ	-6.75	114.14	123.60
1	A	461	LYS	CB-CA-C	-6.75	96.90	110.40
1	A	879	GLU	OE1-CD-OE2	6.75	131.40	123.30
9	K	64	GLU	CG-CD-OE1	6.75	131.80	118.30
2	B	89	GLU	N-CA-C	6.74	129.21	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	710	LEU	CB-CG-CD2	6.73	122.45	111.00
4	E	159	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	A	116	ASP	CB-CG-OD2	6.73	124.36	118.30
3	C	20	PHE	CB-CG-CD1	-6.72	116.10	120.80
1	A	913	LEU	N-CA-CB	-6.71	96.97	110.40
1	A	983	ILE	CG1-CB-CG2	-6.71	96.63	111.40
2	B	1186	ASP	CB-CG-OD2	6.71	124.34	118.30
1	A	22	PHE	CB-CG-CD1	-6.70	116.11	120.80
2	B	661	LEU	CB-CG-CD2	6.70	122.39	111.00
6	H	77	ARG	NH1-CZ-NH2	-6.70	112.03	119.40
2	B	583	ASN	C-N-CA	-6.70	108.24	122.30
2	B	1019	SER	N-CA-CB	6.70	120.54	110.50
1	A	460	VAL	CG1-CB-CG2	-6.69	100.19	110.90
1	A	472	LEU	CB-CG-CD1	6.69	122.37	111.00
1	A	446	ARG	CG-CD-NE	6.68	125.83	111.80
2	B	387	LEU	CA-CB-CG	6.68	130.67	115.30
1	A	266	LEU	CB-CG-CD1	-6.68	99.65	111.00
1	A	107	CYS	N-CA-C	-6.67	92.99	111.00
2	B	642	ASP	C-N-CA	-6.67	105.04	121.70
2	B	542	MET	CG-SD-CE	-6.66	89.54	100.20
2	B	211	VAL	CG1-CB-CG2	-6.66	100.25	110.90
2	B	336	ARG	NE-CZ-NH1	-6.65	116.97	120.30
6	H	111	LEU	CA-CB-CG	6.65	130.60	115.30
5	F	125	LEU	CB-CG-CD1	-6.65	99.70	111.00
3	C	253	LYS	CD-CE-NZ	-6.64	96.42	111.70
5	F	97	ARG	CG-CD-NE	-6.63	97.87	111.80
1	A	396	PRO	N-CD-CG	-6.63	93.25	103.20
2	B	169	ARG	NE-CZ-NH1	6.63	123.61	120.30
2	B	477	ALA	CB-CA-C	6.63	120.05	110.10
2	B	341	LEU	CB-CG-CD1	6.63	122.27	111.00
4	E	112	TYR	CD1-CE1-CZ	6.63	125.77	119.80
1	A	1235	LYS	CD-CE-NZ	6.63	126.94	111.70
4	E	204	THR	CA-CB-OG1	6.62	122.91	109.00
1	A	1136	SER	N-CA-CB	-6.62	100.57	110.50
10	L	48	CYS	N-CA-CB	-6.62	98.68	110.60
1	A	1275	GLY	CA-C-N	-6.62	102.64	117.20
1	A	948	VAL	N-CA-CB	-6.61	96.95	111.50
1	A	144	THR	CA-CB-CG2	6.61	121.66	112.40
2	B	995	ARG	NH1-CZ-NH2	6.61	126.67	119.40
2	B	1101	ASP	CB-CG-OD1	6.61	124.24	118.30
2	B	305	VAL	CG1-CB-CG2	6.60	121.46	110.90
4	E	207	ARG	NH1-CZ-NH2	-6.59	112.15	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	100	THR	OG1-CB-CG2	-6.59	94.84	110.00
8	J	64	ASN	CB-CA-C	6.59	123.57	110.40
9	K	114	LEU	CB-CG-CD1	-6.59	99.80	111.00
4	E	80	VAL	CB-CA-C	-6.58	98.90	111.40
9	K	79	GLU	CB-CA-C	6.58	123.56	110.40
2	B	633	VAL	CG1-CB-CG2	-6.58	100.38	110.90
1	A	56	PRO	O-C-N	6.57	133.21	122.70
1	A	1362	TYR	CZ-CE2-CD2	6.57	125.72	119.80
8	J	31	ASP	CB-CG-OD2	6.57	124.21	118.30
2	B	1026	LEU	CB-CG-CD2	6.56	122.16	111.00
2	B	370	PHE	CB-CA-C	6.56	123.52	110.40
2	B	1023	VAL	CA-CB-CG2	-6.55	101.07	110.90
1	A	138	ILE	CA-CB-CG2	6.55	124.00	110.90
2	B	381	MET	CB-CA-C	-6.55	97.30	110.40
2	B	1108	ARG	N-CA-C	6.55	128.69	111.00
9	K	75	ILE	CA-CB-CG1	6.54	123.43	111.00
1	A	1172	LEU	CB-CA-C	-6.54	97.77	110.20
7	I	24	ARG	N-CA-CB	6.54	122.37	110.60
2	B	975	GLN	CB-CA-C	-6.53	97.33	110.40
7	I	3	THR	O-C-N	6.53	133.15	122.70
7	I	5	ARG	NE-CZ-NH2	6.53	123.57	120.30
1	A	1373	ASP	CB-CG-OD2	6.53	124.17	118.30
2	B	608	ASP	CB-CG-OD2	6.53	124.17	118.30
2	B	477	ALA	N-CA-CB	6.52	119.23	110.10
3	C	230	MET	CG-SD-CE	6.52	110.63	100.20
2	B	332	ASP	CB-CG-OD2	6.52	124.17	118.30
2	B	650	GLU	CG-CD-OE1	-6.52	105.26	118.30
2	B	245	GLU	OE1-CD-OE2	-6.52	115.48	123.30
1	A	66	LYS	CA-CB-CG	6.51	127.73	113.40
7	I	104	LEU	CB-CG-CD1	6.51	122.07	111.00
2	B	789	MET	CG-SD-CE	-6.50	89.80	100.20
1	A	546	VAL	CG1-CB-CG2	-6.50	100.50	110.90
3	C	124	LEU	N-CA-C	6.50	128.54	111.00
7	I	19	ASP	CB-CG-OD2	6.49	124.14	118.30
8	J	47	ARG	NE-CZ-NH1	6.49	123.55	120.30
8	J	46	CYS	CA-CB-SG	-6.49	102.33	114.00
2	B	853	SER	CB-CA-C	-6.48	97.78	110.10
2	B	249	ARG	CD-NE-CZ	6.48	132.67	123.60
1	A	437	MET	CB-CA-C	-6.48	97.44	110.40
8	J	38	ARG	NE-CZ-NH2	-6.48	117.06	120.30
2	B	53	GLN	CA-CB-CG	6.48	127.65	113.40
2	B	365	THR	N-CA-C	-6.48	93.51	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	128	LEU	CB-CG-CD2	6.47	122.01	111.00
1	A	1329	THR	OG1-CB-CG2	-6.47	95.11	110.00
2	B	297	ILE	CA-CB-CG1	6.47	123.30	111.00
4	E	208	TYR	CB-CG-CD1	6.47	124.88	121.00
1	A	305	ASP	CB-CG-OD2	6.47	124.12	118.30
1	A	618	GLU	CG-CD-OE1	-6.47	105.36	118.30
1	A	1370	LEU	CD1-CG-CD2	-6.47	91.09	110.50
5	F	79	ARG	CB-CG-CD	-6.47	94.79	111.60
10	L	63	ARG	N-CA-CB	6.46	122.23	110.60
1	A	571	LEU	CB-CG-CD2	6.46	121.98	111.00
2	B	1069	PHE	CB-CG-CD1	6.46	125.32	120.80
4	E	41	ASP	CB-CG-OD1	6.46	124.11	118.30
7	I	118	ARG	CD-NE-CZ	6.46	132.64	123.60
2	B	591	ARG	NE-CZ-NH2	-6.45	117.07	120.30
2	B	310	MET	CG-SD-CE	6.45	110.52	100.20
1	A	1417	GLU	OE1-CD-OE2	-6.44	115.57	123.30
2	B	737	THR	CA-CB-CG2	-6.44	103.39	112.40
1	A	910	PRO	N-CD-CG	-6.43	93.55	103.20
4	E	17	ARG	CG-CD-NE	-6.43	98.31	111.80
2	B	790	ASP	CB-CA-C	6.42	123.25	110.40
2	B	986	GLN	CA-CB-CG	-6.42	99.27	113.40
4	E	14	ARG	C-N-CA	-6.42	105.64	121.70
4	E	20	LYS	CA-CB-CG	6.42	127.54	113.40
1	A	277	GLU	CA-CB-CG	6.42	127.52	113.40
2	B	401	PHE	CB-CG-CD2	-6.42	116.31	120.80
2	B	731	VAL	N-CA-C	-6.42	93.68	111.00
4	E	137	GLU	OE1-CD-OE2	6.40	130.99	123.30
1	A	420	ARG	NH1-CZ-NH2	-6.40	112.36	119.40
2	B	653	VAL	CB-CA-C	-6.40	99.24	111.40
2	B	249	ARG	NE-CZ-NH2	-6.39	117.10	120.30
4	E	200	ARG	NE-CZ-NH2	-6.39	117.10	120.30
4	E	53	PRO	N-CD-CG	-6.39	93.61	103.20
7	I	83	ASN	CB-CA-C	-6.39	97.62	110.40
10	L	58	LYS	O-C-N	-6.39	112.48	122.70
1	A	566	ILE	CB-CA-C	-6.38	98.83	111.60
1	A	120	GLU	OE1-CD-OE2	6.38	130.96	123.30
2	B	1183	LYS	N-CA-C	-6.38	93.77	111.00
1	A	1196	GLU	CG-CD-OE2	-6.38	105.54	118.30
2	B	1002	THR	OG1-CB-CG2	-6.38	95.33	110.00
7	I	93	LYS	CA-CB-CG	6.38	127.43	113.40
2	B	398	ARG	CB-CA-C	-6.38	97.65	110.40
2	B	582	VAL	CG1-CB-CG2	-6.37	100.72	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1183	LYS	CB-CA-C	6.36	123.13	110.40
2	B	773	MET	CG-SD-CE	6.36	110.38	100.20
1	A	1377	THR	CB-CA-C	-6.36	94.43	111.60
2	B	646	LEU	N-CA-C	6.35	128.15	111.00
1	A	86	LEU	CB-CG-CD2	6.35	121.79	111.00
1	A	1342	GLU	OE1-CD-OE2	6.35	130.92	123.30
10	L	38	LEU	CB-CG-CD2	6.35	121.79	111.00
1	A	840	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	1116	LEU	N-CA-C	-6.34	93.88	111.00
1	A	1228	TRP	CA-CB-CG	6.34	125.75	113.70
10	L	57	LEU	CB-CG-CD2	-6.34	100.22	111.00
3	C	204	SER	N-CA-CB	-6.34	101.00	110.50
4	E	162	ARG	CB-CA-C	6.33	123.07	110.40
2	B	134	LYS	CD-CE-NZ	6.33	126.26	111.70
7	I	98	VAL	CG1-CB-CG2	-6.33	100.78	110.90
2	B	539	LEU	CB-CG-CD2	6.33	121.75	111.00
2	B	1202	LEU	CB-CG-CD1	-6.33	100.25	111.00
1	A	856	THR	N-CA-CB	-6.32	98.28	110.30
1	A	305	ASP	N-CA-C	6.32	128.07	111.00
3	C	262	LEU	CB-CG-CD1	6.32	121.74	111.00
1	A	1223	ASP	OD1-CG-OD2	-6.32	111.30	123.30
2	B	775	LYS	CD-CE-NZ	6.32	126.23	111.70
1	A	664	THR	N-CA-CB	6.31	122.30	110.30
2	B	668	ASP	CB-CG-OD1	6.31	123.98	118.30
8	J	2	ILE	CB-CG1-CD1	-6.30	96.25	113.90
1	A	1382	THR	OG1-CB-CG2	-6.30	95.51	110.00
2	B	1181	GLU	CA-CB-CG	6.30	127.26	113.40
1	A	464	PRO	CA-C-N	6.30	131.05	117.20
1	A	1080	THR	CA-CB-CG2	6.29	121.21	112.40
1	A	469	ARG	CG-CD-NE	-6.29	98.59	111.80
1	A	1368	MET	CG-SD-CE	6.29	110.26	100.20
2	B	1161	HIS	CB-CA-C	6.29	122.97	110.40
3	C	127	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	1203	ASN	CB-CA-C	6.28	122.96	110.40
7	I	75	CYS	N-CA-CB	6.28	121.90	110.60
1	A	110	CYS	CB-CA-C	-6.28	97.85	110.40
2	B	183	GLU	OE1-CD-OE2	-6.27	115.78	123.30
4	E	162	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	A	1290	LYS	CD-CE-NZ	6.27	126.12	111.70
3	C	183	TRP	CA-C-N	6.26	130.97	117.20
3	C	240	VAL	N-CA-C	6.26	127.91	111.00
9	K	71	PHE	N-CA-CB	6.26	121.87	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ARG	NE-CZ-NH1	-6.25	117.17	120.30
3	C	252	GLN	CA-CB-CG	6.25	127.15	113.40
1	A	980	ASP	CB-CA-C	-6.25	97.91	110.40
2	B	297	ILE	CA-CB-CG2	-6.24	98.42	110.90
3	C	254	LYS	CD-CE-NZ	-6.24	97.35	111.70
7	I	118	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	A	1277	GLU	CG-CD-OE2	6.24	130.77	118.30
1	A	1154	TYR	N-CA-C	-6.23	94.17	111.00
1	A	391	LEU	CB-CG-CD1	-6.23	100.41	111.00
2	B	270	LYS	CD-CE-NZ	-6.22	97.38	111.70
6	H	93	TYR	CD1-CE1-CZ	-6.22	114.20	119.80
5	F	115	THR	OG1-CB-CG2	-6.22	95.69	110.00
3	C	153	LEU	CB-CG-CD1	-6.22	100.43	111.00
7	I	74	GLU	CA-CB-CG	6.21	127.07	113.40
2	B	957	ASN	N-CA-CB	-6.21	99.43	110.60
5	F	94	LEU	C-N-CA	-6.21	109.26	122.30
6	H	40	LEU	CB-CG-CD2	6.21	121.55	111.00
2	B	171	PRO	N-CD-CG	-6.21	93.89	103.20
1	A	304	MET	CG-SD-CE	-6.20	90.28	100.20
6	H	38	LEU	CB-CA-C	-6.20	98.42	110.20
1	A	109	HIS	CB-CA-C	6.20	122.79	110.40
1	A	655	PHE	CB-CG-CD2	-6.20	116.46	120.80
1	A	821	ARG	NH1-CZ-NH2	6.20	126.22	119.40
1	A	493	GLN	CB-CG-CD	6.19	127.70	111.60
2	B	252	SER	N-CA-CB	6.19	119.79	110.50
2	B	586	TRP	CB-CA-C	6.19	122.78	110.40
1	A	929	LEU	CB-CG-CD2	-6.19	100.48	111.00
2	B	167	ILE	CB-CA-C	-6.19	99.23	111.60
2	B	1167	GLY	N-CA-C	6.18	128.56	113.10
3	C	33	LEU	CB-CA-C	6.18	121.95	110.20
6	H	46	LEU	CB-CG-CD1	-6.18	100.49	111.00
2	B	890	TYR	CB-CG-CD2	-6.18	117.29	121.00
2	B	749	LEU	CA-CB-CG	-6.18	101.09	115.30
8	J	62	ARG	CG-CD-NE	-6.18	98.83	111.80
1	A	226	GLU	N-CA-CB	6.18	121.72	110.60
2	B	185	THR	OG1-CB-CG2	-6.17	95.81	110.00
4	E	148	GLU	OE1-CD-OE2	-6.17	115.89	123.30
4	E	149	LEU	CA-CB-CG	6.17	129.50	115.30
4	E	30	ILE	CG1-CB-CG2	-6.17	97.83	111.40
2	B	633	VAL	CB-CA-C	-6.17	99.68	111.40
2	B	916	THR	N-CA-C	6.17	127.66	111.00
9	K	79	GLU	OE1-CD-OE2	-6.17	115.90	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1259	MET	N-CA-C	-6.16	94.36	111.00
2	B	267	ARG	O-C-N	-6.16	112.85	122.70
1	A	244	PRO	CA-C-O	-6.15	105.43	120.20
1	A	483	ASP	CB-CG-OD2	6.15	123.84	118.30
1	A	743	VAL	CG1-CB-CG2	-6.15	101.06	110.90
1	A	1271	ILE	CA-CB-CG2	-6.15	98.60	110.90
2	B	485	ARG	CD-NE-CZ	6.15	132.21	123.60
2	B	579	ARG	NH1-CZ-NH2	6.15	126.17	119.40
2	B	895	ASP	N-CA-CB	6.15	121.67	110.60
9	K	22	ASP	OD1-CG-OD2	-6.15	111.61	123.30
1	A	52	GLY	CA-C-O	-6.15	109.53	120.60
1	A	1268	LEU	CB-CG-CD2	6.15	121.45	111.00
1	A	164	ARG	CD-NE-CZ	6.14	132.20	123.60
1	A	1120	LEU	CB-CG-CD1	6.14	121.45	111.00
2	B	373	ARG	NE-CZ-NH1	6.14	123.37	120.30
3	C	9	LYS	CD-CE-NZ	6.14	125.83	111.70
7	I	55	THR	N-CA-CB	-6.14	98.63	110.30
1	A	1161	THR	OG1-CB-CG2	-6.14	95.88	110.00
1	A	1204	ASP	OD1-CG-OD2	-6.14	111.64	123.30
1	A	1411	GLU	OE1-CD-OE2	-6.14	115.94	123.30
2	B	21	GLU	OE1-CD-OE2	-6.14	115.94	123.30
1	A	728	LYS	CB-CG-CD	6.13	127.55	111.60
1	A	752	LYS	CG-CD-CE	-6.13	93.50	111.90
2	B	836	GLU	O-C-N	6.13	132.51	122.70
1	A	1066	VAL	CG1-CB-CG2	-6.13	101.10	110.90
2	B	589	VAL	N-CA-CB	-6.13	98.02	111.50
1	A	1433	MET	N-CA-CB	6.12	121.62	110.60
1	A	291	GLU	CA-CB-CG	6.12	126.87	113.40
1	A	1064	VAL	CA-CB-CG1	6.12	120.08	110.90
2	B	802	PRO	CA-C-O	-6.12	105.51	120.20
3	C	16	ASP	CB-CG-OD1	-6.12	112.79	118.30
2	B	679	TYR	CD1-CE1-CZ	-6.11	114.30	119.80
4	E	202	SER	CB-CA-C	-6.11	98.49	110.10
1	A	1108	ALA	N-CA-CB	-6.11	101.55	110.10
1	A	790	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	1001	ARG	CG-CD-NE	-6.10	99.00	111.80
2	B	768	THR	CA-CB-CG2	-6.10	103.86	112.40
9	K	12	LEU	CA-CB-CG	-6.10	101.28	115.30
1	A	1017	LEU	CB-CG-CD1	6.10	121.36	111.00
1	A	668	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	850	VAL	CG1-CB-CG2	-6.09	101.15	110.90
2	B	615	MET	N-CA-CB	-6.09	99.64	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1418	LEU	CB-CG-CD2	-6.09	100.65	111.00
9	K	105	PHE	CZ-CE2-CD2	-6.09	112.79	120.10
1	A	645	LEU	CB-CG-CD2	6.09	121.35	111.00
1	A	1263	ILE	CG1-CB-CG2	-6.09	98.01	111.40
3	C	226	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	1277	GLU	CG-CD-OE1	-6.08	106.14	118.30
2	B	644	GLU	CB-CG-CD	-6.08	97.79	114.20
2	B	1223	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	1325	THR	N-CA-CB	-6.07	98.76	110.30
1	A	1154	TYR	CD1-CE1-CZ	-6.07	114.34	119.80
1	A	1298	TYR	CG-CD2-CE2	6.07	126.16	121.30
4	E	16	PHE	CB-CA-C	6.07	122.54	110.40
3	C	229	TYR	N-CA-C	6.07	127.38	111.00
8	J	44	TYR	CZ-CE2-CD2	6.07	125.26	119.80
10	L	26	THR	CA-CB-CG2	6.07	120.89	112.40
1	A	992	ASP	N-CA-CB	-6.06	99.69	110.60
2	B	1154	ALA	CB-CA-C	6.06	119.18	110.10
9	K	41	THR	CA-CB-CG2	-6.05	103.92	112.40
10	L	65	VAL	CG1-CB-CG2	6.05	120.59	110.90
10	L	58	LYS	N-CA-C	6.05	127.33	111.00
2	B	576	ASP	CB-CG-OD2	6.05	123.74	118.30
1	A	434	ARG	CD-NE-CZ	6.04	132.06	123.60
4	E	191	LYS	CD-CE-NZ	-6.04	97.80	111.70
1	A	352	VAL	CA-CB-CG1	6.04	119.96	110.90
1	A	664	THR	CB-CA-C	-6.04	95.29	111.60
2	B	381	MET	CG-SD-CE	-6.04	90.54	100.20
3	C	94	LYS	CA-CB-CG	6.04	126.69	113.40
4	E	108	GLY	CA-C-O	6.04	131.47	120.60
1	A	206	GLU	OE1-CD-OE2	6.03	130.54	123.30
1	A	1055	ARG	NE-CZ-NH2	-6.03	117.28	120.30
2	B	408	LEU	N-CA-CB	-6.03	98.33	110.40
2	B	1204	PHE	CB-CG-CD1	6.03	125.02	120.80
6	H	118	PHE	CG-CD1-CE1	6.03	127.44	120.80
2	B	509	ALA	CB-CA-C	6.03	119.15	110.10
1	A	1233	ASP	CB-CG-OD1	-6.03	112.87	118.30
1	A	1209	MET	C-N-CA	-6.03	109.64	122.30
7	I	106	CYS	C-N-CA	6.03	136.77	121.70
1	A	12	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	855	THR	N-CA-CB	6.02	121.74	110.30
1	A	646	PHE	CB-CA-C	-6.02	98.37	110.40
7	I	35	VAL	CA-CB-CG2	-6.01	101.88	110.90
9	K	26	LYS	CG-CD-CE	6.01	129.94	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	406	LEU	CB-CG-CD2	-6.01	100.79	111.00
1	A	914	GLU	CG-CD-OE2	-6.01	106.29	118.30
2	B	797	TYR	CZ-CE2-CD2	6.00	125.20	119.80
2	B	766	ARG	NH1-CZ-NH2	6.00	126.00	119.40
4	E	161	LYS	CA-CB-CG	6.00	126.59	113.40
4	E	176	PRO	CB-CA-C	-6.00	97.00	112.00
2	B	268	THR	CA-CB-CG2	6.00	120.79	112.40
1	A	498	ARG	NE-CZ-NH2	5.99	123.30	120.30
1	A	1135	ARG	CG-CD-NE	-5.99	99.22	111.80
1	A	1317	MET	N-CA-CB	-5.99	99.81	110.60
2	B	568	ASP	OD1-CG-OD2	-5.99	111.92	123.30
3	C	119	VAL	CA-CB-CG2	5.99	119.89	110.90
2	B	823	ALA	CB-CA-C	-5.99	101.12	110.10
2	B	995	ARG	CD-NE-CZ	5.99	131.99	123.60
4	E	172	GLU	CG-CD-OE1	-5.99	106.32	118.30
2	B	522	VAL	N-CA-CB	-5.99	98.33	111.50
1	A	830	LYS	CB-CA-C	-5.99	98.43	110.40
7	I	4	PHE	N-CA-C	5.99	127.16	111.00
8	J	34	THR	OG1-CB-CG2	-5.98	96.24	110.00
1	A	1377	THR	N-CA-CB	5.98	121.67	110.30
2	B	642	ASP	N-CA-CB	5.98	121.37	110.60
2	B	662	MET	CA-CB-CG	-5.98	103.14	113.30
1	A	516	SER	N-CA-CB	-5.98	101.53	110.50
1	A	1409	LEU	CB-CG-CD2	-5.98	100.84	111.00
1	A	1286	LYS	CD-CE-NZ	-5.97	97.96	111.70
2	B	316	PRO	N-CD-CG	-5.97	94.24	103.20
7	I	24	ARG	NE-CZ-NH2	-5.97	117.31	120.30
10	L	50	ASP	CB-CG-OD2	5.97	123.68	118.30
1	A	1299	VAL	CB-CA-C	5.97	122.75	111.40
4	E	112	TYR	CE1-CZ-CE2	-5.97	110.24	119.80
10	L	41	SER	N-CA-C	5.97	127.13	111.00
7	I	75	CYS	CB-CA-C	-5.97	98.46	110.40
1	A	468	PHE	CB-CG-CD2	5.97	124.98	120.80
2	B	654	ARG	NE-CZ-NH2	5.97	123.28	120.30
7	I	20	LYS	CD-CE-NZ	5.96	125.42	111.70
1	A	49	LYS	CD-CE-NZ	5.96	125.42	111.70
2	B	302	CYS	CA-CB-SG	-5.96	103.27	114.00
4	E	198	ILE	CG1-CB-CG2	-5.96	98.28	111.40
9	K	74	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	A	407	ARG	NH1-CZ-NH2	5.96	125.96	119.40
1	A	789	LYS	CD-CE-NZ	-5.96	98.00	111.70
1	A	1158	PRO	CA-C-O	-5.96	105.91	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1409	LEU	CB-CG-CD1	5.95	121.12	111.00
3	C	40	GLU	N-CA-C	5.95	127.07	111.00
2	B	399	ASP	N-CA-C	5.95	127.07	111.00
2	B	909	ASP	OD1-CG-OD2	-5.95	112.00	123.30
2	B	1086	PHE	N-CA-C	-5.95	94.94	111.00
4	E	21	GLU	CB-CA-C	-5.95	98.50	110.40
2	B	242	SER	CB-CA-C	5.95	121.40	110.10
2	B	973	ILE	CG1-CB-CG2	-5.95	98.32	111.40
6	H	87	ARG	CA-CB-CG	5.95	126.48	113.40
6	H	19	ARG	CD-NE-CZ	5.94	131.92	123.60
2	B	711	GLU	CB-CA-C	-5.94	98.51	110.40
2	B	799	PRO	N-CD-CG	-5.94	94.29	103.20
3	C	84	ARG	NH1-CZ-NH2	-5.94	112.86	119.40
10	L	25	ALA	C-N-CA	5.94	136.54	121.70
2	B	1037	LEU	CB-CG-CD1	5.94	121.09	111.00
10	L	40	LEU	CB-CG-CD2	5.94	121.09	111.00
2	B	165	VAL	N-CA-CB	5.93	124.56	111.50
2	B	1078	GLY	N-CA-C	5.93	127.94	113.10
1	A	98	LYS	CG-CD-CE	-5.93	94.11	111.90
2	B	942	ARG	CB-CA-C	-5.93	98.54	110.40
7	I	53	GLY	N-CA-C	5.93	127.93	113.10
1	A	640	GLN	O-C-N	-5.93	113.21	122.70
1	A	1057	VAL	CA-CB-CG2	-5.93	102.00	110.90
8	J	36	LEU	CB-CG-CD1	-5.93	100.92	111.00
1	A	651	LYS	CB-CA-C	5.93	122.26	110.40
6	H	106	GLU	CB-CA-C	5.93	122.26	110.40
1	A	223	GLY	N-CA-C	5.93	127.91	113.10
1	A	696	GLU	OE1-CD-OE2	-5.92	116.19	123.30
5	F	79	ARG	CA-CB-CG	5.92	126.43	113.40
1	A	468	PHE	CG-CD1-CE1	-5.91	114.30	120.80
2	B	694	ASP	CB-CG-OD2	5.91	123.62	118.30
6	H	92	ASP	CB-CG-OD1	5.91	123.62	118.30
8	J	22	LEU	CA-CB-CG	5.91	128.89	115.30
9	K	79	GLU	N-CA-C	-5.91	95.04	111.00
1	A	616	VAL	CG1-CB-CG2	-5.91	101.44	110.90
3	C	35	ARG	CD-NE-CZ	5.91	131.87	123.60
3	C	78	GLU	O-C-N	-5.91	113.25	122.70
2	B	1081	LEU	CB-CG-CD2	5.90	121.03	111.00
7	I	35	VAL	CB-CA-C	-5.90	100.19	111.40
2	B	68	THR	OG1-CB-CG2	-5.90	96.43	110.00
6	H	142	LEU	CA-CB-CG	-5.90	101.73	115.30
1	A	466	SER	N-CA-CB	5.89	119.34	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1058	LEU	CB-CG-CD1	5.89	121.01	111.00
1	A	1077	THR	O-C-N	-5.89	113.28	122.70
2	B	587	HIS	CA-C-N	5.89	127.97	116.20
1	A	942	PHE	CB-CG-CD2	-5.88	116.68	120.80
7	I	111	THR	CB-CA-C	-5.88	95.73	111.60
1	A	1207	LEU	CB-CG-CD2	5.88	120.99	111.00
2	B	990	ILE	CA-CB-CG1	5.88	122.17	111.00
2	B	209	GLU	N-CA-CB	-5.88	100.03	110.60
3	C	11	ARG	NE-CZ-NH2	-5.88	117.36	120.30
3	C	229	TYR	CB-CG-CD2	5.88	124.53	121.00
3	C	3	GLU	C-N-CA	5.87	136.38	121.70
2	B	39	ARG	NE-CZ-NH2	5.87	123.24	120.30
1	A	674	PRO	N-CD-CG	5.87	112.00	103.20
3	C	239	PRO	CA-C-O	5.87	134.28	120.20
7	I	45	ARG	CD-NE-CZ	-5.87	115.39	123.60
1	A	1135	ARG	CD-NE-CZ	5.87	131.81	123.60
6	H	118	PHE	CG-CD2-CE2	-5.87	114.35	120.80
10	L	61	THR	CA-CB-CG2	5.87	120.61	112.40
1	A	1118	VAL	CA-CB-CG1	5.86	119.69	110.90
2	B	436	VAL	CB-CA-C	5.86	122.54	111.40
1	A	987	VAL	CA-CB-CG2	-5.86	102.11	110.90
2	B	953	LEU	CB-CG-CD1	5.86	120.96	111.00
2	B	1168	LEU	CB-CG-CD2	-5.86	101.04	111.00
1	A	293	GLU	OE1-CD-OE2	5.85	130.32	123.30
2	B	1101	ASP	OD1-CG-OD2	-5.85	112.18	123.30
4	E	112	TYR	OH-CZ-CE2	5.85	135.90	120.10
10	L	60	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	A	504	LEU	N-CA-CB	-5.85	98.70	110.40
1	A	244	PRO	N-CD-CG	-5.85	94.43	103.20
2	B	1101	ASP	CB-CG-OD2	5.85	123.56	118.30
2	B	1183	LYS	CA-CB-CG	5.85	126.26	113.40
9	K	78	THR	N-CA-CB	5.84	121.40	110.30
1	A	1299	VAL	N-CA-CB	-5.84	98.66	111.50
1	A	1122	PRO	C-N-CA	-5.84	110.05	122.30
6	H	32	THR	OG1-CB-CG2	-5.84	96.58	110.00
8	J	45	CYS	O-C-N	-5.83	113.36	122.70
3	C	57	VAL	N-CA-CB	-5.83	98.67	111.50
2	B	612	GLU	CA-CB-CG	-5.83	100.57	113.40
7	I	5	ARG	CB-CG-CD	5.83	126.75	111.60
1	A	176	LYS	CD-CE-NZ	5.83	125.10	111.70
1	A	1234	GLU	CB-CA-C	-5.83	98.75	110.40
1	A	739	ASP	CB-CG-OD2	5.83	123.54	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	979	LYS	CD-CE-NZ	-5.83	98.30	111.70
8	J	7	CYS	CB-CA-C	-5.83	98.75	110.40
1	A	279	LEU	CB-CG-CD1	5.82	120.90	111.00
5	F	150	GLU	CG-CD-OE1	-5.82	106.66	118.30
10	L	70	ARG	N-CA-C	5.82	126.71	111.00
5	F	152	ILE	CG1-CB-CG2	-5.82	98.60	111.40
1	A	992	ASP	CB-CG-OD1	-5.82	113.06	118.30
1	A	701	LEU	CB-CG-CD2	-5.81	101.12	111.00
1	A	238	CYS	CA-CB-SG	-5.81	103.55	114.00
2	B	644	GLU	N-CA-CB	-5.80	100.15	110.60
2	B	809	MET	CG-SD-CE	-5.80	90.91	100.20
2	B	914	LYS	CD-CE-NZ	-5.80	98.35	111.70
2	B	538	ASN	N-CA-CB	-5.80	100.16	110.60
1	A	1377	THR	CA-CB-CG2	5.80	120.52	112.40
7	I	91	ARG	N-CA-C	-5.80	95.35	111.00
1	A	462	VAL	CG1-CB-CG2	-5.79	101.63	110.90
2	B	164	LYS	CA-C-N	5.79	129.95	117.20
2	B	365	THR	OG1-CB-CG2	-5.79	96.67	110.00
3	C	72	LEU	CB-CG-CD1	-5.79	101.15	111.00
5	F	143	PHE	CB-CG-CD2	-5.79	116.75	120.80
1	A	858	ASN	CB-CG-OD1	-5.79	110.02	121.60
1	A	497	THR	N-CA-CB	-5.78	99.32	110.30
1	A	923	LEU	CB-CA-C	-5.78	99.22	110.20
1	A	687	LYS	CD-CE-NZ	5.78	124.99	111.70
2	B	61	ASP	CB-CG-OD1	5.78	123.50	118.30
2	B	378	LEU	CB-CG-CD1	-5.78	101.17	111.00
7	I	113	ASP	CB-CG-OD1	5.78	123.50	118.30
2	B	114	PRO	N-CD-CG	5.78	111.86	103.20
2	B	393	LYS	N-CA-CB	5.78	120.99	110.60
3	C	182	PRO	N-CD-CG	-5.78	94.54	103.20
9	K	6	ARG	CD-NE-CZ	5.77	131.68	123.60
1	A	914	GLU	CG-CD-OE1	5.77	129.84	118.30
3	C	20	PHE	N-CA-C	5.77	126.57	111.00
2	B	959	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	12	ARG	CG-CD-NE	-5.76	99.70	111.80
2	B	698	GLU	OE1-CD-OE2	-5.76	116.39	123.30
1	A	49	LYS	CB-CG-CD	5.76	126.57	111.60
1	A	112	LYS	CD-CE-NZ	-5.75	98.46	111.70
1	A	917	SER	CA-CB-OG	-5.75	95.67	111.20
1	A	1004	ASN	N-CA-C	5.75	126.53	111.00
2	B	848	ARG	CG-CD-NE	-5.75	99.73	111.80
1	A	364	VAL	CA-CB-CG2	5.74	119.52	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	904	ARG	NE-CZ-NH1	-5.74	117.43	120.30
4	E	148	GLU	CG-CD-OE2	5.74	129.78	118.30
4	E	141	VAL	CA-CB-CG1	5.74	119.50	110.90
9	K	17	SER	CB-CA-C	-5.74	99.20	110.10
1	A	1141	THR	OG1-CB-CG2	-5.73	96.82	110.00
6	H	53	ASP	CB-CG-OD2	5.73	123.46	118.30
6	H	107	VAL	CA-CB-CG1	5.73	119.50	110.90
1	A	423	ASP	CB-CG-OD1	5.73	123.46	118.30
2	B	391	ASP	N-CA-CB	5.73	120.91	110.60
2	B	948	ILE	CG1-CB-CG2	-5.73	98.80	111.40
1	A	933	TYR	CB-CG-CD2	5.72	124.43	121.00
1	A	1119	TYR	CG-CD1-CE1	-5.72	116.72	121.30
1	A	985	ASP	CB-CG-OD2	5.72	123.44	118.30
1	A	629	LEU	CB-CG-CD2	-5.71	101.29	111.00
3	C	79	GLN	CA-CB-CG	5.71	125.96	113.40
9	K	1	MET	CB-CG-SD	-5.71	95.27	112.40
1	A	893	PHE	CD1-CE1-CZ	5.71	126.95	120.10
2	B	328	GLU	CA-CB-CG	-5.71	100.85	113.40
4	E	9	ILE	CG1-CB-CG2	-5.71	98.85	111.40
1	A	35	ILE	CG1-CB-CG2	-5.70	98.85	111.40
2	B	1031	LEU	CB-CG-CD1	5.70	120.70	111.00
7	I	10	CYS	N-CA-C	5.70	126.39	111.00
2	B	1019	SER	C-N-CA	-5.70	107.45	121.70
1	A	1176	LEU	CB-CG-CD1	5.70	120.69	111.00
4	E	131	THR	CA-CB-CG2	5.70	120.38	112.40
1	A	305	ASP	OD1-CG-OD2	-5.69	112.48	123.30
2	B	429	PHE	N-CA-CB	-5.69	100.35	110.60
1	A	79	GLY	N-CA-C	-5.69	98.87	113.10
1	A	722	LEU	CB-CG-CD1	5.69	120.67	111.00
1	A	1062	GLU	CG-CD-OE1	-5.69	106.92	118.30
2	B	529	GLU	OE1-CD-OE2	5.69	130.13	123.30
2	B	771	SER	N-CA-CB	5.69	119.03	110.50
4	E	192	ARG	CD-NE-CZ	5.69	131.56	123.60
1	A	128	ILE	CA-CB-CG1	5.69	121.80	111.00
1	A	834	THR	CA-CB-CG2	-5.68	104.44	112.40
4	E	112	TYR	CB-CG-CD2	5.68	124.41	121.00
2	B	276	ILE	CG1-CB-CG2	-5.68	98.90	111.40
3	C	18	VAL	N-CA-C	-5.68	95.66	111.00
1	A	705	LYS	N-CA-CB	5.68	120.82	110.60
2	B	1097	HIS	CA-CB-CG	-5.68	103.95	113.60
1	A	1359	ASP	CB-CG-OD2	5.67	123.41	118.30
2	B	35	SER	CB-CA-C	-5.67	99.32	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	29	CYS	CA-CB-SG	5.67	124.21	114.00
1	A	17	VAL	CG1-CB-CG2	-5.67	101.82	110.90
2	B	976	ILE	CG1-CB-CG2	-5.67	98.93	111.40
1	A	555	ASP	OD1-CG-OD2	-5.67	112.53	123.30
1	A	913	LEU	CB-CG-CD2	5.67	120.63	111.00
1	A	376	TYR	CZ-CE2-CD2	-5.66	114.70	119.80
2	B	1201	LYS	CD-CE-NZ	-5.66	98.67	111.70
1	A	938	LYS	CG-CD-CE	-5.66	94.92	111.90
3	C	16	ASP	OD1-CG-OD2	-5.66	112.54	123.30
6	H	52	GLN	CA-C-N	5.66	129.66	117.20
2	B	967	ARG	NE-CZ-NH2	5.66	123.13	120.30
9	K	110	ASN	CB-CA-C	5.66	121.72	110.40
1	A	1325	THR	CA-CB-CG2	5.66	120.32	112.40
2	B	668	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	918	GLU	OE1-CD-OE2	-5.66	116.51	123.30
6	H	112	ILE	CG1-CB-CG2	-5.66	98.96	111.40
1	A	1420	ASP	CB-CG-OD1	-5.65	113.21	118.30
1	A	377	PRO	CA-N-CD	-5.65	103.59	111.50
1	A	1109	LYS	CB-CA-C	5.65	121.70	110.40
2	B	371	GLU	CG-CD-OE1	5.65	129.60	118.30
1	A	801	GLU	CG-CD-OE1	-5.65	107.00	118.30
1	A	96	ILE	CA-CB-CG1	5.64	121.72	111.00
1	A	1405	THR	CA-C-N	-5.64	104.78	117.20
3	C	240	VAL	CB-CA-C	-5.64	100.68	111.40
1	A	825	ILE	CG1-CB-CG2	-5.64	98.99	111.40
1	A	897	TYR	CB-CG-CD2	-5.64	117.61	121.00
6	H	16	ASP	CB-CA-C	-5.64	99.11	110.40
7	I	45	ARG	CB-CA-C	-5.64	99.11	110.40
2	B	858	SER	CA-CB-OG	-5.64	95.97	111.20
1	A	291	GLU	CG-CD-OE1	5.64	129.57	118.30
1	A	65	LEU	CB-CG-CD2	5.64	120.58	111.00
4	E	31	THR	CA-CB-CG2	5.64	120.29	112.40
9	K	96	ASN	N-CA-CB	5.64	120.75	110.60
3	C	76	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	651	LYS	CD-CE-NZ	5.63	124.66	111.70
2	B	680	THR	OG1-CB-CG2	-5.63	97.04	110.00
1	A	843	LYS	CB-CA-C	5.63	121.66	110.40
2	B	668	ASP	OD1-CG-OD2	-5.63	112.61	123.30
2	B	1162	ILE	CG1-CB-CG2	-5.63	99.02	111.40
3	C	193	TYR	CZ-CE2-CD2	-5.63	114.73	119.80
1	A	1043	ASP	OD1-CG-OD2	-5.63	112.61	123.30
1	A	1133	LEU	CB-CG-CD2	-5.63	101.44	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	884	ARG	CG-CD-NE	-5.63	99.98	111.80
1	A	475	THR	CA-CB-CG2	5.62	120.27	112.40
2	B	165	VAL	CG1-CB-CG2	-5.62	101.90	110.90
5	F	120	ILE	CG1-CB-CG2	-5.62	99.03	111.40
1	A	1241	ARG	CD-NE-CZ	5.62	131.47	123.60
2	B	1156	ASP	CB-CG-OD1	5.62	123.36	118.30
4	E	98	ILE	CB-CA-C	5.62	122.84	111.60
9	K	73	LEU	CA-CB-CG	5.62	128.23	115.30
3	C	255	VAL	CB-CA-C	-5.62	100.72	111.40
2	B	131	ASP	CB-CG-OD2	5.62	123.36	118.30
2	B	914	LYS	CB-CA-C	-5.62	99.17	110.40
1	A	890	ASP	CB-CG-OD1	5.61	123.35	118.30
2	B	1020	ARG	CA-CB-CG	5.61	125.74	113.40
1	A	1336	MET	CA-CB-CG	5.61	122.83	113.30
2	B	359	GLU	CB-CA-C	-5.61	99.19	110.40
2	B	641	GLU	CG-CD-OE1	5.61	129.52	118.30
2	B	692	TYR	CB-CG-CD2	-5.61	117.64	121.00
4	E	28	TYR	CD1-CE1-CZ	5.61	124.84	119.80
2	B	1159	ARG	NE-CZ-NH2	-5.60	117.50	120.30
3	C	87	PHE	CD1-CE1-CZ	5.60	126.83	120.10
6	H	91	ASP	CB-CG-OD2	5.60	123.34	118.30
7	I	78	CYS	CA-CB-SG	5.60	124.09	114.00
8	J	39	LEU	CB-CG-CD1	5.60	120.53	111.00
1	A	351	THR	CB-CA-C	-5.60	96.47	111.60
1	A	1012	ARG	CA-CB-CG	5.60	125.72	113.40
1	A	419	LYS	O-C-N	-5.60	113.74	122.70
10	L	50	ASP	CB-CG-OD1	5.60	123.34	118.30
10	L	57	LEU	CB-CA-C	-5.60	99.56	110.20
2	B	1017	ILE	CA-CB-CG1	-5.60	100.37	111.00
1	A	571	LEU	CB-CG-CD1	-5.60	101.49	111.00
2	B	653	VAL	CA-CB-CG1	5.60	119.29	110.90
1	A	945	GLU	OE1-CD-OE2	5.59	130.01	123.30
2	B	327	ARG	NH1-CZ-NH2	5.59	125.55	119.40
8	J	28	ASP	N-CA-CB	5.59	120.67	110.60
1	A	434	ARG	CG-CD-NE	-5.59	100.06	111.80
1	A	1349	TYR	CZ-CE2-CD2	5.59	124.83	119.80
2	B	106	ASP	N-CA-CB	-5.59	100.54	110.60
3	C	47	ASP	CB-CG-OD1	-5.59	113.27	118.30
6	H	110	ASP	OD1-CG-OD2	-5.59	112.68	123.30
1	A	1407	GLU	CB-CA-C	5.59	121.58	110.40
1	A	984	LYS	CA-CB-CG	5.58	125.68	113.40
1	A	1411	GLU	CG-CD-OE1	5.58	129.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1448	GLU	CG-CD-OE1	5.58	129.46	118.30
2	B	407	ASP	OD1-CG-OD2	-5.58	112.69	123.30
4	E	103	LYS	CA-CB-CG	5.58	125.68	113.40
2	B	40	GLU	OE1-CD-OE2	5.58	130.00	123.30
1	A	672	ASP	OD1-CG-OD2	-5.57	112.71	123.30
3	C	183	TRP	O-C-N	-5.57	113.78	122.70
1	A	1334	ASP	CB-CG-OD2	-5.57	113.28	118.30
6	H	5	LEU	CB-CG-CD1	-5.57	101.53	111.00
3	C	35	ARG	CG-CD-NE	-5.56	100.12	111.80
1	A	898	ARG	NH1-CZ-NH2	-5.56	113.28	119.40
1	A	711	ARG	NH1-CZ-NH2	-5.56	113.29	119.40
2	B	324	ILE	CG1-CB-CG2	-5.56	99.17	111.40
2	B	446	LEU	CB-CA-C	5.56	120.77	110.20
9	K	95	ILE	O-C-N	5.56	131.60	122.70
1	A	456	MET	CG-SD-CE	-5.55	91.31	100.20
2	B	451	LYS	CA-C-N	5.55	129.41	117.20
2	B	711	GLU	CG-CD-OE2	5.55	129.40	118.30
2	B	1055	ILE	CA-CB-CG1	5.55	121.55	111.00
8	J	51	LEU	CB-CG-CD1	5.55	120.44	111.00
8	J	31	ASP	OD1-CG-OD2	-5.54	112.77	123.30
2	B	392	ARG	NE-CZ-NH2	-5.54	117.53	120.30
8	J	6	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	A	600	PRO	CA-N-CD	5.54	119.46	111.70
3	C	14	SER	N-CA-C	-5.54	96.04	111.00
8	J	16	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	1271	ILE	N-CA-CB	5.54	123.54	110.80
1	A	63	ARG	NE-CZ-NH2	-5.54	117.53	120.30
8	J	6	ARG	O-C-N	5.54	131.56	122.70
1	A	411	ASP	N-CA-CB	5.53	120.56	110.60
1	A	658	LEU	CB-CG-CD2	-5.53	101.59	111.00
1	A	1362	TYR	CD1-CE1-CZ	-5.53	114.82	119.80
2	B	758	PHE	CB-CG-CD2	5.53	124.67	120.80
5	F	116	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	871	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	678	GLU	OE1-CD-OE2	-5.53	116.67	123.30
2	B	864	LYS	CD-CE-NZ	5.53	124.42	111.70
1	A	597	LEU	CB-CG-CD2	-5.53	101.60	111.00
3	C	25	VAL	CB-CA-C	-5.53	100.90	111.40
1	A	1006	ILE	CA-CB-CG1	5.53	121.50	111.00
2	B	501	PRO	O-C-N	5.53	131.54	122.70
2	B	980	PHE	CG-CD2-CE2	5.53	126.88	120.80
3	C	4	GLU	O-C-N	5.53	132.59	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	895	ASP	OD1-CG-OD2	-5.52	112.80	123.30
2	B	63	ILE	O-C-N	-5.52	113.86	122.70
1	A	1280	GLU	CB-CG-CD	5.52	129.11	114.20
1	A	1145	SER	N-CA-CB	-5.52	102.22	110.50
3	C	119	VAL	CA-CB-CG1	-5.52	102.62	110.90
7	I	72	ASP	OD1-CG-OD2	-5.52	112.81	123.30
3	C	241	ASP	CB-CG-OD1	5.52	123.27	118.30
4	E	57	MET	CG-SD-CE	5.52	109.03	100.20
1	A	1003	LYS	CA-CB-CG	-5.51	101.27	113.40
1	A	1321	GLY	O-C-N	-5.51	113.88	122.70
2	B	811	TYR	CZ-CE2-CD2	-5.51	114.84	119.80
1	A	109	HIS	C-N-CA	5.51	135.48	121.70
2	B	304	ASP	N-CA-CB	5.51	120.52	110.60
2	B	736	THR	N-CA-CB	5.51	120.77	110.30
10	L	63	ARG	CG-CD-NE	5.51	123.37	111.80
2	B	109	THR	N-CA-C	5.51	125.88	111.00
2	B	56	ASP	O-C-N	-5.51	113.89	122.70
2	B	419	THR	OG1-CB-CG2	-5.50	97.34	110.00
1	A	646	PHE	C-N-CA	-5.50	110.75	122.30
1	A	1003	LYS	CB-CG-CD	5.50	125.90	111.60
3	C	23	SER	N-CA-C	-5.50	96.15	111.00
6	H	91	ASP	CA-C-O	5.50	131.65	120.10
3	C	75	MET	CB-CA-C	5.50	121.40	110.40
3	C	248	ILE	CB-CG1-CD1	-5.50	98.50	113.90
4	E	29	PHE	CB-CG-CD1	-5.50	116.95	120.80
1	A	1267	MET	CB-CA-C	5.50	121.39	110.40
7	I	44	TYR	CD1-CE1-CZ	5.50	124.75	119.80
1	A	549	MET	CA-CB-CG	-5.50	103.96	113.30
1	A	1326	ARG	CG-CD-NE	-5.49	100.26	111.80
2	B	936	ASP	CB-CG-OD2	5.49	123.24	118.30
2	B	404	LYS	CD-CE-NZ	-5.49	99.07	111.70
2	B	833	TYR	CB-CG-CD1	5.49	124.29	121.00
1	A	326	ARG	CA-CB-CG	5.49	125.47	113.40
1	A	195	ASP	CB-CG-OD1	5.49	123.24	118.30
2	B	879	ARG	CB-CA-C	-5.49	99.43	110.40
5	F	116	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	840	ARG	CG-CD-NE	-5.48	100.29	111.80
1	A	1034	GLU	OE1-CD-OE2	-5.48	116.73	123.30
2	B	889	THR	N-CA-CB	5.48	120.70	110.30
4	E	28	TYR	CD1-CG-CD2	-5.47	111.88	117.90
4	E	121	MET	CB-CG-SD	5.47	128.82	112.40
9	K	54	ARG	CD-NE-CZ	5.47	131.26	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	68	GLU	CB-CG-CD	5.47	128.98	114.20
6	H	86	ASP	CB-CG-OD2	5.47	123.22	118.30
2	B	961	LEU	CA-CB-CG	5.47	127.88	115.30
3	C	215	GLU	OE1-CD-OE2	-5.47	116.74	123.30
10	L	50	ASP	N-CA-CB	5.46	120.44	110.60
1	A	16	GLU	OE1-CD-OE2	5.46	129.85	123.30
1	A	489	LEU	CB-CG-CD2	5.46	120.28	111.00
2	B	1223	ASP	C-N-CA	5.46	135.35	121.70
4	E	153	HIS	CA-CB-CG	5.46	122.89	113.60
5	F	97	ARG	CB-CG-CD	5.46	125.80	111.60
3	C	95	CYS	CA-CB-SG	5.46	123.82	114.00
10	L	50	ASP	OD1-CG-OD2	-5.45	112.94	123.30
1	A	72	GLU	N-CA-C	5.45	125.72	111.00
4	E	204	THR	N-CA-CB	-5.45	99.95	110.30
5	F	122	MET	CB-CA-C	-5.45	99.51	110.40
1	A	230	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	A	1301	GLU	N-CA-CB	5.45	120.40	110.60
4	E	139	ALA	CB-CA-C	-5.45	101.93	110.10
2	B	698	GLU	CG-CD-OE1	5.44	129.19	118.30
2	B	896	ASP	N-CA-CB	5.44	120.40	110.60
4	E	195	VAL	CG1-CB-CG2	-5.44	102.20	110.90
2	B	969	ARG	CD-NE-CZ	-5.44	115.99	123.60
7	I	4	PHE	CB-CG-CD2	5.44	124.61	120.80
1	A	774	ARG	NH1-CZ-NH2	-5.43	113.42	119.40
1	A	968	GLN	CA-CB-CG	-5.43	101.45	113.40
2	B	389	ALA	N-CA-CB	-5.43	102.50	110.10
1	A	159	THR	N-CA-CB	5.43	120.62	110.30
1	A	1214	GLU	O-C-N	5.43	131.39	122.70
2	B	564	GLU	CG-CD-OE1	-5.43	107.44	118.30
6	H	128	ASN	N-CA-C	5.43	125.66	111.00
1	A	917	SER	N-CA-CB	-5.43	102.36	110.50
2	B	203	PHE	N-CA-CB	-5.43	100.83	110.60
2	B	692	TYR	CB-CG-CD1	5.43	124.26	121.00
2	B	655	LYS	CD-CE-NZ	5.42	124.18	111.70
5	F	73	ALA	N-CA-C	5.42	125.62	111.00
4	E	28	TYR	CB-CG-CD2	5.42	124.25	121.00
6	H	115	TYR	CA-C-N	5.41	129.11	117.20
2	B	964	VAL	CG1-CB-CG2	5.41	119.56	110.90
4	E	167	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	A	474	VAL	CG1-CB-CG2	5.41	119.55	110.90
2	B	994	TYR	CB-CG-CD2	5.40	124.24	121.00
1	A	1012	ARG	NE-CZ-NH2	-5.40	117.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1066	VAL	CA-CB-CG2	-5.40	102.80	110.90
1	A	1201	ALA	N-CA-CB	-5.40	102.54	110.10
1	A	998	LEU	CB-CG-CD1	-5.40	101.83	111.00
4	E	112	TYR	CZ-CE2-CD2	5.40	124.66	119.80
2	B	451	LYS	O-C-N	-5.39	114.07	122.70
1	A	788	SER	CB-CA-C	5.39	120.34	110.10
1	A	802	ASN	N-CA-C	5.39	125.56	111.00
3	C	172	PRO	O-C-N	5.39	131.33	122.70
3	C	175	ALA	N-CA-CB	-5.39	102.55	110.10
1	A	567	LYS	CA-C-O	-5.39	108.78	120.10
3	C	250	THR	OG1-CB-CG2	-5.39	97.60	110.00
2	B	1002	THR	N-CA-CB	-5.39	100.06	110.30
1	A	646	PHE	CB-CG-CD2	-5.38	117.03	120.80
6	H	24	CYS	CB-CA-C	-5.38	99.63	110.40
1	A	686	ALA	N-CA-CB	5.38	117.63	110.10
2	B	108	VAL	CB-CA-C	5.38	121.62	111.40
2	B	328	GLU	CG-CD-OE1	-5.38	107.54	118.30
2	B	699	GLU	CB-CA-C	-5.38	99.64	110.40
1	A	207	ILE	CA-CB-CG1	5.38	121.21	111.00
10	L	69	ALA	CA-C-N	-5.37	105.38	117.20
2	B	1091	TYR	CD1-CE1-CZ	5.37	124.64	119.80
4	E	137	GLU	CG-CD-OE2	-5.37	107.56	118.30
6	H	57	VAL	N-CA-C	5.37	125.49	111.00
1	A	268	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	940	ARG	NH1-CZ-NH2	-5.37	113.50	119.40
1	A	928	LEU	CB-CG-CD1	-5.36	101.88	111.00
7	I	16	PRO	N-CD-CG	-5.36	95.16	103.20
4	E	74	ASP	CB-CG-OD1	5.36	123.13	118.30
1	A	704	ALA	C-N-CA	-5.36	108.30	121.70
6	H	77	ARG	CD-NE-CZ	5.36	131.11	123.60
8	J	13	VAL	CG1-CB-CG2	-5.36	102.32	110.90
9	K	70	ARG	CB-CA-C	5.36	121.12	110.40
1	A	917	SER	CB-CA-C	-5.36	99.92	110.10
2	B	1155	SER	N-CA-CB	5.36	118.54	110.50
7	I	33	SER	N-CA-C	-5.36	96.53	111.00
1	A	200	ARG	NE-CZ-NH1	5.35	122.98	120.30
2	B	990	ILE	CB-CA-C	-5.35	100.89	111.60
4	E	61	GLN	N-CA-C	-5.35	96.55	111.00
7	I	88	SER	CB-CA-C	-5.35	99.93	110.10
1	A	566	ILE	O-C-N	5.35	131.26	122.70
6	H	8	ASP	OD1-CG-OD2	-5.35	113.14	123.30
6	H	80	ARG	N-CA-C	-5.35	96.56	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	125	PRO	N-CA-C	-5.35	98.20	112.10
2	B	558	LEU	CB-CG-CD1	-5.35	101.91	111.00
2	B	104	GLU	OE1-CD-OE2	-5.34	116.89	123.30
9	K	6	ARG	CG-CD-NE	-5.34	100.58	111.80
1	A	469	ARG	CA-CB-CG	5.34	125.15	113.40
3	C	124	LEU	CB-CA-C	-5.34	100.06	110.20
1	A	443	LEU	CB-CG-CD1	-5.34	101.93	111.00
4	E	190	LEU	CB-CA-C	-5.34	100.06	110.20
4	E	81	GLU	N-CA-CB	-5.33	101.00	110.60
7	I	18	GLU	OE1-CD-OE2	5.33	129.70	123.30
8	J	6	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	A	995	GLU	CG-CD-OE1	-5.33	107.64	118.30
1	A	1042	PHE	CB-CG-CD2	-5.33	117.07	120.80
2	B	497	ARG	NH1-CZ-NH2	5.33	125.26	119.40
1	A	985	ASP	OD1-CG-OD2	5.33	133.42	123.30
1	A	295	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	908	LEU	CB-CG-CD1	5.32	120.05	111.00
1	A	764	CYS	N-CA-CB	-5.32	101.02	110.60
2	B	841	MET	CG-SD-CE	5.32	108.71	100.20
2	B	1183	LYS	O-C-N	-5.32	114.16	123.20
1	A	1194	ARG	CA-CB-CG	5.32	125.09	113.40
2	B	601	ARG	NH1-CZ-NH2	5.32	125.25	119.40
1	A	440	ASP	CB-CG-OD2	-5.31	113.52	118.30
3	C	251	LEU	CB-CA-C	-5.31	100.12	110.20
5	F	72	LYS	N-CA-CB	-5.31	101.05	110.60
6	H	103	LYS	CB-CG-CD	5.31	125.40	111.60
2	B	492	LEU	CB-CG-CD2	-5.31	101.98	111.00
9	K	93	SER	CB-CA-C	-5.31	100.02	110.10
1	A	1243	VAL	CA-CB-CG2	5.30	118.86	110.90
8	J	58	GLU	CG-CD-OE2	5.30	128.91	118.30
1	A	123	ARG	N-CA-CB	5.30	120.14	110.60
6	H	120	GLY	N-CA-C	5.30	126.36	113.10
1	A	923	LEU	N-CA-CB	5.30	121.00	110.40
2	B	412	LEU	N-CA-CB	5.30	121.00	110.40
2	B	1007	VAL	N-CA-CB	-5.30	99.84	111.50
3	C	207	CYS	CB-CA-C	-5.30	99.80	110.40
2	B	911	ILE	CA-CB-CG2	5.29	121.49	110.90
1	A	795	GLU	CB-CG-CD	5.29	128.49	114.20
2	B	213	ILE	CG1-CB-CG2	-5.29	99.75	111.40
10	L	28	LYS	O-C-N	-5.29	114.23	122.70
7	I	32	CYS	N-CA-C	-5.29	96.71	111.00
1	A	469	ARG	CD-NE-CZ	5.29	131.00	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	55	ILE	CB-CA-C	-5.29	101.03	111.60
1	A	387	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	653	VAL	CG1-CB-CG2	-5.28	102.44	110.90
1	A	154	SER	CB-CA-C	5.28	120.14	110.10
3	C	10	ILE	CB-CA-C	-5.28	101.04	111.60
4	E	85	GLU	OE1-CD-OE2	5.28	129.64	123.30
2	B	621	GLU	CG-CD-OE2	5.28	128.86	118.30
1	A	684	ALA	CB-CA-C	5.28	118.01	110.10
7	I	120	GLN	N-CA-C	5.28	125.25	111.00
1	A	1170	ILE	CG1-CB-CG2	-5.27	99.80	111.40
2	B	230	ALA	N-CA-C	5.27	125.23	111.00
1	A	1345	ARG	NE-CZ-NH1	5.27	122.94	120.30
5	F	154	ASP	OD1-CG-OD2	-5.27	113.29	123.30
5	F	140	ASP	N-CA-C	5.27	125.22	111.00
4	E	76	GLY	N-CA-C	-5.27	99.93	113.10
1	A	280	GLU	CA-CB-CG	5.26	124.98	113.40
2	B	724	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	790	ASP	OD1-CG-OD2	-5.26	113.30	123.30
2	B	362	PRO	CA-C-O	-5.26	107.57	120.20
2	B	795	ILE	CB-CA-C	-5.26	101.08	111.60
2	B	1183	LYS	CG-CD-CE	5.26	127.69	111.90
4	E	210	SER	N-CA-CB	-5.26	102.61	110.50
1	A	403	LYS	CA-CB-CG	5.26	124.97	113.40
6	H	102	TYR	CA-C-O	5.26	131.15	120.10
10	L	42	ARG	NE-CZ-NH1	5.25	122.93	120.30
2	B	518	HIS	CB-CA-C	-5.25	99.90	110.40
3	C	152	GLU	OE1-CD-OE2	5.25	129.60	123.30
10	L	60	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	A	466	SER	N-CA-C	5.25	125.17	111.00
1	A	926	GLN	N-CA-CB	5.25	120.04	110.60
1	A	416	ARG	CG-CD-NE	-5.24	100.79	111.80
1	A	1146	VAL	N-CA-CB	-5.24	99.96	111.50
2	B	378	LEU	CB-CG-CD2	-5.24	102.09	111.00
2	B	697	GLU	OE1-CD-OE2	5.24	129.59	123.30
5	F	116	ASP	OD1-CG-OD2	-5.24	113.34	123.30
1	A	586	ILE	CG1-CB-CG2	-5.24	99.87	111.40
9	K	53	ASP	OD1-CG-OD2	-5.24	113.34	123.30
1	A	1211	GLN	N-CA-CB	5.24	120.03	110.60
2	B	904	ARG	CG-CD-NE	-5.24	100.80	111.80
3	C	178	PHE	CD1-CE1-CZ	-5.24	113.82	120.10
6	H	124	ARG	CG-CD-NE	-5.24	100.81	111.80
3	C	183	TRP	N-CA-C	-5.23	96.87	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	541	ILE	CG1-CB-CG2	-5.23	99.89	111.40
1	A	1151	GLU	CG-CD-OE1	5.23	128.76	118.30
1	A	1436	ILE	CG1-CB-CG2	-5.23	99.89	111.40
2	B	315	LYS	CB-CA-C	-5.23	99.94	110.40
3	C	14	SER	O-C-N	-5.23	114.33	122.70
2	B	403	LYS	CD-CE-NZ	-5.23	99.68	111.70
1	A	1280	GLU	OE1-CD-OE2	-5.23	117.03	123.30
7	I	24	ARG	CA-CB-CG	5.23	124.90	113.40
2	B	41	LYS	CB-CG-CD	5.22	125.18	111.60
2	B	1224	PHE	CB-CG-CD2	5.22	124.46	120.80
2	B	250	PHE	C-N-CA	5.22	134.75	121.70
1	A	182	VAL	N-CA-C	5.22	125.09	111.00
2	B	942	ARG	CA-CB-CG	5.22	124.88	113.40
6	H	5	LEU	CB-CG-CD2	5.22	119.87	111.00
10	L	70	ARG	NH1-CZ-NH2	-5.22	113.66	119.40
3	C	109	SER	N-CA-CB	-5.22	102.68	110.50
10	L	30	ILE	CG1-CB-CG2	-5.22	99.92	111.40
1	A	521	MET	CG-SD-CE	5.21	108.54	100.20
2	B	56	ASP	N-CA-C	5.21	125.08	111.00
2	B	908	GLU	CG-CD-OE2	5.21	128.73	118.30
2	B	884	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	613	ILE	CA-CB-CG2	5.21	121.32	110.90
2	B	497	ARG	CG-CD-NE	-5.21	100.86	111.80
2	B	598	GLU	CB-CG-CD	5.21	128.27	114.20
1	A	123	ARG	CD-NE-CZ	5.21	130.89	123.60
1	A	1267	MET	CA-CB-CG	-5.21	104.45	113.30
2	B	648	HIS	N-CA-C	5.21	125.06	111.00
2	B	811	TYR	CG-CD1-CE1	-5.21	117.13	121.30
4	E	194	GLU	OE1-CD-OE2	-5.21	117.05	123.30
3	C	263	THR	N-CA-CB	-5.21	100.41	110.30
4	E	12	LEU	CB-CA-C	5.21	120.09	110.20
4	E	87	SER	CB-CA-C	5.20	119.99	110.10
1	A	159	THR	CB-CA-C	-5.20	97.56	111.60
1	A	349	ALA	CB-CA-C	-5.20	102.30	110.10
2	B	578	THR	CA-CB-CG2	-5.20	105.12	112.40
1	A	385	ILE	CG1-CB-CG2	5.20	122.83	111.40
1	A	576	GLN	CB-CA-C	-5.20	100.01	110.40
1	A	482	PHE	CB-CG-CD1	5.20	124.44	120.80
3	C	17	ASN	CB-CA-C	-5.20	100.01	110.40
1	A	97	ALA	CB-CA-C	-5.19	102.31	110.10
1	A	1191	TRP	CD1-NE1-CE2	-5.19	104.33	109.00
2	B	907	GLY	N-CA-C	-5.19	100.12	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	20	ASP	N-CA-CB	5.19	119.94	110.60
4	E	200	ARG	NH1-CZ-NH2	5.19	125.11	119.40
5	F	133	VAL	CA-CB-CG2	-5.19	103.12	110.90
3	C	105	GLY	N-CA-C	-5.19	100.13	113.10
2	B	963	PHE	CB-CG-CD2	-5.19	117.17	120.80
1	A	129	LYS	N-CA-CB	-5.18	101.27	110.60
1	A	1014	ALA	CA-C-O	5.18	130.98	120.10
2	B	860	MET	CB-CA-C	-5.18	100.04	110.40
4	E	3	GLN	N-CA-CB	5.18	119.92	110.60
1	A	90	VAL	N-CA-CB	-5.18	100.11	111.50
1	A	305	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	907	THR	CA-CB-CG2	5.18	119.65	112.40
2	B	1028	GLU	CB-CA-C	-5.17	100.05	110.40
3	C	39	ALA	N-CA-C	5.17	124.97	111.00
1	A	1046	LEU	CB-CG-CD1	-5.17	102.21	111.00
4	E	26	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	1384	VAL	CA-CB-CG1	-5.17	103.15	110.90
9	K	74	ARG	CG-CD-NE	-5.17	100.95	111.80
1	A	602	ASP	C-N-CA	5.16	134.61	121.70
1	A	1062	GLU	CB-CG-CD	5.16	128.13	114.20
2	B	205	ILE	CG1-CB-CG2	-5.16	100.05	111.40
7	I	3	THR	C-N-CA	5.16	134.60	121.70
1	A	636	GLU	CG-CD-OE2	5.16	128.62	118.30
2	B	434	ARG	CA-CB-CG	5.16	124.75	113.40
1	A	413	ILE	CB-CG1-CD1	-5.16	99.46	113.90
2	B	175	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	A	1158	PRO	N-CD-CG	5.15	110.93	103.20
2	B	39	ARG	CG-CD-NE	5.15	122.62	111.80
1	A	41	MET	CG-SD-CE	5.15	108.44	100.20
2	B	995	ARG	CB-CG-CD	-5.15	98.21	111.60
1	A	376	TYR	CD1-CE1-CZ	5.15	124.43	119.80
8	J	18	TRP	CD1-NE1-CE2	-5.15	104.37	109.00
9	K	76	GLN	CB-CA-C	-5.15	100.11	110.40
1	A	146	MET	CA-CB-CG	-5.14	104.56	113.30
2	B	294	ASP	CB-CG-OD1	-5.14	113.67	118.30
8	J	28	ASP	CB-CA-C	-5.14	100.11	110.40
1	A	589	GLN	CB-CA-C	-5.14	100.12	110.40
1	A	685	GLU	N-CA-CB	-5.14	101.35	110.60
6	H	116	TYR	CB-CA-C	-5.14	100.12	110.40
1	A	1417	GLU	CG-CD-OE1	5.14	128.58	118.30
1	A	962	ARG	CG-CD-NE	-5.13	101.02	111.80
3	C	123	ASN	CB-CA-C	5.13	120.67	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1064	TYR	C-N-CA	-5.13	108.87	121.70
2	B	1185	CYS	CB-CA-C	5.13	120.67	110.40
1	A	44	THR	N-CA-CB	5.13	120.05	110.30
1	A	1332	PHE	CG-CD2-CE2	-5.13	115.16	120.80
1	A	1135	ARG	NE-CZ-NH2	5.13	122.86	120.30
2	B	137	TYR	CB-CG-CD1	5.13	124.08	121.00
1	A	681	GLU	OE1-CD-OE2	5.12	129.45	123.30
2	B	595	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	A	833	GLU	OE1-CD-OE2	-5.12	117.15	123.30
6	H	11	GLN	CB-CA-C	-5.12	100.16	110.40
4	E	52	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	1235	LYS	CB-CA-C	5.12	120.64	110.40
2	B	19	GLU	OE1-CD-OE2	-5.12	117.16	123.30
2	B	239	GLU	CB-CA-C	5.11	120.62	110.40
1	A	210	ILE	CG1-CB-CG2	-5.11	100.15	111.40
1	A	1103	GLU	N-CA-CB	-5.11	101.40	110.60
3	C	125	MET	CB-CG-SD	5.11	127.74	112.40
2	B	954	VAL	CB-CA-C	-5.11	101.69	111.40
3	C	24	ASN	CB-CA-C	-5.11	100.18	110.40
7	I	112	SER	N-CA-CB	-5.11	102.83	110.50
1	A	101	LYS	CD-CE-NZ	-5.11	99.96	111.70
1	A	790	ASP	CB-CG-OD2	5.10	122.89	118.30
6	H	34	ASP	CB-CG-OD2	5.10	122.89	118.30
2	B	124	TYR	CD1-CG-CD2	-5.10	112.29	117.90
2	B	494	HIS	CB-CA-C	5.10	120.61	110.40
6	H	102	TYR	N-CA-CB	-5.10	101.41	110.60
1	A	645	LEU	CB-CG-CD1	-5.10	102.33	111.00
2	B	580	VAL	CG1-CB-CG2	-5.10	102.74	110.90
2	B	637	LEU	CB-CG-CD1	-5.10	102.33	111.00
3	C	135	GLN	CA-CB-CG	5.10	124.62	113.40
6	H	130	ARG	NH1-CZ-NH2	5.10	125.01	119.40
10	L	54	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	1107	VAL	CA-CB-CG1	-5.09	103.26	110.90
1	A	1269	GLU	CB-CA-C	-5.09	100.21	110.40
1	A	1279	ILE	CG1-CB-CG2	-5.09	100.19	111.40
4	E	212	ARG	N-CA-CB	-5.09	101.43	110.60
1	A	687	LYS	N-CA-C	5.09	124.74	111.00
1	A	837	ILE	CA-CB-CG1	-5.09	101.33	111.00
1	A	1198	ASP	CB-CA-C	-5.09	100.23	110.40
3	C	3	GLU	CA-CB-CG	-5.09	102.21	113.40
3	C	55	THR	OG1-CB-CG2	-5.08	98.30	110.00
7	I	93	LYS	CD-CE-NZ	5.08	123.39	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	318	VAL	CG1-CB-CG2	-5.08	102.77	110.90
6	H	116	TYR	N-CA-C	5.08	124.73	111.00
1	A	80	HIS	CB-CA-C	5.08	120.56	110.40
4	E	215	MET	N-CA-C	5.08	124.72	111.00
2	B	90	ILE	N-CA-C	5.08	124.71	111.00
2	B	312	GLU	N-CA-CB	-5.08	101.46	110.60
2	B	689	LEU	CB-CG-CD1	-5.08	102.37	111.00
2	B	1130	PHE	CG-CD2-CE2	-5.08	115.21	120.80
4	E	96	PHE	CB-CG-CD2	5.08	124.35	120.80
2	B	855	PHE	CG-CD2-CE2	5.08	126.39	120.80
2	B	684	LEU	CB-CG-CD1	-5.07	102.38	111.00
1	A	896	ARG	CD-NE-CZ	-5.07	116.50	123.60
4	E	85	GLU	CG-CD-OE1	-5.07	108.16	118.30
6	H	18	GLY	O-C-N	-5.07	114.58	122.70
1	A	1158	PRO	CA-C-N	5.07	128.36	117.20
2	B	518	HIS	CA-CB-CG	5.07	122.22	113.60
6	H	110	ASP	C-N-CA	5.07	134.37	121.70
2	B	1154	ALA	N-CA-CB	5.07	117.19	110.10
6	H	63	LEU	CA-CB-CG	5.07	126.96	115.30
1	A	279	LEU	CA-CB-CG	5.07	126.95	115.30
1	A	399	HIS	C-N-CA	5.07	143.28	122.00
4	E	172	GLU	OE1-CD-OE2	5.06	129.38	123.30
1	A	495	GLU	OE1-CD-OE2	-5.06	117.23	123.30
2	B	37	PHE	CB-CG-CD1	-5.06	117.26	120.80
2	B	463	THR	OG1-CB-CG2	-5.06	98.36	110.00
1	A	685	GLU	CG-CD-OE1	5.06	128.42	118.30
2	B	601	ARG	NE-CZ-NH2	-5.06	117.77	120.30
2	B	393	LYS	CD-CE-NZ	-5.06	100.07	111.70
1	A	1000	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	1018	PHE	CZ-CE2-CD2	5.05	126.17	120.10
1	A	1138	ILE	CB-CG1-CD1	-5.05	99.76	113.90
1	A	1318	THR	CA-CB-CG2	5.05	119.47	112.40
1	A	1422	ARG	NH1-CZ-NH2	-5.05	113.84	119.40
2	B	56	ASP	CA-C-N	5.05	128.31	117.20
1	A	121	LEU	CA-CB-CG	5.05	126.91	115.30
2	B	217	ARG	NE-CZ-NH1	-5.05	117.78	120.30
2	B	284	ILE	CA-CB-CG1	5.05	120.59	111.00
4	E	55	ARG	NE-CZ-NH2	5.05	122.82	120.30
8	J	38	ARG	N-CA-C	-5.05	97.38	111.00
8	J	49	MET	N-CA-CB	-5.05	101.52	110.60
2	B	118	ARG	NH1-CZ-NH2	-5.04	113.85	119.40
2	B	477	ALA	O-C-N	-5.04	114.62	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	92	ASN	CB-CA-C	5.04	120.49	110.40
1	A	130	ASP	OD1-CG-OD2	-5.04	113.72	123.30
1	A	933	TYR	CZ-CE2-CD2	5.04	124.34	119.80
2	B	1103	ILE	N-CA-CB	5.04	122.40	110.80
9	K	47	ARG	NH1-CZ-NH2	5.04	124.95	119.40
3	C	184	ASN	C-N-CA	-5.04	109.10	121.70
1	A	1450	LEU	CB-CG-CD2	5.04	119.56	111.00
5	F	84	TYR	CG-CD1-CE1	5.04	125.33	121.30
7	I	52	ILE	CA-C-N	-5.04	106.13	116.20
2	B	21	GLU	CB-CA-C	5.04	120.47	110.40
2	B	512	ARG	N-CA-CB	-5.04	101.54	110.60
7	I	24	ARG	CB-CA-C	-5.04	100.33	110.40
7	I	118	ARG	N-CA-C	5.04	124.60	111.00
1	A	1445	ILE	O-C-N	5.03	130.75	122.70
2	B	828	ALA	N-CA-C	5.03	124.59	111.00
1	A	1443	VAL	CG1-CB-CG2	-5.03	102.85	110.90
9	K	78	THR	CB-CA-C	-5.03	98.02	111.60
1	A	174	ILE	CA-CB-CG1	5.03	120.56	111.00
2	B	1042	GLY	CA-C-O	-5.03	111.55	120.60
1	A	1027	ALA	N-CA-CB	-5.03	103.06	110.10
3	C	163	ILE	CB-CA-C	5.03	121.66	111.60
4	E	75	MET	CB-CA-C	5.03	120.45	110.40
2	B	642	ASP	CA-C-N	-5.02	106.15	117.20
1	A	1111	MET	CG-SD-CE	-5.02	92.17	100.20
2	B	1005	GLY	N-CA-C	5.02	125.66	113.10
1	A	1193	LEU	CB-CG-CD2	-5.02	102.47	111.00
1	A	1227	ILE	CA-CB-CG1	5.02	120.54	111.00
9	K	26	LYS	O-C-N	-5.02	114.67	122.70
9	K	74	ARG	CB-CG-CD	5.02	124.65	111.60
1	A	1214	GLU	CA-C-N	-5.02	106.16	117.20
2	B	129	PHE	N-CA-CB	-5.02	101.57	110.60
1	A	978	PRO	CB-CG-CD	-5.02	86.94	106.50
2	B	741	CYS	CA-CB-SG	5.01	123.02	114.00
3	C	27	LEU	C-N-CA	-5.01	109.16	121.70
2	B	1103	ILE	CA-C-N	-5.01	106.17	117.20
2	B	624	LEU	CB-CG-CD1	5.01	119.52	111.00
2	B	723	VAL	N-CA-CB	5.01	122.53	111.50
1	A	1240	CYS	N-CA-CB	-5.01	101.58	110.60
1	A	519	PRO	N-CD-CG	5.01	110.71	103.20
1	A	1264	GLU	CG-CD-OE2	5.01	128.32	118.30
1	A	95	PHE	N-CA-CB	-5.01	101.59	110.60
3	C	34	ARG	CD-NE-CZ	5.01	130.61	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ASP	N-CA-CB	5.00	119.61	110.60
1	A	1301	GLU	N-CA-C	-5.00	97.49	111.00
2	B	994	TYR	CZ-CE2-CD2	5.00	124.30	119.80
6	H	126	GLU	CA-CB-CG	5.00	124.41	113.40
1	A	1426	GLU	OE1-CD-OE2	-5.00	117.30	123.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	204	THR	CB

All (124) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1015	VAL	Mainchain
1	A	1027	ALA	Mainchain
1	A	1035	TYR	Sidechain
1	A	1046	LEU	Mainchain
1	A	1093	LYS	Peptide
1	A	1119	TYR	Sidechain
1	A	1155	ASP	Mainchain,Peptide
1	A	1218	GLN	Peptide
1	A	1232	ASN	Peptide
1	A	1301	GLU	Mainchain
1	A	1366	ARG	Sidechain
1	A	1375	MET	Mainchain
1	A	1384	VAL	Peptide
1	A	158	PRO	Peptide
1	A	165	GLY	Peptide
1	A	187	LYS	Peptide
1	A	191	THR	Peptide
1	A	194	ALA	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	460	VAL	Peptide
1	A	464	PRO	Mainchain,Peptide
1	A	469	ARG	Mainchain
1	A	555	ASP	Peptide
1	A	60	SER	Peptide

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Mol	Chain	Res	Type	Group
1	A	631	HIS	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	759	ALA	Mainchain
1	A	920	LEU	Mainchain
1	A	936	LEU	Mainchain
1	A	941	LYS	Mainchain
2	B	1009	ASP	Mainchain
2	B	1025	HIS	Sidechain
2	B	104	GLU	Peptide
2	B	107	GLY	Peptide
2	B	109	THR	Peptide
2	B	1097	HIS	Sidechain
2	B	1101	ASP	Peptide
2	B	1102	LYS	Peptide
2	B	1109	GLY	Peptide
2	B	1152	MET	Peptide
2	B	1155	SER	Peptide
2	B	1157	ALA	Peptide
2	B	1166	CYS	Mainchain
2	B	1181	GLU	Peptide
2	B	1221	SER	Peptide
2	B	1222	ARG	Peptide
2	B	199	MET	Mainchain
2	B	202	TYR	Sidechain
2	B	292	ILE	Mainchain
2	B	337	ARG	Sidechain
2	B	369	GLY	Peptide
2	B	431	TYR	Peptide
2	B	501	PRO	Peptide
2	B	517	THR	Mainchain
2	B	518	HIS	Sidechain
2	B	601	ARG	Sidechain
2	B	604	ARG	Sidechain
2	B	642	ASP	Peptide
2	B	643	ASP	Peptide
2	B	644	GLU	Peptide
2	B	667	GLN	Peptide
2	B	732	SER	Peptide

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Mol	Chain	Res	Type	Group
2	B	742	GLU	Mainchain
2	B	808	ALA	Mainchain
2	B	863	GLU	Peptide
2	B	868	MET	Peptide
2	B	882	THR	Peptide
2	B	884	ARG	Peptide
2	B	98	THR	Peptide
2	B	984	HIS	Sidechain
3	C	126	GLY	Peptide
3	C	156	THR	Mainchain
3	C	163	ILE	Mainchain
3	C	184	ASN	Peptide
3	C	190	ASP	Peptide
3	C	194	GLU	Mainchain
3	C	238	ILE	Mainchain
3	C	240	VAL	Mainchain
3	C	261	ALA	Peptide
3	C	267	GLN	Peptide
3	C	34	ARG	Sidechain
3	C	35	ARG	Sidechain
3	C	4	GLU	Peptide
4	E	125	PRO	Peptide
4	E	128	PRO	Peptide
4	E	170	LEU	Peptide
4	E	207	ARG	Mainchain
4	E	212	ARG	Sidechain
4	E	77	SER	Peptide
5	F	122	MET	Mainchain
5	F	144	GLU	Mainchain
6	H	102	TYR	Peptide
6	H	103	LYS	Peptide
6	H	127	GLY	Peptide
6	H	135	LEU	Peptide
6	H	136	LYS	Peptide
6	H	17	PRO	Peptide
6	H	26	ILE	Peptide
6	H	61	SER	Peptide
6	H	62	SER	Peptide
6	H	86	ASP	Peptide
6	H	87	ARG	Peptide
6	H	94	ASP	Peptide
7	I	26	LEU	Peptide

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Mol	Chain	Res	Type	Group
7	I	3	THR	Peptide
7	I	39	GLY	Mainchain
7	I	41	PRO	Mainchain
7	I	43	VAL	Mainchain
7	I	83	ASN	Peptide
8	J	21	TYR	Sidechain
9	K	70	ARG	Mainchain
10	L	35	SER	Peptide
10	L	59	ALA	Peptide

5.2 Too-close contacts [i](#)

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	10635	0	10688	689	0
2	B	8690	0	8715	513	0
3	C	2095	0	2053	155	0
4	E	1760	0	1788	130	0
5	F	670	0	689	44	0
6	H	1068	0	1040	164	0
7	I	990	0	949	71	0
8	J	525	0	537	44	0
9	K	919	0	929	73	0
10	L	364	0	388	65	0
11	A	2	0	0	0	0
12	A	2	0	0	1	0
12	B	1	0	0	1	0
12	C	1	0	0	2	0
12	I	2	0	0	0	0
12	J	1	0	0	2	0
12	L	1	0	0	1	0
13	A	31	0	12	0	0
All	All	27757	0	27788	1823	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (1823) 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:1057:LYS:CE	2:B:1057:LYS:CD	1.75	1.65
1:A:368:LYS:CE	1:A:368:LYS:CD	1.75	1.65
4:E:37:LEU:CD1	4:E:37:LEU:CG	1.75	1.64
1:A:919:ILE:CD1	1:A:919:ILE:CG1	1.75	1.64
1:A:1112:LYS:CE	1:A:1112:LYS:CD	1.74	1.64
4:E:71:LYS:CG	4:E:71:LYS:CD	1.75	1.64
3:C:116:LYS:CE	3:C:116:LYS:CD	1.75	1.64
2:B:436:VAL:CB	2:B:436:VAL:CA	1.76	1.64
1:A:174:ILE:CA	1:A:174:ILE:CB	1.75	1.64
1:A:1385:THR:CB	1:A:1385:THR:CG2	1.76	1.63
4:E:90:VAL:CG1	4:E:90:VAL:CB	1.75	1.63
10:L:64:LEU:CD1	10:L:64:LEU:CG	1.75	1.63
1:A:61:ILE:CB	1:A:61:ILE:CA	1.77	1.63
1:A:1102:LYS:CD	1:A:1102:LYS:CE	1.75	1.63
2:B:883:LEU:CB	2:B:883:LEU:CA	1.75	1.63
1:A:1445:ILE:CG2	1:A:1445:ILE:CB	1.74	1.63
2:B:353:LYS:CD	2:B:353:LYS:CG	1.74	1.62
3:C:205:LYS:CG	3:C:205:LYS:CB	1.74	1.62
1:A:1261:LYS:CD	1:A:1261:LYS:CE	1.77	1.62
1:A:237:THR:CB	1:A:237:THR:CG2	1.75	1.62
1:A:1239:ARG:CD	1:A:1239:ARG:CG	1.75	1.62
2:B:343:ILE:CD1	2:B:343:ILE:CG1	1.75	1.62
1:A:1350:LYS:CD	1:A:1350:LYS:CG	1.76	1.62
1:A:710:LEU:CD2	1:A:710:LEU:CG	1.75	1.62
7:I:1:MET:CG	7:I:1:MET:CB	1.76	1.61
4:E:129:PRO:CD	4:E:129:PRO:CG	1.76	1.61
1:A:1003:LYS:CD	1:A:1003:LYS:CG	1.76	1.61
8:J:38:ARG:CG	8:J:38:ARG:CB	1.75	1.61
2:B:118:ARG:CD	2:B:118:ARG:CG	1.76	1.61
4:E:45:LYS:CE	4:E:45:LYS:CD	1.75	1.61
9:K:25:THR:CB	9:K:25:THR:CG2	1.75	1.61
1:A:123:ARG:CD	1:A:123:ARG:CG	1.76	1.61
1:A:46:THR:CA	1:A:46:THR:CB	1.77	1.61
2:B:347:LYS:CD	2:B:347:LYS:CE	1.77	1.61
3:C:199:LYS:CD	3:C:199:LYS:CG	1.75	1.61
10:L:65:VAL:CB	10:L:65:VAL:CG2	1.78	1.61
2:B:882:THR:CB	2:B:882:THR:CG2	1.75	1.61
1:A:843:LYS:CD	1:A:843:LYS:CG	1.76	1.60
2:B:1163:CYS:CA	2:B:1163:CYS:CB	1.74	1.60
1:A:217:LYS:CD	1:A:217:LYS:CG	1.80	1.60
2:B:358:LYS:CB	2:B:358:LYS:CG	1.75	1.60
1:A:1215:ARG:CG	1:A:1215:ARG:CB	1.75	1.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:9:LYS:CD	3:C:9:LYS:CE	1.75	1.60
7:I:93:LYS:CD	7:I:93:LYS:CG	1.76	1.60
1:A:571:LEU:CD2	1:A:571:LEU:CG	1.78	1.60
1:A:74:MET:CG	1:A:74:MET:CB	1.80	1.60
2:B:425:THR:CG2	2:B:425:THR:CB	1.75	1.60
4:E:52:ARG:CB	4:E:52:ARG:CG	1.75	1.60
2:B:712:PRO:CG	2:B:712:PRO:CD	1.76	1.60
1:A:175:ARG:CB	1:A:175:ARG:CG	1.74	1.59
9:K:102:LYS:CE	9:K:102:LYS:CD	1.74	1.59
4:E:98:ILE:CA	4:E:98:ILE:CB	1.81	1.59
1:A:121:LEU:CG	1:A:121:LEU:CD1	1.75	1.59
1:A:840:ARG:CD	1:A:840:ARG:CG	1.76	1.59
10:L:62:LYS:CD	10:L:62:LYS:CE	1.80	1.59
3:C:94:LYS:CG	3:C:94:LYS:CB	1.75	1.59
2:B:616:ILE:CD1	2:B:616:ILE:CG1	1.79	1.59
10:L:43:THR:CG2	10:L:43:THR:CB	1.75	1.59
1:A:1235:LYS:CE	1:A:1235:LYS:CD	1.79	1.59
3:C:154:LYS:CG	3:C:154:LYS:CB	1.77	1.59
6:H:144:ILE:CG1	6:H:144:ILE:CD1	1.75	1.59
2:B:305:VAL:CB	2:B:305:VAL:CG1	1.79	1.59
2:B:775:LYS:CB	2:B:775:LYS:CG	1.77	1.59
2:B:167:ILE:CD1	2:B:167:ILE:CG1	1.81	1.58
6:H:107:VAL:CB	6:H:107:VAL:CA	1.76	1.58
1:A:941:LYS:CG	1:A:941:LYS:CD	1.75	1.58
4:E:103:LYS:CD	4:E:103:LYS:CE	1.75	1.58
1:A:144:THR:CB	1:A:144:THR:CG2	1.78	1.58
1:A:689:LYS:CE	1:A:689:LYS:CD	1.74	1.58
2:B:961:LEU:CG	2:B:961:LEU:CD1	1.77	1.58
3:C:199:LYS:CE	3:C:199:LYS:CD	1.80	1.58
2:B:1165:ILE:CD1	2:B:1165:ILE:CG1	1.75	1.58
4:E:161:LYS:CD	4:E:161:LYS:CE	1.82	1.58
6:H:19:ARG:CB	6:H:19:ARG:CG	1.77	1.58
5:F:72:LYS:CE	5:F:72:LYS:CD	1.75	1.58
10:L:54:ARG:CG	10:L:54:ARG:CD	1.77	1.58
2:B:418:LYS:CE	2:B:418:LYS:CD	1.74	1.57
3:C:163:ILE:CB	3:C:163:ILE:CG2	1.74	1.57
1:A:1003:LYS:CD	1:A:1003:LYS:CE	1.81	1.57
3:C:9:LYS:CG	3:C:9:LYS:CD	1.76	1.57
1:A:1236:LEU:CG	1:A:1236:LEU:CD2	1.78	1.57
6:H:77:ARG:CB	6:H:77:ARG:CG	1.81	1.57
9:K:111:LEU:CD1	9:K:111:LEU:CG	1.81	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1057:LYS:CD	2:B:1057:LYS:CG	1.80	1.57
3:C:169:LYS:CD	3:C:169:LYS:CE	1.75	1.57
4:E:129:PRO:CG	4:E:129:PRO:CB	1.75	1.57
4:E:191:LYS:CE	4:E:191:LYS:CD	1.75	1.57
9:K:88:LYS:CG	9:K:88:LYS:CD	1.76	1.57
1:A:728:LYS:CE	1:A:728:LYS:NZ	1.67	1.57
1:A:973:ILE:CG2	1:A:973:ILE:CB	1.74	1.57
1:A:66:LYS:CB	1:A:66:LYS:CG	1.76	1.56
1:A:720:ARG:CG	1:A:720:ARG:CD	1.78	1.56
2:B:434:ARG:CG	2:B:434:ARG:CB	1.77	1.56
3:C:15:LYS:CB	3:C:15:LYS:CG	1.75	1.56
7:I:30:ARG:CD	7:I:30:ARG:CG	1.76	1.56
1:A:1102:LYS:CG	1:A:1102:LYS:CD	1.77	1.56
2:B:646:LEU:CD1	2:B:646:LEU:CG	1.79	1.56
2:B:231:PRO:CB	2:B:231:PRO:CG	1.83	1.56
4:E:54:GLN:CG	4:E:54:GLN:CB	1.78	1.56
8:J:26:GLN:CB	8:J:26:GLN:CG	1.75	1.56
1:A:123:ARG:CB	1:A:123:ARG:CG	1.74	1.56
1:A:5:GLN:CG	1:A:5:GLN:CB	1.76	1.56
2:B:344:LYS:CB	2:B:344:LYS:CG	1.83	1.56
2:B:428:ILE:CG1	2:B:428:ILE:CD1	1.80	1.56
6:H:9:ILE:CB	6:H:9:ILE:CA	1.78	1.56
2:B:164:LYS:CE	2:B:164:LYS:CD	1.83	1.56
1:A:191:THR:CA	1:A:191:THR:CB	1.75	1.55
2:B:1097:HIS:CB	2:B:1097:HIS:CA	1.82	1.55
6:H:9:ILE:CD1	6:H:9:ILE:CG1	1.84	1.55
1:A:387:ARG:CG	1:A:387:ARG:CD	1.79	1.55
1:A:518:LYS:CD	1:A:518:LYS:CE	1.81	1.55
1:A:895:LYS:CD	1:A:895:LYS:CG	1.82	1.55
1:A:941:LYS:CD	1:A:941:LYS:CE	1.84	1.55
5:F:129:LYS:CD	5:F:129:LYS:CE	1.78	1.55
10:L:61:THR:CG2	10:L:61:THR:CB	1.83	1.55
2:B:706:GLN:CG	2:B:706:GLN:CB	1.84	1.55
2:B:706:GLN:CG	2:B:706:GLN:CD	1.75	1.55
1:A:1112:LYS:CE	1:A:1112:LYS:NZ	1.70	1.55
9:K:26:LYS:CB	9:K:26:LYS:CG	1.78	1.55
1:A:295:LEU:CG	1:A:295:LEU:CD2	1.83	1.55
5:F:76:LYS:CE	5:F:76:LYS:NZ	1.67	1.55
6:H:91:ASP:C	6:H:91:ASP:CA	1.75	1.55
1:A:1187:GLN:CG	1:A:1187:GLN:CB	1.81	1.55
2:B:399:ASP:CG	2:B:399:ASP:CB	1.75	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:870:ILE:CA	2:B:870:ILE:CB	1.81	1.55
1:A:1144:LYS:CE	1:A:1144:LYS:CD	1.82	1.54
1:A:49:LYS:CD	1:A:49:LYS:CE	1.79	1.54
1:A:274:ILE:CA	1:A:274:ILE:CB	1.80	1.54
4:E:152:LYS:CG	4:E:152:LYS:CD	1.81	1.54
10:L:26:THR:CG2	10:L:26:THR:CB	1.79	1.54
1:A:1222:ASN:CG	1:A:1222:ASN:CB	1.76	1.54
4:E:41:ASP:CB	4:E:41:ASP:CG	1.76	1.54
1:A:1132:LYS:CD	1:A:1132:LYS:CG	1.78	1.54
1:A:830:LYS:CD	1:A:830:LYS:CG	1.85	1.54
1:A:695:LYS:CD	1:A:695:LYS:CE	1.84	1.54
7:I:120:GLN:CG	7:I:120:GLN:CB	1.79	1.54
10:L:62:LYS:NZ	10:L:62:LYS:CE	1.68	1.54
1:A:1132:LYS:CE	1:A:1132:LYS:CD	1.81	1.54
1:A:601:LYS:NZ	1:A:601:LYS:CE	1.70	1.54
2:B:915:THR:CA	2:B:915:THR:CB	1.74	1.54
6:H:136:LYS:C	6:H:136:LYS:CA	1.75	1.54
1:A:1445:ILE:CG1	1:A:1445:ILE:CD1	1.82	1.53
3:C:154:LYS:CG	3:C:154:LYS:CD	1.85	1.53
7:I:49:ILE:CG1	7:I:49:ILE:CD1	1.84	1.53
6:H:52:GLN:CD	6:H:52:GLN:CG	1.76	1.53
1:A:601:LYS:CD	1:A:601:LYS:CE	1.85	1.53
1:A:843:LYS:CE	1:A:843:LYS:CD	1.80	1.53
9:K:26:LYS:CG	9:K:26:LYS:CD	1.80	1.53
2:B:1154:ALA:CA	2:B:1154:ALA:CB	1.83	1.53
1:A:44:THR:CB	1:A:44:THR:CA	1.81	1.53
2:B:962:LYS:CE	2:B:962:LYS:CD	1.85	1.53
10:L:28:LYS:CA	10:L:28:LYS:C	1.76	1.53
1:A:1109:LYS:CG	1:A:1109:LYS:CD	1.87	1.53
1:A:157:ASP:CB	1:A:157:ASP:CG	1.77	1.53
2:B:620:ARG:CG	2:B:620:ARG:CD	1.81	1.53
2:B:227:LYS:CE	2:B:227:LYS:CD	1.79	1.52
10:L:45:ALA:CA	10:L:45:ALA:CB	1.81	1.52
2:B:434:ARG:CG	2:B:434:ARG:CD	1.83	1.52
3:C:102:GLN:CG	3:C:102:GLN:CB	1.86	1.52
1:A:1223:ASP:CG	1:A:1223:ASP:CB	1.75	1.52
2:B:595:ARG:CG	2:B:595:ARG:CD	1.82	1.52
3:C:267:GLN:C	3:C:267:GLN:CA	1.75	1.52
1:A:1290:LYS:NZ	1:A:1290:LYS:CE	1.71	1.52
2:B:415:GLN:CB	2:B:415:GLN:CG	1.83	1.52
1:A:1280:GLU:CD	1:A:1280:GLU:CG	1.75	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LYS:CD	1:A:368:LYS:CG	1.84	1.52
7:I:45:ARG:CD	7:I:45:ARG:CG	1.85	1.51
1:A:199:LEU:CG	1:A:199:LEU:CD1	1.81	1.51
1:A:1109:LYS:CG	1:A:1109:LYS:CB	1.82	1.51
2:B:959:ASP:CG	2:B:959:ASP:CB	1.78	1.51
1:A:566:ILE:CB	1:A:566:ILE:CG2	1.84	1.51
4:E:191:LYS:CE	4:E:191:LYS:NZ	1.72	1.51
2:B:646:LEU:CD2	2:B:646:LEU:CG	1.88	1.51
1:A:248:PRO:CG	1:A:248:PRO:CB	1.77	1.51
2:B:227:LYS:CE	2:B:227:LYS:NZ	1.71	1.51
1:A:1132:LYS:CE	1:A:1132:LYS:NZ	1.68	1.51
2:B:531:GLN:CG	2:B:531:GLN:CB	1.83	1.51
2:B:509:ALA:CA	2:B:509:ALA:CB	1.87	1.51
1:A:1135:ARG:CD	1:A:1135:ARG:CG	1.85	1.51
6:H:131:ASN:CG	6:H:131:ASN:CB	1.74	1.51
2:B:227:LYS:CD	2:B:227:LYS:CG	1.82	1.51
2:B:346:GLU:CG	2:B:346:GLU:CD	1.79	1.50
5:F:87:LYS:CE	5:F:87:LYS:NZ	1.69	1.50
6:H:19:ARG:CD	6:H:19:ARG:CG	1.84	1.50
10:L:48:CYS:CA	10:L:48:CYS:C	1.78	1.50
1:A:1039:LYS:NZ	1:A:1039:LYS:CE	1.68	1.50
2:B:641:GLU:CD	2:B:641:GLU:CG	1.79	1.50
2:B:502:ILE:CB	2:B:502:ILE:CA	1.90	1.50
9:K:20:LYS:CD	9:K:20:LYS:CG	1.85	1.50
1:A:895:LYS:CD	1:A:895:LYS:CE	1.87	1.50
2:B:246:LYS:C	2:B:246:LYS:CA	1.79	1.50
1:A:795:GLU:CD	1:A:795:GLU:CG	1.79	1.50
2:B:1102:LYS:CG	2:B:1102:LYS:CB	1.83	1.50
1:A:217:LYS:CE	1:A:217:LYS:CD	1.90	1.50
2:B:723:VAL:CB	2:B:723:VAL:CG1	1.85	1.50
3:C:160:LYS:CE	3:C:160:LYS:NZ	1.70	1.49
1:A:1171:GLN:CD	1:A:1171:GLN:CG	1.76	1.49
6:H:139:ASN:CB	6:H:139:ASN:CG	1.81	1.49
1:A:644:LYS:CE	1:A:644:LYS:NZ	1.69	1.49
2:B:870:ILE:CG1	2:B:870:ILE:CD1	1.86	1.49
2:B:115:GLN:CD	2:B:115:GLN:CG	1.76	1.49
1:A:1235:LYS:CE	1:A:1235:LYS:NZ	1.71	1.49
2:B:736:THR:CG2	2:B:736:THR:CB	1.89	1.49
1:A:1446:ASP:CB	1:A:1446:ASP:CG	1.77	1.49
2:B:477:ALA:CA	2:B:477:ALA:CB	1.89	1.49
2:B:895:ASP:CB	2:B:895:ASP:CG	1.81	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:THR:CA	1:A:69:THR:C	1.78	1.48
7:I:1:MET:CE	7:I:1:MET:SD	2.01	1.48
2:B:1101:ASP:CB	2:B:1101:ASP:CG	1.78	1.48
1:A:705:LYS:CG	1:A:705:LYS:CB	1.87	1.48
10:L:26:THR:CB	10:L:26:THR:CA	1.89	1.48
1:A:346:ASP:CB	1:A:346:ASP:CG	1.81	1.48
3:C:260:LEU:CG	3:C:260:LEU:CD2	1.86	1.48
2:B:652:LYS:NZ	2:B:652:LYS:CE	1.73	1.48
4:E:50:MET:CG	4:E:50:MET:SD	2.02	1.48
1:A:620:LYS:CE	1:A:620:LYS:CD	1.92	1.48
2:B:1097:HIS:C	2:B:1097:HIS:CA	1.81	1.48
3:C:15:LYS:CD	3:C:15:LYS:CG	1.90	1.47
1:A:1263:ILE:CG1	1:A:1263:ILE:CD1	1.92	1.47
1:A:555:ASP:CG	1:A:555:ASP:CB	1.81	1.47
1:A:423:ASP:CG	1:A:423:ASP:CB	1.81	1.47
4:E:121:MET:SD	4:E:121:MET:CG	2.01	1.47
2:B:315:LYS:CE	2:B:315:LYS:NZ	1.70	1.47
4:E:152:LYS:CE	4:E:152:LYS:CD	1.93	1.47
1:A:752:LYS:CD	1:A:752:LYS:CE	1.93	1.47
4:E:162:ARG:CB	4:E:162:ARG:CG	1.92	1.47
1:A:1111:MET:CG	1:A:1111:MET:SD	2.02	1.47
4:E:131:THR:CG2	4:E:131:THR:CB	1.89	1.47
2:B:962:LYS:CG	2:B:962:LYS:CD	1.91	1.46
6:H:123:MET:SD	6:H:123:MET:CG	2.03	1.46
2:B:432:MET:SD	2:B:432:MET:CE	2.02	1.46
1:A:934:LYS:CE	1:A:934:LYS:CD	1.91	1.46
1:A:597:LEU:CD1	1:A:597:LEU:CG	1.93	1.46
1:A:941:LYS:CE	1:A:941:LYS:NZ	1.76	1.46
1:A:74:MET:SD	1:A:74:MET:CE	2.03	1.46
1:A:938:LYS:CE	1:A:938:LYS:CD	1.87	1.46
4:E:215:MET:SD	4:E:215:MET:CE	2.04	1.45
2:B:233:PRO:CB	2:B:233:PRO:CG	1.75	1.45
2:B:1210:MET:CE	2:B:1210:MET:SD	2.04	1.44
2:B:1169:MET:CE	2:B:1169:MET:SD	2.03	1.44
2:B:531:GLN:CG	2:B:531:GLN:CD	1.84	1.44
2:B:347:LYS:CD	2:B:347:LYS:CG	1.96	1.43
10:L:68:GLU:CD	10:L:68:GLU:CG	1.85	1.43
7:I:17:ARG:CG	7:I:17:ARG:CD	1.94	1.43
2:B:999:MET:CG	2:B:999:MET:SD	2.06	1.43
3:C:154:LYS:CD	3:C:154:LYS:CE	1.95	1.43
1:A:728:LYS:CD	1:A:728:LYS:CG	1.93	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:593:PRO:CG	2:B:593:PRO:CB	1.84	1.43
2:B:598:GLU:CD	2:B:598:GLU:CG	1.87	1.43
5:F:129:LYS:NZ	5:F:129:LYS:CE	1.78	1.42
6:H:104:PHE:C	6:H:104:PHE:CA	1.86	1.42
1:A:978:PRO:CB	1:A:978:PRO:CG	1.88	1.42
2:B:987:LYS:NZ	2:B:987:LYS:CE	1.79	1.42
2:B:1097:HIS:ND1	2:B:1097:HIS:HA	1.29	1.41
1:A:620:LYS:CE	1:A:620:LYS:NZ	1.80	1.41
1:A:676:MET:CG	1:A:676:MET:SD	2.09	1.40
1:A:1444:MET:SD	1:A:1444:MET:CE	2.10	1.40
3:C:29:MET:SD	3:C:29:MET:CE	2.09	1.40
1:A:1294:PRO:CG	1:A:1294:PRO:CB	1.85	1.39
4:E:20:LYS:CE	4:E:20:LYS:NZ	1.84	1.39
4:E:201:LYS:CG	4:E:201:LYS:CD	1.99	1.39
1:A:41:MET:SD	1:A:41:MET:CE	2.10	1.39
2:B:1189:ILE:CG1	2:B:1189:ILE:CD1	2.00	1.38
1:A:1259:MET:CG	1:A:1259:MET:SD	2.12	1.38
7:I:1:MET:CG	7:I:1:MET:SD	2.11	1.38
1:A:1232:ASN:CG	1:A:1232:ASN:CB	1.92	1.38
2:B:986:GLN:CG	2:B:986:GLN:CD	1.92	1.37
1:A:1302:PRO:CB	1:A:1302:PRO:CG	1.90	1.37
4:E:121:MET:CE	4:E:121:MET:SD	2.11	1.36
4:E:162:ARG:CG	4:E:162:ARG:CD	2.06	1.33
1:A:1202:MET:SD	1:A:1202:MET:CE	2.17	1.32
6:H:104:PHE:O	6:H:106:GLU:N	1.62	1.32
1:A:369:SER:OG	9:K:2:ASN:ND2	1.61	1.31
7:I:55:THR:CG2	7:I:55:THR:CB	2.08	1.31
2:B:999:MET:SD	2:B:999:MET:CE	1.20	1.30
3:C:265:MET:SD	3:C:265:MET:CE	2.19	1.29
1:A:728:LYS:CE	1:A:728:LYS:CD	2.11	1.29
8:J:1:MET:CE	8:J:1:MET:SD	2.21	1.28
4:E:93:MET:SD	4:E:93:MET:CE	2.23	1.27
4:E:1:MET:CE	4:E:1:MET:SD	2.23	1.26
1:A:752:LYS:NZ	1:A:752:LYS:CE	1.98	1.25
1:A:487:MET:HE2	1:A:487:MET:CG	1.66	1.25
2:B:1097:HIS:ND1	2:B:1097:HIS:CA	1.97	1.25
1:A:156:ASP:O	1:A:158:PRO:HD3	1.34	1.25
1:A:70:CYS:SG	1:A:80:HIS:NE2	2.12	1.22
1:A:1259:MET:CE	1:A:1259:MET:SD	2.27	1.22
1:A:437:MET:CE	1:A:437:MET:SD	2.28	1.22
3:C:75:MET:SD	3:C:75:MET:CE	2.28	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:792:MET:CE	2:B:792:MET:SD	2.29	1.21
2:B:662:MET:CE	2:B:662:MET:SD	2.30	1.19
2:B:999:MET:HE3	2:B:999:MET:SD	1.78	1.19
2:B:999:MET:SD	2:B:999:MET:HE2	1.78	1.19
3:C:165:LYS:NZ	3:C:165:LYS:CE	2.06	1.18
1:A:487:MET:CE	1:A:487:MET:CG	2.18	1.18
7:I:45:ARG:HH11	7:I:45:ARG:HG2	1.03	1.18
5:F:103:MET:CE	5:F:103:MET:SD	2.31	1.17
3:C:54:ASN:OD1	3:C:56:THR:HB	1.42	1.17
1:A:1402:PHE:O	1:A:1403:GLU:HB2	1.37	1.17
1:A:708:MET:SD	1:A:708:MET:CE	2.33	1.16
7:I:45:ARG:HH11	7:I:45:ARG:CG	1.56	1.16
1:A:535:THR:HG21	1:A:617:VAL:H	1.10	1.14
1:A:567:LYS:HB3	6:H:96:VAL:H	1.15	1.11
6:H:106:GLU:O	6:H:107:VAL:C	1.82	1.11
3:C:125:MET:SD	3:C:125:MET:CE	2.40	1.10
9:K:1:MET:SD	9:K:1:MET:CE	2.40	1.09
2:B:999:MET:HE1	2:B:999:MET:SD	1.78	1.09
2:B:552:MET:SD	2:B:552:MET:CE	2.40	1.09
2:B:955:THR:HG22	10:L:54:ARG:O	1.51	1.08
1:A:487:MET:SD	1:A:487:MET:CE	0.98	1.08
6:H:63:LEU:C	6:H:90:ALA:HB3	1.73	1.08
1:A:42:ASP:OD2	1:A:47:ARG:N	1.86	1.08
6:H:138:GLU:O	6:H:139:ASN:C	1.93	1.07
2:B:999:MET:CG	2:B:999:MET:CE	2.32	1.06
2:B:101:MET:SD	2:B:101:MET:CE	2.44	1.06
1:A:567:LYS:HE2	6:H:95:TYR:CE2	1.88	1.05
2:B:100:PRO:HD2	2:B:180:TYR:CE1	1.92	1.04
1:A:1285:MET:SD	1:A:1285:MET:CE	2.46	1.04
7:I:4:PHE:HE1	7:I:13:MET:HE2	1.21	1.04
1:A:304:MET:CE	1:A:304:MET:SD	2.45	1.04
7:I:4:PHE:HE1	7:I:13:MET:CE	1.71	1.02
6:H:128:ASN:O	6:H:131:ASN:ND2	1.92	1.02
7:I:16:PRO:O	7:I:17:ARG:HD3	1.59	1.02
6:H:106:GLU:O	6:H:107:VAL:O	1.77	1.01
2:B:552:MET:CG	2:B:552:MET:SD	2.49	1.01
1:A:518:LYS:CD	1:A:518:LYS:NZ	2.23	1.00
1:A:487:MET:SD	1:A:487:MET:HE2	1.59	1.00
1:A:567:LYS:HB3	6:H:96:VAL:N	1.76	1.00
1:A:487:MET:HE1	1:A:487:MET:SD	1.59	0.99
1:A:567:LYS:HD3	6:H:95:TYR:HA	1.41	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:MET:HE3	1:A:487:MET:SD	1.59	0.99
2:B:1190:ASP:O	2:B:1191:ILE:HG13	1.63	0.99
1:A:567:LYS:HD3	6:H:95:TYR:CG	1.97	0.98
1:A:1385:THR:HG22	1:A:1385:THR:O	1.61	0.98
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.25	0.98
2:B:620:ARG:NE	2:B:620:ARG:CG	2.27	0.97
9:K:110:ASN:O	9:K:112:GLN:N	1.98	0.97
2:B:428:ILE:HG12	2:B:448:ILE:HD11	1.46	0.97
2:B:885:MET:CE	2:B:885:MET:SD	2.52	0.97
3:C:95:CYS:HG	12:C:3002:ZN:ZN	0.77	0.96
1:A:1079:MET:SD	1:A:1359:ASP:OD2	2.25	0.95
1:A:1233:ASP:O	1:A:1234:GLU:HB3	1.64	0.95
4:E:12:LEU:HD21	4:E:58:MET:SD	2.07	0.94
2:B:1220:ARG:O	2:B:1222:ARG:HD3	1.66	0.94
2:B:643:ASP:O	2:B:644:GLU:HB2	1.64	0.93
3:C:172:PRO:O	3:C:235:VAL:HG12	1.67	0.93
1:A:347:PHE:H	2:B:1107:ALA:HA	1.33	0.93
3:C:163:ILE:CG2	3:C:163:ILE:HB	1.98	0.93
1:A:567:LYS:HG3	1:A:568:PRO:CD	1.98	0.92
1:A:567:LYS:HD3	6:H:95:TYR:CA	1.98	0.92
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	1.85	0.92
4:E:100:ILE:HG22	4:E:101:GLN:N	1.85	0.92
8:J:7:CYS:HG	12:J:3001:ZN:ZN	0.60	0.92
9:K:93:SER:O	9:K:97:LYS:HG3	1.70	0.91
4:E:63:ASN:O	4:E:64:PRO:O	1.88	0.91
7:I:45:ARG:NH1	7:I:45:ARG:HG2	1.85	0.91
1:A:1111:MET:CG	1:A:1111:MET:CE	2.48	0.91
2:B:1097:HIS:CA	2:B:1097:HIS:CG	2.52	0.90
1:A:35:ILE:HD12	1:A:35:ILE:H	1.37	0.90
1:A:567:LYS:CG	1:A:568:PRO:CD	2.48	0.90
7:I:45:ARG:NH1	7:I:45:ARG:CG	2.35	0.90
5:F:81:THR:CG2	5:F:136:ARG:HH11	1.84	0.90
1:A:567:LYS:CD	6:H:95:TYR:HA	2.02	0.90
1:A:567:LYS:CB	6:H:96:VAL:H	1.85	0.89
3:C:86:CYS:HG	3:C:95:CYS:HG	1.15	0.89
4:E:57:MET:SD	4:E:57:MET:CE	2.60	0.89
1:A:148:CYS:HG	12:A:3006:ZN:ZN	0.60	0.89
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.51	0.89
8:J:1:MET:CE	8:J:1:MET:CG	2.51	0.89
2:B:846:ILE:HD12	2:B:974:PRO:HB2	1.53	0.89
2:B:431:TYR:O	2:B:431:TYR:HD2	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:431:TYR:O	2:B:431:TYR:CD2	2.26	0.88
1:A:1402:PHE:O	1:A:1403:GLU:CB	2.18	0.88
1:A:156:ASP:O	1:A:158:PRO:CD	2.20	0.88
6:H:103:LYS:HB3	6:H:105:GLU:OE1	1.73	0.88
1:A:567:LYS:HD2	1:A:568:PRO:HD3	1.55	0.88
10:L:48:CYS:HG	12:L:3005:ZN:ZN	0.77	0.88
1:A:247:ARG:NH1	1:A:263:THR:HG23	1.90	0.87
7:I:4:PHE:CE1	7:I:13:MET:CE	2.56	0.87
1:A:187:LYS:HB2	1:A:194:ALA:HB3	1.57	0.87
6:H:104:PHE:O	6:H:106:GLU:CA	2.22	0.86
2:B:100:PRO:HD2	2:B:180:TYR:CZ	2.10	0.86
4:E:147:HIS:HD2	4:E:149:LEU:H	1.18	0.86
5:F:111:LEU:O	5:F:113:GLY:N	2.08	0.86
2:B:1051:THR:HG22	2:B:1053:GLU:N	1.90	0.86
2:B:104:GLU:OE1	10:L:54:ARG:NE	2.09	0.86
6:H:93:TYR:HB3	6:H:144:ILE:O	1.76	0.86
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.57	0.85
2:B:561:TRP:O	2:B:590:HIS:HE1	1.57	0.85
2:B:680:THR:HG22	2:B:682:SER:H	1.39	0.85
3:C:116:LYS:NZ	3:C:116:LYS:CD	2.37	0.85
10:L:64:LEU:CD1	10:L:64:LEU:HG	2.06	0.85
6:H:130:ARG:C	6:H:130:ARG:HD2	1.95	0.85
3:C:18:VAL:HG23	3:C:240:VAL:HG11	1.59	0.85
1:A:752:LYS:CG	1:A:752:LYS:CE	2.54	0.85
3:C:99:LEU:HD12	3:C:99:LEU:N	1.92	0.85
1:A:369:SER:H	9:K:2:ASN:HD21	1.19	0.85
1:A:752:LYS:HZ3	2:B:1019:SER:H	1.25	0.85
1:A:1079:MET:HG2	1:A:1359:ASP:OD2	1.76	0.84
2:B:1084:GLN:HE22	3:C:192:TRP:H	1.21	0.84
2:B:879:ARG:NH2	2:B:885:MET:CE	2.41	0.84
4:E:79:TRP:HB2	4:E:105:PHE:CE1	2.13	0.84
6:H:63:LEU:C	6:H:90:ALA:CB	2.46	0.84
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.60	0.83
1:A:72:GLU:OE2	2:B:1175:LEU:HD11	1.78	0.83
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.59	0.83
2:B:1182:CYS:HG	2:B:1185:CYS:HB2	1.43	0.83
1:A:73:GLY:O	1:A:75:ASN:N	2.10	0.82
1:A:172:PRO:HG2	1:A:174:ILE:HD11	1.61	0.82
1:A:23:SER:O	1:A:27:VAL:HG23	1.78	0.82
2:B:251:ILE:HG22	2:B:251:ILE:O	1.79	0.82
2:B:542:MET:HG3	2:B:747:MET:HE3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ASN:OD1	1:A:64:ASN:O	1.96	0.82
1:A:1364:ASN:HD22	1:A:1366:ARG:H	1.24	0.82
1:A:61:ILE:CB	1:A:61:ILE:HA	2.07	0.82
4:E:50:MET:CE	4:E:50:MET:SD	2.68	0.82
6:H:5:LEU:O	6:H:133:ASN:ND2	2.12	0.82
7:I:4:PHE:CE1	7:I:13:MET:HE2	2.12	0.82
5:F:77:ASP:O	5:F:78:GLN:HB2	1.79	0.82
7:I:30:ARG:NE	7:I:30:ARG:CG	2.41	0.82
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.45	0.82
1:A:938:LYS:CE	1:A:938:LYS:CG	2.58	0.81
2:B:999:MET:CG	2:B:999:MET:HE3	2.10	0.81
6:H:104:PHE:O	6:H:105:GLU:C	2.19	0.81
1:A:70:CYS:HG	1:A:80:HIS:CE1	1.97	0.81
2:B:1065:GLN:HE22	2:B:1067:ARG:HB2	1.44	0.81
6:H:138:GLU:O	6:H:140:ALA:N	2.13	0.81
2:B:775:LYS:CD	2:B:775:LYS:CB	2.58	0.81
2:B:1084:GLN:NE2	3:C:192:TRP:H	1.77	0.81
3:C:8:VAL:HG12	3:C:9:LYS:H	1.46	0.81
4:E:36:GLU:O	4:E:37:LEU:C	2.17	0.81
2:B:498:THR:CG2	2:B:537:LYS:HB2	2.11	0.81
1:A:120:GLU:HG2	1:A:123:ARG:HH22	1.45	0.80
1:A:107:CYS:SG	1:A:148:CYS:SG	2.79	0.80
1:A:55:ASP:O	1:A:57:ARG:N	2.11	0.80
8:J:14:VAL:HG13	8:J:50:ILE:HD11	1.63	0.80
2:B:294:ASP:H	7:I:12:ASN:ND2	1.79	0.80
1:A:596:THR:HG22	1:A:597:LEU:H	1.47	0.79
2:B:542:MET:HG3	2:B:747:MET:CE	2.12	0.79
3:C:255:VAL:HG12	3:C:255:VAL:O	1.82	0.79
1:A:1364:ASN:ND2	1:A:1366:ARG:H	1.81	0.79
1:A:941:LYS:CD	1:A:941:LYS:NZ	2.45	0.79
1:A:108:MET:H	1:A:171:GLN:HE22	1.27	0.79
4:E:98:ILE:HA	4:E:98:ILE:CB	2.05	0.79
1:A:187:LYS:HG3	1:A:194:ALA:CB	2.13	0.79
4:E:129:PRO:CG	4:E:129:PRO:CA	2.61	0.79
1:A:711:ARG:HE	7:I:95:THR:HG22	1.48	0.79
6:H:123:MET:HE1	6:H:142:LEU:HD22	1.65	0.78
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.31	0.78
1:A:46:THR:HB	1:A:46:THR:CA	2.10	0.78
1:A:567:LYS:CD	1:A:568:PRO:HD3	2.13	0.78
1:A:1079:MET:CG	1:A:1359:ASP:OD2	2.31	0.78
1:A:55:ASP:N	1:A:56:PRO:CD	2.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:LEU:O	2:B:965:LYS:NZ	2.17	0.78
1:A:174:ILE:CA	1:A:174:ILE:HB	2.09	0.78
1:A:247:ARG:HH11	1:A:263:THR:HG23	1.42	0.78
1:A:1445:ILE:CG2	1:A:1445:ILE:CA	2.61	0.78
2:B:428:ILE:CG1	2:B:448:ILE:HD11	2.14	0.78
6:H:89:LEU:O	6:H:91:ASP:N	2.16	0.78
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.24	0.78
1:A:901:LEU:H	1:A:926:GLN:NE2	1.82	0.78
1:A:1259:MET:CB	1:A:1259:MET:SD	2.71	0.77
1:A:535:THR:HG21	1:A:617:VAL:N	1.95	0.77
2:B:643:ASP:O	2:B:644:GLU:CB	2.32	0.77
2:B:877:PRO:O	2:B:878:GLN:HG2	1.84	0.77
3:C:167:HIS:HD2	3:C:169:LYS:H	1.30	0.77
9:K:111:LEU:CB	9:K:111:LEU:CD1	2.62	0.77
6:H:89:LEU:HB3	6:H:91:ASP:OD1	1.85	0.77
2:B:879:ARG:HH21	2:B:885:MET:HE1	1.47	0.77
1:A:369:SER:CB	9:K:2:ASN:ND2	2.46	0.77
1:A:110:CYS:SG	1:A:167:CYS:SG	2.82	0.77
2:B:1077:THR:HG22	2:B:1079:LYS:H	1.47	0.77
1:A:571:LEU:CD2	1:A:571:LEU:CD1	2.59	0.77
1:A:909:ASP:OD1	1:A:911:SER:N	2.16	0.77
2:B:217:ARG:HD3	2:B:407:ASP:OD2	1.84	0.77
5:F:75:PRO:O	5:F:77:ASP:O	2.03	0.77
2:B:1097:HIS:C	2:B:1097:HIS:HA	2.00	0.77
2:B:114:PRO:HD3	2:B:124:TYR:CE1	2.20	0.77
1:A:849:MET:HE2	1:A:1061:GLY:HA2	1.67	0.77
4:E:90:VAL:CG1	4:E:90:VAL:HB	2.11	0.77
10:L:47:ARG:HG2	10:L:48:CYS:H	1.50	0.77
1:A:199:LEU:CD2	1:A:199:LEU:CD1	2.61	0.77
2:B:417:PHE:CD2	2:B:417:PHE:O	2.39	0.77
2:B:593:PRO:HG2	2:B:617:ARG:NH2	1.99	0.77
9:K:35:PHE:HE1	9:K:73:LEU:HD12	1.48	0.77
3:C:120:ILE:H	3:C:120:ILE:HD12	1.48	0.76
1:A:282:ASN:C	1:A:283:GLY:O	2.21	0.76
1:A:413:ILE:HD13	1:A:413:ILE:N	2.00	0.76
6:H:105:GLU:HB3	6:H:107:VAL:HG23	1.67	0.76
1:A:555:ASP:OD1	9:K:26:LYS:HE3	1.86	0.76
2:B:879:ARG:NH2	2:B:885:MET:HE1	1.99	0.76
3:C:196:ASP:HB3	3:C:199:LYS:HG3	1.67	0.76
4:E:79:TRP:HB2	4:E:105:PHE:CD1	2.20	0.76
7:I:4:PHE:CE1	7:I:13:MET:HE1	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1350:LYS:CB	1:A:1350:LYS:CD	2.63	0.76
2:B:1163:CYS:HA	2:B:1163:CYS:CB	2.11	0.76
1:A:555:ASP:OD1	9:K:26:LYS:CE	2.34	0.76
1:A:1385:THR:CA	1:A:1385:THR:CG2	2.62	0.76
1:A:567:LYS:CD	6:H:95:TYR:CG	2.68	0.76
1:A:32:VAL:HG23	1:A:33:ALA:H	1.49	0.76
1:A:446:ARG:CG	1:A:446:ARG:HH11	1.99	0.76
1:A:61:ILE:O	1:A:62:ASP:HB2	1.87	0.75
10:L:28:LYS:HA	10:L:28:LYS:C	2.03	0.75
1:A:903:ASN:C	1:A:903:ASN:HD22	1.88	0.75
3:C:73:GLN:HE21	3:C:75:MET:H	1.32	0.75
1:A:1233:ASP:O	1:A:1234:GLU:CB	2.29	0.75
2:B:477:ALA:CB	2:B:477:ALA:HA	2.13	0.75
2:B:393:LYS:NZ	2:B:621:GLU:OE2	2.17	0.75
10:L:34:CYS:CB	10:L:51:CYS:HB3	2.17	0.75
1:A:1161:THR:CG2	1:A:1163:ILE:H	1.99	0.75
1:A:567:LYS:CG	1:A:568:PRO:HD3	2.17	0.75
2:B:1025:HIS:HE1	2:B:1090:THR:HG21	1.50	0.75
3:C:167:HIS:HE1	10:L:70:ARG:O	1.69	0.75
6:H:6:PHE:CD2	6:H:7:ASP:N	2.55	0.75
1:A:567:LYS:CE	6:H:95:TYR:CE2	2.63	0.75
1:A:541:ILE:N	1:A:541:ILE:HD12	2.02	0.75
1:A:571:LEU:HG	1:A:571:LEU:CD2	2.12	0.75
10:L:34:CYS:HB3	10:L:51:CYS:CB	2.16	0.75
3:C:169:LYS:CG	3:C:169:LYS:CE	2.64	0.75
1:A:973:ILE:CG2	1:A:973:ILE:HB	2.11	0.75
6:H:91:ASP:CA	6:H:92:ASP:N	2.48	0.75
2:B:515:HIS:H	2:B:518:HIS:HD2	1.33	0.74
2:B:955:THR:HG23	10:L:55:ILE:HA	1.69	0.74
1:A:1385:THR:C	1:A:1385:THR:CG2	2.56	0.74
2:B:1166:CYS:O	2:B:1168:LEU:N	2.20	0.74
1:A:351:THR:CG2	2:B:1103:ILE:CG1	2.66	0.74
2:B:1128:LEU:HD12	2:B:1128:LEU:C	2.06	0.74
5:F:81:THR:HG23	5:F:136:ARG:HH11	1.50	0.74
6:H:107:VAL:CB	6:H:107:VAL:HA	2.10	0.74
1:A:369:SER:N	9:K:2:ASN:HD21	1.85	0.74
2:B:595:ARG:CB	2:B:595:ARG:CD	2.64	0.74
2:B:90:ILE:N	2:B:90:ILE:HD12	2.03	0.74
1:A:1404:GLU:HG3	1:A:1405:THR:HB	1.69	0.74
3:C:169:LYS:NZ	3:C:169:LYS:CD	2.51	0.74
6:H:77:ARG:O	6:H:78:SER:O	2.04	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:163:ILE:CG1	3:C:163:ILE:CG2	2.65	0.74
9:K:82:ASP:OD1	9:K:83:PRO:HG2	1.86	0.74
1:A:710:LEU:CD2	1:A:710:LEU:HG	2.13	0.74
2:B:305:VAL:CG1	2:B:305:VAL:CA	2.65	0.74
1:A:895:LYS:CD	1:A:895:LYS:NZ	2.50	0.74
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.17	0.74
1:A:174:ILE:CG2	1:A:174:ILE:CA	2.62	0.73
1:A:487:MET:HE2	1:A:487:MET:HG3	1.69	0.73
2:B:282:ILE:H	2:B:282:ILE:HD13	1.53	0.73
7:I:32:CYS:HB2	7:I:34:TYR:H	1.52	0.73
1:A:237:THR:CA	1:A:237:THR:CG2	2.64	0.73
8:J:7:CYS:SG	8:J:10:CYS:SG	2.86	0.73
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.69	0.73
1:A:555:ASP:OD1	9:K:26:LYS:NZ	2.21	0.73
2:B:484:ASN:OD1	2:B:486:TYR:CE1	2.41	0.73
5:F:73:ALA:HB2	5:F:143:PHE:CZ	2.23	0.73
2:B:498:THR:HG21	2:B:537:LYS:HB2	1.71	0.73
6:H:96:VAL:HG22	6:H:143:LEU:HD23	1.70	0.73
2:B:357:GLN:NE2	2:B:368:GLU:HG2	2.04	0.73
8:J:38:ARG:CD	8:J:38:ARG:CB	2.64	0.73
2:B:213:ILE:HD12	2:B:213:ILE:N	2.03	0.73
1:A:588:LEU:HD23	1:A:588:LEU:C	2.08	0.72
2:B:744:HIS:HD2	2:B:746:SER:H	1.37	0.72
7:I:30:ARG:CD	7:I:30:ARG:CB	2.67	0.72
1:A:121:LEU:HG	1:A:121:LEU:CD1	2.10	0.72
1:A:351:THR:CG2	2:B:1103:ILE:HG12	2.19	0.72
2:B:1222:ARG:HH11	2:B:1222:ARG:HB2	1.53	0.72
2:B:251:ILE:O	2:B:251:ILE:CG2	2.37	0.72
7:I:116:ASN:HD21	7:I:118:ARG:HB2	1.54	0.72
1:A:547:LEU:HB3	9:K:58:PHE:CE1	2.25	0.72
10:L:58:LYS:O	10:L:59:ALA:HB3	1.90	0.72
1:A:31:SER:CB	1:A:83:HIS:HD2	2.02	0.72
2:B:915:THR:CA	2:B:915:THR:HB	2.11	0.72
4:E:127:ILE:N	4:E:128:PRO:CD	2.53	0.72
1:A:709:THR:HG22	1:A:712:GLU:H	1.54	0.71
10:L:65:VAL:CG2	10:L:65:VAL:CA	2.67	0.71
1:A:119:ASN:O	1:A:120:GLU:HB2	1.91	0.71
1:A:351:THR:HG21	2:B:1103:ILE:HG12	1.71	0.71
2:B:1154:ALA:HA	2:B:1154:ALA:CB	2.14	0.71
1:A:1151:GLU:OE2	7:I:45:ARG:HD3	1.90	0.71
1:A:206:GLU:O	1:A:210:ILE:HD13	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:ILE:HA	2:B:133:LYS:O	1.91	0.71
3:C:50:GLU:HB3	10:L:64:LEU:HD13	1.70	0.71
8:J:7:CYS:SG	8:J:46:CYS:SG	2.89	0.71
2:B:58:THR:O	2:B:62:ILE:HG12	1.90	0.71
3:C:8:VAL:CG1	3:C:9:LYS:H	2.04	0.71
5:F:109:VAL:CG1	5:F:110:ASP:N	2.53	0.71
2:B:1177:HIS:HB2	2:B:1179:GLN:NE2	2.06	0.71
2:B:654:ARG:H	2:B:657:HIS:HD2	1.37	0.70
4:E:98:ILE:CA	4:E:98:ILE:HB	2.15	0.70
1:A:265:LYS:HD3	1:A:302:THR:HG22	1.72	0.70
1:A:566:ILE:CA	1:A:566:ILE:CG2	2.69	0.70
2:B:883:LEU:CA	2:B:883:LEU:HB2	2.15	0.70
2:B:549:THR:HG22	2:B:628:THR:HB	1.70	0.70
2:B:883:LEU:HB3	2:B:883:LEU:CA	2.15	0.70
10:L:48:CYS:HA	10:L:48:CYS:C	2.03	0.70
1:A:120:GLU:HG2	1:A:123:ARG:NH2	2.06	0.70
1:A:587:HIS:HD2	1:A:966:ASN:OD1	1.73	0.70
1:A:636:GLU:OE1	1:A:966:ASN:ND2	2.24	0.70
4:E:37:LEU:CD1	4:E:37:LEU:HG	2.11	0.70
1:A:1151:GLU:CG	7:I:45:ARG:HD2	2.22	0.70
2:B:167:ILE:HG22	2:B:167:ILE:O	1.91	0.70
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.74	0.70
2:B:644:GLU:OE1	2:B:646:LEU:HB2	1.92	0.70
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.26	0.70
1:A:120:GLU:CG	1:A:123:ARG:HH22	2.03	0.70
1:A:840:ARG:NE	1:A:840:ARG:CG	2.53	0.70
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.73	0.70
6:H:91:ASP:O	6:H:91:ASP:OD1	2.08	0.70
2:B:1084:GLN:HE22	3:C:192:TRP:N	1.87	0.70
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.74	0.69
1:A:535:THR:CG2	1:A:617:VAL:H	1.97	0.69
1:A:446:ARG:HH11	1:A:446:ARG:HG2	1.57	0.69
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.56	0.69
4:E:152:LYS:CB	4:E:152:LYS:CD	2.70	0.69
1:A:567:LYS:HD2	1:A:568:PRO:CD	2.22	0.69
2:B:1222:ARG:NH1	2:B:1222:ARG:HG2	2.07	0.69
2:B:914:LYS:H	2:B:938:SER:HB2	1.57	0.69
1:A:184:SER:HB2	1:A:199:LEU:HD23	1.74	0.69
1:A:795:GLU:HG2	2:B:731:VAL:HG21	1.74	0.69
2:B:879:ARG:NH2	2:B:885:MET:HE2	2.06	0.69
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:313:MET:CE	2:B:386:LEU:HD22	2.22	0.69
2:B:531:GLN:H	2:B:531:GLN:CD	1.95	0.69
1:A:1135:ARG:CG	1:A:1135:ARG:NE	2.54	0.69
1:A:1385:THR:CG2	1:A:1385:THR:O	2.39	0.69
6:H:26:ILE:HD12	6:H:42:ILE:HD12	1.74	0.69
2:B:663:ALA:O	2:B:667:GLN:HG3	1.92	0.69
8:J:45:CYS:HG	12:J:3001:ZN:ZN	1.03	0.69
2:B:294:ASP:H	7:I:12:ASN:HD22	1.40	0.69
2:B:436:VAL:HB	2:B:436:VAL:CA	2.16	0.69
3:C:8:VAL:HG12	3:C:9:LYS:N	2.08	0.69
8:J:1:MET:C	8:J:2:ILE:HD12	2.14	0.69
2:B:487:THR:HG22	2:B:490:SER:H	1.59	0.68
3:C:267:GLN:C	3:C:267:GLN:HA	2.06	0.68
1:A:886:ILE:HD12	1:A:943:LEU:HB3	1.76	0.68
2:B:99:LYS:HB3	2:B:100:PRO:HD3	1.75	0.68
5:F:76:LYS:O	5:F:79:ARG:HD2	1.93	0.68
6:H:123:MET:CE	6:H:123:MET:CG	2.72	0.68
1:A:567:LYS:CG	6:H:96:VAL:H	2.07	0.68
1:A:834:THR:HG21	1:A:1077:THR:OG1	1.94	0.68
2:B:315:LYS:NZ	2:B:315:LYS:CD	2.51	0.68
2:B:620:ARG:CG	2:B:620:ARG:HE	2.05	0.68
2:B:1220:ARG:O	2:B:1222:ARG:CD	2.41	0.68
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.33	0.68
3:C:260:LEU:O	3:C:260:LEU:HD12	1.92	0.68
6:H:107:VAL:HB	6:H:107:VAL:CA	2.15	0.68
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.24	0.68
1:A:265:LYS:HZ3	1:A:302:THR:HG21	1.58	0.67
1:A:752:LYS:HG3	1:A:753:GLY:N	2.09	0.67
2:B:358:LYS:CA	2:B:358:LYS:CG	2.70	0.67
3:C:199:LYS:NZ	3:C:199:LYS:CD	2.56	0.67
6:H:89:LEU:C	6:H:91:ASP:H	1.97	0.67
9:K:35:PHE:CE1	9:K:73:LEU:HD12	2.30	0.67
1:A:1039:LYS:NZ	1:A:1039:LYS:CD	2.56	0.67
2:B:787:VAL:O	2:B:787:VAL:CG1	2.42	0.67
1:A:1259:MET:HB2	1:A:1259:MET:SD	2.35	0.67
2:B:227:LYS:CB	2:B:227:LYS:CD	2.69	0.67
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.29	0.67
1:A:503:GLN:NE2	5:F:90:ARG:NH2	2.43	0.67
9:K:88:LYS:CB	9:K:88:LYS:CD	2.72	0.67
1:A:941:LYS:CB	1:A:941:LYS:CD	2.67	0.67
2:B:1182:CYS:HG	2:B:1185:CYS:CB	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:209:TYR:H	3:C:209:TYR:HD1	1.43	0.67
6:H:106:GLU:O	6:H:108:SER:N	2.27	0.67
1:A:1162:VAL:HG12	1:A:1162:VAL:O	1.94	0.67
1:A:535:THR:O	1:A:575:LYS:HE2	1.94	0.67
1:A:587:HIS:CE1	1:A:969:GLN:HG2	2.29	0.67
1:A:174:ILE:CB	1:A:174:ILE:HA	2.15	0.67
1:A:537:ARG:NH2	1:A:600:PRO:O	2.27	0.67
2:B:1222:ARG:NH1	2:B:1222:ARG:CG	2.57	0.67
6:H:130:ARG:HB2	6:H:133:ASN:HB3	1.76	0.67
9:K:102:LYS:CE	9:K:102:LYS:CG	2.72	0.67
3:C:86:CYS:HG	12:C:3002:ZN:ZN	1.07	0.67
5:F:77:ASP:O	5:F:78:GLN:CB	2.41	0.67
2:B:1008:PRO:HG2	2:B:1011:ILE:HD11	1.77	0.66
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.24	0.66
1:A:1350:LYS:CG	1:A:1350:LYS:CE	2.72	0.66
1:A:596:THR:HG22	1:A:597:LEU:HD12	1.78	0.66
2:B:884:ARG:O	2:B:936:ASP:HB3	1.95	0.66
1:A:901:LEU:HD22	1:A:919:ILE:HD13	1.77	0.66
9:K:65:HIS:HD2	9:K:67:PHE:H	1.44	0.66
2:B:883:LEU:HA	2:B:883:LEU:CB	2.15	0.66
5:F:109:VAL:HG12	5:F:110:ASP:N	2.09	0.66
1:A:11:LEU:HD11	2:B:1195:HIS:CD2	2.31	0.66
2:B:645:SER:OG	2:B:646:LEU:N	2.28	0.66
5:F:129:LYS:CG	5:F:129:LYS:CE	2.70	0.66
1:A:35:ILE:HD12	1:A:35:ILE:N	2.10	0.66
2:B:515:HIS:H	2:B:518:HIS:CD2	2.12	0.66
4:E:71:LYS:NZ	4:E:160:GLU:OE2	2.23	0.66
6:H:123:MET:CE	6:H:142:LEU:HD22	2.26	0.66
6:H:131:ASN:HD22	6:H:131:ASN:H	1.43	0.66
5:F:81:THR:HG23	5:F:136:ARG:NH1	2.11	0.66
1:A:531:ILE:O	1:A:535:THR:HB	1.94	0.66
1:A:369:SER:CB	9:K:2:ASN:HD21	2.07	0.66
10:L:40:LEU:HD22	10:L:44:ASP:OD1	1.95	0.66
6:H:105:GLU:H	6:H:105:GLU:CD	1.99	0.66
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.78	0.65
2:B:1222:ARG:HH11	2:B:1222:ARG:CG	2.08	0.65
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.94	0.65
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.31	0.65
1:A:534:LEU:O	1:A:574:GLY:HA3	1.96	0.65
1:A:144:THR:CG2	1:A:144:THR:HB	2.17	0.65
2:B:417:PHE:CD2	2:B:417:PHE:C	2.69	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:LYS:C	2:B:246:LYS:HA	2.06	0.65
2:B:431:TYR:CE1	2:B:447:ALA:HB1	2.31	0.65
1:A:46:THR:C	1:A:46:THR:CB	2.63	0.65
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.32	0.65
2:B:806:THR:HG23	2:B:808:ALA:H	1.61	0.65
2:B:870:ILE:HA	2:B:870:ILE:CB	2.15	0.65
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.32	0.65
4:E:83:CYS:O	4:E:113:GLN:NE2	2.30	0.65
5:F:81:THR:CG2	5:F:136:ARG:NH1	2.59	0.65
4:E:117:THR:O	4:E:119:SER:N	2.30	0.65
6:H:19:ARG:CG	6:H:19:ARG:CA	2.73	0.65
6:H:27:GLU:OE1	6:H:39:THR:OG1	2.07	0.65
1:A:869:GLY:O	4:E:204:THR:HG21	1.96	0.65
4:E:116:ILE:HG22	4:E:120:ALA:HB3	1.78	0.65
2:B:1025:HIS:CE1	2:B:1090:THR:HG21	2.31	0.64
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.80	0.64
3:C:209:TYR:CD1	3:C:209:TYR:N	2.65	0.64
1:A:567:LYS:HD3	6:H:95:TYR:CD2	2.31	0.64
2:B:424:LEU:HD23	2:B:424:LEU:C	2.18	0.64
2:B:436:VAL:CB	2:B:436:VAL:HA	2.17	0.64
1:A:503:GLN:NE2	5:F:90:ARG:HH21	1.96	0.64
1:A:636:GLU:OE2	1:A:962:ARG:HD2	1.97	0.64
6:H:130:ARG:HB2	6:H:133:ASN:CB	2.27	0.64
6:H:6:PHE:CG	6:H:7:ASP:N	2.65	0.64
2:B:754:SER:O	2:B:806:THR:HG21	1.97	0.64
2:B:792:MET:SD	2:B:857:ARG:NH2	2.71	0.64
2:B:99:LYS:HB3	2:B:100:PRO:CD	2.28	0.64
2:B:118:ARG:NE	2:B:118:ARG:CG	2.53	0.64
4:E:147:HIS:CD2	4:E:149:LEU:H	2.08	0.64
6:H:103:LYS:NZ	6:H:105:GLU:OE2	2.27	0.64
3:C:252:GLN:HE22	9:K:99:GLY:HA2	1.62	0.64
1:A:567:LYS:CB	1:A:568:PRO:CD	2.76	0.64
4:E:153:HIS:CE1	4:E:184:VAL:HG11	2.32	0.64
6:H:91:ASP:CG	6:H:91:ASP:C	2.56	0.64
7:I:120:GLN:O	7:I:121:PHE:HB2	1.98	0.64
6:H:123:MET:CB	6:H:123:MET:SD	2.84	0.64
2:B:531:GLN:HE21	2:B:532:ALA:H	1.44	0.64
1:A:1198:ASP:OD1	1:A:1200:ALA:HB3	1.97	0.63
1:A:144:THR:O	1:A:146:MET:HG2	1.99	0.63
6:H:63:LEU:HB2	6:H:90:ALA:HB2	1.79	0.63
2:B:132:VAL:HG12	2:B:133:LYS:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:CB	6:H:95:TYR:HA	2.29	0.63
1:A:589:GLN:HB2	1:A:961:ARG:HH22	1.61	0.63
2:B:915:THR:C	2:B:915:THR:CB	2.63	0.63
4:E:191:LYS:CD	4:E:191:LYS:NZ	2.62	0.63
1:A:472:LEU:O	1:A:475:THR:HB	1.98	0.63
2:B:1166:CYS:O	2:B:1167:GLY:C	2.36	0.63
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.01	0.63
2:B:916:THR:N	2:B:935:ARG:O	2.32	0.63
1:A:41:MET:O	1:A:50:ILE:HD11	1.99	0.63
1:A:596:THR:HG22	1:A:597:LEU:N	2.13	0.63
1:A:69:THR:C	1:A:69:THR:HA	2.05	0.63
1:A:844:ALA:HB2	1:A:1384:VAL:HG12	1.81	0.63
2:B:916:THR:HB	2:B:935:ARG:HB2	1.81	0.63
7:I:64:SER:O	7:I:66:PRO:HD3	1.99	0.63
1:A:369:SER:H	9:K:2:ASN:ND2	1.93	0.63
1:A:567:LYS:CD	1:A:568:PRO:CD	2.76	0.63
2:B:1222:ARG:HH11	2:B:1222:ARG:CB	2.10	0.63
9:K:49:GLU:HG2	9:K:94:ILE:HD11	1.79	0.63
2:B:846:ILE:CD1	2:B:974:PRO:HB2	2.28	0.62
6:H:103:LYS:O	6:H:115:TYR:HD1	1.81	0.62
10:L:34:CYS:SG	10:L:36:SER:OG	2.57	0.62
1:A:172:PRO:HG2	1:A:174:ILE:CD1	2.29	0.62
1:A:644:LYS:NZ	1:A:644:LYS:CD	2.62	0.62
1:A:1077:THR:HG22	1:A:1078:GLN:NE2	2.13	0.62
1:A:744:LYS:HD3	1:A:748:MET:CE	2.29	0.62
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.63	0.62
3:C:152:GLU:OE2	3:C:154:LYS:HD2	1.99	0.62
6:H:91:ASP:C	6:H:91:ASP:CB	2.64	0.62
8:J:1:MET:CE	8:J:1:MET:CB	2.77	0.62
1:A:858:ASN:HD21	1:A:860:LEU:HB2	1.64	0.62
6:H:104:PHE:C	6:H:104:PHE:HA	2.10	0.62
9:K:49:GLU:CG	9:K:94:ILE:HD11	2.29	0.62
3:C:40:GLU:OE2	3:C:254:LYS:NZ	2.32	0.62
1:A:744:LYS:HD3	1:A:748:MET:SD	2.39	0.62
3:C:54:ASN:OD1	3:C:56:THR:CB	2.35	0.62
8:J:2:ILE:O	8:J:3:VAL:C	2.38	0.62
1:A:265:LYS:CD	1:A:302:THR:HG22	2.30	0.62
1:A:535:THR:CG2	1:A:616:VAL:HA	2.29	0.62
2:B:435:THR:HG23	2:B:437:GLU:HB2	1.81	0.62
9:K:12:LEU:N	9:K:12:LEU:HD12	2.14	0.62
6:H:89:LEU:C	6:H:91:ASP:N	2.53	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:53:HIS:HE1	8:J:55:ASP:HA	1.65	0.62
1:A:1144:LYS:NZ	1:A:1144:LYS:CD	2.60	0.61
1:A:533:LYS:NZ	1:A:745:GLN:HE22	1.97	0.61
2:B:498:THR:HG22	2:B:537:LYS:HB2	1.81	0.61
2:B:269:ILE:HB	2:B:282:ILE:HD12	1.82	0.61
1:A:804:TYR:O	2:B:761:HIS:ND1	2.31	0.61
3:C:252:GLN:HE22	9:K:99:GLY:CA	2.13	0.61
1:A:752:LYS:NZ	2:B:1019:SER:H	1.96	0.61
3:C:209:TYR:N	3:C:209:TYR:HD1	1.99	0.61
5:F:87:LYS:CD	5:F:87:LYS:NZ	2.62	0.61
1:A:689:LYS:CG	1:A:689:LYS:CE	2.74	0.61
3:C:116:LYS:CE	3:C:116:LYS:CG	2.75	0.61
6:H:144:ILE:CB	6:H:144:ILE:CD1	2.72	0.61
1:A:518:LYS:CG	1:A:518:LYS:CE	2.78	0.61
4:E:129:PRO:N	4:E:129:PRO:CG	2.62	0.61
1:A:164:ARG:O	1:A:166:GLY:N	2.33	0.61
1:A:26:GLU:HA	1:A:29:ALA:HB3	1.83	0.61
4:E:36:GLU:O	4:E:38:PRO:N	2.32	0.61
1:A:973:ILE:HD11	1:A:1038:THR:HG23	1.82	0.61
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.01	0.61
1:A:982:THR:HG22	1:A:985:ASP:H	1.64	0.61
2:B:1051:THR:CG2	2:B:1053:GLU:H	2.05	0.61
2:B:1097:HIS:CE1	2:B:1102:LYS:HG3	2.35	0.61
2:B:561:TRP:O	2:B:590:HIS:CE1	2.48	0.61
1:A:57:ARG:O	1:A:68:GLN:NE2	2.32	0.61
1:A:187:LYS:CB	1:A:194:ALA:HB3	2.29	0.61
1:A:605:MET:HE2	1:A:607:ILE:HD11	1.83	0.60
2:B:757:PRO:HD2	2:B:984:HIS:HE1	1.66	0.60
3:C:169:LYS:NZ	10:L:69:ALA:O	2.31	0.60
1:A:752:LYS:HG2	1:A:752:LYS:CE	2.30	0.60
1:A:73:GLY:C	1:A:75:ASN:N	2.54	0.60
2:B:1152:MET:CE	2:B:1152:MET:HA	2.31	0.60
1:A:1111:MET:CG	1:A:1111:MET:HE2	2.31	0.60
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.82	0.60
1:A:351:THR:CG2	2:B:1103:ILE:HG13	2.29	0.60
4:E:98:ILE:O	4:E:101:GLN:HB3	2.01	0.60
1:A:1239:ARG:NE	1:A:1239:ARG:CG	2.61	0.60
1:A:42:ASP:OD2	1:A:47:ARG:CA	2.50	0.60
4:E:45:LYS:CG	4:E:45:LYS:CE	2.79	0.60
6:H:115:TYR:O	6:H:123:MET:O	2.19	0.60
6:H:127:GLY:O	6:H:128:ASN:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:CD	6:H:95:TYR:CD1	2.84	0.60
8:J:53:HIS:ND1	8:J:54:VAL:N	2.48	0.60
2:B:242:SER:HG	2:B:363:HIS:HD1	1.46	0.60
2:B:955:THR:CG2	10:L:55:ILE:HA	2.31	0.60
1:A:982:THR:HB	1:A:985:ASP:OD2	2.01	0.60
1:A:752:LYS:HE2	2:B:1019:SER:OG	2.01	0.60
1:A:351:THR:HG21	2:B:1103:ILE:CG1	2.30	0.60
2:B:25:ILE:HD11	2:B:651:LEU:HD12	1.83	0.60
2:B:357:GLN:HE21	2:B:368:GLU:HG2	1.66	0.60
2:B:98:THR:HB	2:B:99:LYS:O	2.02	0.60
1:A:46:THR:HB	1:A:46:THR:O	2.02	0.60
1:A:535:THR:HG23	1:A:616:VAL:HA	1.83	0.60
2:B:206:ASN:OD1	2:B:458:LYS:CE	2.50	0.60
2:B:616:ILE:CB	2:B:616:ILE:CD1	2.73	0.60
2:B:643:ASP:HB3	2:B:644:GLU:C	2.22	0.59
2:B:63:ILE:HG12	2:B:95:ILE:HD11	1.83	0.59
3:C:181:ASP:OD2	3:C:186:LEU:HB2	2.02	0.59
3:C:196:ASP:CB	3:C:199:LYS:HG3	2.32	0.59
6:H:105:GLU:HG2	6:H:136:LYS:NZ	2.17	0.59
1:A:63:ARG:HA	1:A:74:MET:SD	2.42	0.59
2:B:566:LEU:HD13	2:B:588:GLY:HA2	1.82	0.59
1:A:72:GLU:OE2	2:B:1175:LEU:CD1	2.51	0.59
2:B:418:LYS:CE	2:B:418:LYS:CG	2.80	0.59
1:A:1112:LYS:CE	1:A:1112:LYS:CG	2.79	0.59
1:A:63:ARG:HA	1:A:74:MET:HG2	1.84	0.59
6:H:107:VAL:CG2	6:H:107:VAL:CA	2.78	0.59
1:A:1282:VAL:HG22	1:A:1308:THR:HG22	1.84	0.59
1:A:1315:GLU:O	1:A:1318:THR:HG22	2.02	0.59
10:L:26:THR:CG2	10:L:27:LEU:H	2.16	0.59
1:A:1287:TYR:CD1	1:A:1305:VAL:HG21	2.37	0.59
1:A:956:LEU:HB3	1:A:957:PRO:HD2	1.84	0.59
2:B:118:ARG:HH22	2:B:194:GLU:CG	2.14	0.59
2:B:906:SER:O	2:B:907:GLY:C	2.40	0.59
1:A:55:ASP:OD1	1:A:55:ASP:O	2.21	0.59
1:A:903:ASN:C	1:A:903:ASN:ND2	2.56	0.59
2:B:185:THR:HG23	2:B:188:ASP:OD2	2.03	0.59
7:I:55:THR:CG2	7:I:55:THR:HB	2.26	0.59
2:B:425:THR:CG2	2:B:425:THR:HB	2.17	0.59
2:B:531:GLN:NE2	2:B:532:ALA:H	2.00	0.59
10:L:26:THR:HB	10:L:26:THR:CA	2.19	0.59
1:A:844:ALA:CB	1:A:1384:VAL:HG12	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:GLY:N	1:A:674:PRO:HD2	2.17	0.59
6:H:47:PHE:CZ	6:H:146:ARG:HD2	2.38	0.59
8:J:2:ILE:HD11	8:J:57:ILE:HD12	1.83	0.59
8:J:7:CYS:HG	8:J:45:CYS:HG	1.50	0.59
1:A:446:ARG:CG	1:A:446:ARG:NH1	2.65	0.58
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.31	0.58
3:C:267:GLN:CA	3:C:268:ASP:N	2.64	0.58
8:J:26:GLN:CA	8:J:26:GLN:CG	2.75	0.58
1:A:351:THR:HG23	2:B:1103:ILE:CG1	2.33	0.58
1:A:518:LYS:CD	1:A:518:LYS:HZ2	2.15	0.58
1:A:903:ASN:ND2	1:A:905:ASP:H	2.02	0.58
2:B:1198:TYR:CE1	2:B:1201:LYS:HD2	2.38	0.58
2:B:995:ARG:HD2	2:B:997:GLU:OE2	2.04	0.58
9:K:12:LEU:HD12	9:K:12:LEU:H	1.69	0.58
1:A:295:LEU:CB	1:A:295:LEU:CD2	2.78	0.58
2:B:775:LYS:CA	2:B:775:LYS:CG	2.73	0.58
1:A:1172:LEU:O	1:A:1173:HIS:CD2	2.56	0.58
1:A:174:ILE:N	1:A:174:ILE:CB	2.59	0.58
1:A:265:LYS:NZ	1:A:302:THR:HG21	2.17	0.58
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.37	0.58
1:A:741:ASN:HD22	1:A:741:ASN:C	2.06	0.58
1:A:587:HIS:NE2	1:A:969:GLN:HG2	2.18	0.58
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.85	0.58
3:C:205:LYS:CG	3:C:205:LYS:CA	2.74	0.58
6:H:76:THR:HG22	6:H:76:THR:O	2.04	0.58
8:J:53:HIS:HE1	8:J:55:ASP:CA	2.16	0.58
8:J:2:ILE:HD12	8:J:2:ILE:N	2.18	0.58
3:C:252:GLN:NE2	9:K:99:GLY:N	2.52	0.58
1:A:123:ARG:CA	1:A:123:ARG:CG	2.76	0.58
2:B:1162:ILE:HD11	2:B:1169:MET:HG2	1.85	0.58
2:B:1002:THR:HG21	2:B:1006:ILE:HB	1.85	0.57
2:B:1077:THR:CG2	2:B:1079:LYS:H	2.15	0.57
4:E:6:GLU:OE2	4:E:43:LYS:NZ	2.37	0.57
6:H:81:PRO:HB2	6:H:82:PRO:HD2	1.86	0.57
1:A:365:GLY:HA2	1:A:461:LYS:O	2.04	0.57
2:B:95:ILE:HG22	2:B:96:TYR:N	2.18	0.57
3:C:11:ARG:NE	3:C:209:TYR:CE2	2.72	0.57
3:C:29:MET:HB2	3:C:29:MET:CE	2.34	0.57
2:B:1002:THR:CG2	2:B:1006:ILE:HB	2.33	0.57
2:B:127:GLY:HA2	2:B:168:GLY:O	2.05	0.57
6:H:93:TYR:CD1	6:H:93:TYR:N	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HD3	6:H:95:TYR:CB	2.34	0.57
2:B:134:LYS:O	2:B:135:ARG:HG3	2.05	0.57
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.40	0.57
3:C:8:VAL:CG1	3:C:9:LYS:N	2.67	0.57
7:I:4:PHE:CZ	7:I:13:MET:HE1	2.39	0.57
2:B:862:GLN:HE22	2:B:961:LEU:HD13	1.70	0.57
1:A:567:LYS:HE2	6:H:95:TYR:CD2	2.40	0.57
2:B:101:MET:HA	2:B:110:HIS:O	2.05	0.57
2:B:341:LEU:HD12	2:B:342:GLY:H	1.69	0.57
1:A:1215:ARG:CD	1:A:1215:ARG:CB	2.76	0.57
2:B:914:LYS:CD	2:B:937:ALA:HB3	2.35	0.57
6:H:47:PHE:CB	6:H:95:TYR:HD1	2.18	0.57
3:C:252:GLN:HE22	9:K:99:GLY:N	2.02	0.57
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.22	0.57
2:B:249:ARG:CZ	2:B:415:GLN:HG3	2.34	0.57
2:B:210:LYS:HE3	2:B:461:LEU:O	2.04	0.57
5:F:114:GLU:HB2	5:F:120:ILE:CD1	2.35	0.57
10:L:51:CYS:SG	10:L:53:HIS:HB2	2.44	0.57
1:A:1404:GLU:O	1:A:1404:GLU:HG3	2.00	0.57
1:A:103:CYS:SG	1:A:207:ILE:HD12	2.45	0.57
1:A:858:ASN:ND2	1:A:862:ASN:H	2.01	0.57
3:C:208:GLU:O	3:C:210:GLU:N	2.38	0.57
6:H:105:GLU:C	6:H:107:VAL:N	2.57	0.57
2:B:955:THR:CG2	10:L:54:ARG:O	2.40	0.57
1:A:941:LYS:HD3	1:A:941:LYS:NZ	2.19	0.57
2:B:261:ARG:O	2:B:264:SER:N	2.38	0.57
2:B:916:THR:HB	2:B:935:ARG:CB	2.34	0.57
2:B:228:LYS:O	2:B:261:ARG:NH2	2.28	0.56
2:B:680:THR:HG22	2:B:682:SER:N	2.16	0.56
3:C:255:VAL:CG1	3:C:255:VAL:O	2.51	0.56
4:E:103:LYS:CG	4:E:103:LYS:CE	2.76	0.56
9:K:78:THR:HG22	9:K:79:GLU:H	1.70	0.56
1:A:1146:VAL:O	1:A:1146:VAL:CG1	2.53	0.56
1:A:346:ASP:O	1:A:347:PHE:HB2	2.05	0.56
2:B:1198:TYR:OH	2:B:1201:LYS:NZ	2.37	0.56
3:C:56:THR:HG22	3:C:58:LEU:H	1.69	0.56
1:A:1236:LEU:C	1:A:1237:ILE:HD12	2.25	0.56
1:A:175:ARG:CA	1:A:175:ARG:CG	2.74	0.56
1:A:57:ARG:HB3	1:A:68:GLN:HG2	1.86	0.56
2:B:68:THR:HG23	2:B:91:SER:HB3	1.86	0.56
1:A:187:LYS:CG	1:A:194:ALA:CB	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:52:GLN:NE2	6:H:52:GLN:CG	2.64	0.56
7:I:10:CYS:SG	7:I:29:CYS:SG	3.04	0.56
1:A:1151:GLU:HG3	7:I:45:ARG:HD2	1.88	0.56
4:E:39:LEU:O	4:E:42:PHE:HB3	2.05	0.56
6:H:103:LYS:HG2	6:H:105:GLU:OE2	2.05	0.56
1:A:599:SER:HB2	1:A:602:ASP:H	1.70	0.56
3:C:15:LYS:CB	3:C:15:LYS:CD	2.84	0.56
2:B:293:PRO:HA	7:I:12:ASN:HD21	1.71	0.56
7:I:98:VAL:HG22	7:I:99:LEU:N	2.19	0.56
1:A:200:ARG:NH2	1:A:206:GLU:OE2	2.39	0.56
6:H:136:LYS:C	6:H:136:LYS:HA	2.11	0.56
1:A:261:ASP:OD1	1:A:261:ASP:N	2.39	0.56
2:B:120:ARG:NH2	2:B:956:THR:O	2.35	0.56
4:E:2:ASP:HB3	4:E:6:GLU:HB2	1.88	0.56
9:K:20:LYS:CE	9:K:20:LYS:CG	2.82	0.56
1:A:274:ILE:C	1:A:274:ILE:CB	2.70	0.56
7:I:49:ILE:HG22	7:I:49:ILE:O	2.06	0.56
1:A:1263:ILE:CD1	1:A:1263:ILE:CB	2.79	0.56
2:B:425:THR:CG2	2:B:425:THR:CA	2.77	0.56
2:B:864:LYS:O	2:B:961:LEU:HD23	2.06	0.56
2:B:882:THR:CG2	2:B:882:THR:HB	2.18	0.56
1:A:1261:LYS:CD	1:A:1261:LYS:NZ	2.66	0.55
2:B:787:VAL:O	2:B:787:VAL:HG12	2.06	0.55
2:B:841:MET:SD	2:B:846:ILE:HD11	2.46	0.55
2:B:999:MET:HB3	2:B:1000:PRO:HD2	1.88	0.55
6:H:44:VAL:O	6:H:44:VAL:HG13	2.05	0.55
9:K:55:LYS:HB3	9:K:81:TYR:HD1	1.71	0.55
10:L:68:GLU:O	10:L:69:ALA:HB3	2.06	0.55
1:A:1132:LYS:CB	1:A:1132:LYS:CD	2.78	0.55
1:A:606:LEU:HD11	1:A:608:ILE:HD11	1.88	0.55
3:C:15:LYS:O	3:C:240:VAL:CG2	2.55	0.55
3:C:252:GLN:NE2	9:K:99:GLY:H	2.05	0.55
4:E:161:LYS:CG	4:E:161:LYS:CE	2.75	0.55
1:A:768:GLN:NE2	1:A:816:HIS:HA	2.22	0.55
2:B:961:LEU:CD2	2:B:961:LEU:CD1	2.81	0.55
3:C:239:PRO:O	3:C:242:GLN:HB2	2.06	0.55
4:E:116:ILE:H	4:E:116:ILE:HD12	1.71	0.55
4:E:117:THR:OG1	4:E:120:ALA:CB	2.55	0.55
1:A:1151:GLU:CG	7:I:45:ARG:CD	2.83	0.55
1:A:31:SER:HB3	1:A:83:HIS:HD2	1.71	0.55
2:B:167:ILE:CG2	2:B:424:LEU:HD13	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:142:LEU:HG	6:H:143:LEU:N	2.17	0.55
7:I:116:ASN:ND2	7:I:118:ARG:HB2	2.21	0.55
2:B:1128:LEU:O	2:B:1128:LEU:HG	2.07	0.55
1:A:858:ASN:HD22	1:A:858:ASN:C	2.10	0.55
2:B:46:GLN:HG3	2:B:47:GLN:H	1.71	0.55
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.06	0.55
2:B:642:ASP:HB3	2:B:649:LYS:HG3	1.89	0.55
2:B:999:MET:HE3	2:B:999:MET:HG2	1.89	0.55
3:C:56:THR:CG2	3:C:58:LEU:H	2.19	0.55
9:K:24:ASP:OD1	9:K:74:ARG:NH1	2.40	0.55
10:L:38:LEU:HG	10:L:39:SER:H	1.72	0.55
1:A:1171:GLN:NE2	1:A:1171:GLN:CG	2.63	0.55
1:A:1224:LEU:HG	1:A:1225:PHE:N	2.21	0.55
1:A:150:THR:HA	1:A:166:GLY:HA2	1.89	0.55
1:A:279:LEU:HB3	1:A:289:ILE:HD11	1.87	0.55
1:A:494:SER:OG	1:A:497:THR:HB	2.07	0.55
2:B:353:LYS:CD	2:B:353:LYS:CB	2.77	0.55
3:C:131:HIS:O	3:C:132:PRO:C	2.44	0.55
6:H:27:GLU:OE1	6:H:39:THR:CG2	2.54	0.55
2:B:1002:THR:HG22	2:B:1006:ILE:N	2.21	0.55
3:C:40:GLU:OE1	3:C:254:LYS:NZ	2.40	0.55
8:J:42:LYS:HG3	8:J:43:ARG:N	2.22	0.55
1:A:1265:ASN:O	1:A:1266:THR:C	2.42	0.54
1:A:150:THR:HG22	1:A:151:ASP:OD2	2.07	0.54
1:A:175:ARG:CD	1:A:175:ARG:CB	2.83	0.54
1:A:843:LYS:CE	1:A:843:LYS:CG	2.85	0.54
4:E:116:ILE:HG22	4:E:120:ALA:CB	2.36	0.54
10:L:47:ARG:HG2	10:L:48:CYS:N	2.19	0.54
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.20	0.54
2:B:956:THR:HA	2:B:961:LEU:O	2.07	0.54
1:A:562:THR:CG2	6:H:98:TYR:CD2	2.90	0.54
8:J:2:ILE:HD11	8:J:57:ILE:CD1	2.37	0.54
1:A:89:PRO:HB2	1:A:204:THR:HG21	1.90	0.54
2:B:282:ILE:N	2:B:282:ILE:HD13	2.22	0.54
2:B:744:HIS:CD2	2:B:746:SER:H	2.21	0.54
1:A:1325:THR:O	4:E:148:GLU:HG2	2.06	0.54
4:E:71:LYS:CG	4:E:71:LYS:CE	2.80	0.54
7:I:109:ILE:HD12	7:I:109:ILE:N	2.21	0.54
2:B:435:THR:O	2:B:435:THR:HG22	2.07	0.54
2:B:1163:CYS:SG	2:B:1163:CYS:CA	2.95	0.54
2:B:1163:CYS:CB	2:B:1182:CYS:SG	2.96	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1163:CYS:HB2	2:B:1182:CYS:SG	2.48	0.54
3:C:33:LEU:HD13	3:C:248:ILE:HD13	1.88	0.54
4:E:61:GLN:HB2	4:E:79:TRP:HE3	1.71	0.54
9:K:46:ILE:O	9:K:47:ARG:C	2.35	0.54
1:A:507:VAL:N	1:A:508:PRO:CD	2.70	0.54
2:B:1182:CYS:SG	2:B:1185:CYS:SG	3.06	0.54
8:J:4:PRO:HD3	8:J:53:HIS:HD2	1.72	0.54
1:A:1203:ASN:O	1:A:1205:LYS:N	2.41	0.54
2:B:509:ALA:N	2:B:509:ALA:CB	2.65	0.54
4:E:47:CYS:SG	4:E:52:ARG:O	2.66	0.54
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.73	0.54
10:L:32:ALA:HB2	10:L:55:ILE:HG22	1.90	0.54
10:L:65:VAL:CG2	10:L:65:VAL:HB	2.17	0.54
2:B:900:ALA:O	2:B:901:PRO:C	2.44	0.54
4:E:61:GLN:HB2	4:E:79:TRP:CE3	2.43	0.54
6:H:95:TYR:CE2	6:H:97:MET:HG3	2.43	0.54
1:A:217:LYS:CD	1:A:217:LYS:CB	2.81	0.54
3:C:15:LYS:CA	3:C:15:LYS:CG	2.80	0.54
6:H:47:PHE:CG	6:H:95:TYR:HD1	2.26	0.54
1:A:846:GLU:HA	1:A:1066:VAL:HG23	1.88	0.53
1:A:1146:VAL:HG12	1:A:1197:LEU:HD22	1.90	0.53
1:A:55:ASP:N	1:A:56:PRO:HD2	2.22	0.53
2:B:463:THR:HG21	2:B:465:ASN:OD1	2.08	0.53
4:E:55:ARG:O	4:E:56:LYS:C	2.46	0.53
6:H:44:VAL:O	6:H:44:VAL:CG1	2.56	0.53
10:L:54:ARG:NE	10:L:54:ARG:CG	2.62	0.53
1:A:1318:THR:HG23	4:E:11:ARG:HH12	1.73	0.53
1:A:42:ASP:OD2	1:A:46:THR:C	2.45	0.53
2:B:1177:HIS:HB2	2:B:1179:GLN:HE21	1.71	0.53
2:B:984:HIS:CD2	2:B:1025:HIS:HA	2.42	0.53
1:A:852:TYR:CD2	5:F:136:ARG:HD3	2.43	0.53
1:A:672:ASP:HB3	1:A:674:PRO:HG2	1.89	0.53
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.44	0.53
2:B:89:GLU:HB2	2:B:137:TYR:HB2	1.90	0.53
2:B:436:VAL:CA	2:B:436:VAL:CG1	2.78	0.53
10:L:48:CYS:HB3	10:L:51:CYS:O	2.09	0.53
1:A:55:ASP:C	1:A:57:ARG:H	2.04	0.53
6:H:9:ILE:HA	6:H:9:ILE:CB	2.17	0.53
1:A:1445:ILE:CG2	1:A:1445:ILE:HA	2.36	0.53
1:A:191:THR:CB	1:A:191:THR:HA	2.18	0.53
6:H:9:ILE:HB	6:H:9:ILE:CA	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:16:PRO:O	7:I:17:ARG:CD	2.46	0.53
1:A:1298:TYR:O	1:A:1299:VAL:HG23	2.08	0.53
1:A:919:ILE:CD1	1:A:919:ILE:CB	2.81	0.53
2:B:755:ILE:CG2	2:B:755:ILE:O	2.56	0.53
4:E:116:ILE:N	4:E:116:ILE:HD12	2.24	0.53
6:H:100:THR:O	6:H:116:TYR:HA	2.08	0.53
8:J:6:ARG:HD2	8:J:11:GLY:O	2.08	0.53
1:A:1226:VAL:HG12	1:A:1227:ILE:N	2.20	0.53
3:C:133:ILE:C	3:C:134:ILE:HG12	2.28	0.53
6:H:138:GLU:HG2	6:H:139:ASN:N	2.23	0.53
6:H:59:ILE:HG22	6:H:60:ALA:N	2.24	0.53
1:A:1166:ASP:OD2	1:A:1239:ARG:NH2	2.22	0.53
2:B:98:THR:OG1	2:B:127:GLY:O	2.26	0.53
2:B:169:ARG:O	2:B:457:LEU:HD12	2.08	0.53
2:B:103:ASN:HB2	2:B:169:ARG:HH22	1.73	0.52
6:H:130:ARG:O	6:H:130:ARG:HD2	2.07	0.52
7:I:120:GLN:O	7:I:121:PHE:CB	2.56	0.52
1:A:1162:VAL:CG1	1:A:1162:VAL:O	2.57	0.52
2:B:1152:MET:HE2	2:B:1152:MET:HA	1.91	0.52
2:B:313:MET:HE3	2:B:386:LEU:CD2	2.35	0.52
7:I:71:SER:OG	7:I:83:ASN:ND2	2.41	0.52
1:A:476:SER:N	1:A:477:PRO:HD2	2.24	0.52
2:B:453:ILE:HG22	2:B:454:THR:N	2.23	0.52
5:F:72:LYS:CG	5:F:72:LYS:CE	2.84	0.52
3:C:167:HIS:CE1	10:L:70:ARG:O	2.58	0.52
1:A:1155:ASP:O	1:A:1241:ARG:NH2	2.42	0.52
1:A:274:ILE:CA	1:A:274:ILE:CG1	2.82	0.52
1:A:658:LEU:HD12	1:A:658:LEU:O	2.10	0.52
1:A:636:GLU:OE2	1:A:962:ARG:CD	2.57	0.52
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.92	0.52
6:H:98:TYR:C	6:H:118:PHE:HD2	2.13	0.52
9:K:25:THR:CG2	9:K:25:THR:CA	2.78	0.52
1:A:1293:SER:HB2	1:A:1294:PRO:HD2	1.92	0.52
1:A:278:THR:O	1:A:278:THR:HG22	2.09	0.52
1:A:42:ASP:OD2	1:A:47:ARG:CG	2.58	0.52
2:B:1057:LYS:NZ	2:B:1057:LYS:CD	2.66	0.52
2:B:516:ASN:H	2:B:516:ASN:HD22	1.55	0.52
3:C:19:ASP:C	3:C:19:ASP:OD1	2.48	0.52
4:E:176:PRO:O	4:E:212:ARG:HA	2.09	0.52
6:H:103:LYS:CB	6:H:105:GLU:OE1	2.51	0.52
9:K:18:LYS:HE3	9:K:38:GLU:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASP:HB3	1:A:299:HIS:CD2	2.44	0.52
2:B:360:PHE:O	2:B:361:LEU:C	2.48	0.52
6:H:96:VAL:HA	6:H:142:LEU:O	2.10	0.52
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.09	0.52
2:B:658:ILE:O	2:B:658:ILE:HG22	2.10	0.52
4:E:127:ILE:H	4:E:128:PRO:HD3	1.74	0.52
2:B:294:ASP:N	7:I:12:ASN:HD22	2.08	0.52
6:H:37:LYS:O	6:H:125:LEU:HA	2.10	0.52
1:A:741:ASN:ND2	1:A:741:ASN:C	2.62	0.52
6:H:114:VAL:HG11	6:H:134:ASN:ND2	2.25	0.52
4:E:152:LYS:NZ	4:E:152:LYS:CD	2.70	0.52
4:E:71:LYS:CB	4:E:71:LYS:CD	2.78	0.52
8:J:16:ASP:OD1	8:J:17:LYS:HG3	2.10	0.52
1:A:107:CYS:HB2	1:A:148:CYS:HB2	1.92	0.51
2:B:1097:HIS:CB	2:B:1097:HIS:N	2.69	0.51
2:B:117:ALA:HA	2:B:122:LEU:HB2	1.91	0.51
2:B:43:LEU:HD11	2:B:811:TYR:O	2.10	0.51
3:C:40:GLU:CD	3:C:254:LYS:NZ	2.64	0.51
1:A:1195:LEU:HD11	1:A:1267:MET:HE1	1.91	0.51
1:A:1287:TYR:HD1	1:A:1305:VAL:HG21	1.76	0.51
1:A:901:LEU:H	1:A:926:GLN:HE22	1.54	0.51
1:A:1111:MET:CB	1:A:1111:MET:SD	2.89	0.51
2:B:531:GLN:CG	2:B:531:GLN:CA	2.84	0.51
4:E:37:LEU:CB	4:E:37:LEU:CD1	2.79	0.51
3:C:154:LYS:CG	3:C:154:LYS:CA	2.82	0.51
5:F:114:GLU:HB2	5:F:120:ILE:HD11	1.93	0.51
6:H:91:ASP:C	6:H:91:ASP:OD1	2.48	0.51
1:A:356:ASP:OD2	1:A:469:ARG:HD3	2.11	0.51
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.10	0.51
1:A:55:ASP:N	1:A:56:PRO:HD3	2.24	0.51
2:B:399:ASP:CA	2:B:399:ASP:CG	2.67	0.51
2:B:46:GLN:HG3	2:B:47:GLN:N	2.25	0.51
1:A:567:LYS:HB2	6:H:95:TYR:HA	1.92	0.51
1:A:1172:LEU:O	1:A:1173:HIS:CG	2.64	0.51
1:A:378:GLU:OE1	1:A:434:ARG:HD3	2.10	0.51
1:A:562:THR:HG22	6:H:98:TYR:CD2	2.45	0.51
4:E:79:TRP:HE1	4:E:81:GLU:HB2	1.76	0.51
1:A:567:LYS:CE	6:H:95:TYR:CD2	2.94	0.51
1:A:852:TYR:CE2	5:F:136:ARG:HD3	2.45	0.51
2:B:864:LYS:O	2:B:961:LEU:CD2	2.59	0.51
1:A:982:THR:HB	1:A:985:ASP:CG	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.46	0.51
2:B:788:ARG:HD3	2:B:790:ASP:OD1	2.10	0.51
3:C:124:LEU:HD23	3:C:124:LEU:N	2.26	0.51
3:C:8:VAL:O	3:C:9:LYS:HB2	2.11	0.51
6:H:105:GLU:HG2	6:H:136:LYS:HZ2	1.75	0.51
1:A:237:THR:HB	1:A:237:THR:CG2	2.18	0.51
1:A:605:MET:HE2	1:A:607:ILE:CD1	2.40	0.51
2:B:353:LYS:CG	2:B:353:LYS:CE	2.82	0.51
2:B:424:LEU:O	2:B:428:ILE:HG13	2.09	0.51
1:A:247:ARG:HH11	1:A:263:THR:CG2	2.19	0.50
5:F:109:VAL:HG11	5:F:123:LYS:HG2	1.93	0.50
1:A:191:THR:CA	1:A:191:THR:HB	2.18	0.50
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.75	0.50
3:C:7:GLN:OE1	9:K:104:ASN:ND2	2.44	0.50
4:E:127:ILE:N	4:E:128:PRO:HD3	2.24	0.50
1:A:1166:ASP:O	1:A:1170:ILE:HD13	2.11	0.50
1:A:597:LEU:H	1:A:597:LEU:HD12	1.76	0.50
2:B:1195:HIS:C	2:B:1196:ILE:HG23	2.31	0.50
2:B:502:ILE:HD13	2:B:502:ILE:HA	1.93	0.50
2:B:775:LYS:CB	2:B:775:LYS:HD2	2.39	0.50
3:C:47:ASP:CG	3:C:47:ASP:O	2.49	0.50
8:J:3:VAL:HA	8:J:53:HIS:CD2	2.46	0.50
1:A:1122:PRO:O	1:A:1123:GLY:C	2.48	0.50
4:E:93:MET:HE3	4:E:116:ILE:HG21	1.93	0.50
6:H:118:PHE:O	6:H:119:GLY:C	2.44	0.50
6:H:8:ASP:OD2	6:H:9:ILE:N	2.39	0.50
10:L:48:CYS:CA	10:L:49:LYS:N	2.67	0.50
1:A:189:ARG:HG2	1:A:189:ARG:O	2.11	0.50
1:A:463:ILE:CD1	1:A:469:ARG:HG3	2.42	0.50
1:A:752:LYS:HZ3	2:B:1019:SER:N	2.03	0.50
1:A:903:ASN:ND2	1:A:905:ASP:N	2.59	0.50
2:B:365:THR:HG22	2:B:367:LEU:H	1.77	0.50
2:B:820:GLY:HA3	2:B:1091:TYR:CZ	2.47	0.50
1:A:61:ILE:CG1	1:A:61:ILE:CA	2.83	0.50
2:B:910:VAL:C	2:B:911:ILE:HD12	2.32	0.50
3:C:120:ILE:N	3:C:120:ILE:HD12	2.24	0.50
7:I:41:PRO:HD2	7:I:42:LEU:H	1.77	0.50
10:L:34:CYS:CB	10:L:51:CYS:CB	2.81	0.50
2:B:544:CYS:HB2	2:B:634:TYR:CE1	2.46	0.50
10:L:43:THR:CG2	10:L:43:THR:CA	2.82	0.50
2:B:393:LYS:HZ1	2:B:621:GLU:CD	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:240:VAL:C	3:C:242:GLN:N	2.64	0.50
6:H:11:GLN:NE2	6:H:52:GLN:HG2	2.27	0.50
7:I:74:GLU:HA	7:I:80:SER:O	2.12	0.50
9:K:102:LYS:O	9:K:106:GLU:HB2	2.12	0.50
1:A:1258:HIS:O	1:A:1259:MET:C	2.50	0.50
1:A:1256:GLU:HB3	1:A:1259:MET:HE2	1.93	0.50
1:A:587:HIS:CE1	1:A:609:ASP:H	2.30	0.50
2:B:344:LYS:CG	2:B:344:LYS:CA	2.84	0.50
2:B:428:ILE:HG12	2:B:448:ILE:CD1	2.30	0.50
3:C:178:PHE:C	3:C:178:PHE:CD2	2.86	0.50
4:E:14:ARG:O	4:E:15:ALA:C	2.46	0.50
9:K:26:LYS:CB	9:K:26:LYS:CD	2.89	0.50
1:A:526:ASP:OD1	2:B:1013:ASN:ND2	2.40	0.49
3:C:73:GLN:HE21	3:C:75:MET:N	2.06	0.49
6:H:32:THR:HG22	6:H:33:GLN:CD	2.32	0.49
8:J:10:CYS:SG	8:J:45:CYS:SG	3.10	0.49
1:A:1127:ASP:HB3	1:A:1130:GLN:H	1.77	0.49
1:A:89:PRO:HB2	1:A:204:THR:CG2	2.42	0.49
1:A:353:ILE:HD13	1:A:487:MET:HE3	1.93	0.49
1:A:605:MET:CE	1:A:607:ILE:HG13	2.42	0.49
2:B:1058:LEU:O	2:B:1062:HIS:HD2	1.95	0.49
2:B:830:TYR:O	2:B:831:SER:CB	2.60	0.49
2:B:243:ALA:C	2:B:244:LEU:HG	2.32	0.49
7:I:16:PRO:HG3	7:I:27:PHE:CE2	2.47	0.49
8:J:1:MET:CE	8:J:1:MET:HG3	2.38	0.49
8:J:53:HIS:HD1	8:J:54:VAL:N	2.09	0.49
2:B:516:ASN:ND2	2:B:516:ASN:H	2.11	0.49
5:F:109:VAL:HG22	5:F:127:GLU:OE1	2.11	0.49
1:A:247:ARG:NH1	1:A:263:THR:CG2	2.70	0.49
2:B:755:ILE:HG22	2:B:755:ILE:O	2.11	0.49
2:B:957:ASN:OD1	2:B:959:ASP:HB2	2.12	0.49
6:H:138:GLU:CG	6:H:139:ASN:N	2.74	0.49
9:K:49:GLU:C	9:K:51:LEU:N	2.65	0.49
10:L:43:THR:CG2	10:L:43:THR:HB	2.20	0.49
10:L:47:ARG:CG	10:L:48:CYS:H	2.22	0.49
1:A:387:ARG:O	1:A:388:LEU:C	2.51	0.49
1:A:605:MET:CE	1:A:607:ILE:HD11	2.43	0.49
2:B:1008:PRO:CG	2:B:1011:ILE:HD11	2.43	0.49
8:J:14:VAL:CG1	8:J:50:ILE:HD11	2.39	0.49
1:A:46:THR:O	1:A:48:ALA:N	2.46	0.49
2:B:436:VAL:CG2	2:B:436:VAL:CA	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:595:ARG:CD	2:B:595:ARG:HB2	2.43	0.49
3:C:53:THR:O	3:C:153:LEU:HA	2.13	0.49
1:A:1383:SER:OG	1:A:1384:VAL:N	2.44	0.49
1:A:215:SER:OG	1:A:218:ASP:HB2	2.13	0.49
3:C:244:VAL:O	3:C:248:ILE:HG12	2.13	0.49
4:E:161:LYS:CE	4:E:172:GLU:OE2	2.61	0.49
6:H:99:GLY:N	6:H:118:PHE:CD2	2.81	0.49
9:K:25:THR:OG1	9:K:25:THR:CG2	2.54	0.49
1:A:1445:ILE:CG2	1:A:1445:ILE:HB	2.19	0.49
1:A:44:THR:CA	1:A:44:THR:HB	2.20	0.49
1:A:693:VAL:HG21	1:A:721:PHE:CE1	2.44	0.49
2:B:1065:GLN:NE2	2:B:1067:ARG:HB2	2.22	0.49
4:E:117:THR:O	4:E:118:PRO:C	2.51	0.49
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.48	0.49
10:L:31:CYS:SG	10:L:51:CYS:SG	3.10	0.49
1:A:1209:MET:O	1:A:1210:GLY:C	2.48	0.49
1:A:1236:LEU:HG	1:A:1236:LEU:CD2	2.19	0.49
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.48	0.49
1:A:597:LEU:CD1	1:A:597:LEU:HG	2.24	0.49
2:B:1051:THR:O	2:B:1055:ILE:HG12	2.13	0.49
8:J:53:HIS:CE1	8:J:54:VAL:C	2.86	0.49
9:K:55:LYS:HB2	9:K:81:TYR:CE1	2.48	0.49
9:K:49:GLU:HG3	9:K:94:ILE:CD1	2.43	0.49
1:A:230:ARG:NH1	1:A:232:GLU:OE2	2.43	0.48
2:B:1097:HIS:C	2:B:1097:HIS:ND1	2.67	0.48
1:A:771:GLU:CD	2:B:510:LYS:HZ3	2.15	0.48
2:B:515:HIS:N	2:B:518:HIS:HD2	2.05	0.48
2:B:914:LYS:HD2	2:B:937:ALA:HB3	1.93	0.48
4:E:52:ARG:HG3	4:E:53:PRO:HD3	1.95	0.48
1:A:14:VAL:N	1:A:1432:GLN:HE22	2.05	0.48
1:A:362:ASP:OD1	1:A:459:ARG:HD3	2.13	0.48
1:A:901:LEU:HB2	1:A:926:GLN:HE21	1.77	0.48
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.95	0.48
4:E:60:PHE:CD1	4:E:60:PHE:C	2.87	0.48
9:K:98:LEU:O	9:K:99:GLY:C	2.51	0.48
1:A:119:ASN:O	1:A:120:GLU:CB	2.58	0.48
1:A:1290:LYS:HA	1:A:1299:VAL:O	2.12	0.48
2:B:130:VAL:CG2	2:B:167:ILE:HD11	2.44	0.48
2:B:121:ASN:HD21	2:B:965:LYS:NZ	2.11	0.48
2:B:167:ILE:CD1	2:B:167:ILE:CB	2.80	0.48
2:B:286:PHE:HB3	2:B:297:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:103:LYS:HE3	6:H:135:LEU:O	2.13	0.48
1:A:1111:MET:CE	1:A:1111:MET:CB	2.91	0.48
2:B:1163:CYS:SG	2:B:1165:ILE:HG12	2.53	0.48
3:C:56:THR:CG2	3:C:57:VAL:N	2.75	0.48
1:A:1157:ASP:O	1:A:1160:SER:O	2.32	0.48
1:A:110:CYS:SG	1:A:167:CYS:CB	3.02	0.48
2:B:1057:LYS:CB	2:B:1057:LYS:CD	2.81	0.48
3:C:186:LEU:HD12	3:C:186:LEU:HA	1.53	0.48
5:F:111:LEU:C	5:F:113:GLY:N	2.66	0.48
5:F:73:ALA:HB2	5:F:143:PHE:CE1	2.49	0.48
6:H:105:GLU:N	6:H:105:GLU:CD	2.67	0.48
6:H:47:PHE:CB	6:H:95:TYR:CD1	2.96	0.48
8:J:38:ARG:CG	8:J:38:ARG:CA	2.82	0.48
9:K:18:LYS:HE3	9:K:36:GLU:O	2.13	0.48
1:A:399:HIS:HE1	1:A:436:ILE:O	1.97	0.48
1:A:464:PRO:O	1:A:465:TYR:O	2.32	0.48
2:B:1085:ILE:HD12	2:B:1085:ILE:N	2.29	0.48
6:H:114:VAL:HG11	6:H:134:ASN:HD22	1.79	0.48
8:J:26:GLN:CB	8:J:26:GLN:CD	2.77	0.48
1:A:1362:TYR:C	1:A:1362:TYR:CD2	2.85	0.48
1:A:3:GLY:CA	1:A:76:GLU:HG2	2.43	0.48
1:A:834:THR:HG21	1:A:1077:THR:CA	2.43	0.48
1:A:913:LEU:HD11	1:A:981:LEU:O	2.13	0.48
2:B:436:VAL:CB	2:B:436:VAL:N	2.66	0.48
4:E:63:ASN:O	4:E:64:PRO:C	2.46	0.48
6:H:6:PHE:C	6:H:6:PHE:CD2	2.87	0.48
2:B:451:LYS:HA	2:B:454:THR:HB	1.96	0.48
2:B:69:LEU:O	2:B:70:ILE:HD13	2.13	0.48
2:B:90:ILE:N	2:B:90:ILE:CD1	2.76	0.48
4:E:31:THR:OG1	4:E:34:GLU:HB2	2.14	0.48
1:A:1164:PRO:O	1:A:1167:GLU:HG3	2.14	0.48
2:B:1213:THR:HG21	2:B:1215:ARG:NH2	2.29	0.48
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.79	0.47
2:B:128:LEU:O	2:B:167:ILE:N	2.43	0.47
6:H:123:MET:HE3	6:H:123:MET:CG	2.44	0.47
6:H:26:ILE:CD1	6:H:42:ILE:HD12	2.44	0.47
3:C:166:GLU:HB2	9:K:10:PHE:HE2	1.79	0.47
10:L:58:LYS:O	10:L:59:ALA:CB	2.44	0.47
1:A:1266:THR:O	1:A:1267:MET:C	2.53	0.47
2:B:502:ILE:CG1	2:B:502:ILE:CA	2.85	0.47
1:A:771:GLU:CD	2:B:510:LYS:NZ	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.43	0.47
7:I:51:ASN:HB2	7:I:118:ARG:CZ	2.44	0.47
9:K:18:LYS:CE	9:K:38:GLU:OE2	2.62	0.47
9:K:55:LYS:HB3	9:K:81:TYR:CD1	2.49	0.47
10:L:38:LEU:HD13	10:L:48:CYS:HA	1.95	0.47
1:A:35:ILE:HG22	1:A:270:LEU:HD21	1.95	0.47
2:B:531:GLN:HE21	2:B:532:ALA:N	2.11	0.47
2:B:914:LYS:HD3	2:B:937:ALA:HB3	1.94	0.47
10:L:38:LEU:O	10:L:39:SER:HB2	2.13	0.47
1:A:1172:LEU:C	1:A:1173:HIS:CD2	2.87	0.47
1:A:853:ASP:OD2	1:A:857:ARG:NH2	2.47	0.47
2:B:859:TYR:CD1	2:B:859:TYR:N	2.82	0.47
3:C:248:ILE:N	3:C:248:ILE:HD13	2.25	0.47
4:E:36:GLU:O	4:E:38:PRO:CD	2.62	0.47
4:E:43:LYS:O	4:E:47:CYS:HB3	2.13	0.47
4:E:94:LYS:O	4:E:98:ILE:HD13	2.14	0.47
6:H:113:ALA:CB	6:H:124:ARG:HH21	2.28	0.47
8:J:62:ARG:HE	8:J:62:ARG:HB3	1.25	0.47
1:A:1192:LEU:HD11	1:A:1239:ARG:HB2	1.96	0.47
1:A:304:MET:HB2	1:A:304:MET:CE	2.44	0.47
1:A:35:ILE:H	1:A:35:ILE:CD1	2.16	0.47
2:B:128:LEU:HD13	2:B:128:LEU:N	2.29	0.47
2:B:94:LYS:HG2	2:B:96:TYR:CE1	2.49	0.47
4:E:63:ASN:C	4:E:64:PRO:O	2.52	0.47
1:A:187:LYS:HG3	1:A:194:ALA:HB3	1.96	0.47
1:A:187:LYS:CG	1:A:194:ALA:HB3	2.43	0.47
1:A:40:THR:HG23	1:A:54:ASN:ND2	2.30	0.47
1:A:66:LYS:CB	1:A:66:LYS:CD	2.86	0.47
1:A:704:ALA:HB1	1:A:708:MET:O	2.15	0.47
2:B:1004:GLU:HB2	2:B:1006:ILE:HD13	1.96	0.47
4:E:118:PRO:O	4:E:121:MET:SD	2.73	0.47
8:J:51:LEU:O	8:J:51:LEU:HG	2.15	0.47
8:J:1:MET:HG3	8:J:60:PHE:HE2	1.80	0.47
1:A:925:LEU:HA	1:A:925:LEU:HD23	1.72	0.47
2:B:227:LYS:CE	2:B:227:LYS:CG	2.90	0.47
2:B:291:ILE:HG22	2:B:297:ILE:HD13	1.95	0.47
2:B:900:ALA:O	2:B:903:VAL:HG23	2.14	0.47
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.45	0.47
6:H:27:GLU:OE1	6:H:39:THR:HG23	2.12	0.47
8:J:53:HIS:C	8:J:53:HIS:ND1	2.66	0.47
1:A:1148:ILE:HD12	1:A:1196:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1260:LEU:HA	1:A:1260:LEU:HD12	1.68	0.47
1:A:279:LEU:H	1:A:281:HIS:H	1.61	0.47
1:A:840:ARG:CB	1:A:840:ARG:CD	2.86	0.47
2:B:424:LEU:HD21	2:B:428:ILE:HD11	1.96	0.47
2:B:529:GLU:O	2:B:531:GLN:NE2	2.48	0.47
3:C:42:PRO:HG3	3:C:163:ILE:HD11	1.96	0.47
4:E:79:TRP:NE1	4:E:81:GLU:HB2	2.29	0.47
10:L:65:VAL:CG2	10:L:65:VAL:N	2.78	0.47
3:C:43:THR:CG2	3:C:44:LEU:N	2.78	0.47
1:A:216:VAL:HG22	1:A:219:PHE:CZ	2.49	0.47
1:A:979:SER:OG	1:A:981:LEU:HB2	2.15	0.47
9:K:77:THR:OG1	9:K:83:PRO:HD3	2.15	0.47
9:K:88:LYS:CG	9:K:88:LYS:CE	2.83	0.47
1:A:1151:GLU:HG2	7:I:45:ARG:HD2	1.96	0.47
1:A:279:LEU:HB3	1:A:289:ILE:CD1	2.45	0.47
2:B:132:VAL:CG1	2:B:133:LYS:N	2.78	0.47
2:B:592:ASN:O	2:B:593:PRO:C	2.52	0.47
2:B:864:LYS:HG3	2:B:865:LYS:N	2.28	0.47
2:B:914:LYS:N	2:B:938:SER:HB2	2.27	0.47
3:C:63:ILE:HG23	3:C:63:ILE:HD12	1.42	0.47
1:A:664:THR:HG22	1:A:742:ASN:HB3	1.96	0.46
1:A:752:LYS:CE	2:B:1019:SER:OG	2.63	0.46
5:F:105:ALA:HB1	5:F:106:PRO:HD2	1.97	0.46
6:H:106:GLU:HB2	6:H:113:ALA:HB3	1.96	0.46
6:H:123:MET:HE1	6:H:142:LEU:HD13	1.97	0.46
10:L:44:ASP:O	10:L:45:ALA:CB	2.63	0.46
1:A:588:LEU:C	1:A:588:LEU:CD2	2.82	0.46
1:A:744:LYS:HD3	1:A:748:MET:HE2	1.97	0.46
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	2.50	0.46
2:B:646:LEU:CD2	2:B:646:LEU:CD1	2.90	0.46
1:A:550:LEU:HD13	1:A:556:TRP:CZ2	2.50	0.46
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.51	0.46
2:B:431:TYR:CE1	2:B:447:ALA:CB	2.97	0.46
2:B:167:ILE:CG2	2:B:424:LEU:CD1	2.93	0.46
3:C:163:ILE:HG21	3:C:163:ILE:HD13	1.96	0.46
3:C:180:TYR:CD1	3:C:180:TYR:C	2.88	0.46
3:C:262:LEU:HA	3:C:262:LEU:HD23	1.70	0.46
6:H:76:THR:CG2	6:H:76:THR:O	2.63	0.46
7:I:75:CYS:SG	7:I:106:CYS:SG	3.14	0.46
1:A:903:ASN:HD21	1:A:905:ASP:HB2	1.80	0.46
1:A:938:LYS:HE2	1:A:938:LYS:CG	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:LYS:HZ3	2:B:1018:PRO:HD2	1.81	0.46
2:B:424:LEU:CD2	2:B:424:LEU:C	2.82	0.46
6:H:95:TYR:CD2	6:H:95:TYR:C	2.88	0.46
1:A:46:THR:O	1:A:46:THR:CB	2.63	0.46
3:C:124:LEU:O	3:C:127:ARG:HG3	2.15	0.46
4:E:129:PRO:CD	4:E:130:ALA:H	2.28	0.46
4:E:31:THR:O	4:E:32:GLN:C	2.52	0.46
1:A:1449:SER:HB2	5:F:149:GLU:OE2	2.15	0.46
1:A:1236:LEU:CD2	1:A:1236:LEU:CD1	2.80	0.46
1:A:217:LYS:O	1:A:221:SER:HB2	2.15	0.46
1:A:565:ILE:HG22	1:A:569:LYS:O	2.16	0.46
2:B:1161:HIS:HA	2:B:1192:TYR:O	2.16	0.46
1:A:444:PHE:CE2	1:A:470:LEU:HD21	2.51	0.46
1:A:664:THR:HG21	1:A:746:MET:CE	2.46	0.46
1:A:982:THR:HG22	1:A:984:LYS:N	2.31	0.46
4:E:118:PRO:HA	4:E:121:MET:SD	2.56	0.46
4:E:80:VAL:HG12	4:E:81:GLU:N	2.31	0.46
1:A:1151:GLU:HG2	7:I:45:ARG:CD	2.46	0.46
9:K:101:LEU:C	9:K:101:LEU:HD13	2.36	0.46
1:A:64:ASN:O	1:A:66:LYS:N	2.49	0.46
1:A:830:LYS:CD	1:A:830:LYS:CB	2.82	0.46
1:A:920:LEU:HD22	1:A:921:GLY:N	2.30	0.46
3:C:152:GLU:OE2	3:C:154:LYS:CD	2.64	0.46
6:H:93:TYR:HD1	6:H:93:TYR:N	2.12	0.46
1:A:1146:VAL:O	1:A:1146:VAL:HG13	2.17	0.45
1:A:122:MET:CE	1:A:138:ILE:HD13	2.46	0.45
1:A:1232:ASN:ND2	1:A:1232:ASN:CB	2.73	0.45
1:A:237:THR:C	1:A:237:THR:CG2	2.84	0.45
1:A:512:VAL:HG11	1:A:635:ARG:HH21	1.81	0.45
1:A:640:GLN:O	1:A:641:VAL:C	2.53	0.45
2:B:662:MET:CE	2:B:662:MET:CG	2.90	0.45
4:E:168:TYR:O	4:E:169:ARG:C	2.51	0.45
6:H:135:LEU:HD13	6:H:139:ASN:O	2.16	0.45
9:K:27:ALA:HB1	9:K:28:PRO:CD	2.46	0.45
1:A:588:LEU:HD23	1:A:589:GLN:N	2.31	0.45
1:A:596:THR:CG2	1:A:597:LEU:N	2.78	0.45
2:B:1153:GLU:HB3	2:B:1155:SER:HB3	1.98	0.45
4:E:36:GLU:O	4:E:38:PRO:HD3	2.16	0.45
6:H:32:THR:CG2	6:H:33:GLN:OE1	2.64	0.45
10:L:28:LYS:O	10:L:59:ALA:HB3	2.15	0.45
1:A:106:VAL:HG21	1:A:214:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1182:CYS:HB3	2:B:1185:CYS:HB2	1.97	0.45
6:H:138:GLU:O	6:H:139:ASN:O	2.35	0.45
1:A:1204:ASP:OD1	1:A:1205:LYS:HE2	2.17	0.45
1:A:1224:LEU:HD23	1:A:1226:VAL:CG2	2.47	0.45
1:A:63:ARG:HA	1:A:74:MET:CG	2.45	0.45
1:A:973:ILE:HA	1:A:973:ILE:HD13	1.64	0.45
2:B:882:THR:HG1	2:B:933:SER:N	2.14	0.45
3:C:207:CYS:O	3:C:208:GLU:C	2.55	0.45
3:C:18:VAL:CG2	3:C:240:VAL:CG1	2.91	0.45
4:E:16:PHE:CZ	4:E:20:LYS:HE2	2.51	0.45
7:I:65:ASP:C	7:I:65:ASP:OD1	2.55	0.45
9:K:18:LYS:HE2	9:K:38:GLU:OE2	2.15	0.45
1:A:1222:ASN:ND2	1:A:1222:ASN:CB	2.69	0.45
1:A:545:GLN:O	1:A:546:VAL:C	2.53	0.45
2:B:121:ASN:HD21	2:B:965:LYS:CE	2.30	0.45
2:B:130:VAL:HG23	2:B:167:ILE:HD11	1.99	0.45
1:A:1138:ILE:HD13	1:A:1138:ILE:HG21	1.54	0.45
1:A:1263:ILE:HA	1:A:1263:ILE:CD1	2.46	0.45
1:A:274:ILE:CD1	1:A:274:ILE:CA	2.95	0.45
1:A:351:THR:HG23	2:B:1103:ILE:HG12	1.94	0.45
4:E:96:PHE:CZ	4:E:100:ILE:CD1	2.98	0.45
6:H:77:ARG:C	6:H:78:SER:O	2.54	0.45
9:K:33:ILE:CD1	9:K:87:LEU:HD22	2.47	0.45
9:K:49:GLU:HG3	9:K:94:ILE:HD11	1.99	0.45
1:A:423:ASP:CG	1:A:423:ASP:O	2.55	0.45
1:A:868:TYR:CE1	1:A:1064:VAL:HG13	2.51	0.45
2:B:95:ILE:CG2	2:B:96:TYR:N	2.80	0.45
4:E:169:ARG:HD3	5:F:140:ASP:OD2	2.17	0.45
1:A:1263:ILE:O	1:A:1267:MET:HG3	2.17	0.45
1:A:304:MET:HB2	1:A:304:MET:HE2	1.99	0.45
2:B:773:MET:O	2:B:774:GLY:C	2.53	0.45
3:C:102:GLN:CA	3:C:102:GLN:CG	2.84	0.45
4:E:161:LYS:NZ	4:E:172:GLU:OE2	2.49	0.45
7:I:40:SER:CB	7:I:41:PRO:CD	2.95	0.45
8:J:53:HIS:C	8:J:53:HIS:HD1	2.20	0.45
9:K:55:LYS:CB	9:K:81:TYR:CD1	2.99	0.45
2:B:387:LEU:HD12	2:B:387:LEU:HA	1.68	0.45
2:B:428:ILE:CD1	2:B:448:ILE:HD11	2.47	0.45
2:B:898:LEU:HB2	10:L:58:LYS:HE2	1.98	0.45
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	1.98	0.45
4:E:90:VAL:CG1	4:E:90:VAL:CG2	2.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1164:PRO:O	1:A:1167:GLU:CG	2.65	0.45
1:A:924:LYS:HB2	1:A:924:LYS:HE2	1.81	0.45
2:B:1097:HIS:CA	2:B:1098:MET:N	2.67	0.45
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.99	0.45
2:B:425:THR:CG2	2:B:425:THR:C	2.85	0.45
3:C:166:GLU:HB2	9:K:10:PHE:CE2	2.52	0.45
1:A:786:HIS:HE1	2:B:742:GLU:OE2	2.00	0.44
2:B:1212:ILE:O	2:B:1214:PRO:HD3	2.16	0.44
3:C:56:THR:HG23	3:C:57:VAL:N	2.30	0.44
1:A:134:ARG:HD2	1:A:221:SER:O	2.17	0.44
1:A:884:ASP:O	1:A:886:ILE:N	2.50	0.44
2:B:724:ASP:O	2:B:725:PRO:C	2.55	0.44
4:E:93:MET:CE	4:E:116:ILE:HG21	2.47	0.44
2:B:294:ASP:N	7:I:12:ASN:ND2	2.57	0.44
1:A:64:ASN:O	1:A:64:ASN:CG	2.55	0.44
1:A:853:ASP:O	1:A:854:ASN:HB2	2.15	0.44
2:B:102:VAL:O	2:B:109:THR:HA	2.17	0.44
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.67	0.44
4:E:191:LYS:O	4:E:192:ARG:C	2.49	0.44
6:H:102:TYR:O	6:H:104:PHE:N	2.49	0.44
1:A:673:GLY:N	1:A:674:PRO:CD	2.80	0.44
2:B:429:PHE:O	2:B:429:PHE:CD2	2.69	0.44
2:B:526:GLU:HG2	2:B:538:ASN:ND2	2.33	0.44
3:C:43:THR:O	3:C:161:LYS:HA	2.17	0.44
1:A:1242:VAL:HG11	1:A:1259:MET:CE	2.47	0.44
1:A:90:VAL:HG22	1:A:297:GLN:HB2	2.00	0.44
4:E:74:ASP:N	4:E:74:ASP:OD1	2.49	0.44
6:H:136:LYS:CA	6:H:137:GLN:N	2.66	0.44
1:A:1023:ARG:HD3	1:A:1023:ARG:HH21	1.62	0.44
1:A:148:CYS:SG	1:A:167:CYS:SG	3.16	0.44
1:A:44:THR:CB	1:A:44:THR:C	2.81	0.44
1:A:896:ARG:HD3	1:A:897:TYR:CZ	2.52	0.44
1:A:903:ASN:HD22	1:A:905:ASP:N	2.15	0.44
2:B:345:LYS:O	2:B:346:GLU:C	2.50	0.44
3:C:260:LEU:CD2	3:C:260:LEU:HG	2.23	0.44
4:E:129:PRO:HD2	4:E:130:ALA:H	1.82	0.44
5:F:83:PRO:HA	5:F:146:TRP:CZ3	2.53	0.44
1:A:1111:MET:HE1	1:A:1331:SER:HB2	1.99	0.44
1:A:243:PRO:CB	1:A:245:PRO:HD2	2.42	0.44
1:A:274:ILE:CD1	1:A:274:ILE:HA	2.48	0.44
2:B:1182:CYS:HG	12:B:3007:ZN:ZN	1.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:129:PRO:CD	4:E:130:ALA:N	2.81	0.44
6:H:113:ALA:HA	6:H:125:LEU:O	2.18	0.44
6:H:138:GLU:CG	6:H:139:ASN:H	2.31	0.44
1:A:1263:ILE:HG23	1:A:1263:ILE:CD1	2.47	0.44
2:B:282:ILE:HD11	2:B:317:CYS:SG	2.58	0.44
2:B:420:LEU:HB3	2:B:453:ILE:HD13	1.99	0.44
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.65	0.44
2:B:724:ASP:O	2:B:726:ALA:N	2.51	0.44
1:A:567:LYS:HG2	6:H:96:VAL:O	2.18	0.44
1:A:59:GLY:C	1:A:60:SER:OG	2.57	0.44
1:A:913:LEU:HD12	1:A:913:LEU:HA	1.62	0.44
3:C:86:CYS:SG	3:C:92:CYS:SG	3.16	0.44
4:E:117:THR:OG1	4:E:120:ALA:HB3	2.16	0.44
8:J:1:MET:O	8:J:2:ILE:HD12	2.18	0.44
2:B:1065:GLN:NE2	2:B:1067:ARG:N	2.63	0.43
2:B:68:THR:CG2	2:B:91:SER:HB3	2.48	0.43
1:A:503:GLN:HE21	5:F:90:ARG:HH21	1.65	0.43
7:I:104:LEU:HA	7:I:104:LEU:HD23	1.80	0.43
3:C:52:GLU:HA	10:L:64:LEU:HD21	2.00	0.43
1:A:846:GLU:HA	1:A:1066:VAL:CG2	2.48	0.43
1:A:916:GLY:O	1:A:919:ILE:HD12	2.18	0.43
2:B:1153:GLU:OE1	2:B:1153:GLU:HA	2.18	0.43
2:B:1189:ILE:HG22	2:B:1190:ASP:N	2.33	0.43
2:B:121:ASN:ND2	2:B:965:LYS:NZ	2.65	0.43
1:A:140:THR:HA	1:A:143:LYS:HD3	2.01	0.43
1:A:908:LEU:O	1:A:909:ASP:C	2.55	0.43
2:B:826:ALA:HB3	2:B:1011:ILE:HD12	2.01	0.43
2:B:118:ARG:NH2	2:B:194:GLU:CD	2.71	0.43
2:B:569:TYR:CE2	2:B:571:PRO:HG3	2.54	0.43
3:C:260:LEU:CD1	3:C:260:LEU:CD2	2.89	0.43
4:E:117:THR:OG1	4:E:120:ALA:HB2	2.17	0.43
7:I:41:PRO:CD	7:I:42:LEU:H	2.30	0.43
7:I:65:ASP:HA	7:I:66:PRO:HD2	1.81	0.43
1:A:1280:GLU:OE1	1:A:1280:GLU:CG	2.53	0.43
1:A:557:ASP:O	1:A:559:VAL:N	2.51	0.43
1:A:88:LYS:HB3	1:A:89:PRO:HD2	2.01	0.43
1:A:938:LYS:CE	1:A:938:LYS:HG3	2.46	0.43
3:C:29:MET:CB	3:C:29:MET:CE	2.97	0.43
4:E:117:THR:C	4:E:119:SER:N	2.71	0.43
4:E:7:ARG:O	4:E:8:ASN:C	2.57	0.43
1:A:1293:SER:CB	1:A:1294:PRO:HD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:TYR:CD2	9:K:62:LYS:HD3	2.53	0.43
6:H:95:TYR:HB3	6:H:144:ILE:HB	2.00	0.43
1:A:809:THR:HB	1:A:810:PRO:CD	2.48	0.43
2:B:839:MET:CE	2:B:1010:LEU:HD11	2.48	0.43
6:H:55:LEU:HD22	6:H:144:ILE:HG23	2.00	0.43
9:K:82:ASP:HA	9:K:83:PRO:HD2	1.75	0.43
1:A:138:ILE:HD12	1:A:142:CYS:SG	2.58	0.43
1:A:599:SER:O	1:A:600:PRO:C	2.57	0.43
1:A:973:ILE:CG2	1:A:973:ILE:CA	2.84	0.43
1:A:497:THR:HG21	2:B:1149:GLU:OE1	2.19	0.43
2:B:418:LYS:CD	2:B:418:LYS:NZ	2.66	0.43
3:C:102:GLN:N	3:C:102:GLN:CG	2.81	0.43
3:C:55:THR:O	3:C:151:GLN:HG2	2.19	0.43
5:F:81:THR:HB	5:F:144:GLU:OE1	2.19	0.43
6:H:123:MET:CE	6:H:142:LEU:HD13	2.49	0.43
6:H:63:LEU:H	6:H:63:LEU:HD12	1.81	0.43
7:I:45:ARG:CD	7:I:45:ARG:CB	2.86	0.43
1:A:711:ARG:NE	7:I:95:THR:HG22	2.25	0.43
9:K:65:HIS:CD2	9:K:67:PHE:H	2.28	0.43
10:L:44:ASP:O	10:L:45:ALA:HB3	2.18	0.43
2:B:26:THR:O	2:B:27:ALA:C	2.57	0.43
2:B:324:ILE:N	2:B:324:ILE:HD12	2.34	0.43
2:B:458:LYS:O	2:B:459:TYR:C	2.53	0.43
4:E:30:ILE:HG23	4:E:30:ILE:HD12	1.64	0.43
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.54	0.43
1:A:110:CYS:SG	1:A:167:CYS:HB3	2.59	0.43
2:B:296:GLU:O	2:B:300:HIS:CD2	2.72	0.43
2:B:365:THR:HG21	2:B:370:PHE:CG	2.54	0.43
2:B:642:ASP:HA	2:B:643:ASP:HA	1.12	0.43
5:F:120:ILE:HD12	5:F:120:ILE:HG23	1.71	0.43
6:H:105:GLU:C	6:H:107:VAL:H	2.22	0.43
8:J:7:CYS:SG	8:J:46:CYS:N	2.92	0.43
1:A:53:LEU:HD23	1:A:54:ASN:N	2.34	0.43
2:B:292:ILE:HD12	2:B:292:ILE:N	2.33	0.43
2:B:417:PHE:C	2:B:417:PHE:HD2	2.20	0.43
6:H:47:PHE:CG	6:H:95:TYR:CD1	3.07	0.43
1:A:567:LYS:CD	6:H:95:TYR:CD2	3.00	0.43
8:J:6:ARG:HH11	8:J:6:ARG:HD2	1.62	0.43
1:A:1074:GLU:O	1:A:1077:THR:HB	2.18	0.42
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.69	0.42
1:A:74:MET:H	1:A:74:MET:HG3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:GLN:HE21	1:A:816:HIS:HA	1.84	0.42
2:B:1012:ILE:HD12	2:B:1012:ILE:C	2.39	0.42
2:B:293:PRO:HA	7:I:12:ASN:ND2	2.34	0.42
2:B:712:PRO:HA	2:B:733:HIS:NE2	2.34	0.42
3:C:69:LEU:O	8:J:6:ARG:NH2	2.49	0.42
8:J:20:SER:O	8:J:24:LEU:HG	2.18	0.42
1:A:369:SER:CA	9:K:2:ASN:HD21	2.32	0.42
1:A:587:HIS:CD2	1:A:966:ASN:OD1	2.62	0.42
2:B:259:TYR:OH	2:B:279:ASP:OD2	2.35	0.42
2:B:297:ILE:HG23	2:B:297:ILE:HD12	1.83	0.42
4:E:117:THR:C	4:E:119:SER:H	2.22	0.42
4:E:37:LEU:HA	4:E:38:PRO:HD2	1.80	0.42
4:E:5:ASN:O	4:E:9:ILE:HG13	2.18	0.42
6:H:9:ILE:C	6:H:9:ILE:CB	2.73	0.42
1:A:1287:TYR:O	1:A:1302:PRO:HA	2.19	0.42
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	2.00	0.42
1:A:1446:ASP:OD1	1:A:1448:GLU:HG3	2.19	0.42
1:A:203:SER:OG	1:A:206:GLU:HG2	2.18	0.42
1:A:216:VAL:HA	1:A:219:PHE:CZ	2.53	0.42
1:A:35:ILE:N	1:A:35:ILE:CD1	2.79	0.42
2:B:1162:ILE:HD13	2:B:1162:ILE:HA	1.77	0.42
2:B:1166:CYS:SG	2:B:1182:CYS:SG	3.17	0.42
3:C:73:GLN:HA	3:C:133:ILE:HD11	2.01	0.42
6:H:97:MET:HE2	6:H:142:LEU:HD23	2.01	0.42
1:A:1263:ILE:HG23	1:A:1263:ILE:HD12	2.01	0.42
1:A:391:LEU:HA	1:A:391:LEU:HD23	1.71	0.42
1:A:446:ARG:HG2	1:A:478:TYR:O	2.19	0.42
1:A:807:GLY:CA	2:B:761:HIS:CE1	3.01	0.42
2:B:1010:LEU:HD12	2:B:1010:LEU:HA	1.52	0.42
2:B:104:GLU:HB2	2:B:108:VAL:HA	2.02	0.42
1:A:1438:THR:HB	2:B:1142:GLY:O	2.18	0.42
2:B:118:ARG:NH2	2:B:194:GLU:CG	2.82	0.42
2:B:658:ILE:CG2	2:B:658:ILE:O	2.66	0.42
6:H:8:ASP:CG	6:H:9:ILE:H	2.22	0.42
1:A:507:VAL:HB	1:A:508:PRO:HD3	2.02	0.42
1:A:61:ILE:CA	1:A:61:ILE:CG2	2.91	0.42
2:B:648:HIS:HB2	2:B:649:LYS:H	1.64	0.42
3:C:15:LYS:O	3:C:240:VAL:HG23	2.19	0.42
3:C:80:LEU:HA	3:C:80:LEU:HD12	1.49	0.42
1:A:1004:ASN:OD1	4:E:167:ARG:HG3	2.18	0.42
6:H:105:GLU:O	6:H:107:VAL:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1264:GLU:OE2	7:I:46:HIS:HD2	2.02	0.42
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	2.02	0.42
2:B:65:GLU:HG2	2:B:66:ASP:N	2.34	0.42
2:B:705:MET:HB3	2:B:706:GLN:HE21	1.84	0.42
3:C:100:THR:HG22	3:C:101:LEU:N	2.34	0.42
1:A:858:ASN:ND2	1:A:858:ASN:C	2.73	0.42
2:B:1022:THR:HG23	2:B:1022:THR:O	2.20	0.42
2:B:770:GLN:HE22	2:B:1093:GLN:HE22	1.68	0.42
2:B:555:ILE:HG23	2:B:555:ILE:HD12	1.84	0.42
2:B:706:GLN:CG	2:B:706:GLN:OE1	2.50	0.42
2:B:830:TYR:O	2:B:831:SER:OG	2.33	0.42
2:B:969:ARG:HH11	2:B:969:ARG:HD3	1.44	0.42
3:C:148:ARG:NH1	8:J:64:ASN:HA	2.34	0.42
3:C:181:ASP:CG	3:C:181:ASP:O	2.56	0.42
4:E:37:LEU:HD23	4:E:42:PHE:HB2	2.01	0.42
6:H:18:GLY:O	6:H:19:ARG:HB2	2.20	0.42
10:L:38:LEU:HG	10:L:39:SER:N	2.35	0.42
1:A:1006:ILE:HG23	1:A:1006:ILE:HD12	1.53	0.42
1:A:1120:LEU:HD21	1:A:1131:ALA:HB2	2.02	0.42
1:A:908:LEU:HD23	1:A:908:LEU:HA	1.73	0.42
2:B:1182:CYS:CB	2:B:1185:CYS:HB2	2.49	0.42
2:B:961:LEU:HG	2:B:961:LEU:CD1	2.21	0.42
3:C:242:GLN:NE2	3:C:246:ARG:HE	2.18	0.42
1:A:1004:ASN:CG	4:E:167:ARG:HG3	2.40	0.42
4:E:179:GLN:H	4:E:179:GLN:HG2	1.44	0.42
1:A:1239:ARG:CD	1:A:1239:ARG:CB	2.78	0.42
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.40	0.42
1:A:606:LEU:HD23	1:A:613:ILE:HG21	2.01	0.42
2:B:1163:CYS:HB3	2:B:1166:CYS:SG	2.60	0.42
2:B:269:ILE:HB	2:B:282:ILE:CD1	2.49	0.42
2:B:65:GLU:O	2:B:67:SER:N	2.53	0.42
2:B:737:THR:O	2:B:738:PHE:C	2.55	0.42
2:B:806:THR:HG23	2:B:808:ALA:N	2.33	0.42
3:C:55:THR:O	3:C:55:THR:HG22	2.19	0.42
4:E:28:TYR:CE1	4:E:75:MET:CE	3.03	0.42
6:H:103:LYS:CE	6:H:135:LEU:O	2.67	0.42
1:A:1003:LYS:CG	1:A:1003:LYS:CE	2.94	0.42
1:A:54:ASN:C	1:A:56:PRO:HD2	2.41	0.42
1:A:533:LYS:HZ3	1:A:745:GLN:HE22	1.66	0.42
2:B:1084:GLN:C	2:B:1085:ILE:HD12	2.41	0.42
2:B:915:THR:CA	2:B:915:THR:CG2	2.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:50:ALA:HB3	6:H:53:ASP:OD2	2.20	0.42
1:A:113:LEU:O	1:A:164:ARG:NH2	2.51	0.41
1:A:1134:ILE:HG22	1:A:1306:LEU:HD11	2.02	0.41
1:A:49:LYS:CG	1:A:49:LYS:CE	2.88	0.41
1:A:571:LEU:HA	1:A:571:LEU:HD12	1.76	0.41
1:A:62:ASP:C	1:A:64:ASN:H	2.24	0.41
1:A:913:LEU:HD12	1:A:913:LEU:C	2.30	0.41
2:B:189:LEU:HA	2:B:189:LEU:HD23	1.88	0.41
2:B:384:ARG:NH2	2:B:396:ASP:OD2	2.53	0.41
9:K:10:PHE:HD1	9:K:11:LEU:HD13	1.84	0.41
10:L:64:LEU:HD23	10:L:64:LEU:HA	1.87	0.41
1:A:1242:VAL:HG11	1:A:1259:MET:HE3	2.02	0.41
1:A:1263:ILE:HD13	1:A:1263:ILE:HA	2.01	0.41
1:A:71:GLN:O	1:A:72:GLU:O	2.37	0.41
1:A:913:LEU:HD12	1:A:914:GLU:N	2.34	0.41
1:A:587:HIS:HE2	1:A:969:GLN:HG2	1.81	0.41
2:B:1064:TYR:O	2:B:1065:GLN:C	2.57	0.41
2:B:235:SER:OG	2:B:236:HIS:HD2	2.03	0.41
2:B:451:LYS:O	2:B:452:THR:C	2.59	0.41
2:B:744:HIS:CD2	2:B:745:PRO:HD2	2.55	0.41
2:B:896:ASP:OD2	10:L:29:TYR:OH	2.24	0.41
3:C:46:ILE:HD12	3:C:72:LEU:HD11	2.02	0.41
1:A:1336:MET:HE2	1:A:1381:LEU:HG	2.02	0.41
2:B:113:TYR:CD2	2:B:192:LEU:CD2	3.03	0.41
2:B:1221:SER:OG	5:F:72:LYS:HD2	2.20	0.41
2:B:758:PHE:N	2:B:759:PRO:CD	2.82	0.41
3:C:145:CYS:SG	3:C:146:LYS:N	2.94	0.41
7:I:15:TYR:CD1	7:I:30:ARG:HG3	2.55	0.41
2:B:955:THR:HG21	10:L:55:ILE:HD13	2.02	0.41
1:A:187:LYS:HD2	1:A:194:ALA:HB2	2.02	0.41
1:A:476:SER:N	1:A:477:PRO:CD	2.83	0.41
1:A:84:ILE:CG2	1:A:241:VAL:CG2	2.98	0.41
2:B:121:ASN:HD22	2:B:121:ASN:N	2.17	0.41
2:B:788:ARG:HD3	2:B:788:ARG:HH11	1.65	0.41
10:L:34:CYS:SG	10:L:51:CYS:HB3	2.60	0.41
2:B:1002:THR:O	2:B:1003:ALA:C	2.55	0.41
2:B:1194:ILE:HG13	2:B:1194:ILE:O	2.20	0.41
6:H:32:THR:HB	6:H:33:GLN:OE1	2.20	0.41
7:I:111:THR:HG21	7:I:113:ASP:HB2	2.02	0.41
7:I:40:SER:HB2	7:I:41:PRO:CD	2.50	0.41
10:L:48:CYS:SG	10:L:51:CYS:SG	3.13	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1150:SER:OG	7:I:46:HIS:HB3	2.20	0.41
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.21	0.41
1:A:176:LYS:NZ	1:A:178:GLY:O	2.32	0.41
1:A:867:ILE:HD13	1:A:867:ILE:HG21	1.68	0.41
2:B:1050:ILE:H	2:B:1050:ILE:HD12	1.86	0.41
2:B:25:ILE:N	2:B:25:ILE:HD13	2.35	0.41
3:C:265:MET:CG	3:C:265:MET:CE	2.96	0.41
4:E:78:LEU:HG	4:E:79:TRP:N	2.34	0.41
7:I:98:VAL:HG21	7:I:113:ASP:HB2	2.02	0.41
1:A:523:ILE:CB	1:A:622:VAL:HG13	2.47	0.41
1:A:837:ILE:O	1:A:838:GLN:C	2.57	0.41
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	3.03	0.41
2:B:99:LYS:NZ	2:B:183:GLU:OE1	2.53	0.41
3:C:266:ASP:OD1	3:C:266:ASP:N	2.52	0.41
6:H:32:THR:CG2	6:H:33:GLN:CD	2.89	0.41
6:H:59:ILE:CG2	6:H:60:ALA:N	2.82	0.41
9:K:59:ALA:HA	9:K:74:ARG:O	2.20	0.41
1:A:1364:ASN:HD22	1:A:1366:ARG:N	2.04	0.41
4:E:52:ARG:CG	4:E:53:PRO:HD3	2.51	0.41
10:L:34:CYS:HB3	10:L:51:CYS:SG	2.61	0.41
1:A:1356:ILE:HG21	1:A:1356:ILE:HD13	1.74	0.41
1:A:19:PHE:HB2	1:A:1417:GLU:O	2.21	0.41
1:A:595:THR:HG22	1:A:596:THR:N	2.35	0.41
1:A:722:LEU:HA	1:A:722:LEU:HD23	1.93	0.41
1:A:899:VAL:CG1	1:A:929:LEU:HD13	2.51	0.41
1:A:964:ILE:HA	1:A:964:ILE:HD13	1.66	0.41
2:B:1165:ILE:CD1	2:B:1165:ILE:CB	2.84	0.41
7:I:14:LEU:HB3	7:I:27:PHE:HB3	2.03	0.41
1:A:1035:TYR:O	1:A:1036:ARG:HB2	2.21	0.41
1:A:1111:MET:HE1	1:A:1331:SER:CB	2.50	0.41
1:A:1127:ASP:OD2	1:A:1130:GLN:HB2	2.20	0.41
1:A:30:ILE:HG13	1:A:30:ILE:O	2.20	0.41
1:A:325:ILE:HG22	1:A:325:ILE:O	2.21	0.41
1:A:676:MET:CB	1:A:676:MET:SD	3.01	0.41
1:A:689:LYS:O	1:A:693:VAL:HG23	2.20	0.41
2:B:749:LEU:HD23	2:B:749:LEU:HA	1.82	0.41
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.35	0.41
3:C:43:THR:HG23	3:C:44:LEU:H	1.85	0.41
4:E:37:LEU:C	4:E:38:PRO:O	2.58	0.41
5:F:109:VAL:HG13	5:F:110:ASP:N	2.31	0.41
6:H:130:ARG:HB2	6:H:133:ASN:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1098:VAL:N	1:A:1099:PRO:CD	2.84	0.41
1:A:1264:GLU:O	1:A:1264:GLU:HG2	2.19	0.41
1:A:1436:ILE:O	1:A:1437:GLY:C	2.57	0.41
1:A:325:ILE:HD13	1:A:325:ILE:HG21	1.60	0.41
1:A:55:ASP:H	1:A:56:PRO:HD3	1.85	0.41
2:B:1077:THR:HG22	2:B:1079:LYS:N	2.24	0.41
2:B:564:GLU:OE2	2:B:591:ARG:HD2	2.21	0.41
2:B:885:MET:HB3	2:B:885:MET:CE	2.50	0.41
2:B:952:VAL:HG22	2:B:966:VAL:HG22	2.03	0.41
3:C:55:THR:HB	3:C:152:GLU:H	1.86	0.41
3:C:240:VAL:HG23	3:C:240:VAL:H	1.48	0.41
4:E:41:ASP:O	4:E:42:PHE:C	2.59	0.41
6:H:47:PHE:O	6:H:47:PHE:CD2	2.74	0.41
1:A:265:LYS:CE	1:A:302:THR:CG2	2.99	0.40
1:A:457:ALA:HB3	1:A:506:ALA:HA	2.02	0.40
2:B:100:PRO:CD	2:B:180:TYR:CZ	2.94	0.40
2:B:259:TYR:HB2	2:B:268:THR:HG22	2.03	0.40
2:B:435:THR:O	2:B:435:THR:CG2	2.69	0.40
3:C:11:ARG:O	3:C:12:GLU:HG3	2.21	0.40
3:C:32:SER:O	3:C:36:VAL:HG23	2.21	0.40
4:E:168:TYR:O	4:E:169:ARG:HB2	2.21	0.40
5:F:128:LYS:HA	5:F:128:LYS:HD3	1.83	0.40
1:A:1319:VAL:HA	1:A:1320:PRO:HD3	1.88	0.40
1:A:42:ASP:OD2	1:A:47:ARG:HG2	2.21	0.40
1:A:541:ILE:HG22	1:A:546:VAL:HG23	2.03	0.40
1:A:560:ILE:O	1:A:561:PRO:C	2.59	0.40
1:A:672:ASP:HB3	1:A:674:PRO:HD2	2.03	0.40
1:A:92:HIS:HD2	1:A:94:GLY:N	2.19	0.40
2:B:324:ILE:HG13	2:B:329:THR:HG22	2.03	0.40
1:A:871:ASP:CB	4:E:204:THR:HG23	2.42	0.40
6:H:139:ASN:CB	6:H:139:ASN:ND2	2.72	0.40
9:K:100:ALA:O	9:K:103:THR:HB	2.20	0.40
1:A:601:LYS:CD	1:A:601:LYS:NZ	2.81	0.40
1:A:884:ASP:O	1:A:885:THR:C	2.59	0.40
2:B:121:ASN:H	2:B:121:ASN:HD22	1.68	0.40
2:B:423:LYS:O	2:B:426:LYS:N	2.53	0.40
3:C:33:LEU:O	3:C:37:MET:HG3	2.21	0.40
3:C:77:ILE:HD12	3:C:77:ILE:HA	1.82	0.40
5:F:93:ILE:HD13	5:F:93:ILE:HG21	1.78	0.40
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	2.04	0.40
1:A:241:VAL:HA	1:A:242:PRO:HD2	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:LEU:O	1:A:547:LEU:HG	2.20	0.40
1:A:699:ALA:HA	7:I:112:SER:O	2.21	0.40
2:B:25:ILE:H	2:B:25:ILE:HD13	1.85	0.40
2:B:35:SER:HA	2:B:811:TYR:CE2	2.56	0.40
2:B:639:ILE:HD12	2:B:639:ILE:HG23	1.70	0.40
2:B:789:MET:CE	2:B:965:LYS:HB3	2.51	0.40
3:C:167:HIS:CD2	3:C:169:LYS:HG2	2.57	0.40
7:I:16:PRO:HG3	7:I:27:PHE:HE2	1.86	0.40
1:A:59:GLY:C	1:A:60:SER:HG	2.25	0.40
1:A:633:VAL:O	1:A:634:THR:C	2.58	0.40
2:B:1197:PRO:O	2:B:1200:ALA:HB3	2.22	0.40
2:B:296:GLU:O	2:B:300:HIS:HD2	2.05	0.40
2:B:90:ILE:HG22	2:B:90:ILE:O	2.18	0.40
3:C:114:TYR:HB3	3:C:140:ASN:O	2.21	0.40
3:C:99:LEU:CD1	3:C:99:LEU:N	2.71	0.40
3:C:9:LYS:CB	3:C:9:LYS:CD	2.83	0.40
1:A:1151:GLU:HA	7:I:44:TYR:O	2.21	0.40
3:C:84:ARG:HD2	9:K:11:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1335/1733 (77%)	1187 (89%)	91 (7%)	57 (4%)	2	20
2	B	1071/1224 (88%)	924 (86%)	104 (10%)	43 (4%)	3	21
3	C	264/318 (83%)	231 (88%)	23 (9%)	10 (4%)	3	22
4	E	213/215 (99%)	183 (86%)	16 (8%)	14 (7%)	1	9
5	F	81/155 (52%)	73 (90%)	6 (7%)	2 (2%)	5	32
6	H	129/146 (88%)	89 (69%)	19 (15%)	21 (16%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	I	119/122 (98%)	110 (92%)	8 (7%)	1 (1%)	19	58
8	J	62/70 (89%)	58 (94%)	4 (6%)	0	100	100
9	K	112/120 (93%)	98 (88%)	12 (11%)	2 (2%)	8	41
10	L	44/70 (63%)	24 (54%)	13 (30%)	7 (16%)	0	0
All	All	3430/4173 (82%)	2977 (87%)	296 (9%)	157 (5%)	2	18

All (157) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	45	GLN
1	A	47	ARG
1	A	59	GLY
1	A	60	SER
1	A	62	ASP
1	A	65	LEU
1	A	69	THR
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	286	HIS
1	A	326	ARG
1	A	400	PRO
1	A	418	SER
1	A	465	TYR
1	A	567	LYS
1	A	672	ASP
1	A	707	GLY
1	A	1080	THR
1	A	1221	LYS
1	A	1403	GLU
1	A	1448	GLU
2	B	66	ASP
2	B	105	SER
2	B	108	VAL
2	B	109	THR
2	B	165	VAL
2	B	230	ALA

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Mol	Chain	Res	Type
2	B	645	SER
2	B	646	LEU
2	B	733	HIS
2	B	864	LYS
2	B	879	ARG
2	B	957	ASN
2	B	1108	ARG
2	B	1128	LEU
2	B	1167	GLY
3	C	4	GLU
3	C	9	LYS
3	C	206	ASN
4	E	48	ASP
4	E	64	PRO
5	F	73	ALA
6	H	32	THR
6	H	52	GLN
6	H	77	ARG
6	H	78	SER
6	H	90	ALA
6	H	104	PHE
6	H	105	GLU
6	H	107	VAL
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
10	L	58	LYS
1	A	57	ARG
1	A	193	ASP
1	A	464	PRO
1	A	885	THR
1	A	1405	THR
2	B	432	MET
2	B	436	VAL
2	B	451	LYS
2	B	643	ASP
2	B	869	SER

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Mol	Chain	Res	Type
2	B	887	HIS
2	B	940	PRO
2	B	1078	GLY
2	B	1097	HIS
2	B	1105	ALA
2	B	1158	PHE
3	C	56	THR
3	C	126	GLY
3	C	267	GLN
4	E	45	LYS
4	E	50	MET
4	E	56	LYS
4	E	118	PRO
4	E	126	SER
6	H	81	PRO
6	H	82	PRO
6	H	86	ASP
6	H	116	TYR
9	K	99	GLY
1	A	56	PRO
1	A	74	MET
1	A	75	ASN
1	A	278	THR
1	A	279	LEU
1	A	1204	ASP
1	A	1223	ASP
1	A	1234	GLU
1	A	1255	GLU
1	A	1280	GLU
1	A	1359	ASP
2	B	266	ALA
2	B	466	TRP
2	B	831	SER
2	B	1155	SER
3	C	209	TYR
3	C	231	ASN
4	E	59	SER
6	H	18	GLY
6	H	53	ASP
6	H	128	ASN
6	H	135	LEU
1	A	32	VAL

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Mol	Chain	Res	Type
1	A	38	PRO
1	A	196	GLU
1	A	408	ASP
1	A	915	SER
2	B	865	LYS
2	B	1189	ILE
2	B	1190	ASP
2	B	1221	SER
2	B	1222	ARG
4	E	2	ASP
4	E	74	ASP
10	L	41	SER
1	A	599	SER
1	A	706	HIS
1	A	958	VAL
1	A	1123	GLY
1	A	1263	ILE
2	B	90	ILE
2	B	106	ASP
2	B	424	LEU
3	C	18	VAL
4	E	127	ILE
6	H	19	ARG
6	H	89	LEU
6	H	119	GLY
10	L	46	VAL
1	A	52	GLY
2	B	56	ASP
3	C	217	ASP
4	E	44	ALA
5	F	76	LYS
2	B	1017	ILE
1	A	55	ASP
1	A	78	PRO
1	A	1122	PRO
2	B	364	ILE
4	E	37	LEU
1	A	158	PRO
4	E	128	PRO
2	B	1099	VAL
2	B	1214	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	1184/1520 (78%)	998 (84%)	186 (16%)	2	12
2	B	947/1061 (89%)	806 (85%)	141 (15%)	3	14
3	C	234/274 (85%)	194 (83%)	40 (17%)	2	10
4	E	197/197 (100%)	152 (77%)	45 (23%)	1	4
5	F	73/137 (53%)	64 (88%)	9 (12%)	4	21
6	H	117/128 (91%)	73 (62%)	44 (38%)	0	0
7	I	115/116 (99%)	91 (79%)	24 (21%)	1	6
8	J	59/65 (91%)	49 (83%)	10 (17%)	2	10
9	K	99/102 (97%)	80 (81%)	19 (19%)	1	8
10	L	40/57 (70%)	21 (52%)	19 (48%)	0	0
All	All	3065/3657 (84%)	2528 (82%)	537 (18%)	2	9

All (537) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	11	LEU
1	A	15	LYS
1	A	22	PHE
1	A	34	LYS
1	A	36	ARG
1	A	39	GLU
1	A	41	MET
1	A	44	THR
1	A	49	LYS
1	A	54	ASN
1	A	58	LEU
1	A	60	SER
1	A	62	ASP
1	A	68	GLN
1	A	70	CYS

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Mol	Chain	Res	Type
1	A	74	MET
1	A	84	ILE
1	A	90	VAL
1	A	93	VAL
1	A	96	ILE
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	138	ILE
1	A	141	LEU
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
1	A	174	ILE
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	237	THR
1	A	239	LEU
1	A	247	ARG
1	A	261	ASP
1	A	263	THR
1	A	265	LYS
1	A	270	LEU
1	A	274	ILE

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Mol	Chain	Res	Type
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	382	PRO
1	A	412	ARG
1	A	416	ARG
1	A	418	SER
1	A	419	LYS
1	A	434	ARG
1	A	436	ILE
1	A	446	ARG
1	A	451	HIS
1	A	461	LYS
1	A	466	SER
1	A	468	PHE
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
1	A	513	SER
1	A	535	THR
1	A	537	ARG
1	A	543	LEU
1	A	571	LEU
1	A	586	ILE
1	A	588	LEU
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	636	GLU
1	A	651	LYS
1	A	666	ILE
1	A	681	GLU

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Mol	Chain	Res	Type
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	794	PRO
1	A	810	PRO
1	A	821	ARG
1	A	830	LYS
1	A	840	ARG
1	A	843	LYS
1	A	858	ASN
1	A	895	LYS
1	A	903	ASN
1	A	907	THR
1	A	909	ASP
1	A	919	ILE
1	A	920	LEU
1	A	973	ILE
1	A	974	ASP
1	A	979	SER
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	1102	LYS
1	A	1109	LYS
1	A	1120	LEU
1	A	1129	GLU
1	A	1133	LEU
1	A	1134	ILE

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Mol	Chain	Res	Type
1	A	1161	THR
1	A	1165	GLU
1	A	1171	GLN
1	A	1176	LEU
1	A	1187	GLN
1	A	1204	ASP
1	A	1208	THR
1	A	1217	LYS
1	A	1219	THR
1	A	1222	ASN
1	A	1225	PHE
1	A	1229	SER
1	A	1230	GLU
1	A	1233	ASP
1	A	1235	LYS
1	A	1236	LEU
1	A	1237	ILE
1	A	1239	ARG
1	A	1255	GLU
1	A	1258	HIS
1	A	1259	MET
1	A	1267	MET
1	A	1269	GLU
1	A	1277	GLU
1	A	1281	ARG
1	A	1291	VAL
1	A	1293	SER
1	A	1309	ASP
1	A	1318	THR
1	A	1325	THR
1	A	1350	LYS
1	A	1359	ASP
1	A	1366	ARG
1	A	1376	THR
1	A	1377	THR
1	A	1384	VAL
1	A	1404	GLU
1	A	1405	THR
1	A	1411	GLU
1	A	1426	GLU
1	A	1438	THR
1	A	1445	ILE

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Mol	Chain	Res	Type
1	A	1448	GLU
1	A	1449	SER
2	B	18	PHE
2	B	20	ASP
2	B	25	ILE
2	B	46	GLN
2	B	63	ILE
2	B	65	GLU
2	B	68	THR
2	B	69	LEU
2	B	89	GLU
2	B	92	PHE
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	179	CYS
2	B	194	GLU
2	B	199	MET
2	B	217	ARG
2	B	228	LYS
2	B	240	ILE
2	B	242	SER
2	B	244	LEU
2	B	248	SER
2	B	252	SER
2	B	261	ARG
2	B	264	SER
2	B	276	ILE
2	B	277	LYS
2	B	282	ILE
2	B	305	VAL
2	B	358	LYS
2	B	367	LEU
2	B	373	ARG
2	B	387	LEU

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Mol	Chain	Res	Type
2	B	417	PHE
2	B	422	LYS
2	B	423	LYS
2	B	425	THR
2	B	434	ARG
2	B	435	THR
2	B	448	ILE
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	589	VAL
2	B	591	ARG
2	B	595	ARG
2	B	598	GLU
2	B	606	LYS
2	B	612	GLU
2	B	641	GLU
2	B	645	SER
2	B	648	HIS
2	B	653	VAL
2	B	680	THR
2	B	691	GLU
2	B	693	ILE
2	B	706	GLN
2	B	710	LEU
2	B	722	ASP
2	B	723	VAL
2	B	733	HIS
2	B	736	THR
2	B	775	LYS
2	B	806	THR
2	B	838	SER

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Mol	Chain	Res	Type
2	B	839	MET
2	B	864	LYS
2	B	865	LYS
2	B	868	MET
2	B	870	ILE
2	B	871	THR
2	B	875	GLU
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	942	ARG
2	B	955	THR
2	B	958	GLN
2	B	962	LYS
2	B	974	PRO
2	B	975	GLN
2	B	987	LYS
2	B	996	ARG
2	B	997	GLU
2	B	1007	VAL
2	B	1056	SER
2	B	1060	ARG
2	B	1065	GLN
2	B	1077	THR
2	B	1097	HIS
2	B	1099	VAL
2	B	1101	ASP
2	B	1103	ILE
2	B	1106	ARG
2	B	1129	ARG

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Mol	Chain	Res	Type
2	B	1150	ARG
2	B	1152	MET
2	B	1155	SER
2	B	1156	ASP
2	B	1159	ARG
2	B	1163	CYS
2	B	1165	ILE
2	B	1174	LYS
2	B	1175	LEU
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	9	LYS
3	C	14	SER
3	C	23	SER
3	C	25	VAL
3	C	26	ASP
3	C	29	MET
3	C	33	LEU
3	C	43	THR
3	C	56	THR
3	C	57	VAL
3	C	86	CYS
3	C	93	ASP
3	C	102	GLN
3	C	119	VAL
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	154	LYS
3	C	163	ILE
3	C	178	PHE
3	C	184	ASN
3	C	185	LYS
3	C	186	LEU

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Mol	Chain	Res	Type
3	C	197	SER
3	C	199	LYS
3	C	205	LYS
3	C	209	TYR
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	251	LEU
3	C	264	GLN
3	C	265	MET
3	C	266	ASP
3	C	268	ASP
4	E	3	GLN
4	E	10	SER
4	E	33	GLU
4	E	34	GLU
4	E	37	LEU
4	E	49	SER
4	E	50	MET
4	E	52	ARG
4	E	53	PRO
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	82	PHE
4	E	84	ASP
4	E	90	VAL
4	E	91	LYS
4	E	92	THR
4	E	98	ILE
4	E	100	ILE
4	E	101	GLN
4	E	102	GLU
4	E	103	LYS

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Mol	Chain	Res	Type
4	E	107	THR
4	E	116	ILE
4	E	118	PRO
4	E	121	MET
4	E	123	LEU
4	E	129	PRO
4	E	134	THR
4	E	137	GLU
4	E	149	LEU
4	E	158	SER
4	E	159	ASP
4	E	161	LYS
4	E	162	ARG
4	E	171	LYS
4	E	192	ARG
4	E	196	VAL
4	E	200	ARG
4	E	212	ARG
5	F	72	LYS
5	F	77	ASP
5	F	81	THR
5	F	82	THR
5	F	87	LYS
5	F	97	ARG
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	27	GLU
6	H	34	ASP
6	H	35	GLN
6	H	36	CYS
6	H	40	LEU
6	H	42	ILE
6	H	45	GLU
6	H	46	LEU
6	H	52	GLN
6	H	53	ASP

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Mol	Chain	Res	Type
6	H	54	SER
6	H	56	THR
6	H	63	LEU
6	H	77	ARG
6	H	78	SER
6	H	80	ARG
6	H	86	ASP
6	H	87	ARG
6	H	88	SER
6	H	89	LEU
6	H	91	ASP
6	H	92	ASP
6	H	93	TYR
6	H	105	GLU
6	H	106	GLU
6	H	108	SER
6	H	109	LYS
6	H	110	ASP
6	H	111	LEU
6	H	112	ILE
6	H	121	LEU
6	H	126	GLU
6	H	129	TYR
6	H	130	ARG
6	H	131	ASN
6	H	136	LYS
6	H	137	GLN
6	H	144	ILE
6	H	146	ARG
7	I	1	MET
7	I	2	THR
7	I	10	CYS
7	I	18	GLU
7	I	21	GLU
7	I	31	THR
7	I	32	CYS
7	I	40	SER
7	I	45	ARG
7	I	46	HIS
7	I	55	THR
7	I	61	ASP
7	I	75	CYS

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Mol	Chain	Res	Type
7	I	76	PRO
7	I	77	LYS
7	I	78	CYS
7	I	82	GLU
7	I	84	VAL
7	I	95	THR
7	I	116	ASN
7	I	117	LYS
7	I	118	ARG
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	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	63	VAL
9	K	70	ARG
9	K	73	LEU
9	K	75	ILE
9	K	78	THR
9	K	93	SER
9	K	110	ASN
9	K	112	GLN
9	K	113	THR
9	K	114	LEU
10	L	27	LEU
10	L	28	LYS

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Mol	Chain	Res	Type
10	L	33	GLU
10	L	36	SER
10	L	38	LEU
10	L	42	ARG
10	L	44	ASP
10	L	46	VAL
10	L	49	LYS
10	L	50	ASP
10	L	51	CYS
10	L	54	ARG
10	L	58	LYS
10	L	60	ARG
10	L	61	THR
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 (71) such sidechains are listed below:

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

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Mol	Chain	Res	Type
1	A	994	GLN
1	A	1078	GLN
1	A	1173	HIS
1	A	1364	ASN
1	A	1432	GLN
2	B	121	ASN
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS
2	B	300	HIS
2	B	366	GLN
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
2	B	958	GLN
2	B	984	HIS
2	B	1015	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	5	ASN
4	E	147	HIS
6	H	11	GLN

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Mol	Chain	Res	Type
6	H	131	ASN
7	I	12	ASN
7	I	46	HIS
7	I	83	ASN
7	I	116	ASN
8	J	53	HIS
9	K	2	ASN
9	K	65	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	ATP	A	3011	11	26,33,33	1.14	2 (7%)	31,52,52	1.57	4 (12%)

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	ATP	A	3011	11	-	2/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	3011	ATP	C2-N3	4.13	1.38	1.32
13	A	3011	ATP	C2-N1	2.67	1.38	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	3011	ATP	N3-C2-N1	-5.48	120.11	128.68
13	A	3011	ATP	PB-O3B-PG	-3.45	120.99	132.83
13	A	3011	ATP	PA-O3A-PB	-3.40	121.17	132.83
13	A	3011	ATP	C3'-C2'-C1'	2.89	105.32	100.98

There are no chirality outliers.

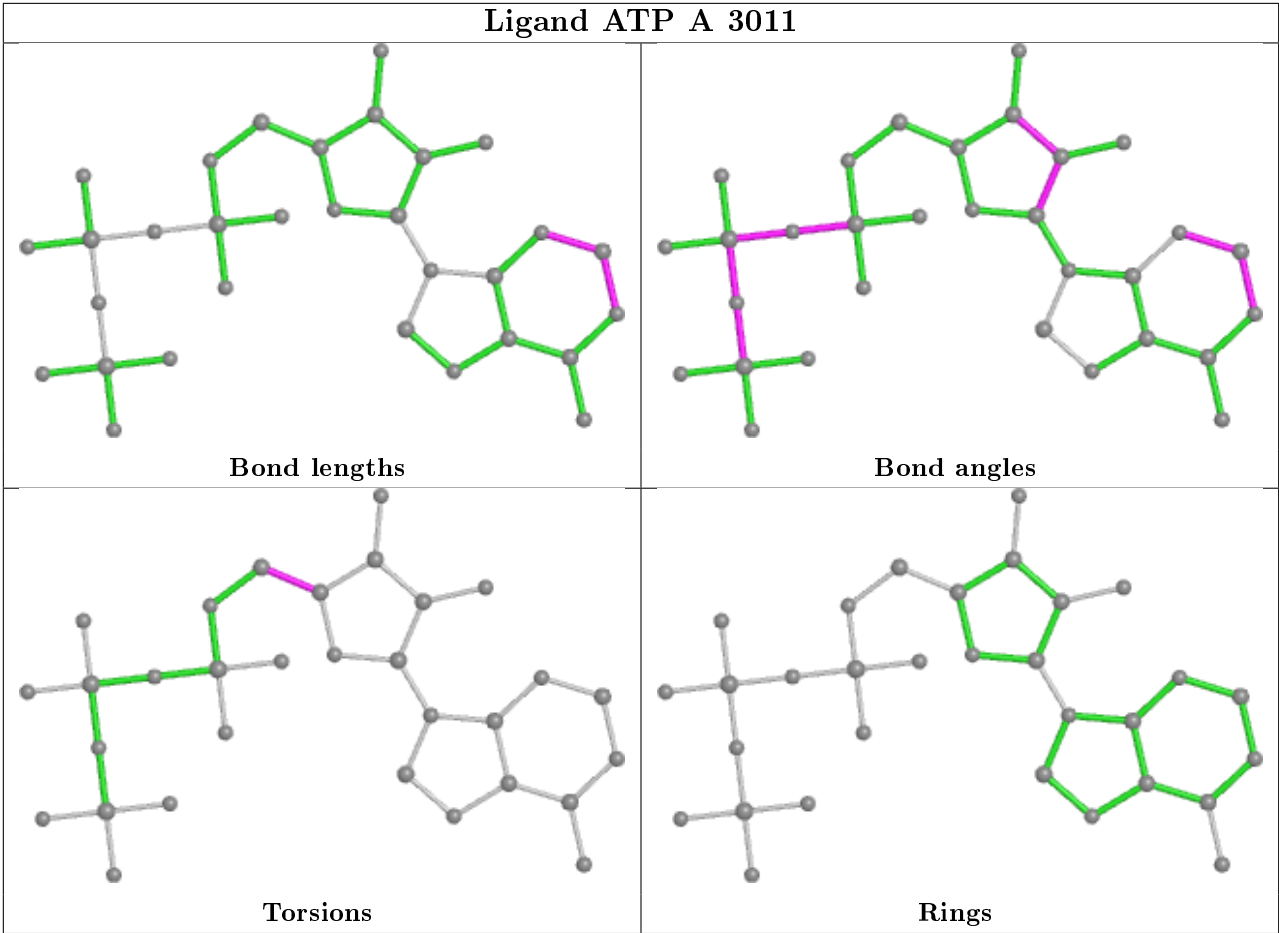
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	3011	ATP	O4'-C4'-C5'-O5'
13	A	3011	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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
1	A	5
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	686:ALA	C	687:LYS	N	1.20
1	A	1064:VAL	C	1065:GLY	N	1.20
1	B	632:ARG	C	633:VAL	N	1.20
1	A	366:VAL	C	367:PRO	N	1.19

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1195:LEU	C	1196:GLU	N	1.19
1	A	464:PRO	C	465:TYR	N	1.15

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	1352/1733 (78%)	-0.36	27 (1%) 65 51	9, 38, 105, 151	0
2	B	1091/1224 (89%)	-0.26	50 (4%) 32 20	10, 36, 111, 138	0
3	C	266/318 (83%)	-0.45	2 (0%) 86 78	21, 42, 72, 123	0
4	E	215/215 (100%)	-0.25	5 (2%) 60 47	13, 51, 102, 134	0
5	F	83/155 (53%)	-0.37	2 (2%) 59 44	18, 36, 64, 73	0
6	H	133/146 (91%)	0.21	6 (4%) 33 21	41, 79, 121, 132	0
7	I	121/122 (99%)	-0.21	2 (1%) 70 57	23, 44, 78, 108	0
8	J	64/70 (91%)	-0.55	0 100 100	21, 35, 61, 76	0
9	K	114/120 (95%)	-0.30	0 100 100	21, 50, 72, 81	0
10	L	46/70 (65%)	0.26	3 (6%) 18 11	39, 89, 118, 121	0
All	All	3485/4173 (83%)	-0.30	97 (2%) 53 37	9, 41, 107, 151	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1109	GLY	9.4
1	A	69	THR	7.7
2	B	1110	PRO	7.4
1	A	248	PRO	7.1
6	H	85	GLY	6.8
2	B	882	THR	6.6
2	B	1223	ASP	6.1
1	A	188	ASP	6.0
3	C	268	ASP	5.4
2	B	247	GLY	5.3
2	B	1105	ALA	5.3
2	B	869	SER	5.2
4	E	1	MET	5.0

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Mol	Chain	Res	Type	RSRZ
2	B	246	LYS	4.9
2	B	870	ILE	4.9
2	B	137	TYR	4.8
2	B	1104	HIS	4.6
1	A	191	THR	4.5
1	A	1450	LEU	4.5
2	B	136	THR	4.4
1	A	44	THR	4.3
2	B	871	THR	4.2
1	A	1449	SER	4.2
1	A	45	GLN	4.1
2	B	1106	ARG	4.1
2	B	89	GLU	4.0
2	B	433	GLN	4.0
2	B	1224	PHE	3.9
2	B	1176	ASN	3.9
2	B	90	ILE	3.8
1	A	1448	GLU	3.7
1	A	3	GLY	3.6
2	B	68	THR	3.5
2	B	1102	LYS	3.5
2	B	432	MET	3.4
2	B	436	VAL	3.4
2	B	733	HIS	3.4
1	A	190	ALA	3.4
6	H	132	LEU	3.2
2	B	135	ARG	3.1
2	B	1108	ARG	3.1
2	B	935	ARG	3.1
2	B	1179	GLN	3.0
7	I	79	HIS	2.9
6	H	86	ASP	2.9
10	L	50	ASP	2.9
1	A	192	GLY	2.9
1	A	37	PHE	2.9
2	B	883	LEU	2.8
2	B	887	HIS	2.8
2	B	70	ILE	2.8
3	C	267	GLN	2.8
1	A	43	GLU	2.8
1	A	157	ASP	2.7
2	B	868	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	71	GLN	2.7
2	B	867	GLY	2.7
10	L	26	THR	2.6
6	H	84	ALA	2.6
2	B	1100	ASP	2.6
1	A	1222	ASN	2.6
2	B	1101	ASP	2.6
4	E	52	ARG	2.6
1	A	1243	VAL	2.6
2	B	250	PHE	2.6
1	A	1446	ASP	2.6
10	L	25	ALA	2.6
1	A	62	ASP	2.5
2	B	1103	ILE	2.5
2	B	245	GLU	2.5
2	B	881	ASN	2.5
6	H	131	ASN	2.5
2	B	248	SER	2.4
5	F	110	ASP	2.4
2	B	866	TYR	2.4
1	A	66	LYS	2.4
1	A	46	THR	2.3
2	B	1221	SER	2.3
4	E	50	MET	2.2
2	B	106	ASP	2.2
1	A	189	ARG	2.1
4	E	51	GLY	2.1
2	B	138	GLU	2.1
2	B	1178	ASN	2.1
1	A	1092	LYS	2.1
1	A	41	MET	2.1
4	E	102	GLU	2.1
2	B	103	ASN	2.1
2	B	915	THR	2.1
6	H	127	GLY	2.1
1	A	1403	GLU	2.1
2	B	133	LYS	2.1
2	B	448	ILE	2.0
7	I	74	GLU	2.0
1	A	1176	LEU	2.0
5	F	112	GLU	2.0
2	B	132	VAL	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](#)

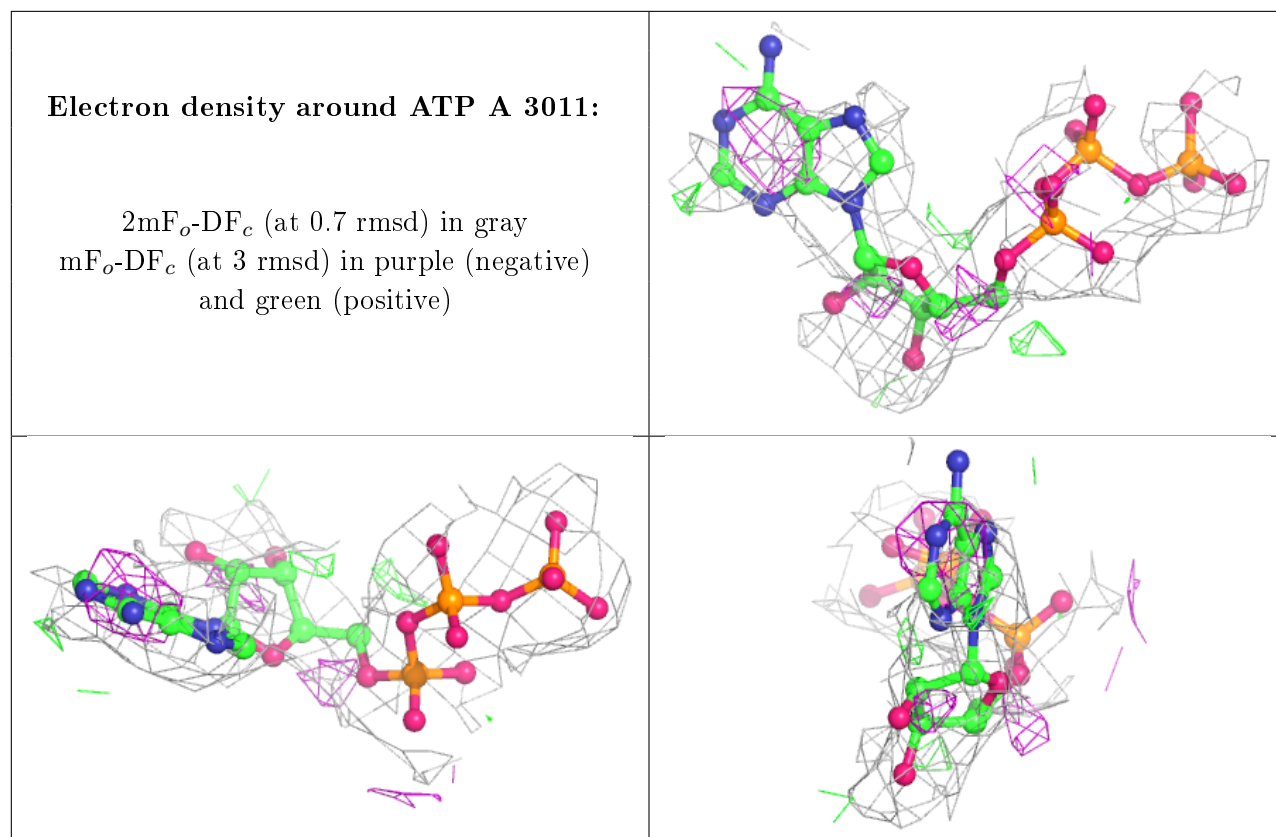
There are no carbohydrates in this entry.

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
12	ZN	L	3005	1/1	0.69	0.06	139,139,139,139	0
12	ZN	I	3003	1/1	0.87	0.06	144,144,144,144	0
13	ATP	A	3011	31/31	0.89	0.23	69,74,83,83	0
12	ZN	B	3007	1/1	0.93	0.06	108,108,108,108	0
12	ZN	A	3006	1/1	0.96	0.04	124,124,124,124	0
12	ZN	I	3004	1/1	0.97	0.05	144,144,144,144	0
11	MN	A	3010	1/1	0.97	0.12	29,29,29,29	0
12	ZN	A	3008	1/1	0.97	0.03	96,96,96,96	0
11	MN	A	3009	1/1	0.98	0.12	24,24,24,24	0
12	ZN	C	3002	1/1	0.98	0.06	78,78,78,78	0
12	ZN	J	3001	1/1	0.99	0.08	84,84,84,84	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 [i](#)

There are no such residues in this entry.