



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:55 PM UTC

PDB ID : 1TWC / pdb_00001twc
Title : RNA polymerase II complexed with GTP
Authors : Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2004-06-30
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

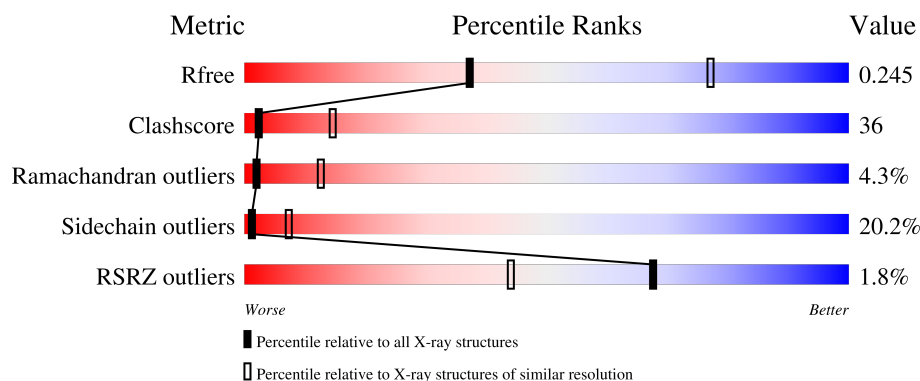
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1733	11% 37% 22% 8% 22%
2	B	1224	2% 10% 42% 26% 10% 11%
3	C	318	8% 40% 26% 10% 16%
4	E	215	11% 35% 40% 14%
5	F	155	6% 24% 18% 5% 46%

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Mol	Chain	Length	Quality of chain
6	H	146	
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
13	GTP	B	3008	X	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 27772 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	1351	Total	C	N	O	S	0	0	0
			10625	6704	1844	2019	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 14.2KD 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 ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total	Zn	0	0
			2	2		
11	B	1	Total	Zn	0	0
			1	1		
11	C	1	Total	Zn	0	0
			1	1		
11	I	2	Total	Zn	0	0
			2	2		
11	J	1	Total	Zn	0	0
			1	1		

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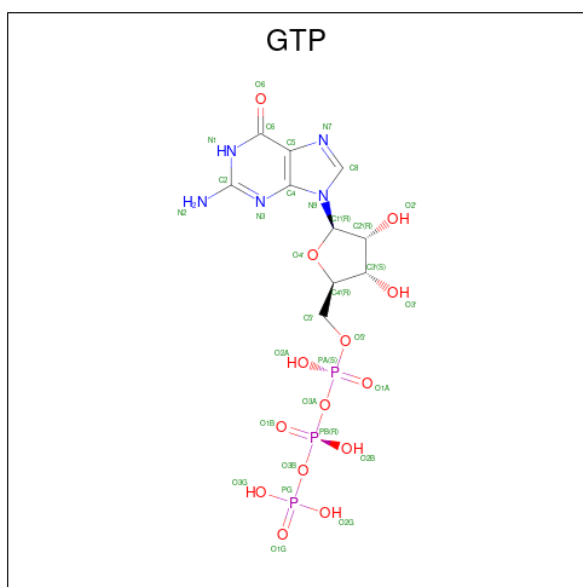
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	1	Total	Zn	0	0
			1	1		

- Molecule 12 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 13 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	N	O	P	
			32	10	5	14	3	0

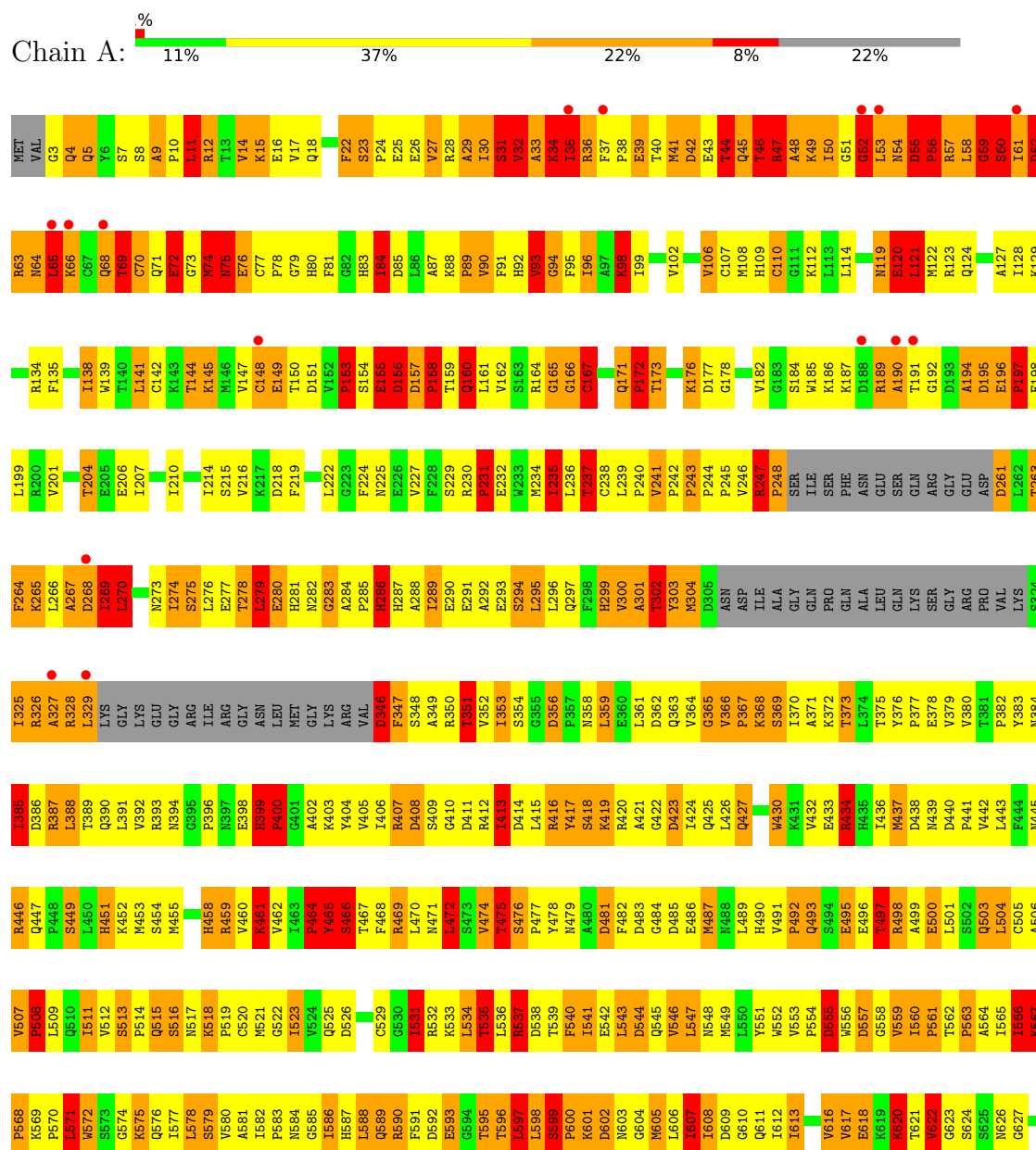
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	11	Total	O	0	0
			11	11		
14	B	11	Total	O	0	0
			11	11		
14	F	1	Total	O	0	0
			1	1		
14	L	1	Total	O	0	0
			1	1		

3 Residue-property plots

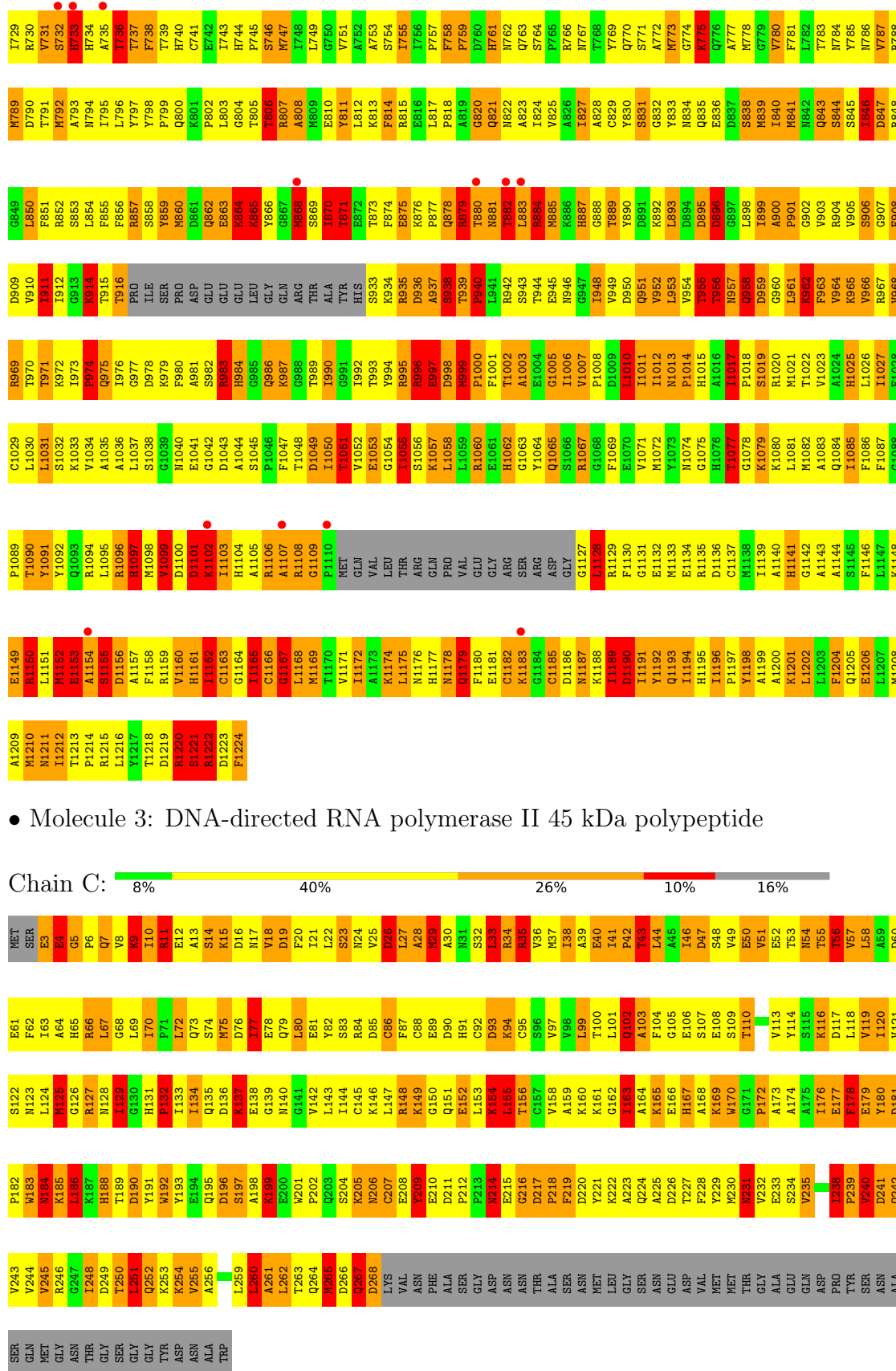
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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



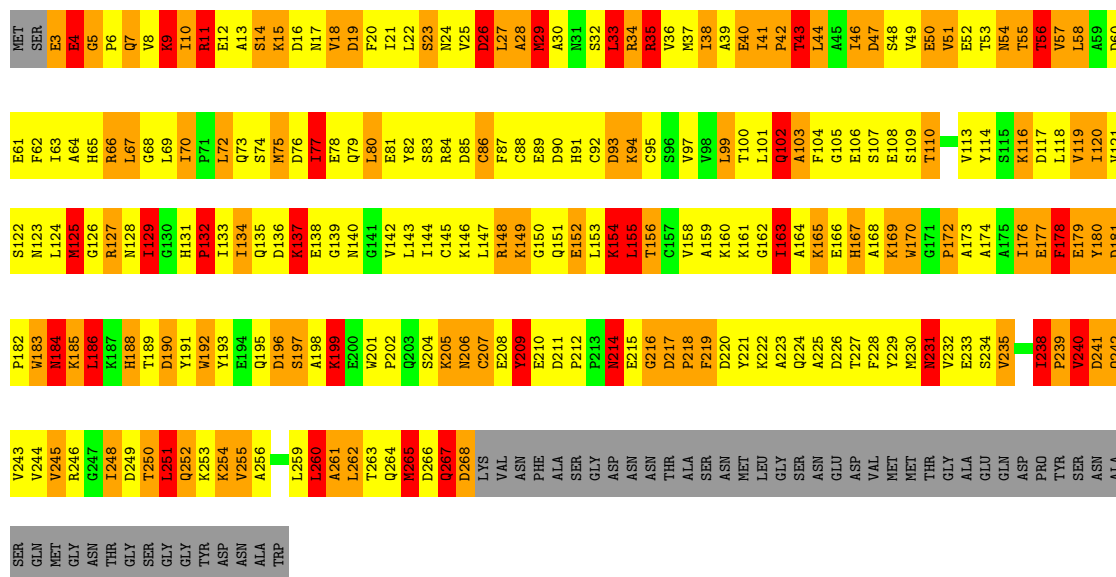
SER	LEU	L1418	S1358	T1295	K1235	SER	S1115	L993	Y933	M873	B812	S751	L691	I630
PRO	VAL	D1419	D1359	G1296	L1236	L1176	L1116	Q994	K994	D874	F813	K752	D692	H631
GLY	ASN	D1420	S1360	E1297	I1237	LEU	T1117	E995	Q995	A875	F814	G753	D693	T634
PHE	ALA	C1421	S1361	Y1298	I1238	ASP	Y1118	N996	L936	A876	F815	G754	T694	
SER	ASP	G1422	Y1362	I1299	G1239	GLU	Y1119	N997	V937	H877	R816	F755	K695	K635
PRO	LEU	G1423	Y1363	K1300	C1240	GLU	L1120	L998	K938	H878	A817	F756	K696	E636
THR	ASP	V1424	R1241	E1301	R1241	ALA	E1121	V999	D939	E879	M818	F757	K697	K637
SER	VAL	S1425	Y1365	P1302	V1242	GLU	F1122	L1000	R940	K880	G819	I758	Q698	G638
PRO	LYS	E1426	R1366	E1303	V1243	GLN	G1123	L1001	K941	Q881	G820	A759	A699	P639
THR	ASP	N1427	H1367	E1304	ARG	SER	H1124	K1002	F942	S882	R821	G760	N700	Q640
THR	GLU	V1428	M1368	V1305	PRO	PHE	A1125	K1003	L943	L883		M761	L701	V641
SER	LEU	I1429	A1369	L1306	LYS	ASP	A1126	K1004	R944	L884	L824	G762	T702	C642
PRO	MET		L1370	E1307	SER	Q1187	D1127	N1005	E945	T885	I825	A763	T703	A643
THR	PHE		L1371	T1308	LEU	Q1188	G1128	I1006	V946	I886	D826	C764	A704	K644
SER	SER		Y1372	D1309	ASP	S1189	E1129	I1007	F947	G887	T827	V765	K705	L645
PRO	PRO	A1434	D1373	G1310	ALA	P1190	Q1130	Q908	V948	G888	A828	G772	E712	V652
ALA	LEU	P1435	Y1374	V1311	GLU	W1191	A1131	N1009	D949	S889	V829	Q767	G707	G647
TYR	VAL	I1436	M1375	N1312	THR	L1192	K1132	A1010	Q950	D890	K830	Q768	M708	N648
SER	ASP	G1437	T1376	L1313	GLU	L1193	L1133	Q1011	E951	A891	T831	S769	T709	I649
PRO	SER		T1377	S1314		R1194	I1134	R1012	A952	A892	A832	V770	L710	Q650
THR	GLY		Q1378	E1315		L1195	A1135	D1013	N953	F893	E833	E771	K611	L657
SER	PRO	A1440	G1379	V1316	E1255	E1196	S1136	C1019	N960	D900	R840	G778	V718	L658
PRO	ASN	F1441	G1380	M1317	D1257	L1197	A1137	V1015	N965	K895	T834	G779	V719	H659
SER	ASP	D1442	L1381	T1318	H1258	R1198	I1138	T1016	L956	R896	Y836	R774	F714	N654
ALA	ASP	V1443	T1382	V1319	M1259	D1199	E1139	L1017	P957	Y897	I837	I775	E715	F655
SER	MET	M1444	S1383	F1320	L1260	A1200	H1140	F1018	V958	R898	Q838	A776	D716	M656
PRO	ALA	T1445	Y1384	G1321	K1261	A1201	T1141	C1019	N959	V899	R840	F777	N717	L657
THR	GLY	D1446	T1385	I1322	K1262	M1202	T1142	G1020	P960	D900	R840	G778	V718	L658
SER	GLY	E1447	G1386	D1323	E1263	N1203	L1143	L1021	R961	L901	L841	G779	V719	H659
PRO	PHE	A1448	HIS	P1324	E1264	D1204	K1144	L1022	R962	L902	V842	V780	K720	N650
THR	THR	S1449	GLY	T1325	N1265	K1205	S1145	R1023	I963	K903	K843	D781	F721	G661
SER	ALA	L1450	PHE	R1326	T1266	D1206	F1168	S1024	I964	T894	A844	R782	L722	F662
SER	TYR		ASN	I1327	M1267	L1207	T1147	R1025	Q965	D905	L845	T783	M723	S663
PRO	GLY		ARG	Y1328	L1268	T1208	I1148	L1026	N966	H906	E846	G784	E724	G665
THR	GLY		SER	T1329	E1269	M1209	A1149	A1027	A967	T907	D847	F785	A725	G665
SER	ALA		ASN	N1330	N1270	G1210	S1150	T1028	Q968	L908	I848	H786	R726	I666
PRO	ASP		THR	S1331	I1271	Q1211	E1151	R1029	Q969	D909	M849	F787	D727	G667
SER	TYR		GLY	F1332	T1272	V1212	I1152	R1030	T970	P910	V850	S788	K728	D668
TYR	GLY		ALA	I1333	L1273	G1213	Y1153	L1031	F971	S911	H851	K789	A729	T669
SER	GLU		LEU	D1334	R1274	E1214	Y1154	L1032	H972	L912	Y852	D790	G730	I670
PRO	ALA		MET	I1335	G1275	R1215	D1155	Q1033	I973	L913	D853	D791	R731	A671
THR	THR		ARG	M1336	V1276	I1216	P1156	E1034	D974	E914	N854	Y792	L732	D672
SER	SER		CYS	E1337	E1277	K1217	D1157	Y1035	H975	S915	T855	S793	A733	G673
PRO	PRO		ILE	V1338	N1278	Q1218	P1158	L1036	T976	G916	T856	F794	E734	P674
SER	PHE		PHE	L1339	I1279	T1219	R1159	L1037	K977	S917	R857	E795	V735	T675
TYR	GLY		GLU	G1340	E1280	F1220	S1160	T1038	P978	E918	N858	S796	N736	M676
SER	ALA		GLU	I1341	R1281	K1221	T1161	K1039	S979	I919	S859	K797	L737	R677
PRO	TYR		GLN	E1342	V1282	N1222	V1162	D980	L920	L860	L860	K797	K738	E678
THR	GLY		ASP	A1343	V1283	D1223	I1163	Q1040	L981	G921	G861	V800	D739	I679
SER	GLU		GLY	G1344	M1284	L1224	P1164						L740	T680
PRO	ALA		GLY	R1345	M1285	F1225	E1168	W1044	T982	D922	N862	N802	M741	E681
PRO	PRO		VAL	A1346	K1286	V1226	D1166	L1045	N983	L923	V863	S803	N742	T682
TYR	THR		THR	A1347	Y1287	I1227	E1167	L1046	K984	K924	I864	N803	M742	I682
SER	SER		PRO	L1348	D1288	W1228	A1168	S1047	D985	L925	Q865	Y804	V743	I683
PRO	PRO		TYR	I1349	R1289	S1229	I1169	N1048	I986	Q926	F866	L805	K744	A684
THR	GLY		SER	G1350	K1290	E1230	N1170	E1050	V987	V927	I867	R806	Q745	E685
SER	PHE		ASN		V1291	D1231	M1111	A1051	G988	L929	G868	G807	M746	A686
PRO	GLY		GLU		P1292	M1232	K1112	Q1052	V990	D930	E870	T809	M748	K688
SER	VAL		SER		S1293	D1233	T1113	F1053	K991	E931	D871	P810	K749	K689
TYR	SER		GLY		P1294	E1234	P1114	L1054	D992	E932	G872	Q811	G750	V690



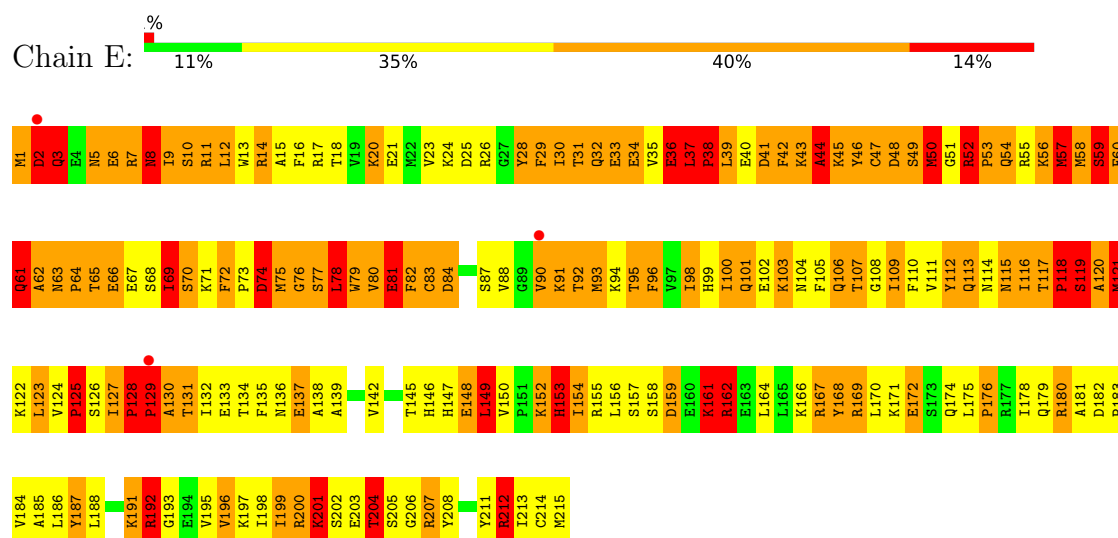


• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide

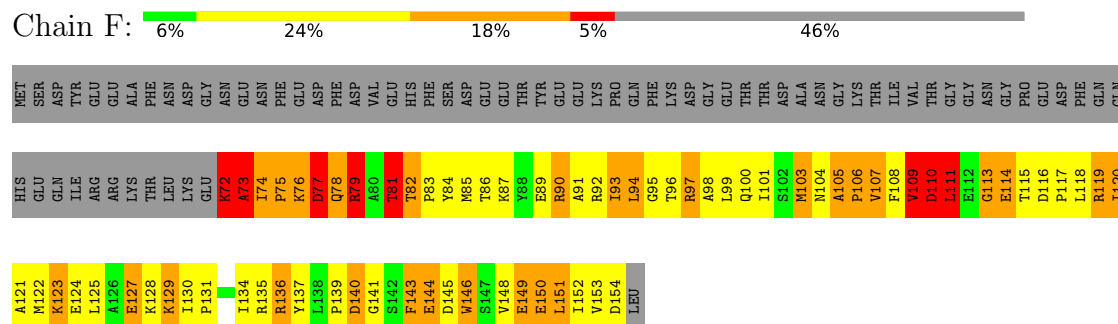
Chain C: 8% 40% 26% 10% 16%



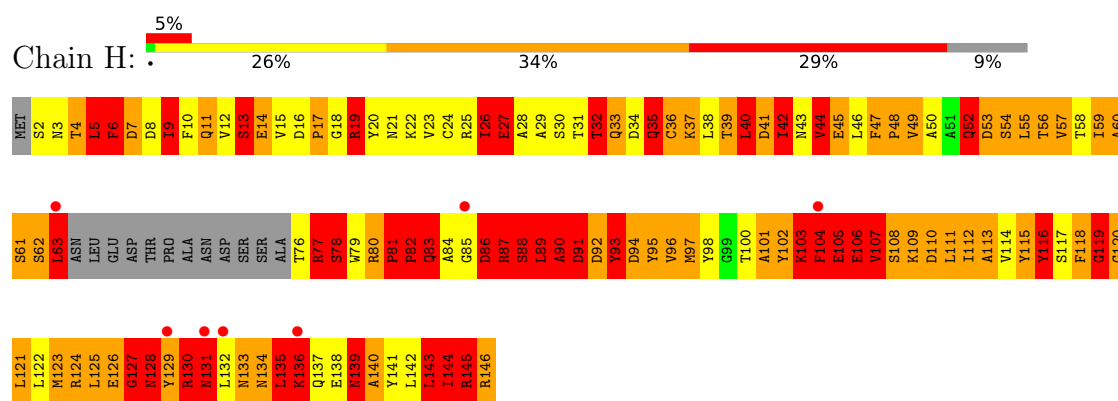
• Molecule 4: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide



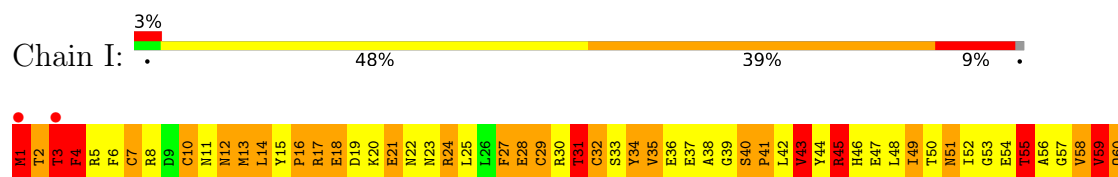
- Molecule 5: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

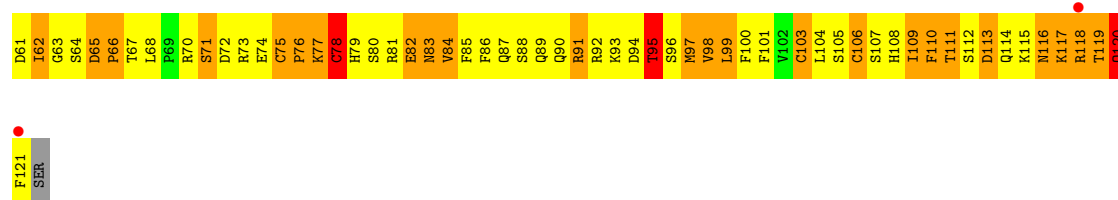


- Molecule 6: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



- Molecule 7: DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE





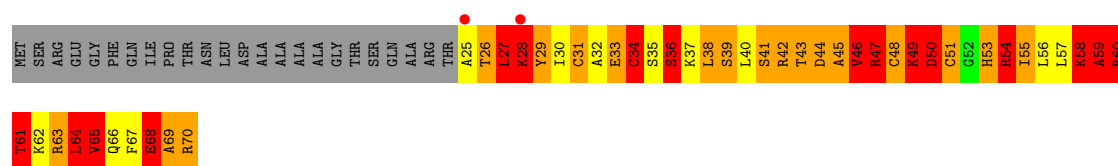
- Molecule 8: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.23Å 223.61Å 374.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 40.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.00) 89.0 (40.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.255 0.207 , 0.245	Depositor DCC
R_{free} test set	3424 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	56.3	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.0	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	0.93	EDS
Total number of atoms	27772	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: MN, GTP, ZN

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	3.75	1712/10811 (15.8%)	2.67	938/14626 (6.4%)
2	B	3.92	1505/8860 (17.0%)	2.64	734/11945 (6.1%)
3	C	4.03	377/2133 (17.7%)	2.81	194/2891 (6.7%)
4	E	3.92	285/1796 (15.9%)	2.63	161/2416 (6.7%)
5	F	3.72	111/682 (16.3%)	2.70	55/922 (6.0%)
6	H	3.95	177/1086 (16.3%)	2.66	106/1470 (7.2%)
7	I	4.06	207/1009 (20.5%)	2.80	114/1357 (8.4%)
8	J	3.48	70/533 (13.1%)	2.87	61/715 (8.5%)
9	K	3.75	154/937 (16.4%)	2.77	84/1265 (6.6%)
10	L	4.29	72/366 (19.7%)	2.97	45/485 (9.3%)
All	All	3.86	4670/28213 (16.6%)	2.69	2492/38092 (6.5%)

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	28
2	B	0	32
3	C	0	13
4	E	1	7
6	H	0	13
7	I	0	3
9	K	0	2
10	L	0	4
All	All	1	102

All (4670) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	50	MET	SD-CE	36.31	2.70	1.79
2	B	552	MET	SD-CE	30.20	2.55	1.79
2	B	885	MET	SD-CE	30.02	2.54	1.79
1	A	487	MET	SD-CE	-28.01	1.09	1.79
4	E	57	MET	SD-CE	27.29	2.47	1.79
2	B	552	MET	CG-SD	27.01	2.48	1.80
1	A	1285	MET	SD-CE	26.69	2.46	1.79
3	C	181	ASP	C-O	-26.38	1.11	1.23
2	B	792	MET	SD-CE	25.08	2.42	1.79
1	A	775	ILE	CG1-CD1	24.70	2.48	1.51
3	C	181	ASP	CA-C	-24.70	1.37	1.53
2	B	705	MET	SD-CE	-24.44	1.18	1.79
2	B	870	ILE	CA-CB	24.16	1.87	1.54
2	B	723	VAL	CA-CB	24.02	1.84	1.54
2	B	999	MET	SD-CE	-23.79	1.20	1.79
1	A	507	VAL	CA-CB	23.53	1.67	1.54
1	A	708	MET	SD-CE	23.11	2.37	1.79
2	B	101	MET	SD-CE	22.55	2.35	1.79
6	H	104	PHE	CA-C	22.45	1.82	1.52
9	K	1	MET	SD-CE	22.26	2.35	1.79
5	F	103	MET	SD-CE	21.69	2.33	1.79
10	L	26	THR	CA-CB	21.09	1.89	1.53
2	B	1154	ALA	CA-CB	20.94	1.87	1.53
4	E	162	ARG	NE-CZ	20.72	1.55	1.33
2	B	662	MET	SD-CE	20.68	2.31	1.79
10	L	48	CYS	CA-C	20.52	1.77	1.53
1	A	549	MET	SD-CE	-20.03	1.29	1.79
2	B	542	MET	SD-CE	-19.99	1.29	1.79
3	C	125	MET	SD-CE	19.15	2.27	1.79
2	B	1150	ARG	CZ-NH1	19.11	1.59	1.32
3	C	97	VAL	C-O	-19.08	1.01	1.24
1	A	728	LYS	CD-CE	18.89	2.09	1.52
1	A	274	ILE	CA-CB	18.88	1.78	1.54
10	L	28	LYS	CA-C	18.63	1.77	1.52
2	B	747	MET	SD-CE	-18.61	1.33	1.79
1	A	304	MET	SD-CE	18.42	2.25	1.79
3	C	75	MET	SD-CE	18.33	2.25	1.79
2	B	246	LYS	CA-C	18.19	1.76	1.52
1	A	464	PRO	C-O	-18.19	1.00	1.24
2	B	313	MET	SD-CE	-18.12	1.34	1.79
4	E	98	ILE	CA-CB	17.57	1.79	1.54
2	B	1150	ARG	CZ-NH2	17.44	1.56	1.33
2	B	436	VAL	CA-CB	17.35	1.78	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	165	LYS	CE-NZ	17.26	2.01	1.49
1	A	498	ARG	NE-CZ	-17.18	1.14	1.33
6	H	9	ILE	CA-CB	16.94	1.76	1.54
2	B	626	ILE	C-O	-16.80	1.06	1.24
1	A	593	GLU	C-O	16.75	1.45	1.24
4	E	1	MET	SD-CE	16.64	2.21	1.79
1	A	1135	ARG	CZ-NH2	16.60	1.55	1.33
1	A	69	THR	CA-C	16.50	1.74	1.52
4	E	162	ARG	CG-CD	16.41	2.01	1.52
1	A	481	ASP	CA-CB	-16.13	1.32	1.54
5	F	122	MET	SD-CE	-16.05	1.39	1.79
7	I	91	ARG	CA-C	-16.01	1.27	1.53
1	A	771	GLU	CD-OE2	15.91	1.55	1.25
7	I	55	THR	CB-CG2	15.90	2.05	1.52
6	H	91	ASP	CA-C	15.87	1.72	1.52
2	B	245	GLU	CA-C	15.86	1.74	1.52
1	A	849	MET	SD-CE	-15.84	1.40	1.79
1	A	1355	VAL	CA-CB	-15.82	1.36	1.54
1	A	622	VAL	CA-CB	-15.75	1.37	1.54
1	A	1336	MET	C-O	-15.72	1.04	1.24
3	C	267	GLN	CA-C	15.65	1.73	1.52
9	K	94	ILE	CA-CB	15.64	1.72	1.54
2	B	1097	HIS	CA-CB	15.61	1.79	1.53
2	B	1002	THR	CA-C	15.60	1.73	1.52
1	A	1259	MET	SD-CE	15.58	2.18	1.79
1	A	437	MET	SD-CE	15.51	2.18	1.79
6	H	19	ARG	CG-CD	15.46	1.98	1.52
2	B	448	ILE	N-CA	15.39	1.64	1.46
2	B	1097	HIS	CA-C	15.31	1.73	1.52
2	B	1106	ARG	CA-C	15.31	1.72	1.52
3	C	154	LYS	CD-CE	15.27	1.98	1.52
1	A	61	ILE	CA-CB	15.21	1.75	1.54
2	B	347	LYS	CG-CD	15.19	1.98	1.52
1	A	1232	ASN	CB-CG	15.13	1.89	1.52
7	I	92	ARG	C-O	15.06	1.43	1.23
1	A	585	GLY	C-O	15.04	1.43	1.24
1	A	1433	MET	SD-CE	-14.95	1.42	1.79
2	B	1154	ALA	CA-C	14.93	1.73	1.52
6	H	11	GLN	CA-C	-14.92	1.34	1.52
2	B	230	ALA	CA-CB	14.90	1.76	1.53
9	K	17	SER	C-O	-14.82	1.05	1.23
3	C	134	ILE	CA-CB	-14.82	1.35	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	128	PRO	CA-C	14.79	1.66	1.52
2	B	594	ALA	CA-CB	-14.75	1.28	1.53
2	B	1101	ASP	CA-C	14.71	1.73	1.52
2	B	620	ARG	CZ-NH2	14.70	1.52	1.33
2	B	240	ILE	C-O	-14.68	1.08	1.23
3	C	89	GLU	C-O	14.66	1.42	1.24
9	K	111	LEU	C-O	14.64	1.42	1.24
2	B	957	ASN	CA-C	14.62	1.72	1.52
5	F	93	ILE	C-O	-14.60	1.06	1.24
2	B	1171	VAL	C-O	14.52	1.38	1.24
2	B	531	GLN	CG-CD	14.49	1.88	1.52
4	E	192	ARG	NE-CZ	14.48	1.49	1.33
2	B	204	ILE	CA-CB	-14.45	1.36	1.53
2	B	436	VAL	CA-C	14.35	1.71	1.52
1	A	1442	ASP	CA-C	-14.30	1.35	1.52
2	B	733	HIS	CA-C	14.21	1.71	1.52
1	A	938	LYS	CD-CE	14.20	1.95	1.52
3	C	143	LEU	C-O	-14.16	1.07	1.24
1	A	1045	VAL	CA-CB	-14.16	1.38	1.54
4	E	131	THR	CB-CG2	14.15	1.99	1.52
1	A	1214	GLU	C-O	14.13	1.42	1.24
1	A	1444	MET	SD-CE	14.12	2.14	1.79
1	A	44	THR	CA-CB	14.11	1.77	1.53
3	C	186	LEU	CA-C	14.10	1.72	1.52
6	H	132	LEU	CA-CB	14.03	1.69	1.52
1	A	1152	ILE	CA-CB	-14.02	1.37	1.54
1	A	919	ILE	CA-CB	13.95	1.70	1.54
6	H	27	GLU	CA-C	13.95	1.71	1.52
2	B	466	TRP	CA-C	13.93	1.71	1.52
3	C	225	ALA	CA-CB	-13.90	1.35	1.53
7	I	42	LEU	C-O	-13.88	1.08	1.24
2	B	458	LYS	C-O	-13.87	1.07	1.24
1	A	677	ARG	NE-CZ	13.84	1.48	1.33
1	A	346	ASP	CB-CG	13.83	1.86	1.52
6	H	121	LEU	C-O	13.81	1.40	1.24
4	E	201	LYS	CG-CD	13.81	1.93	1.52
9	K	61	TYR	C-O	-13.79	1.06	1.23
6	H	6	PHE	CA-C	-13.79	1.35	1.52
1	A	733	ALA	C-O	-13.68	1.08	1.24
6	H	139	ASN	CB-CG	13.68	1.86	1.52
1	A	780	VAL	C-O	13.66	1.36	1.23
1	A	1232	ASN	C-O	13.60	1.41	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	28	ALA	C-O	13.59	1.40	1.24
6	H	19	ARG	NE-CZ	13.58	1.48	1.33
8	J	49	MET	SD-CE	-13.52	1.45	1.79
2	B	729	ILE	C-O	-13.51	1.10	1.24
10	L	68	GLU	CG-CD	13.48	1.85	1.52
1	A	728	LYS	CG-CD	13.45	1.92	1.52
1	A	347	PHE	N-CA	13.42	1.66	1.46
1	A	821	ARG	CD-NE	-13.36	1.27	1.46
2	B	1102	LYS	N-CA	13.34	1.61	1.46
1	A	1014	ALA	CA-CB	-13.28	1.30	1.53
7	I	1	MET	CG-SD	13.26	2.13	1.80
3	C	63	ILE	CA-CB	13.22	1.69	1.54
2	B	975	GLN	CD-NE2	13.22	1.61	1.33
1	A	1138	ILE	C-O	13.20	1.37	1.23
2	B	184	ALA	C-O	-13.18	1.08	1.23
1	A	1080	THR	CA-CB	13.17	1.75	1.53
2	B	736	THR	CB-CG2	13.16	1.96	1.52
2	B	883	LEU	CA-CB	13.14	1.73	1.53
3	C	254	LYS	CA-C	-13.14	1.36	1.52
4	E	121	MET	CG-SD	13.14	2.13	1.80
9	K	2	ASN	C-O	13.12	1.41	1.24
1	A	1280	GLU	C-O	-13.12	1.07	1.24
7	I	17	ARG	CG-CD	13.12	1.91	1.52
4	E	131	THR	CA-CB	13.03	1.74	1.53
1	A	1381	LEU	C-O	-13.03	1.07	1.24
10	L	65	VAL	CA-C	-13.02	1.36	1.52
2	B	512	ARG	CA-C	12.98	1.70	1.52
3	C	97	VAL	CA-CB	-12.98	1.38	1.54
1	A	644	LYS	C-O	-12.88	1.08	1.24
7	I	21	GLU	C-O	-12.88	1.08	1.24
1	A	1448	GLU	CA-C	12.85	1.70	1.52
1	A	912	LEU	CA-C	-12.84	1.34	1.52
1	A	1005	GLU	CD-OE1	12.83	1.49	1.25
3	C	159	ALA	C-O	-12.80	1.06	1.23
3	C	78	GLU	C-O	-12.78	1.07	1.24
2	B	246	LYS	N-CA	12.75	1.62	1.46
1	A	1080	THR	CA-C	12.73	1.69	1.52
2	B	1168	LEU	CA-C	-12.70	1.37	1.52
1	A	705	LYS	CB-CG	12.68	1.90	1.52
1	A	419	LYS	C-O	-12.65	1.07	1.24
3	C	84	ARG	C-O	-12.65	1.07	1.24
8	J	3	VAL	CA-CB	-12.63	1.34	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	392	VAL	CA-CB	-12.62	1.39	1.54
1	A	842	VAL	C-O	-12.58	1.09	1.24
2	B	106	ASP	CA-C	12.56	1.69	1.52
3	C	15	LYS	CG-CD	12.56	1.90	1.52
1	A	975	HIS	CA-C	12.50	1.69	1.52
1	A	446	ARG	CZ-NH1	12.47	1.50	1.32
6	H	107	VAL	CA-CB	12.44	1.71	1.54
1	A	729	ALA	CA-CB	-12.42	1.32	1.53
2	B	1155	SER	N-CA	12.42	1.62	1.46
9	K	92	ASN	N-CA	12.42	1.60	1.46
2	B	692	TYR	C-O	-12.38	1.09	1.23
2	B	27	ALA	CA-CB	-12.36	1.32	1.53
1	A	14	VAL	C-O	-12.35	1.09	1.24
2	B	531	GLN	CD-OE1	12.34	1.47	1.23
2	B	703	ILE	C-O	12.33	1.36	1.24
3	C	29	MET	SD-CE	12.32	2.10	1.79
1	A	900	ASP	C-O	12.32	1.38	1.24
2	B	172	ILE	CA-CB	-12.28	1.39	1.54
7	I	99	LEU	C-O	-12.28	1.09	1.23
1	A	496	GLU	CD-OE1	12.27	1.48	1.25
2	B	39	ARG	C-O	-12.26	1.09	1.24
2	B	662	MET	C-O	-12.26	1.08	1.24
3	C	120	ILE	CA-CB	-12.24	1.41	1.54
2	B	1091	TYR	C-O	-12.22	1.09	1.24
2	B	110	HIS	CA-C	12.22	1.67	1.52
1	A	811	GLN	N-CA	-12.22	1.31	1.46
2	B	607	GLY	C-O	-12.20	1.08	1.24
2	B	1108	ARG	CA-C	12.20	1.69	1.52
1	A	1338	VAL	CA-CB	-12.18	1.40	1.54
7	I	56	ALA	C-O	-12.17	1.09	1.23
1	A	1237	ILE	N-CA	-12.17	1.31	1.46
1	A	792	TYR	CA-C	-12.16	1.36	1.52
5	F	143	PHE	C-O	-12.16	1.08	1.23
1	A	69	THR	CA-CB	12.14	1.74	1.53
1	A	1287	TYR	C-O	12.14	1.38	1.23
1	A	839	ARG	NE-CZ	12.13	1.46	1.33
1	A	74	MET	SD-CE	12.12	2.09	1.79
2	B	733	HIS	N-CA	12.12	1.61	1.46
2	B	169	ARG	NE-CZ	12.11	1.46	1.33
1	A	908	LEU	C-O	-12.11	1.09	1.24
1	A	843	LYS	C-O	-12.09	1.10	1.24
1	A	738	LYS	C-O	-12.09	1.08	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	49	VAL	C-O	-12.07	1.11	1.24
4	E	36	GLU	C-O	-12.06	1.08	1.24
1	A	1419	ASP	CG-OD1	12.02	1.48	1.25
10	L	37	LYS	C-O	-12.01	1.08	1.24
2	B	901	PRO	C-O	-12.00	1.08	1.23
4	E	47	CYS	CA-C	12.00	1.66	1.52
2	B	870	ILE	N-CA	11.99	1.61	1.46
1	A	1227	ILE	C-O	-11.96	1.09	1.23
2	B	184	ALA	CA-CB	-11.95	1.34	1.53
1	A	1149	ALA	CA-CB	-11.95	1.33	1.53
2	B	330	ALA	CA-CB	-11.93	1.34	1.53
1	A	990	VAL	CA-CB	-11.92	1.38	1.54
3	C	198	ALA	CA-CB	-11.92	1.34	1.53
7	I	50	THR	CA-C	-11.91	1.38	1.52
4	E	71	LYS	N-CA	11.90	1.61	1.46
1	A	695	LYS	CD-CE	11.90	1.88	1.52
7	I	91	ARG	C-O	-11.88	1.07	1.23
1	A	620	LYS	CE-NZ	11.88	1.84	1.49
5	F	153	VAL	CA-C	-11.87	1.39	1.52
1	A	874	ASP	CA-C	-11.86	1.38	1.52
1	A	941	LYS	CD-CE	11.85	1.88	1.52
2	B	735	ALA	N-CA	11.85	1.60	1.46
4	E	20	LYS	CE-NZ	11.85	1.84	1.49
1	A	421	ALA	CA-CB	-11.84	1.34	1.53
1	A	830	LYS	CG-CD	11.83	1.88	1.52
1	A	39	GLU	CA-C	11.82	1.67	1.52
4	E	180	ARG	CG-CD	11.82	1.88	1.52
2	B	962	LYS	CG-CD	11.81	1.87	1.52
1	A	589	GLN	CA-C	-11.81	1.38	1.52
1	A	684	ALA	CA-CB	11.81	1.72	1.53
6	H	23	VAL	CA-CB	-11.81	1.38	1.54
1	A	843	LYS	CG-CD	11.80	1.87	1.52
1	A	1146	VAL	C-O	-11.80	1.10	1.24
2	B	25	ILE	CA-CB	11.79	1.70	1.54
1	A	1424	VAL	C-O	11.78	1.38	1.24
2	B	1200	ALA	C-O	-11.77	1.10	1.24
3	C	119	VAL	CA-CB	11.77	1.68	1.54
1	A	1284	MET	CA-C	-11.76	1.37	1.52
2	B	1183	LYS	CA-C	11.74	1.68	1.52
1	A	917	SER	CA-C	-11.73	1.38	1.52
2	B	967	ARG	N-CA	-11.73	1.31	1.46
6	H	111	LEU	CA-C	11.72	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1209	MET	SD-CE	-11.70	1.50	1.79
1	A	359	LEU	CA-CB	-11.69	1.35	1.53
4	E	93	MET	SD-CE	11.69	2.08	1.79
4	E	78	LEU	N-CA	-11.66	1.32	1.46
7	I	61	ASP	C-O	-11.66	1.08	1.24
2	B	582	VAL	C-O	-11.66	1.12	1.24
3	C	163	ILE	CA-CB	-11.65	1.37	1.55
1	A	1101	LEU	N-CA	-11.65	1.31	1.46
1	A	1105	LEU	C-O	-11.64	1.08	1.24
3	C	70	ILE	N-CA	11.61	1.60	1.46
2	B	572	HIS	C-O	-11.60	1.09	1.24
1	A	1038	THR	CA-C	-11.60	1.37	1.53
2	B	608	ASP	C-O	-11.57	1.09	1.24
1	A	1015	VAL	CB-CG2	-11.57	1.14	1.52
1	A	934	LYS	CD-CE	11.56	1.87	1.52
2	B	529	GLU	CD-OE2	11.56	1.47	1.25
2	B	194	GLU	CD-OE1	11.55	1.47	1.25
2	B	993	THR	CA-C	-11.55	1.39	1.52
2	B	448	ILE	CA-CB	11.54	1.68	1.54
2	B	613	VAL	CA-CB	11.54	1.67	1.54
4	E	110	PHE	N-CA	-11.53	1.32	1.46
2	B	759	PRO	C-O	11.53	1.39	1.24
3	C	240	VAL	CA-C	-11.53	1.39	1.52
2	B	218	SER	C-O	-11.52	1.08	1.23
10	L	26	THR	N-CA	11.52	1.61	1.46
2	B	682	SER	CA-C	-11.51	1.37	1.52
1	A	1302	PRO	C-O	11.51	1.36	1.23
9	K	71	PHE	C-O	11.51	1.38	1.23
1	A	946	VAL	CA-CB	-11.50	1.39	1.54
4	E	121	MET	SD-CE	11.49	2.08	1.79
1	A	1326	ARG	C-O	-11.49	1.08	1.24
1	A	466	SER	CB-OG	-11.48	1.19	1.42
2	B	361	LEU	C-N	-11.47	1.21	1.34
4	E	65	THR	C-O	11.46	1.37	1.23
4	E	162	ARG	CB-CG	11.46	1.86	1.52
2	B	882	THR	N-CA	11.45	1.60	1.46
1	A	1259	MET	CG-SD	11.44	2.09	1.80
2	B	462	ALA	CA-CB	-11.43	1.34	1.53
2	B	389	ALA	CA-CB	-11.42	1.34	1.53
2	B	108	VAL	CA-CB	11.40	1.70	1.54
3	C	212	PRO	C-O	-11.40	1.11	1.24
3	C	179	GLU	C-O	-11.39	1.09	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	904	ARG	C-O	-11.38	1.10	1.23
1	A	620	LYS	CD-CE	11.38	1.86	1.52
7	I	48	LEU	C-O	-11.36	1.10	1.24
2	B	983	ARG	CD-NE	-11.33	1.30	1.46
2	B	174	LEU	C-O	-11.32	1.10	1.23
1	A	994	GLN	CA-C	-11.32	1.37	1.52
2	B	259	TYR	C-O	-11.30	1.10	1.23
9	K	81	TYR	C-O	-11.29	1.11	1.24
5	F	98	ALA	C-O	-11.28	1.09	1.24
8	J	1	MET	SD-CE	11.28	2.07	1.79
1	A	1225	PHE	C-O	-11.28	1.10	1.24
1	A	1309	ASP	CA-C	-11.28	1.38	1.52
1	A	1120	LEU	C-O	-11.27	1.09	1.23
3	C	158	VAL	CA-CB	-11.26	1.40	1.54
4	E	152	LYS	CD-CE	11.25	1.86	1.52
8	J	21	TYR	CA-CB	11.25	1.71	1.53
2	B	382	ILE	CG1-CD1	11.24	1.95	1.51
1	A	956	LEU	C-O	-11.23	1.14	1.24
2	B	790	ASP	CA-C	-11.23	1.38	1.52
5	F	77	ASP	C-O	11.23	1.38	1.23
1	A	506	ALA	C-O	-11.22	1.09	1.23
2	B	734	HIS	C-N	11.21	1.47	1.33
3	C	17	ASN	C-O	-11.21	1.09	1.23
1	A	1268	LEU	N-CA	-11.21	1.32	1.46
1	A	671	ALA	CA-CB	-11.20	1.36	1.53
1	A	836	TYR	CA-C	11.20	1.67	1.52
1	A	985	ASP	CG-OD2	11.19	1.46	1.25
1	A	610	GLY	C-O	11.18	1.39	1.24
1	A	45	GLN	CA-C	11.18	1.67	1.52
2	B	567	GLU	C-O	-11.17	1.09	1.24
1	A	1277	GLU	CD-OE2	11.15	1.46	1.25
7	I	1	MET	SD-CE	11.14	2.07	1.79
2	B	19	GLU	N-CA	11.14	1.60	1.46
3	C	158	VAL	C-O	-11.13	1.12	1.24
4	E	106	GLN	CG-CD	11.13	1.79	1.52
2	B	173	MET	C-O	-11.13	1.10	1.24
2	B	617	ARG	C-O	-11.11	1.10	1.24
7	I	14	LEU	C-O	-11.11	1.10	1.23
1	A	905	ASP	N-CA	-11.10	1.32	1.46
1	A	1023	ARG	CA-C	-11.10	1.37	1.52
6	H	48	PRO	C-O	11.09	1.37	1.23
1	A	1359	ASP	N-CA	11.09	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	711	ARG	C-O	-11.08	1.10	1.24
10	L	45	ALA	CA-CB	11.07	1.72	1.53
1	A	1418	LEU	C-O	-11.07	1.10	1.24
2	B	267	ARG	C-O	-11.07	1.10	1.23
1	A	618	GLU	CD-OE2	11.07	1.46	1.25
2	B	732	SER	CA-C	11.05	1.67	1.52
2	B	56	ASP	C-O	-11.03	1.09	1.24
1	A	32	VAL	CA-C	11.01	1.66	1.52
3	C	166	GLU	CD-OE2	11.01	1.46	1.25
6	H	37	LYS	CA-C	11.01	1.66	1.52
2	B	265	SER	CA-C	11.00	1.66	1.52
2	B	188	ASP	C-O	11.00	1.38	1.24
1	A	1038	THR	C-O	-10.99	1.09	1.23
10	L	59	ALA	N-CA	10.95	1.60	1.46
6	H	136	LYS	CA-C	10.95	1.67	1.52
1	A	291	GLU	C-O	-10.94	1.10	1.24
2	B	766	ARG	NE-CZ	10.94	1.45	1.33
1	A	895	LYS	CD-CE	10.93	1.85	1.52
1	A	238	CYS	C-O	-10.92	1.11	1.23
1	A	264	PHE	CA-C	10.92	1.67	1.52
2	B	1128	LEU	N-CA	10.92	1.60	1.46
3	C	167	HIS	CA-C	-10.92	1.38	1.52
1	A	697	ALA	CA-CB	-10.91	1.35	1.53
1	A	617	VAL	CA-CB	-10.90	1.41	1.54
7	I	120	GLN	CA-C	10.90	1.63	1.53
2	B	641	GLU	CG-CD	10.89	1.79	1.52
1	A	1204	ASP	CB-CG	10.88	1.79	1.52
1	A	1279	ILE	N-CA	-10.87	1.33	1.46
2	B	249	ARG	NE-CZ	10.87	1.45	1.33
2	B	986	GLN	CA-C	10.86	1.65	1.52
1	A	358	ASN	CA-C	-10.84	1.38	1.52
3	C	261	ALA	C-O	-10.84	1.10	1.23
1	A	1141	THR	C-O	10.84	1.36	1.23
2	B	626	ILE	CA-CB	-10.83	1.40	1.54
2	B	1087	PHE	C-O	-10.82	1.11	1.23
1	A	414	ASP	C-O	-10.80	1.10	1.24
1	A	536	LEU	CA-C	10.80	1.67	1.53
2	B	219	ALA	CA-CB	10.80	1.70	1.53
4	E	185	ALA	N-CA	-10.80	1.33	1.46
4	E	205	SER	C-O	-10.79	1.10	1.24
2	B	604	ARG	N-CA	10.78	1.59	1.46
2	B	882	THR	CA-CB	10.77	1.71	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	143	LEU	CA-C	-10.77	1.39	1.52
2	B	1164	GLY	C-O	10.75	1.37	1.24
2	B	271	ALA	CA-CB	-10.75	1.34	1.53
1	A	390	GLN	C-O	10.74	1.36	1.24
6	H	37	LYS	C-O	10.74	1.37	1.23
1	A	350	ARG	C-O	-10.74	1.11	1.23
1	A	880	LYS	C-O	-10.73	1.11	1.24
2	B	299	GLU	CD-OE1	10.73	1.45	1.25
9	K	64	GLU	C-O	-10.73	1.10	1.24
1	A	1228	TRP	CA-C	-10.71	1.39	1.52
2	B	706	GLN	CB-CG	10.71	1.84	1.52
2	B	1165	ILE	CA-CB	10.69	1.66	1.55
2	B	987	LYS	CE-NZ	10.69	1.81	1.49
1	A	555	ASP	CB-CG	10.69	1.78	1.52
6	H	32	THR	CA-CB	10.69	1.71	1.53
1	A	711	ARG	CA-C	-10.68	1.38	1.52
4	E	142	VAL	C-O	10.67	1.36	1.24
2	B	846	ILE	CA-CB	10.66	1.69	1.54
6	H	131	ASN	CA-CB	10.65	1.70	1.53
1	A	722	LEU	C-O	-10.65	1.10	1.24
2	B	414	ALA	CA-CB	-10.64	1.36	1.54
2	B	90	ILE	N-CA	10.62	1.59	1.46
3	C	172	PRO	CA-C	-10.62	1.37	1.52
1	A	1027	ALA	C-O	10.61	1.37	1.23
2	B	105	SER	CA-C	10.61	1.67	1.52
1	A	1187	GLN	CB-CG	10.61	1.84	1.52
3	C	60	ASP	CA-C	-10.61	1.39	1.52
1	A	705	LYS	CA-CB	10.60	1.70	1.52
1	A	373	THR	C-O	-10.57	1.10	1.24
7	I	28	GLU	CD-OE2	10.56	1.45	1.25
1	A	491	VAL	C-O	-10.55	1.11	1.24
2	B	1097	HIS	CD2-NE2	10.54	1.49	1.37
1	A	961	ARG	CZ-NH2	10.54	1.47	1.33
1	A	361	LEU	C-O	-10.54	1.10	1.24
1	A	626	ASN	CG-ND2	10.54	1.55	1.33
1	A	597	LEU	CG-CD1	10.53	1.87	1.52
1	A	677	ARG	CZ-NH2	10.53	1.47	1.33
1	A	1382	THR	C-O	10.53	1.36	1.24
1	A	1349	TYR	C-O	-10.52	1.11	1.24
9	K	36	GLU	CA-CB	-10.51	1.36	1.53
1	A	613	ILE	CA-CB	10.50	1.64	1.55
1	A	673	GLY	C-O	-10.50	1.09	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	GLU	CD-OE1	10.49	1.45	1.25
7	I	75	CYS	CA-C	-10.46	1.38	1.52
2	B	115	GLN	CG-CD	10.46	1.78	1.52
2	B	910	VAL	C-O	-10.46	1.11	1.24
2	B	1083	ALA	CA-CB	-10.46	1.37	1.53
1	A	546	VAL	CA-CB	-10.45	1.42	1.54
3	C	39	ALA	CA-CB	-10.44	1.38	1.53
1	A	693	VAL	CA-CB	-10.43	1.40	1.54
2	B	194	GLU	C-O	-10.42	1.11	1.24
2	B	1221	SER	N-CA	10.41	1.59	1.46
1	A	1110	ASN	CB-CG	10.41	1.78	1.52
1	A	1290	LYS	CE-NZ	10.41	1.80	1.49
2	B	963	PHE	CE1-CZ	10.41	1.69	1.38
2	B	130	VAL	CA-C	10.40	1.66	1.52
2	B	547	VAL	N-CA	10.40	1.57	1.46
2	B	841	MET	CA-C	10.40	1.65	1.52
2	B	1032	SER	C-O	10.39	1.36	1.24
3	C	127	ARG	N-CA	10.39	1.58	1.46
2	B	854	LEU	CA-C	-10.38	1.39	1.52
4	E	99	HIS	N-CA	10.37	1.59	1.46
3	C	66	ARG	NE-CZ	-10.36	1.21	1.33
2	B	282	ILE	CA-CB	-10.36	1.40	1.54
1	A	770	VAL	C-O	-10.36	1.12	1.24
9	K	26	LYS	CA-C	10.36	1.66	1.52
8	J	22	LEU	CA-C	10.35	1.65	1.52
2	B	587	HIS	C-O	-10.35	1.10	1.24
8	J	56	LEU	N-CA	-10.35	1.32	1.46
1	A	871	ASP	C-O	-10.34	1.10	1.24
1	A	875	ALA	CA-CB	-10.34	1.35	1.53
1	A	576	GLN	CA-C	-10.33	1.38	1.52
1	A	985	ASP	CA-C	10.33	1.66	1.52
3	C	265	MET	SD-CE	10.33	2.05	1.79
7	I	6	PHE	C-O	-10.32	1.10	1.23
1	A	1349	TYR	CG-CD2	-10.31	1.17	1.39
1	A	1275	GLY	C-O	10.31	1.35	1.23
2	B	595	ARG	NE-CZ	10.31	1.44	1.33
2	B	573	GLN	C-O	-10.29	1.10	1.24
2	B	1050	ILE	C-O	-10.29	1.11	1.24
3	C	61	GLU	N-CA	10.29	1.59	1.46
9	K	111	LEU	CG-CD1	10.29	1.86	1.52
1	A	1093	LYS	N-CA	10.29	1.59	1.46
4	E	155	ARG	NE-CZ	10.27	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	481	ASP	CG-OD2	10.27	1.44	1.25
1	A	41	MET	SD-CE	10.26	2.05	1.79
2	B	789	MET	SD-CE	10.26	2.05	1.79
1	A	366	VAL	C-N	-10.26	1.20	1.33
2	B	485	ARG	NE-CZ	-10.26	1.21	1.33
2	B	1101	ASP	CB-CG	10.26	1.77	1.52
6	H	56	THR	CA-CB	10.25	1.66	1.53
3	C	205	LYS	N-CA	10.24	1.58	1.46
1	A	1164	PRO	CA-C	10.24	1.67	1.52
1	A	471	ASN	CA-C	-10.23	1.40	1.52
1	A	1117	THR	CA-CB	-10.23	1.39	1.53
2	B	344	LYS	CA-C	10.23	1.65	1.52
2	B	974	PRO	C-O	-10.23	1.11	1.23
1	A	1118	VAL	N-CA	-10.22	1.34	1.46
1	A	958	VAL	CA-CB	-10.21	1.40	1.54
1	A	367	PRO	CA-C	-10.21	1.41	1.52
3	C	239	PRO	C-N	-10.21	1.21	1.33
2	B	945	GLU	CD-OE1	10.21	1.44	1.25
1	A	1229	SER	C-O	10.21	1.36	1.23
1	A	1188	GLN	CA-C	10.20	1.65	1.52
2	B	381	MET	SD-CE	-10.20	1.54	1.79
2	B	346	GLU	CG-CD	10.19	1.77	1.52
1	A	676	MET	SD-CE	10.19	2.05	1.79
3	C	253	LYS	C-O	10.19	1.36	1.24
2	B	119	LEU	CA-CB	-10.18	1.37	1.53
6	H	116	TYR	N-CA	10.18	1.59	1.46
3	C	256	ALA	CA-CB	-10.17	1.37	1.53
9	K	108	GLU	CD-OE2	10.17	1.44	1.25
1	A	599	SER	CA-C	-10.17	1.40	1.52
2	B	792	MET	C-O	-10.17	1.11	1.23
2	B	1169	MET	SD-CE	10.17	2.04	1.79
2	B	249	ARG	C-O	10.16	1.36	1.24
6	H	117	SER	C-O	10.16	1.35	1.23
3	C	50	GLU	CG-CD	10.16	1.77	1.52
7	I	45	ARG	CG-CD	10.15	1.82	1.52
2	B	269	ILE	CA-CB	-10.15	1.42	1.54
1	A	555	ASP	CA-CB	10.14	1.66	1.53
3	C	22	LEU	C-O	-10.13	1.11	1.23
2	B	1079	LYS	CA-C	-10.12	1.39	1.52
6	H	139	ASN	CA-CB	10.12	1.70	1.53
1	A	751	SER	CB-OG	10.12	1.62	1.42
3	C	228	PHE	C-O	-10.12	1.12	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	154	LYS	CG-CD	10.11	1.82	1.52
1	A	1416	ALA	C-O	-10.11	1.10	1.23
2	B	415	GLN	CB-CG	10.11	1.82	1.52
2	B	1146	PHE	C-O	-10.10	1.12	1.24
2	B	962	LYS	CD-CE	10.09	1.82	1.52
1	A	1159	ARG	NE-CZ	10.09	1.44	1.33
7	I	87	GLN	CA-C	-10.08	1.39	1.53
2	B	592	ASN	CG-OD1	10.08	1.42	1.23
2	B	164	LYS	CD-CE	10.07	1.82	1.52
1	A	1330	ASN	C-O	-10.06	1.11	1.24
2	B	1135	ARG	NE-CZ	-10.06	1.22	1.33
1	A	485	ASP	C-O	-10.06	1.12	1.23
4	E	162	ARG	CZ-NH1	10.06	1.46	1.32
2	B	24	PRO	CA-CB	-10.06	1.41	1.53
9	K	2	ASN	CA-C	10.06	1.66	1.52
1	A	544	ASP	CB-CG	10.05	1.77	1.52
2	B	266	ALA	CA-CB	10.04	1.70	1.53
2	B	869	SER	CA-C	10.03	1.66	1.52
2	B	353	LYS	C-O	-10.02	1.12	1.24
1	A	888	GLY	CA-C	-10.02	1.40	1.52
3	C	267	GLN	N-CA	10.01	1.59	1.46
4	E	49	SER	CA-C	10.01	1.65	1.52
6	H	91	ASP	C-O	10.01	1.35	1.24
3	C	57	VAL	CA-CB	-10.00	1.41	1.54
2	B	1102	LYS	CA-C	10.00	1.62	1.52
2	B	477	ALA	CA-CB	10.00	1.85	1.52
4	E	195	VAL	CA-CB	-9.99	1.42	1.54
9	K	72	LYS	C-O	-9.99	1.12	1.23
1	A	942	PHE	C-O	-9.99	1.12	1.24
2	B	1128	LEU	CA-C	9.98	1.66	1.52
2	B	371	GLU	CA-C	-9.98	1.39	1.52
2	B	25	ILE	C-O	-9.98	1.12	1.24
10	L	67	PHE	C-O	-9.98	1.11	1.23
1	A	1189	SER	C-O	-9.98	1.11	1.24
4	E	41	ASP	CB-CG	9.98	1.76	1.52
2	B	1082	MET	CA-C	-9.97	1.39	1.52
2	B	89	GLU	CA-C	9.96	1.73	1.52
1	A	1356	ILE	CA-CB	-9.96	1.42	1.54
1	A	801	GLU	CD-OE1	9.96	1.44	1.25
2	B	1137	CYS	C-O	-9.96	1.12	1.24
4	E	152	LYS	CG-CD	9.95	1.82	1.52
2	B	32	ALA	CA-CB	9.95	1.69	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	87	ARG	CA-C	9.95	1.64	1.52
6	H	103	LYS	CA-C	-9.95	1.39	1.52
2	B	1223	ASP	CA-C	9.94	1.66	1.52
4	E	182	ASP	CA-C	-9.94	1.43	1.53
1	A	377	PRO	C-O	-9.94	1.16	1.24
1	A	16	GLU	N-CA	9.93	1.57	1.46
2	B	735	ALA	CA-C	-9.92	1.41	1.52
4	E	138	ALA	C-O	-9.92	1.11	1.24
3	C	9	LYS	CG-CD	9.91	1.82	1.52
3	C	174	ALA	N-CA	-9.90	1.38	1.46
1	A	1422	ARG	NE-CZ	9.89	1.44	1.33
1	A	601	LYS	CD-CE	9.89	1.82	1.52
1	A	1145	SER	C-O	-9.88	1.11	1.24
1	A	509	LEU	C-O	-9.88	1.09	1.24
1	A	1111	MET	CG-SD	9.88	2.05	1.80
7	I	62	ILE	C-O	-9.87	1.10	1.24
1	A	241	VAL	CA-C	-9.87	1.45	1.53
1	A	466	SER	N-CA	9.87	1.58	1.46
1	A	702	LEU	N-CA	-9.87	1.34	1.45
1	A	801	GLU	CD-OE2	9.87	1.44	1.25
2	B	266	ALA	C-O	9.87	1.36	1.24
4	E	185	ALA	CA-CB	-9.87	1.38	1.53
9	K	86	ALA	CA-CB	-9.87	1.36	1.53
1	A	1112	LYS	CB-CG	9.86	1.82	1.52
2	B	531	GLN	CD-NE2	9.86	1.53	1.33
4	E	90	VAL	CA-C	9.86	1.65	1.52
7	I	83	ASN	CB-CG	-9.85	1.27	1.52
1	A	1108	ALA	N-CA	-9.85	1.33	1.46
2	B	219	ALA	CA-C	-9.84	1.40	1.52
2	B	1108	ARG	N-CA	9.84	1.58	1.46
1	A	1222	ASN	CA-CB	9.83	1.69	1.53
1	A	725	ALA	CA-CB	-9.82	1.38	1.53
2	B	1096	ARG	C-O	-9.81	1.10	1.23
1	A	603	ASN	CA-C	-9.81	1.40	1.52
1	A	661	GLY	CA-C	9.81	1.62	1.51
4	E	23	VAL	N-CA	-9.81	1.35	1.46
2	B	999	MET	CG-SD	9.79	2.05	1.80
1	A	763	ALA	CA-CB	-9.79	1.37	1.53
1	A	1283	VAL	CA-C	9.79	1.64	1.52
2	B	798	TYR	CA-CB	9.79	1.64	1.53
1	A	264	PHE	CB-CG	9.78	1.73	1.50
2	B	793	ALA	C-O	-9.78	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	391	ASP	C-O	-9.78	1.09	1.23
2	B	1019	SER	CB-OG	-9.78	1.22	1.42
1	A	768	GLN	C-O	-9.78	1.11	1.23
1	A	1311	VAL	N-CA	-9.78	1.34	1.46
9	K	54	ARG	NE-CZ	9.78	1.43	1.33
4	E	30	ILE	C-O	-9.78	1.14	1.24
4	E	26	ARG	CB-CG	-9.77	1.23	1.52
2	B	479	VAL	C-O	-9.77	1.10	1.24
3	C	34	ARG	CD-NE	-9.77	1.32	1.46
3	C	199	LYS	CA-C	-9.76	1.39	1.52
1	A	481	ASP	CB-CG	9.76	1.76	1.52
7	I	85	PHE	C-O	-9.76	1.11	1.23
1	A	476	SER	C-O	-9.75	1.11	1.24
2	B	91	SER	C-O	9.75	1.34	1.23
1	A	830	LYS	N-CA	9.74	1.58	1.46
2	B	604	ARG	C-O	-9.74	1.12	1.24
7	I	28	GLU	CA-C	-9.73	1.41	1.52
1	A	423	ASP	CB-CG	9.73	1.76	1.52
2	B	822	ASN	C-O	-9.73	1.12	1.24
4	E	23	VAL	C-O	9.73	1.35	1.24
2	B	598	GLU	CG-CD	9.72	1.76	1.52
1	A	1280	GLU	CD-OE2	9.72	1.43	1.25
2	B	1194	ILE	CA-C	-9.72	1.41	1.52
1	A	647	GLY	CA-C	9.72	1.63	1.52
1	A	1328	TYR	C-O	-9.71	1.11	1.23
4	E	57	MET	C-O	9.71	1.36	1.24
3	C	55	THR	C-O	9.70	1.37	1.24
1	A	828	ALA	CA-CB	-9.70	1.38	1.53
6	H	9	ILE	C-O	9.70	1.33	1.24
1	A	1171	GLN	CG-CD	9.70	1.76	1.52
1	A	673	GLY	CA-C	-9.69	1.38	1.51
1	A	1281	ARG	NE-CZ	9.69	1.43	1.33
2	B	775	LYS	CB-CG	9.69	1.81	1.52
1	A	244	PRO	CA-C	9.68	1.61	1.52
1	A	1345	ARG	NE-CZ	-9.68	1.22	1.33
2	B	239	GLU	CD-OE2	9.68	1.43	1.25
3	C	100	THR	C-O	9.68	1.36	1.23
6	H	2	SER	CA-C	9.67	1.73	1.52
6	H	135	LEU	CA-C	9.67	1.65	1.52
1	A	489	LEU	C-O	-9.67	1.12	1.23
6	H	77	ARG	CB-CG	9.65	1.81	1.52
7	I	97	MET	N-CA	-9.65	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	767	GLN	CA-CB	-9.64	1.38	1.53
2	B	509	ALA	CA-CB	9.64	1.84	1.52
4	E	52	ARG	C-O	9.63	1.36	1.24
1	A	623	GLY	C-O	9.63	1.32	1.23
7	I	11	ASN	CG-OD1	-9.63	1.05	1.23
1	A	603	ASN	N-CA	-9.62	1.34	1.45
1	A	1222	ASN	CB-CG	9.62	1.76	1.52
1	A	52	GLY	C-O	-9.62	1.10	1.23
7	I	37	GLU	CD-OE1	9.62	1.43	1.25
1	A	795	GLU	CG-CD	9.61	1.76	1.52
1	A	1061	GLY	CA-C	9.60	1.64	1.51
2	B	224	GLN	C-O	-9.60	1.13	1.23
5	F	148	VAL	C-O	9.60	1.35	1.24
9	K	73	LEU	C-O	9.59	1.35	1.24
1	A	718	VAL	CA-CB	-9.59	1.41	1.54
6	H	131	ASN	N-CA	9.59	1.58	1.46
1	A	521	MET	SD-CE	-9.58	1.55	1.79
1	A	880	LYS	N-CA	-9.58	1.34	1.46
5	F	108	PHE	N-CA	-9.57	1.34	1.46
2	B	211	VAL	CB-CG1	-9.57	1.21	1.52
2	B	337	ARG	CD-NE	-9.57	1.32	1.46
10	L	68	GLU	CD-OE1	9.57	1.43	1.25
1	A	830	LYS	CD-CE	9.57	1.81	1.52
4	E	191	LYS	C-O	-9.57	1.11	1.23
4	E	145	THR	CA-CB	-9.56	1.37	1.53
2	B	352	ALA	CA-CB	-9.56	1.38	1.53
7	I	28	GLU	C-O	-9.56	1.11	1.23
1	A	976	THR	CA-CB	9.55	1.66	1.53
6	H	19	ARG	CD-NE	9.55	1.59	1.46
1	A	676	MET	CG-SD	9.55	2.04	1.80
2	B	660	LYS	CD-CE	-9.54	1.23	1.52
1	A	558	GLY	C-O	-9.54	1.11	1.23
2	B	650	GLU	CD-OE2	9.54	1.43	1.25
3	C	81	GLU	C-O	9.53	1.35	1.23
1	A	581	ALA	CA-C	-9.53	1.40	1.52
1	A	885	THR	N-CA	-9.53	1.33	1.46
2	B	951	GLN	N-CA	-9.53	1.34	1.46
1	A	1419	ASP	CB-CG	9.52	1.75	1.52
1	A	874	ASP	CG-OD2	9.52	1.43	1.25
2	B	186	GLU	C-O	9.51	1.35	1.24
2	B	191	LYS	CB-CG	9.51	1.80	1.52
1	A	1291	VAL	CA-C	-9.51	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	117	SER	N-CA	9.50	1.57	1.46
2	B	268	THR	C-O	-9.50	1.11	1.23
3	C	108	GLU	C-O	9.49	1.35	1.24
2	B	764	SER	C-O	-9.49	1.15	1.24
1	A	469	ARG	CD-NE	-9.49	1.32	1.46
2	B	876	LYS	C-O	-9.49	1.12	1.24
1	A	611	GLN	CA-C	-9.48	1.41	1.52
2	B	617	ARG	CA-C	-9.48	1.41	1.52
7	I	98	VAL	C-O	-9.47	1.12	1.24
2	B	1181	GLU	N-CA	9.47	1.57	1.46
4	E	200	ARG	NE-CZ	-9.47	1.22	1.33
2	B	1072	MET	SD-CE	-9.47	1.55	1.79
2	B	986	GLN	CG-CD	9.46	1.75	1.52
2	B	498	THR	CA-CB	9.45	1.72	1.54
4	E	35	VAL	CA-CB	-9.44	1.43	1.54
1	A	500	GLU	C-O	-9.44	1.13	1.24
2	B	597	MET	SD-CE	-9.44	1.55	1.79
1	A	686	ALA	C-O	-9.44	1.12	1.24
1	A	1132	LYS	CG-CD	9.44	1.80	1.52
2	B	459	TYR	CG-CD2	9.43	1.59	1.39
1	A	940	ARG	CD-NE	-9.43	1.33	1.46
1	A	1026	LEU	C-O	-9.43	1.11	1.23
2	B	880	THR	CA-C	9.42	1.65	1.52
1	A	274	ILE	N-CA	9.42	1.57	1.46
1	A	1227	ILE	CA-C	-9.40	1.42	1.52
1	A	1237	ILE	CA-CB	-9.40	1.42	1.54
1	A	1288	ASP	CG-OD1	9.40	1.43	1.25
2	B	499	ASN	C-O	-9.40	1.12	1.23
6	H	50	ALA	N-CA	9.40	1.57	1.45
2	B	109	THR	CA-CB	9.40	1.69	1.53
1	A	90	VAL	C-O	-9.39	1.14	1.24
1	A	923	LEU	C-O	9.39	1.35	1.24
3	C	214	ASN	N-CA	9.39	1.57	1.46
4	E	31	THR	CA-CB	9.39	1.67	1.53
2	B	958	GLN	N-CA	9.39	1.58	1.46
2	B	432	MET	SD-CE	9.39	2.03	1.79
2	B	1133	MET	SD-CE	-9.38	1.56	1.79
1	A	1196	GLU	CD-OE1	9.38	1.43	1.25
2	B	351	TYR	C-O	9.38	1.35	1.24
1	A	299	HIS	C-O	-9.37	1.12	1.24
1	A	1049	ILE	CA-CB	-9.37	1.43	1.54
2	B	482	VAL	C-O	-9.37	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	SER	C-O	9.37	1.35	1.23
3	C	18	VAL	CA-C	-9.37	1.40	1.52
2	B	546	SER	C-O	-9.37	1.12	1.23
2	B	789	MET	CA-C	-9.36	1.43	1.53
2	B	865	LYS	CA-CB	9.36	1.69	1.53
2	B	870	ILE	C-O	9.35	1.35	1.24
1	A	1256	GLU	N-CA	9.34	1.58	1.46
2	B	165	VAL	N-CA	9.34	1.58	1.46
1	A	900	ASP	N-CA	9.34	1.58	1.46
2	B	337	ARG	NE-CZ	-9.34	1.22	1.33
1	A	1438	THR	CB-CG2	-9.34	1.21	1.52
2	B	366	GLN	C-O	-9.33	1.11	1.24
2	B	857	ARG	C-O	-9.33	1.12	1.24
1	A	1419	ASP	CG-OD2	9.32	1.43	1.25
1	A	956	LEU	N-CA	9.32	1.54	1.45
6	H	78	SER	C-O	-9.32	1.12	1.24
1	A	16	GLU	CD-OE2	9.32	1.43	1.25
2	B	1097	HIS	ND1-CE1	9.32	1.41	1.32
2	B	199	MET	SD-CE	9.31	2.02	1.79
2	B	230	ALA	CA-C	9.31	1.64	1.52
6	H	132	LEU	CA-C	9.30	1.64	1.53
1	A	734	GLU	CD-OE2	9.30	1.43	1.25
1	A	808	LEU	N-CA	-9.30	1.34	1.45
2	B	780	VAL	C-O	-9.30	1.13	1.24
2	B	972	LYS	CA-CB	-9.29	1.40	1.53
1	A	1232	ASN	CG-OD1	9.29	1.41	1.23
7	I	31	THR	N-CA	-9.28	1.33	1.46
2	B	304	ASP	N-CA	9.28	1.58	1.46
1	A	1239	ARG	N-CA	-9.27	1.34	1.46
2	B	970	THR	CA-CB	-9.27	1.35	1.53
3	C	84	ARG	NE-CZ	9.27	1.43	1.33
2	B	758	PHE	CE2-CZ	-9.27	1.10	1.38
4	E	39	LEU	CA-C	-9.27	1.41	1.53
7	I	56	ALA	CA-CB	-9.27	1.37	1.53
1	A	540	PHE	C-O	-9.27	1.11	1.23
7	I	27	PHE	C-O	-9.27	1.12	1.24
6	H	19	ARG	N-CA	9.26	1.58	1.46
2	B	529	GLU	N-CA	9.26	1.57	1.45
6	H	111	LEU	N-CA	9.26	1.56	1.45
10	L	27	LEU	CA-C	9.25	1.64	1.52
1	A	411	ASP	C-O	-9.25	1.12	1.23
1	A	496	GLU	CD-OE2	9.25	1.43	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	529	CYS	C-O	-9.25	1.13	1.24
2	B	95	ILE	CA-C	-9.25	1.41	1.52
6	H	88	SER	N-CA	9.24	1.58	1.46
1	A	1446	ASP	CA-CB	9.23	1.65	1.52
1	A	1019	CYS	CA-CB	-9.23	1.38	1.53
2	B	711	GLU	CA-C	9.23	1.64	1.52
7	I	103	CYS	C-O	-9.23	1.12	1.23
1	A	5	GLN	CB-CG	9.22	1.80	1.52
1	A	662	PHE	CA-C	-9.22	1.40	1.52
1	A	1445	ILE	CB-CG2	9.22	1.82	1.52
6	H	21	ASN	C-O	-9.22	1.10	1.23
1	A	1157	ASP	C-O	9.22	1.35	1.24
6	H	131	ASN	CA-C	9.21	1.64	1.52
1	A	370	ILE	C-O	-9.21	1.13	1.24
1	A	1302	PRO	CB-CG	9.21	1.95	1.49
2	B	966	VAL	C-O	-9.21	1.14	1.24
6	H	104	PHE	C-O	9.21	1.35	1.24
1	A	474	VAL	C-O	-9.20	1.14	1.24
5	F	152	ILE	N-CA	-9.21	1.34	1.46
1	A	892	ALA	CA-CB	-9.20	1.38	1.53
2	B	723	VAL	CB-CG1	9.19	1.82	1.52
3	C	188	HIS	CA-C	9.19	1.65	1.52
1	A	983	ILE	C-N	-9.19	1.21	1.34
3	C	113	VAL	C-O	-9.17	1.14	1.24
1	A	44	THR	N-CA	9.17	1.58	1.46
1	A	237	THR	CB-CG2	9.17	1.82	1.52
1	A	1356	ILE	CA-C	-9.17	1.41	1.52
1	A	882	SER	C-O	-9.16	1.12	1.24
1	A	497	THR	CB-CG2	-9.16	1.22	1.52
3	C	10	ILE	CA-CB	-9.16	1.42	1.54
2	B	60	GLN	C-O	-9.16	1.13	1.24
1	A	1118	VAL	C-O	-9.15	1.14	1.24
1	A	1225	PHE	CD1-CE1	9.15	1.66	1.38
2	B	308	TRP	CA-C	-9.15	1.39	1.52
4	E	54	GLN	CA-CB	9.15	1.64	1.53
1	A	1109	LYS	CG-CD	9.14	1.79	1.52
2	B	949	VAL	CA-CB	-9.14	1.43	1.54
1	A	712	GLU	C-O	-9.14	1.12	1.24
1	A	1208	THR	C-O	9.14	1.35	1.23
2	B	200	GLY	C-O	-9.14	1.12	1.23
2	B	1010	LEU	CA-C	-9.13	1.40	1.52
4	E	192	ARG	CD-NE	9.13	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	951	GLN	CG-CD	9.13	1.74	1.52
1	A	774	ARG	CD-NE	-9.12	1.33	1.46
1	A	839	ARG	C-O	-9.12	1.12	1.24
1	A	873	MET	SD-CE	-9.12	1.56	1.79
2	B	39	ARG	NE-CZ	9.12	1.43	1.33
3	C	116	LYS	CD-CE	9.12	1.79	1.52
6	H	52	GLN	CG-CD	9.12	1.74	1.52
8	J	42	LYS	C-O	9.12	1.36	1.23
2	B	420	LEU	CA-C	-9.11	1.40	1.52
3	C	174	ALA	CA-CB	-9.11	1.38	1.52
1	A	744	LYS	CA-C	-9.09	1.40	1.52
2	B	563	MET	SD-CE	-9.09	1.56	1.79
2	B	997	GLU	N-CA	9.09	1.57	1.46
8	J	28	ASP	CA-C	-9.09	1.41	1.52
6	H	45	GLU	CD-OE1	9.08	1.42	1.25
2	B	1139	ILE	C-O	-9.07	1.13	1.24
1	A	373	THR	CB-CG2	-9.07	1.22	1.52
1	A	1417	GLU	CA-CB	9.07	1.67	1.53
1	A	1303	GLU	C-O	-9.07	1.12	1.23
2	B	640	VAL	C-O	-9.06	1.14	1.24
1	A	1318	THR	C-O	-9.06	1.11	1.23
2	B	478	GLY	N-CA	9.06	1.59	1.45
3	C	252	GLN	CD-OE1	9.06	1.40	1.23
2	B	731	VAL	CA-C	-9.06	1.41	1.52
1	A	462	VAL	CA-CB	-9.05	1.43	1.54
5	F	152	ILE	C-O	-9.05	1.14	1.24
4	E	179	GLN	CD-OE1	9.05	1.40	1.23
1	A	53	LEU	N-CA	9.05	1.59	1.46
1	A	1385	THR	CA-C	9.05	1.72	1.52
2	B	396	ASP	C-O	9.05	1.35	1.23
4	E	204	THR	CA-CB	-9.05	1.40	1.53
1	A	1109	LYS	CB-CG	9.04	1.79	1.52
1	A	1130	GLN	CG-CD	9.04	1.74	1.52
2	B	126	SER	CA-CB	-9.04	1.38	1.54
2	B	271	ALA	C-O	-9.03	1.12	1.23
3	C	214	ASN	C-O	9.03	1.34	1.24
2	B	231	PRO	CA-C	9.03	1.68	1.52
2	B	173	MET	SD-CE	-9.01	1.57	1.79
1	A	837	ILE	CA-CB	-9.00	1.43	1.54
3	C	244	VAL	CA-CB	-9.00	1.43	1.54
2	B	1154	ALA	N-CA	9.00	1.57	1.46
7	I	90	GLN	C-O	-9.00	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	459	ARG	CA-C	9.00	1.64	1.52
2	B	497	ARG	CZ-NH1	8.99	1.45	1.32
1	A	653	VAL	C-O	-8.99	1.13	1.24
1	A	1428	VAL	C-O	-8.98	1.14	1.24
3	C	54	ASN	C-O	-8.98	1.14	1.23
1	A	653	VAL	CB-CG2	-8.98	1.23	1.52
1	A	720	ARG	CG-CD	8.98	1.79	1.52
1	A	973	ILE	CA-CB	8.98	1.65	1.54
1	A	1241	ARG	CA-C	-8.97	1.41	1.52
2	B	959	ASP	CB-CG	8.97	1.74	1.52
2	B	848	ARG	NE-CZ	-8.97	1.23	1.33
2	B	96	TYR	CG-CD1	8.96	1.58	1.39
2	B	30	SER	C-O	-8.96	1.13	1.24
1	A	451	HIS	CA-CB	-8.96	1.37	1.53
2	B	959	ASP	CA-CB	8.96	1.69	1.53
2	B	261	ARG	NE-CZ	8.96	1.43	1.33
2	B	1027	ILE	CA-CB	-8.96	1.41	1.54
1	A	724	GLU	CD-OE1	8.95	1.42	1.25
2	B	865	LYS	CA-C	8.95	1.64	1.52
4	E	63	ASN	CA-C	8.95	1.64	1.52
2	B	624	LEU	CA-CB	-8.95	1.39	1.53
1	A	1170	ILE	CA-CB	8.95	1.66	1.54
1	A	911	SER	C-O	8.94	1.35	1.24
2	B	49	ASP	C-O	-8.94	1.13	1.24
10	L	33	GLU	CA-C	8.94	1.64	1.52
2	B	958	GLN	CG-CD	8.93	1.74	1.52
7	I	29	CYS	C-O	8.93	1.34	1.23
7	I	67	THR	C-O	-8.93	1.11	1.24
2	B	711	GLU	CA-CB	-8.93	1.39	1.53
2	B	67	SER	CA-C	8.93	1.64	1.52
2	B	240	ILE	CA-C	-8.92	1.42	1.52
7	I	72	ASP	CB-CG	8.92	1.74	1.52
2	B	368	GLU	CA-CB	8.92	1.67	1.53
2	B	323	VAL	C-O	-8.90	1.12	1.24
2	B	764	SER	CB-OG	-8.90	1.24	1.42
1	A	1447	GLU	CA-C	8.90	1.64	1.52
3	C	104	PHE	CD2-CE2	8.90	1.65	1.38
1	A	293	GLU	N-CA	8.89	1.57	1.46
1	A	240	PRO	C-O	8.89	1.34	1.23
1	A	992	ASP	C-O	-8.89	1.13	1.24
1	A	553	VAL	C-N	-8.88	1.23	1.33
3	C	10	ILE	C-O	-8.88	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1420	ASP	CG-OD2	8.88	1.42	1.25
1	A	961	ARG	NE-CZ	8.87	1.42	1.33
9	K	30	ALA	CA-C	-8.87	1.41	1.52
1	A	1209	MET	N-CA	-8.86	1.36	1.46
7	I	111	THR	C-O	-8.86	1.13	1.23
2	B	971	THR	N-CA	-8.86	1.35	1.46
2	B	103	ASN	CA-CB	8.85	1.68	1.53
4	E	26	ARG	CD-NE	8.85	1.58	1.46
1	A	445	ASN	C-O	8.85	1.34	1.23
2	B	250	PHE	N-CA	8.84	1.57	1.46
8	J	42	LYS	CD-CE	8.84	1.78	1.52
2	B	348	ARG	C-O	-8.83	1.14	1.24
1	A	371	ALA	CA-C	-8.83	1.40	1.52
1	A	1202	MET	C-O	8.83	1.34	1.24
1	A	1350	LYS	CG-CD	8.83	1.78	1.52
2	B	1189	ILE	CA-C	8.83	1.64	1.52
1	A	924	LYS	CA-C	8.83	1.64	1.52
2	B	63	ILE	CA-C	8.82	1.64	1.52
2	B	301	ILE	CA-C	8.82	1.64	1.52
1	A	925	LEU	N-CA	-8.82	1.35	1.46
3	C	63	ILE	CA-C	8.82	1.63	1.52
1	A	1433	MET	CA-C	-8.81	1.41	1.52
2	B	657	HIS	C-N	-8.81	1.23	1.33
2	B	695	ALA	CA-CB	-8.81	1.38	1.53
1	A	498	ARG	CZ-NH2	-8.80	1.22	1.33
2	B	434	ARG	CG-CD	8.80	1.78	1.52
2	B	483	LEU	C-O	-8.80	1.13	1.24
1	A	601	LYS	C-O	-8.80	1.12	1.24
1	A	37	PHE	C-O	-8.80	1.12	1.23
4	E	7	ARG	NE-CZ	8.80	1.42	1.33
2	B	646	LEU	CG-CD2	8.80	1.81	1.52
2	B	1129	ARG	NE-CZ	8.80	1.42	1.33
1	A	681	GLU	CD-OE2	8.79	1.42	1.25
1	A	1080	THR	N-CA	8.79	1.57	1.46
4	E	137	GLU	CD-OE1	8.79	1.42	1.25
2	B	642	ASP	CA-C	-8.79	1.42	1.52
3	C	226	ASP	C-O	-8.79	1.13	1.24
5	F	78	GLN	C-O	-8.79	1.12	1.24
1	A	860	LEU	C-O	-8.78	1.12	1.24
1	A	1327	ILE	N-CA	-8.78	1.35	1.46
6	H	78	SER	CA-C	-8.78	1.41	1.52
2	B	1221	SER	CA-C	8.78	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	499	ASN	CA-C	-8.78	1.41	1.52
2	B	864	LYS	CA-C	8.77	1.64	1.52
4	E	129	PRO	CG-CD	8.77	1.75	1.51
1	A	1211	GLN	CA-C	-8.77	1.41	1.52
4	E	164	LEU	CA-C	-8.76	1.41	1.52
4	E	54	GLN	CB-CG	8.76	1.78	1.52
1	A	734	GLU	CD-OE1	8.76	1.42	1.25
1	A	635	ARG	C-O	-8.76	1.13	1.24
9	K	21	ILE	C-O	-8.76	1.14	1.24
1	A	35	ILE	CA-C	8.75	1.63	1.52
2	B	589	VAL	CA-CB	-8.75	1.42	1.54
2	B	845	SER	C-O	8.75	1.34	1.24
3	C	97	VAL	CA-C	-8.75	1.42	1.52
2	B	1036	ALA	CA-CB	8.74	1.67	1.53
7	I	17	ARG	CA-C	-8.74	1.42	1.52
7	I	10	CYS	CB-SG	-8.74	1.52	1.81
1	A	1195	LEU	N-CA	8.74	1.56	1.46
1	A	1414	ALA	CA-C	-8.74	1.40	1.52
3	C	248	ILE	CA-CB	-8.74	1.43	1.54
7	I	65	ASP	N-CA	8.74	1.58	1.46
5	F	105	ALA	CA-CB	-8.73	1.38	1.53
1	A	699	ALA	C-O	-8.73	1.12	1.24
1	A	892	ALA	C-O	-8.73	1.13	1.24
9	K	5	ASP	CG-OD2	8.72	1.42	1.25
3	C	220	ASP	CB-CG	8.71	1.73	1.52
8	J	48	ARG	CZ-NH2	-8.71	1.22	1.33
1	A	596	THR	CA-C	-8.71	1.41	1.52
2	B	367	LEU	CA-C	8.71	1.64	1.53
1	A	788	SER	C-O	-8.71	1.12	1.23
1	A	525	GLN	CG-CD	8.70	1.73	1.52
1	A	1350	LYS	CE-NZ	8.71	1.75	1.49
3	C	66	ARG	CZ-NH1	-8.71	1.20	1.32
8	J	53	HIS	CG-CD2	-8.71	1.26	1.35
2	B	882	THR	CA-C	8.70	1.64	1.52
2	B	973	ILE	N-CA	-8.70	1.35	1.46
2	B	690	VAL	C-O	-8.70	1.14	1.23
2	B	787	VAL	N-CA	-8.70	1.35	1.46
2	B	1030	LEU	CA-C	-8.70	1.41	1.52
7	I	111	THR	CA-CB	-8.69	1.38	1.53
2	B	434	ARG	CB-CG	8.69	1.78	1.52
6	H	131	ASN	CB-CG	8.69	1.73	1.52
3	C	165	LYS	N-CA	8.68	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	31	THR	CA-C	8.68	1.64	1.52
1	A	297	GLN	C-O	-8.68	1.13	1.24
1	A	670	ILE	CA-CB	-8.68	1.44	1.54
1	A	368	LYS	C-O	-8.68	1.14	1.24
2	B	646	LEU	CG-CD1	8.67	1.81	1.52
1	A	1376	THR	C-O	-8.67	1.11	1.24
2	B	349	ILE	CA-CB	-8.67	1.44	1.54
2	B	895	ASP	CB-CG	8.66	1.73	1.52
4	E	37	LEU	CG-CD1	8.66	1.81	1.52
2	B	1183	LYS	CA-CB	8.66	1.68	1.53
1	A	847	ASP	CG-OD1	8.65	1.41	1.25
1	A	1003	LYS	CB-CG	8.65	1.78	1.52
2	B	346	GLU	CD-OE1	8.65	1.41	1.25
3	C	23	SER	CB-OG	8.65	1.59	1.42
1	A	264	PHE	CA-CB	8.64	1.68	1.53
1	A	1446	ASP	CB-CG	8.64	1.73	1.52
1	A	1048	ASN	N-CA	-8.64	1.36	1.46
2	B	249	ARG	CA-C	8.64	1.64	1.52
5	F	90	ARG	NE-CZ	-8.64	1.23	1.33
2	B	257	LYS	C-O	-8.63	1.13	1.24
1	A	775	ILE	CA-CB	-8.63	1.43	1.54
1	A	346	ASP	CG-OD2	8.62	1.41	1.25
3	C	102	GLN	C-O	8.63	1.34	1.23
1	A	505	CYS	C-O	-8.62	1.12	1.23
2	B	868	MET	SD-CE	8.62	2.01	1.79
1	A	1014	ALA	C-N	-8.62	1.23	1.33
2	B	525	ALA	C-O	8.62	1.35	1.23
2	B	1191	ILE	CA-CB	-8.62	1.42	1.55
1	A	795	GLU	C-O	-8.62	1.14	1.24
5	F	103	MET	C-O	-8.62	1.10	1.23
2	B	973	ILE	CA-CB	8.61	1.65	1.54
2	B	1148	LYS	C-O	-8.61	1.14	1.24
3	C	9	LYS	C-O	-8.61	1.13	1.24
1	A	675	THR	CA-C	8.61	1.64	1.52
2	B	1219	ASP	CB-CG	8.61	1.73	1.52
2	B	736	THR	CA-CB	8.60	1.65	1.53
2	B	564	GLU	CD-OE1	8.60	1.41	1.25
1	A	974	ASP	N-CA	8.60	1.56	1.46
2	B	401	PHE	C-O	-8.59	1.12	1.24
2	B	1102	LYS	CB-CG	8.59	1.78	1.52
1	A	929	LEU	N-CA	-8.59	1.35	1.46
2	B	275	TYR	CE2-CZ	-8.59	1.17	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	931	GLU	CG-CD	8.58	1.73	1.52
1	A	1216	ILE	CA-CB	-8.57	1.44	1.54
1	A	1105	LEU	CA-C	-8.57	1.40	1.52
7	I	52	ILE	CA-C	-8.57	1.43	1.52
4	E	109	ILE	CA-CB	8.57	1.66	1.54
1	A	586	ILE	CA-C	-8.57	1.42	1.52
4	E	81	GLU	N-CA	-8.57	1.36	1.46
8	J	24	LEU	CA-CB	-8.57	1.38	1.53
1	A	1027	ALA	N-CA	-8.56	1.35	1.45
3	C	102	GLN	CB-CG	8.56	1.78	1.52
1	A	66	LYS	CB-CG	8.55	1.78	1.52
2	B	1008	PRO	CA-CB	-8.56	1.42	1.53
5	F	148	VAL	CA-CB	-8.55	1.44	1.54
9	K	40	HIS	CA-CB	8.55	1.66	1.53
10	L	42	ARG	NE-CZ	8.56	1.42	1.33
1	A	11	LEU	C-O	-8.55	1.13	1.24
1	A	74	MET	CB-CG	8.55	1.78	1.52
1	A	408	ASP	C-O	8.54	1.34	1.24
1	A	1210	GLY	C-O	8.54	1.35	1.23
1	A	1135	ARG	CG-CD	8.54	1.78	1.52
1	A	1443	VAL	C-O	-8.53	1.14	1.24
4	E	50	MET	CG-SD	8.53	2.02	1.80
7	I	5	ARG	C-O	8.53	1.34	1.23
2	B	373	ARG	CZ-NH1	8.53	1.44	1.32
1	A	461	LYS	CA-CB	-8.51	1.40	1.53
4	E	93	MET	CG-SD	8.51	2.02	1.80
1	A	797	LYS	CA-C	-8.51	1.42	1.52
1	A	1001	ARG	N-CA	-8.51	1.34	1.45
2	B	69	LEU	CA-C	8.51	1.65	1.53
1	A	24	PRO	CA-C	8.50	1.65	1.52
1	A	917	SER	C-O	-8.50	1.14	1.24
1	A	1162	VAL	CB-CG1	8.50	1.80	1.52
1	A	1372	VAL	CA-C	8.50	1.63	1.52
1	A	50	ILE	N-CA	8.50	1.57	1.46
1	A	1339	LEU	CA-CB	-8.50	1.41	1.54
6	H	136	LYS	N-CA	8.50	1.57	1.46
2	B	529	GLU	CD-OE1	8.49	1.41	1.25
1	A	1001	ARG	C-O	8.49	1.35	1.24
2	B	1154	ALA	C-N	8.49	1.45	1.33
5	F	98	ALA	CA-CB	-8.49	1.39	1.53
2	B	253	THR	CA-CB	-8.48	1.42	1.53
6	H	136	LYS	CA-CB	8.48	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	46	ILE	CA-CB	-8.48	1.45	1.54
1	A	47	ARG	CA-C	8.48	1.64	1.52
1	A	1195	LEU	C-N	-8.48	1.22	1.33
1	A	1286	LYS	C-O	-8.47	1.13	1.24
3	C	43	THR	C-O	8.47	1.33	1.23
1	A	387	ARG	CA-C	8.47	1.64	1.52
3	C	13	ALA	C-O	-8.47	1.13	1.23
2	B	481	GLN	C-O	8.46	1.34	1.23
3	C	176	ILE	C-O	-8.46	1.14	1.24
2	B	899	ILE	CA-CB	-8.46	1.43	1.54
2	B	357	GLN	CA-C	-8.46	1.41	1.52
6	H	28	ALA	CA-C	8.45	1.63	1.52
1	A	1348	LEU	C-O	-8.45	1.14	1.24
9	K	26	LYS	CG-CD	8.45	1.77	1.52
2	B	1156	ASP	CA-CB	8.45	1.67	1.53
2	B	1210	MET	SD-CE	8.45	2.00	1.79
1	A	464	PRO	C-N	-8.44	1.21	1.33
1	A	41	MET	CA-C	8.44	1.64	1.52
2	B	241	ARG	NE-CZ	8.44	1.42	1.33
3	C	143	LEU	CA-CB	-8.44	1.41	1.53
4	E	7	ARG	CD-NE	8.44	1.58	1.46
4	E	79	TRP	C-O	-8.44	1.13	1.24
1	A	660	ASN	CA-C	-8.43	1.41	1.52
1	A	826	ASP	CG-OD2	8.43	1.41	1.25
1	A	1406	VAL	CA-C	-8.43	1.42	1.52
5	F	121	ALA	CA-CB	-8.43	1.40	1.53
1	A	1102	LYS	CD-CE	8.43	1.77	1.52
4	E	150	VAL	CA-C	8.43	1.60	1.53
4	E	50	MET	CA-C	8.43	1.64	1.52
1	A	279	LEU	CA-C	-8.42	1.41	1.52
2	B	1100	ASP	CA-CB	8.42	1.67	1.53
4	E	44	ALA	C-O	8.42	1.34	1.24
1	A	1238	ILE	C-O	-8.42	1.14	1.24
1	A	1260	LEU	C-O	-8.42	1.14	1.24
7	I	117	LYS	CA-C	8.42	1.64	1.52
2	B	466	TRP	C-O	8.41	1.34	1.24
3	C	197	SER	CB-OG	8.41	1.58	1.42
3	C	228	PHE	CA-C	-8.41	1.42	1.52
7	I	70	ARG	NE-CZ	-8.41	1.23	1.33
3	C	26	ASP	CG-OD1	8.41	1.41	1.25
1	A	1415	SER	CB-OG	-8.41	1.25	1.42
4	E	162	ARG	CA-CB	8.40	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	931	GLU	CD-OE2	8.40	1.41	1.25
1	A	1405	THR	CA-CB	8.40	1.77	1.54
2	B	315	LYS	CA-CB	-8.40	1.42	1.53
1	A	1077	THR	C-O	-8.40	1.13	1.24
2	B	643	ASP	CB-CG	8.40	1.73	1.52
3	C	123	ASN	CA-CB	8.40	1.63	1.53
2	B	737	THR	C-O	-8.39	1.12	1.24
5	F	97	ARG	CA-CB	-8.39	1.40	1.53
9	K	111	LEU	CA-C	8.39	1.64	1.52
9	K	16	GLU	C-O	-8.39	1.13	1.23
1	A	967	ALA	CA-CB	-8.38	1.39	1.53
2	B	531	GLN	CB-CG	8.38	1.77	1.52
2	B	624	LEU	C-O	-8.38	1.14	1.24
6	H	83	GLN	CA-C	8.38	1.64	1.52
2	B	815	ARG	CZ-NH2	8.38	1.44	1.33
4	E	34	GLU	CD-OE2	8.38	1.41	1.25
2	B	612	GLU	C-O	-8.37	1.12	1.24
1	A	37	PHE	CA-C	8.37	1.62	1.53
1	A	686	ALA	C-N	-8.37	1.23	1.34
3	C	42	PRO	CA-CB	-8.37	1.42	1.53
2	B	646	LEU	CB-CG	8.36	1.70	1.53
2	B	1018	PRO	CA-C	-8.36	1.40	1.52
5	F	120	ILE	CA-CB	8.36	1.64	1.54
1	A	1434	ALA	CA-CB	-8.36	1.36	1.53
2	B	619	ILE	CA-CB	-8.36	1.43	1.54
4	E	77	SER	N-CA	-8.36	1.34	1.46
1	A	518	LYS	CD-CE	8.36	1.77	1.52
9	K	20	LYS	CG-CD	8.36	1.77	1.52
1	A	89	PRO	C-O	-8.35	1.14	1.23
2	B	165	VAL	CA-CB	8.35	1.65	1.54
2	B	788	ARG	CD-NE	-8.34	1.34	1.46
1	A	579	SER	CA-C	-8.34	1.40	1.52
1	A	1132	LYS	CE-NZ	8.34	1.74	1.49
2	B	823	ALA	CA-C	-8.34	1.42	1.52
9	K	91	CYS	CA-C	8.34	1.63	1.52
3	C	13	ALA	CA-C	-8.32	1.41	1.52
1	A	1006	ILE	CA-CB	8.32	1.63	1.54
2	B	620	ARG	CG-CD	8.32	1.77	1.52
2	B	1182	CYS	CA-C	8.32	1.64	1.52
3	C	241	ASP	CA-CB	8.32	1.67	1.53
1	A	999	VAL	N-CA	-8.31	1.37	1.46
2	B	1130	PHE	CA-C	-8.31	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	709	ASP	CA-C	-8.31	1.41	1.52
4	E	30	ILE	CA-CB	8.31	1.67	1.54
2	B	193	LYS	CA-C	8.31	1.64	1.52
2	B	479	VAL	CA-CB	-8.31	1.42	1.54
2	B	105	SER	CA-CB	8.31	1.67	1.53
3	C	37	MET	CA-CB	-8.30	1.40	1.53
3	C	155	LEU	C-O	8.30	1.33	1.23
1	A	1193	LEU	C-N	-8.30	1.23	1.33
3	C	24	ASN	CA-C	8.30	1.63	1.53
2	B	104	GLU	CA-C	8.30	1.63	1.52
2	B	665	GLU	CA-C	-8.30	1.42	1.52
1	A	578	LEU	N-CA	8.29	1.56	1.46
2	B	208	SER	C-O	8.29	1.34	1.24
2	B	1063	GLY	C-O	-8.29	1.13	1.24
6	H	130	ARG	CA-C	8.29	1.66	1.52
7	I	119	THR	N-CA	8.29	1.56	1.46
1	A	549	MET	C-O	-8.28	1.13	1.24
1	A	1052	GLN	N-CA	-8.29	1.36	1.46
2	B	18	PHE	CB-CG	8.29	1.69	1.50
2	B	68	THR	CA-CB	8.29	1.66	1.53
5	F	144	GLU	CA-C	-8.29	1.42	1.52
4	E	106	GLN	CA-C	8.28	1.64	1.52
2	B	224	GLN	N-CA	-8.28	1.35	1.46
2	B	617	ARG	CA-CB	-8.28	1.41	1.53
9	K	50	LEU	C-O	-8.28	1.13	1.24
1	A	511	ILE	CA-C	-8.27	1.42	1.52
7	I	120	GLN	CA-CB	8.27	1.63	1.53
1	A	986	ILE	C-O	-8.27	1.15	1.24
1	A	17	VAL	CA-CB	-8.26	1.44	1.54
2	B	838	SER	CB-OG	-8.26	1.25	1.42
1	A	618	GLU	CD-OE1	8.26	1.41	1.25
1	A	1256	GLU	CA-C	8.26	1.63	1.52
1	A	1417	GLU	N-CA	8.25	1.56	1.46
1	A	1265	ASN	CA-C	8.25	1.63	1.52
3	C	17	ASN	CA-C	-8.25	1.42	1.52
2	B	706	GLN	CG-CD	8.25	1.72	1.52
2	B	1029	CYS	CA-C	8.25	1.63	1.52
3	C	90	ASP	N-CA	8.24	1.56	1.46
1	A	966	ASN	CA-C	-8.24	1.42	1.52
1	A	1347	ALA	C-O	-8.24	1.14	1.24
2	B	943	SER	CA-C	8.24	1.63	1.52
2	B	899	ILE	CA-C	-8.24	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	984	HIS	C-O	-8.23	1.11	1.24
4	E	90	VAL	CA-CB	8.23	1.65	1.54
5	F	130	ILE	CA-C	-8.23	1.46	1.53
1	A	1286	LYS	CB-CG	8.23	1.77	1.52
2	B	348	ARG	NE-CZ	-8.23	1.24	1.33
2	B	223	VAL	C-O	-8.23	1.13	1.24
1	A	446	ARG	NE-CZ	-8.22	1.24	1.33
1	A	815	PHE	C-O	-8.22	1.14	1.24
2	B	275	TYR	CA-CB	8.22	1.64	1.53
2	B	803	LEU	CA-CB	-8.21	1.39	1.53
1	A	1036	ARG	C-O	-8.21	1.13	1.23
2	B	821	GLN	CA-C	-8.21	1.42	1.52
1	A	908	LEU	CA-C	-8.21	1.42	1.52
1	A	1006	ILE	N-CA	-8.21	1.36	1.46
1	A	1135	ARG	NE-CZ	8.20	1.42	1.33
2	B	1155	SER	CA-CB	8.20	1.67	1.53
1	A	33	ALA	C-O	-8.19	1.14	1.23
2	B	199	MET	C-O	-8.20	1.13	1.24
1	A	1051	ALA	CA-C	8.19	1.63	1.52
1	A	836	TYR	CZ-OH	8.19	1.55	1.38
2	B	252	SER	N-CA	8.18	1.56	1.46
2	B	320	ASP	CB-CG	8.18	1.72	1.52
5	F	149	GLU	C-O	8.18	1.33	1.24
1	A	724	GLU	N-CA	-8.18	1.35	1.46
8	J	19	GLU	CA-C	-8.18	1.42	1.52
1	A	1187	GLN	CG-CD	8.17	1.72	1.52
1	A	1270	ASN	CA-CB	8.17	1.64	1.53
1	A	1417	GLU	CD-OE1	8.17	1.40	1.25
1	A	666	ILE	CA-CB	-8.17	1.41	1.54
7	I	83	ASN	C-O	8.17	1.34	1.23
3	C	7	GLN	CB-CG	8.17	1.76	1.52
3	C	110	THR	CA-C	-8.16	1.42	1.52
3	C	82	TYR	C-O	-8.16	1.13	1.23
2	B	305	VAL	CB-CG1	8.16	1.79	1.52
2	B	1002	THR	CA-CB	-8.16	1.40	1.53
1	A	836	TYR	CG-CD2	8.16	1.56	1.39
1	A	1285	MET	CA-C	-8.15	1.42	1.52
2	B	239	GLU	CG-CD	8.15	1.72	1.52
3	C	199	LYS	CD-CE	8.15	1.76	1.52
6	H	52	GLN	CA-C	8.15	1.63	1.52
3	C	20	PHE	C-O	-8.15	1.13	1.24
2	B	20	ASP	CA-C	-8.15	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	975	GLN	CB-CG	-8.15	1.28	1.52
2	B	274	PRO	CA-C	8.14	1.62	1.52
2	B	1027	ILE	N-CA	-8.14	1.34	1.46
1	A	1308	THR	N-CA	-8.14	1.35	1.45
1	A	1282	VAL	CA-CB	-8.14	1.44	1.54
1	A	1372	VAL	CB-CG1	-8.14	1.25	1.52
2	B	618	ASP	CG-OD1	8.14	1.40	1.25
3	C	158	VAL	N-CA	-8.13	1.36	1.46
6	H	140	ALA	CA-CB	-8.13	1.40	1.53
9	K	54	ARG	CD-NE	8.13	1.57	1.46
2	B	983	ARG	NE-CZ	-8.13	1.24	1.33
1	A	358	ASN	C-O	-8.12	1.12	1.24
1	A	769	SER	CA-C	8.12	1.62	1.52
2	B	272	THR	CA-C	-8.12	1.42	1.53
1	A	380	VAL	C-O	8.12	1.33	1.24
1	A	1417	GLU	CD-OE2	8.12	1.40	1.25
2	B	20	ASP	C-O	-8.12	1.14	1.23
2	B	995	ARG	CD-NE	-8.12	1.34	1.46
1	A	974	ASP	CA-C	-8.11	1.42	1.52
1	A	1223	ASP	CB-CG	8.11	1.72	1.52
1	A	1256	GLU	CA-CB	8.11	1.67	1.53
2	B	166	PHE	C-O	-8.12	1.14	1.23
10	L	40	LEU	CB-CG	8.11	1.69	1.53
2	B	970	THR	C-O	-8.11	1.14	1.23
7	I	75	CYS	C-O	-8.11	1.14	1.23
1	A	1055	ARG	CG-CD	8.11	1.76	1.52
2	B	579	ARG	NE-CZ	-8.11	1.24	1.33
2	B	653	VAL	CB-CG2	-8.11	1.25	1.52
1	A	1289	ARG	NE-CZ	-8.11	1.24	1.33
2	B	112	LEU	C-O	-8.11	1.14	1.24
1	A	696	GLU	N-CA	-8.10	1.36	1.46
1	A	1119	TYR	CE2-CZ	-8.10	1.18	1.38
5	F	72	LYS	CD-CE	8.10	1.76	1.52
1	A	897	TYR	N-CA	8.10	1.56	1.46
9	K	82	ASP	C-O	-8.10	1.13	1.24
2	B	397	ASP	C-O	8.09	1.33	1.23
2	B	773	MET	C-O	-8.09	1.14	1.24
1	A	1093	LYS	CB-CG	8.09	1.76	1.52
8	J	53	HIS	CE1-NE2	-8.09	1.24	1.32
3	C	145	CYS	N-CA	-8.08	1.36	1.46
1	A	1111	MET	SD-CE	-8.08	1.59	1.79
2	B	243	ALA	CA-CB	8.08	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	888	GLY	N-CA	8.08	1.51	1.44
7	I	59	VAL	C-O	-8.08	1.14	1.23
1	A	48	ALA	CA-C	8.08	1.63	1.52
1	A	943	LEU	C-O	-8.08	1.14	1.24
1	A	1007	ILE	CA-CB	-8.08	1.44	1.54
9	K	32	VAL	CB-CG2	-8.08	1.25	1.52
2	B	251	ILE	CA-CB	8.07	1.65	1.54
1	A	290	GLU	CD-OE2	8.07	1.40	1.25
1	A	393	ARG	CA-C	-8.07	1.42	1.52
9	K	69	ALA	CA-CB	-8.07	1.42	1.52
2	B	755	ILE	C-O	8.06	1.33	1.24
1	A	681	GLU	CD-OE1	8.06	1.40	1.25
2	B	644	GLU	CA-C	8.06	1.63	1.52
3	C	267	GLN	C-O	8.06	1.34	1.24
1	A	1264	GLU	CA-C	-8.06	1.42	1.52
2	B	488	TYR	C-O	8.06	1.33	1.24
2	B	397	ASP	CG-OD1	8.06	1.40	1.25
1	A	759	ALA	N-CA	-8.05	1.36	1.46
1	A	1307	GLU	C-O	-8.05	1.14	1.23
4	E	66	GLU	CD-OE2	8.05	1.40	1.25
9	K	66	PRO	C-O	-8.05	1.13	1.24
7	I	118	ARG	CA-C	8.05	1.63	1.52
1	A	808	LEU	C-O	-8.04	1.14	1.23
2	B	347	LYS	CD-CE	8.04	1.76	1.52
1	A	1336	MET	CG-SD	-8.04	1.60	1.80
6	H	135	LEU	CA-CB	8.04	1.67	1.53
2	B	235	SER	N-CA	-8.03	1.35	1.46
8	J	59	LYS	CA-C	-8.03	1.41	1.52
1	A	750	GLY	C-O	-8.03	1.12	1.24
2	B	404	LYS	N-CA	-8.03	1.35	1.45
2	B	791	THR	N-CA	-8.02	1.36	1.46
2	B	1077	THR	C-O	-8.02	1.13	1.24
10	L	38	LEU	N-CA	-8.02	1.37	1.46
2	B	892	LYS	C-O	-8.01	1.13	1.24
2	B	1034	VAL	CA-CB	-8.01	1.44	1.54
7	I	114	GLN	C-O	-8.01	1.13	1.24
9	K	78	THR	CA-CB	-8.01	1.40	1.53
6	H	12	VAL	N-CA	8.01	1.55	1.46
1	A	672	ASP	CA-CB	8.01	1.67	1.53
2	B	557	PHE	N-CA	-8.01	1.36	1.46
1	A	1303	GLU	N-CA	-8.00	1.35	1.46
5	F	154	ASP	CB-CG	8.00	1.72	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	896	ARG	CA-C	-8.00	1.42	1.52
7	I	70	ARG	N-CA	8.00	1.55	1.45
1	A	925	LEU	C-O	-8.00	1.14	1.24
9	K	48	ALA	CA-CB	-8.00	1.40	1.53
1	A	711	ARG	N-CA	-7.99	1.36	1.46
9	K	47	ARG	CZ-NH1	7.99	1.44	1.32
2	B	1007	VAL	CB-CG1	-7.99	1.26	1.52
1	A	1236	LEU	C-O	-7.98	1.14	1.24
1	A	1192	LEU	C-O	-7.98	1.14	1.24
2	B	660	LYS	N-CA	-7.98	1.36	1.46
1	A	1292	PRO	C-O	7.98	1.32	1.23
1	A	795	GLU	CD-OE2	7.98	1.40	1.25
1	A	244	PRO	C-O	7.97	1.33	1.24
4	E	103	LYS	CA-CB	7.97	1.64	1.53
8	J	57	ILE	CA-CB	-7.97	1.43	1.54
6	H	90	ALA	CA-CB	-7.97	1.40	1.53
1	A	247	ARG	C-O	7.97	1.34	1.24
7	I	77	LYS	C-O	-7.97	1.15	1.24
1	A	867	ILE	CB-CG1	-7.96	1.37	1.53
1	A	940	ARG	C-O	-7.96	1.14	1.24
9	K	37	LYS	CA-CB	-7.96	1.39	1.53
1	A	1277	GLU	CG-CD	7.96	1.72	1.52
7	I	63	GLY	C-O	-7.96	1.13	1.23
2	B	556	THR	C-O	7.95	1.33	1.24
1	A	1439	GLY	C-O	-7.95	1.16	1.24
3	C	32	SER	C-O	7.95	1.33	1.24
4	E	172	GLU	C-O	-7.95	1.14	1.24
2	B	1095	LEU	CA-C	-7.95	1.42	1.52
1	A	292	ALA	CA-CB	7.94	1.65	1.53
2	B	743	ILE	CA-CB	7.94	1.64	1.54
2	B	1085	ILE	C-O	-7.94	1.15	1.24
8	J	48	ARG	CZ-NH1	-7.94	1.21	1.32
2	B	889	THR	N-CA	7.94	1.56	1.46
2	B	1012	ILE	CA-CB	-7.94	1.43	1.54
4	E	111	VAL	C-O	-7.94	1.15	1.24
4	E	161	LYS	CD-CE	7.94	1.76	1.52
2	B	55	VAL	N-CA	-7.94	1.36	1.46
2	B	368	GLU	N-CA	7.94	1.55	1.46
2	B	1215	ARG	C-O	-7.93	1.14	1.24
10	L	41	SER	CA-C	7.93	1.63	1.52
3	C	195	GLN	CG-CD	7.93	1.71	1.52
2	B	1212	ILE	CA-CB	-7.92	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	122	LYS	CA-CB	7.92	1.66	1.53
1	A	1121	GLU	CA-C	-7.92	1.45	1.53
3	C	195	GLN	C-O	-7.92	1.14	1.23
1	A	557	ASP	CA-C	7.92	1.62	1.52
3	C	55	THR	CB-OG1	-7.92	1.31	1.43
2	B	211	VAL	N-CA	-7.91	1.37	1.46
2	B	227	LYS	C-O	-7.91	1.13	1.23
2	B	745	PRO	CA-CB	-7.91	1.42	1.53
10	L	54	ARG	CG-CD	7.90	1.76	1.52
1	A	843	LYS	CD-CE	7.90	1.76	1.52
1	A	423	ASP	CG-OD1	7.90	1.40	1.25
1	A	1131	ALA	CA-CB	-7.90	1.40	1.53
6	H	112	ILE	CA-C	7.90	1.62	1.52
1	A	1235	LYS	CA-C	7.90	1.62	1.52
9	K	69	ALA	N-CA	7.90	1.56	1.46
8	J	21	TYR	C-O	-7.90	1.14	1.23
2	B	958	GLN	CB-CG	7.89	1.76	1.52
7	I	15	TYR	C-O	-7.89	1.13	1.24
2	B	31	TRP	CD2-CE2	-7.89	1.27	1.41
7	I	45	ARG	CD-NE	7.89	1.57	1.46
1	A	979	SER	CA-C	-7.89	1.42	1.53
1	A	1203	ASN	CA-C	7.88	1.62	1.52
1	A	724	GLU	CG-CD	7.88	1.71	1.52
2	B	367	LEU	CA-CB	7.88	1.66	1.53
1	A	364	VAL	CA-C	-7.88	1.43	1.52
1	A	889	SER	C-O	-7.87	1.13	1.23
2	B	239	GLU	C-O	7.87	1.33	1.23
2	B	552	MET	CA-CB	-7.87	1.42	1.53
3	C	30	ALA	C-O	-7.87	1.15	1.24
1	A	801	GLU	CA-CB	-7.87	1.40	1.53
2	B	315	LYS	CE-NZ	7.87	1.73	1.49
2	B	582	VAL	CA-C	-7.86	1.43	1.52
10	L	41	SER	N-CA	7.86	1.56	1.46
1	A	406	ILE	CA-CB	-7.86	1.44	1.54
1	A	1261	LYS	CD-CE	7.86	1.76	1.52
2	B	360	PHE	C-O	7.86	1.33	1.24
2	B	887	HIS	CA-C	7.86	1.63	1.52
3	C	234	SER	C-O	7.85	1.34	1.23
8	J	59	LYS	C-O	7.85	1.34	1.24
1	A	909	ASP	C-O	-7.85	1.15	1.24
7	I	24	ARG	C-O	7.85	1.33	1.23
2	B	115	GLN	CB-CG	7.85	1.75	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	371	GLU	C-O	-7.85	1.12	1.23
2	B	541	LEU	CA-C	-7.85	1.42	1.52
8	J	53	HIS	C-O	-7.84	1.14	1.23
1	A	1326	ARG	CA-C	7.84	1.62	1.52
3	C	79	GLN	N-CA	-7.84	1.36	1.46
2	B	452	THR	CA-CB	7.83	1.66	1.53
2	B	1149	GLU	C-O	-7.83	1.14	1.24
3	C	176	ILE	CA-C	-7.83	1.43	1.52
3	C	230	MET	SD-CE	-7.83	1.59	1.79
1	A	571	LEU	CG-CD2	7.83	1.78	1.52
1	A	818	MET	SD-CE	-7.83	1.59	1.79
9	K	107	THR	C-O	7.83	1.33	1.24
2	B	217	ARG	CZ-NH1	-7.82	1.21	1.32
1	A	1215	ARG	CB-CG	7.82	1.75	1.52
7	I	36	GLU	CA-CB	-7.82	1.40	1.53
2	B	592	ASN	CG-ND2	7.82	1.49	1.33
5	F	136	ARG	N-CA	-7.82	1.36	1.46
2	B	250	PHE	CA-C	7.81	1.63	1.52
1	A	643	ALA	CA-CB	-7.81	1.40	1.53
1	A	770	VAL	N-CA	-7.81	1.36	1.46
1	A	293	GLU	C-O	-7.81	1.14	1.24
1	A	995	GLU	CD-OE2	7.81	1.40	1.25
2	B	586	TRP	C-O	-7.81	1.14	1.24
2	B	1040	ASN	CB-CG	-7.81	1.32	1.52
1	A	1001	ARG	NE-CZ	-7.81	1.24	1.33
1	A	1162	VAL	CA-C	-7.80	1.42	1.52
2	B	518	HIS	CE1-NE2	-7.80	1.24	1.32
2	B	1219	ASP	CA-C	7.80	1.61	1.52
1	A	286	HIS	CB-CG	7.80	1.61	1.50
2	B	1081	LEU	CA-C	-7.80	1.43	1.52
1	A	652	VAL	CA-C	-7.80	1.43	1.52
1	A	1156	PRO	C-O	7.79	1.34	1.24
1	A	1285	MET	CG-SD	7.79	2.00	1.80
1	A	1155	ASP	N-CA	7.79	1.54	1.46
2	B	434	ARG	NE-CZ	7.79	1.41	1.33
1	A	301	ALA	C-O	-7.79	1.14	1.24
2	B	399	ASP	CB-CG	7.79	1.71	1.52
2	B	896	ASP	CA-C	-7.78	1.42	1.52
2	B	41	LYS	CE-NZ	7.78	1.72	1.49
7	I	92	ARG	CA-C	7.78	1.62	1.52
2	B	730	ARG	C-O	-7.78	1.14	1.23
1	A	776	ALA	CA-CB	-7.78	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1132	LYS	CB-CG	7.78	1.75	1.52
2	B	219	ALA	C-O	-7.77	1.14	1.23
7	I	74	GLU	CA-C	-7.77	1.43	1.52
1	A	833	GLU	C-O	7.77	1.33	1.24
5	F	92	ARG	CA-CB	-7.77	1.40	1.53
1	A	782	ARG	C-O	-7.77	1.14	1.23
2	B	549	THR	C-O	7.77	1.33	1.23
1	A	371	ALA	CA-CB	-7.77	1.40	1.53
2	B	118	ARG	CZ-NH1	-7.76	1.21	1.32
2	B	194	GLU	CD-OE2	7.76	1.40	1.25
3	C	78	GLU	CD-OE2	7.76	1.40	1.25
1	A	89	PRO	CA-C	-7.76	1.42	1.52
3	C	5	GLY	CA-C	7.76	1.63	1.51
2	B	137	TYR	CA-C	7.76	1.63	1.52
2	B	883	LEU	CB-CG	7.76	1.69	1.53
2	B	521	LEU	CA-C	7.76	1.62	1.52
10	L	47	ARG	C-O	-7.75	1.17	1.23
1	A	43	GLU	CA-C	7.75	1.62	1.52
1	A	1224	LEU	C-O	-7.75	1.13	1.23
1	A	941	LYS	CA-CB	7.75	1.65	1.53
1	A	384	ASN	CA-C	7.75	1.62	1.52
2	B	482	VAL	CA-C	-7.75	1.44	1.52
1	A	458	HIS	C-O	7.74	1.33	1.23
2	B	857	ARG	NE-CZ	7.74	1.41	1.33
1	A	17	VAL	C-O	7.74	1.32	1.24
1	A	491	VAL	CA-CB	-7.74	1.44	1.54
1	A	1012	ARG	NE-CZ	7.74	1.41	1.33
2	B	106	ASP	CB-CG	7.74	1.71	1.52
3	C	120	ILE	C-O	-7.74	1.14	1.24
9	K	54	ARG	C-O	-7.74	1.14	1.24
2	B	1206	GLU	CD-OE1	7.73	1.40	1.25
1	A	56	PRO	C-O	7.73	1.34	1.24
2	B	958	GLN	CA-CB	7.73	1.65	1.53
1	A	469	ARG	CZ-NH2	-7.73	1.23	1.33
2	B	310	MET	C-O	7.73	1.32	1.24
2	B	1031	LEU	CA-CB	-7.73	1.40	1.53
2	B	126	SER	CA-C	-7.72	1.43	1.52
2	B	128	LEU	N-CA	-7.72	1.36	1.46
1	A	731	ARG	C-O	-7.72	1.15	1.24
2	B	210	LYS	C-O	-7.72	1.14	1.24
1	A	288	ALA	CA-CB	7.72	1.65	1.53
1	A	919	ILE	N-CA	7.72	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1434	ALA	CA-C	-7.72	1.44	1.53
5	F	129	LYS	CE-NZ	7.72	1.72	1.49
2	B	463	THR	CA-C	7.72	1.63	1.52
1	A	973	ILE	C-O	7.72	1.33	1.24
1	A	1079	MET	CA-C	7.72	1.65	1.52
7	I	82	GLU	CA-C	7.72	1.63	1.53
2	B	628	THR	CA-C	7.71	1.62	1.52
1	A	37	PHE	CG-CD2	7.71	1.55	1.38
1	A	1078	GLN	CG-CD	7.71	1.71	1.52
2	B	1161	HIS	CA-C	7.71	1.64	1.53
1	A	513	SER	C-N	-7.71	1.25	1.34
2	B	860	MET	SD-CE	7.71	1.98	1.79
3	C	47	ASP	CG-OD2	7.71	1.40	1.25
7	I	118	ARG	NE-CZ	7.71	1.41	1.33
1	A	46	THR	CA-CB	7.70	1.77	1.53
1	A	965	GLN	CD-NE2	7.70	1.49	1.33
2	B	459	TYR	C-O	-7.70	1.15	1.24
5	F	122	MET	C-O	-7.70	1.14	1.24
1	A	1034	GLU	CA-CB	-7.70	1.41	1.53
2	B	19	GLU	CA-CB	7.70	1.66	1.53
1	A	49	LYS	N-CA	7.70	1.56	1.46
2	B	786	ASN	C-O	-7.70	1.14	1.24
1	A	1140	HIS	N-CA	7.70	1.55	1.46
1	A	53	LEU	CA-CB	7.70	1.64	1.53
2	B	1135	ARG	N-CA	-7.69	1.37	1.46
1	A	1092	LYS	CA-C	7.69	1.69	1.52
2	B	397	ASP	CA-CB	7.69	1.62	1.52
2	B	1223	ASP	N-CA	7.69	1.56	1.46
3	C	159	ALA	N-CA	-7.69	1.35	1.45
1	A	437	MET	C-O	-7.69	1.14	1.23
4	E	191	LYS	CE-NZ	7.69	1.72	1.49
2	B	297	ILE	CA-CB	-7.69	1.44	1.54
2	B	999	MET	C-O	-7.69	1.14	1.23
1	A	857	ARG	C-O	7.68	1.33	1.23
1	A	1301	GLU	C-O	-7.68	1.18	1.25
2	B	103	ASN	CB-CG	7.68	1.71	1.52
1	A	285	PRO	C-O	-7.68	1.13	1.23
1	A	1123	GLY	CA-C	7.68	1.62	1.51
2	B	785	TYR	CA-C	-7.68	1.42	1.52
3	C	41	ILE	CA-CB	-7.67	1.44	1.54
3	C	70	ILE	CA-C	-7.67	1.44	1.52
3	C	255	VAL	CA-CB	-7.67	1.42	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1214	GLU	CD-OE1	7.67	1.40	1.25
1	A	897	TYR	C-O	-7.67	1.14	1.24
4	E	215	MET	SD-CE	7.67	1.98	1.79
3	C	57	VAL	CA-C	7.66	1.63	1.52
5	F	73	ALA	N-CA	7.66	1.56	1.46
7	I	31	THR	CA-CB	-7.66	1.41	1.54
1	A	912	LEU	C-N	-7.66	1.23	1.33
1	A	1327	ILE	C-O	-7.66	1.16	1.24
6	H	49	VAL	CA-CB	-7.66	1.46	1.55
1	A	1200	ALA	C-O	7.66	1.33	1.24
7	I	72	ASP	CG-OD2	7.65	1.39	1.25
1	A	840	ARG	CG-CD	7.65	1.75	1.52
1	A	1023	ARG	C-O	-7.65	1.14	1.24
4	E	1	MET	CG-SD	7.65	1.99	1.80
2	B	550	ASP	C-O	7.65	1.35	1.23
2	B	397	ASP	CG-OD2	7.65	1.39	1.25
1	A	356	ASP	CA-C	-7.64	1.43	1.52
2	B	651	LEU	CG-CD2	-7.64	1.27	1.52
2	B	1196	ILE	CA-CB	-7.64	1.42	1.54
1	A	1003	LYS	C-O	7.64	1.33	1.24
4	E	38	PRO	CA-C	-7.64	1.41	1.52
1	A	37	PHE	CD1-CE1	7.64	1.61	1.38
2	B	1132	GLU	CD-OE1	7.64	1.39	1.25
9	K	7	PHE	CB-CG	-7.64	1.33	1.50
9	K	83	PRO	C-O	-7.64	1.13	1.24
1	A	792	TYR	C-O	-7.64	1.13	1.24
2	B	825	VAL	CA-CB	-7.64	1.45	1.54
8	J	18	TRP	CA-CB	-7.64	1.41	1.53
8	J	38	ARG	N-CA	-7.64	1.36	1.46
9	K	70	ARG	C-O	-7.64	1.13	1.23
2	B	466	TRP	C-N	7.63	1.44	1.33
3	C	204	SER	C-O	7.63	1.33	1.23
5	F	148	VAL	CA-C	-7.63	1.43	1.52
2	B	31	TRP	CZ3-CH2	-7.63	1.21	1.40
2	B	734	HIS	CA-C	7.63	1.65	1.52
2	B	1069	PHE	CA-C	7.63	1.62	1.52
2	B	857	ARG	CA-C	-7.62	1.43	1.52
1	A	1234	GLU	CD-OE1	7.62	1.39	1.25
3	C	191	TYR	N-CA	-7.62	1.36	1.46
4	E	72	PHE	CE2-CZ	7.62	1.61	1.38
2	B	190	TYR	CA-CB	-7.62	1.41	1.53
1	A	368	LYS	CG-CD	7.62	1.75	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	525	GLN	C-O	-7.62	1.14	1.24
2	B	969	ARG	NE-CZ	-7.62	1.24	1.33
10	L	27	LEU	CB-CG	7.61	1.68	1.53
10	L	66	GLN	C-O	-7.61	1.14	1.23
3	C	148	ARG	CD-NE	7.61	1.56	1.46
3	C	191	TYR	C-O	-7.61	1.14	1.24
2	B	292	ILE	CA-CB	7.60	1.64	1.54
4	E	200	ARG	CA-C	-7.60	1.43	1.52
2	B	136	THR	C-O	7.60	1.33	1.23
1	A	672	ASP	CB-CG	-7.60	1.33	1.52
3	C	216	GLY	C-O	7.60	1.34	1.23
1	A	295	LEU	CG-CD2	7.60	1.77	1.52
1	A	1074	GLU	CD-OE2	7.60	1.39	1.25
2	B	1030	LEU	C-O	-7.60	1.15	1.24
7	I	87	GLN	C-O	-7.60	1.13	1.23
10	L	50	ASP	CB-CG	7.59	1.71	1.52
1	A	1441	PHE	C-O	-7.59	1.14	1.23
1	A	977	LYS	CB-CG	7.59	1.75	1.52
2	B	226	PHE	CE2-CZ	7.59	1.61	1.38
1	A	1009	ASN	CG-OD1	7.58	1.38	1.23
1	A	668	ASP	CA-CB	-7.58	1.40	1.53
2	B	813	LYS	C-N	-7.58	1.22	1.33
2	B	1220	ARG	NE-CZ	7.58	1.41	1.33
1	A	1152	ILE	C-O	-7.58	1.15	1.24
2	B	784	ASN	N-CA	-7.58	1.37	1.46
1	A	960	ILE	CG1-CD1	-7.58	1.22	1.51
1	A	1426	GLU	C-O	7.58	1.32	1.24
1	A	1129	GLU	CA-CB	7.57	1.65	1.53
3	C	87	PHE	CD2-CE2	7.57	1.61	1.38
2	B	497	ARG	CA-C	-7.57	1.42	1.53
2	B	843	GLN	CG-CD	-7.57	1.33	1.52
1	A	469	ARG	NE-CZ	-7.57	1.24	1.33
2	B	512	ARG	CZ-NH1	7.57	1.43	1.32
2	B	710	LEU	CG-CD1	-7.56	1.27	1.52
1	A	655	PHE	N-CA	7.56	1.55	1.46
3	C	11	ARG	CA-C	-7.56	1.42	1.52
1	A	1300	LYS	C-O	-7.55	1.14	1.24
5	F	122	MET	CA-C	-7.55	1.42	1.52
1	A	1446	ASP	N-CA	7.55	1.56	1.46
1	A	964	ILE	C-O	7.55	1.32	1.24
1	A	411	ASP	CA-C	-7.55	1.42	1.52
1	A	1191	TRP	C-O	7.55	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	8	ARG	C-O	-7.55	1.15	1.24
1	A	776	ALA	C-O	-7.54	1.13	1.23
6	H	127	GLY	N-CA	7.54	1.56	1.45
2	B	230	ALA	N-CA	7.54	1.56	1.46
1	A	1140	HIS	CB-CG	-7.54	1.39	1.50
2	B	496	ARG	N-CA	-7.54	1.37	1.46
2	B	370	PHE	CD1-CE1	7.53	1.61	1.38
1	A	913	LEU	CA-CB	7.53	1.66	1.53
5	F	139	PRO	C-O	-7.53	1.14	1.24
10	L	44	ASP	C-O	7.53	1.33	1.24
2	B	222	ILE	N-CA	-7.53	1.37	1.46
2	B	996	ARG	NE-CZ	-7.52	1.24	1.33
7	I	118	ARG	CD-NE	7.52	1.56	1.46
2	B	1106	ARG	CA-CB	7.52	1.62	1.52
2	B	92	PHE	N-CA	7.52	1.55	1.46
1	A	604	GLY	CA-C	-7.52	1.41	1.52
1	A	1117	THR	N-CA	7.52	1.55	1.46
5	F	78	GLN	CA-C	7.52	1.62	1.52
2	B	1020	ARG	CA-C	7.52	1.62	1.52
3	C	125	MET	CA-C	7.52	1.62	1.52
2	B	822	ASN	CA-C	-7.51	1.43	1.52
1	A	1262	LYS	CG-CD	7.51	1.75	1.52
4	E	211	TYR	C-O	7.51	1.32	1.23
1	A	883	LEU	C-O	7.50	1.32	1.24
1	A	287	HIS	CA-C	7.50	1.63	1.52
1	A	885	THR	CA-CB	7.50	1.66	1.53
2	B	1140	ALA	C-O	7.50	1.32	1.24
1	A	669	THR	CA-CB	7.50	1.65	1.53
2	B	1057	LYS	CG-CD	7.50	1.75	1.52
1	A	1411	GLU	CG-CD	7.50	1.70	1.52
2	B	227	LYS	CG-CD	7.50	1.75	1.52
1	A	1188	GLN	N-CA	7.49	1.55	1.46
6	H	56	THR	N-CA	-7.49	1.36	1.46
1	A	771	GLU	CA-C	-7.49	1.43	1.53
1	A	797	LYS	N-CA	7.49	1.54	1.46
4	E	102	GLU	N-CA	-7.49	1.36	1.46
2	B	319	GLU	CG-CD	7.49	1.70	1.52
2	B	357	GLN	C-O	-7.49	1.14	1.24
1	A	460	VAL	N-CA	-7.48	1.37	1.46
2	B	610	ASN	C-O	7.48	1.33	1.24
3	C	12	GLU	CD-OE2	7.48	1.39	1.25
7	I	120	GLN	CB-CG	7.48	1.74	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	28	GLU	CD-OE1	7.48	1.39	1.25
1	A	462	VAL	CA-C	-7.48	1.44	1.52
1	A	956	LEU	C-N	-7.48	1.23	1.33
1	A	1282	VAL	C-O	-7.48	1.16	1.24
2	B	1106	ARG	NE-CZ	7.47	1.41	1.33
3	C	188	HIS	C-O	7.47	1.33	1.24
2	B	1156	ASP	CB-CG	7.46	1.70	1.52
1	A	375	THR	C-O	-7.46	1.14	1.23
1	A	1241	ARG	C-O	-7.46	1.14	1.23
3	C	177	GLU	CD-OE2	7.46	1.39	1.25
2	B	517	THR	CA-C	-7.46	1.42	1.52
4	E	162	ARG	N-CA	7.46	1.55	1.46
2	B	226	PHE	CD1-CE1	7.45	1.61	1.38
2	B	621	GLU	CD-OE2	7.45	1.39	1.25
1	A	592	ASP	CG-OD1	7.45	1.39	1.25
2	B	968	VAL	CB-CG2	-7.45	1.27	1.52
1	A	864	ILE	N-CA	-7.45	1.36	1.46
1	A	1420	ASP	CG-OD1	7.45	1.39	1.25
1	A	10	PRO	CA-C	7.45	1.61	1.52
1	A	742	ASN	C-O	-7.44	1.14	1.24
2	B	310	MET	N-CA	-7.44	1.37	1.46
3	C	173	ALA	C-O	-7.44	1.14	1.23
1	A	966	ASN	N-CA	-7.43	1.37	1.46
1	A	487	MET	CG-SD	7.43	1.99	1.80
1	A	584	ASN	N-CA	7.43	1.55	1.45
2	B	244	LEU	CA-C	7.43	1.61	1.52
1	A	690	VAL	CA-C	-7.43	1.43	1.52
1	A	1316	VAL	CA-C	7.43	1.62	1.52
1	A	1448	GLU	N-CA	7.43	1.55	1.46
1	A	451	HIS	C-O	-7.42	1.14	1.23
1	A	603	ASN	CB-CG	-7.42	1.33	1.52
4	E	16	PHE	CA-C	-7.42	1.42	1.52
1	A	1273	LEU	CA-C	7.42	1.62	1.52
2	B	1011	ILE	C-O	-7.42	1.15	1.24
1	A	589	GLN	CG-CD	7.42	1.70	1.52
1	A	1384	VAL	C-O	-7.41	1.15	1.23
1	A	883	LEU	CA-CB	-7.41	1.43	1.53
2	B	639	ILE	CA-CB	-7.41	1.45	1.54
1	A	806	ARG	CZ-NH1	7.41	1.43	1.32
1	A	1355	VAL	N-CA	-7.41	1.38	1.46
1	A	367	PRO	CA-CB	-7.41	1.44	1.53
2	B	1155	SER	C-O	7.41	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1221	SER	CA-CB	7.41	1.66	1.53
1	A	640	GLN	CD-OE1	7.41	1.37	1.23
2	B	519	TRP	CD2-CE2	-7.40	1.28	1.41
1	A	941	LYS	CG-CD	7.40	1.74	1.52
8	J	24	LEU	C-O	-7.40	1.14	1.24
1	A	74	MET	CG-SD	7.40	1.99	1.80
1	A	769	SER	C-O	-7.39	1.14	1.23
10	L	43	THR	CB-CG2	7.39	1.76	1.52
1	A	1081	LEU	CG-CD2	7.39	1.76	1.52
1	A	1127	ASP	CA-CB	7.39	1.62	1.52
1	A	515	GLN	CA-C	-7.39	1.43	1.52
3	C	252	GLN	C-O	-7.39	1.15	1.24
6	H	117	SER	CA-C	-7.39	1.43	1.52
9	K	47	ARG	C-O	-7.38	1.15	1.24
10	L	66	GLN	CD-NE2	7.38	1.48	1.33
2	B	840	ILE	C-O	-7.38	1.16	1.24
2	B	703	ILE	CA-CB	-7.38	1.45	1.54
4	E	63	ASN	CA-CB	7.37	1.64	1.53
1	A	777	PHE	CA-CB	7.37	1.63	1.52
2	B	1020	ARG	CZ-NH2	-7.37	1.23	1.33
1	A	291	GLU	CG-CD	7.37	1.70	1.52
3	C	127	ARG	C-O	7.37	1.32	1.23
2	B	479	VAL	CA-C	-7.37	1.41	1.52
7	I	35	VAL	C-O	-7.37	1.14	1.23
10	L	56	LEU	CA-C	-7.37	1.43	1.52
2	B	277	LYS	N-CA	-7.36	1.37	1.46
1	A	1362	TYR	N-CA	7.36	1.55	1.46
2	B	371	GLU	CD-OE1	7.36	1.39	1.25
2	B	643	ASP	CA-CB	7.36	1.68	1.53
10	L	67	PHE	CA-C	-7.36	1.43	1.52
1	A	1429	ILE	C-O	-7.36	1.15	1.24
3	C	135	GLN	CG-CD	7.35	1.70	1.52
3	C	174	ALA	C-O	-7.35	1.14	1.24
10	L	40	LEU	CA-CB	7.35	1.63	1.54
1	A	980	ASP	C-O	7.35	1.34	1.24
3	C	252	GLN	CB-CG	7.35	1.74	1.52
1	A	889	SER	CA-C	-7.34	1.43	1.53
1	A	1376	THR	CB-CG2	-7.34	1.28	1.52
1	A	1346	ALA	CA-CB	-7.34	1.41	1.53
2	B	593	PRO	CB-CG	7.34	1.86	1.49
3	C	191	TYR	CB-CG	7.34	1.67	1.51
7	I	47	GLU	C-O	-7.34	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	ASP	CA-CB	7.33	1.66	1.53
2	B	908	GLU	CA-CB	7.33	1.63	1.53
4	E	74	ASP	CA-C	7.33	1.62	1.52
2	B	812	LEU	C-O	-7.33	1.14	1.24
6	H	130	ARG	NE-CZ	-7.33	1.25	1.33
1	A	896	ARG	CZ-NH1	7.33	1.43	1.32
2	B	699	GLU	C-O	-7.32	1.14	1.24
4	E	17	ARG	C-O	7.32	1.32	1.24
1	A	1203	ASN	C-O	7.32	1.32	1.24
1	A	1314	SER	CA-CB	-7.32	1.41	1.53
2	B	611	PRO	C-O	-7.32	1.14	1.24
10	L	58	LYS	CA-C	-7.31	1.43	1.52
1	A	1304	TRP	CA-C	-7.31	1.43	1.52
1	A	372	LYS	N-CA	7.31	1.55	1.46
1	A	947	PHE	C-O	-7.31	1.13	1.23
6	H	61	SER	CA-C	-7.31	1.43	1.52
10	L	43	THR	CA-CB	7.31	1.66	1.53
1	A	356	ASP	C-N	-7.31	1.25	1.34
1	A	1013	ASP	CG-OD2	7.30	1.39	1.25
2	B	735	ALA	CA-CB	-7.30	1.41	1.53
1	A	475	THR	C-O	-7.30	1.14	1.24
2	B	489	SER	C-O	-7.30	1.14	1.24
2	B	1040	ASN	CA-CB	-7.30	1.43	1.53
2	B	224	GLN	CA-C	-7.30	1.43	1.52
1	A	1287	TYR	CA-C	7.29	1.61	1.52
2	B	195	CYS	C-N	-7.29	1.25	1.33
1	A	1196	GLU	CA-C	7.29	1.61	1.52
3	C	211	ASP	CG-OD2	7.29	1.39	1.25
2	B	706	GLN	CD-NE2	7.29	1.48	1.33
2	B	1097	HIS	CB-CG	-7.29	1.40	1.50
4	E	91	LYS	CA-CB	7.28	1.64	1.53
8	J	35	ALA	N-CA	-7.28	1.37	1.46
1	A	438	ASP	N-CA	-7.28	1.36	1.46
1	A	895	LYS	CG-CD	7.28	1.74	1.52
6	H	41	ASP	CB-CG	7.28	1.70	1.52
1	A	351	THR	CA-CB	7.28	1.65	1.53
1	A	1149	ALA	C-O	7.27	1.32	1.23
1	A	1422	ARG	CZ-NH1	7.27	1.43	1.32
1	A	1093	LYS	CG-CD	7.27	1.74	1.52
2	B	1153	GLU	CA-C	7.27	1.62	1.53
1	A	955	PRO	CA-C	-7.27	1.44	1.52
2	B	172	ILE	C-O	7.27	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	72	PHE	CG-CD1	7.27	1.54	1.38
5	F	74	ILE	CA-CB	7.26	1.59	1.54
1	A	675	THR	C-O	-7.26	1.15	1.24
2	B	380	TYR	N-CA	-7.26	1.37	1.46
2	B	975	GLN	C-O	-7.26	1.15	1.23
1	A	1449	SER	CA-C	7.26	1.61	1.52
2	B	963	PHE	CB-CG	-7.25	1.33	1.50
4	E	78	LEU	C-O	7.25	1.33	1.23
9	K	61	TYR	CG-CD2	-7.24	1.24	1.39
1	A	824	LEU	CA-C	-7.24	1.43	1.52
1	A	1200	ALA	CA-C	7.24	1.62	1.52
2	B	137	TYR	CB-CG	7.24	1.67	1.51
1	A	501	LEU	N-CA	-7.24	1.37	1.46
1	A	1279	ILE	C-O	-7.24	1.16	1.24
2	B	369	GLY	CA-C	7.23	1.62	1.51
7	I	72	ASP	CG-OD1	7.23	1.39	1.25
8	J	6	ARG	CZ-NH1	-7.23	1.22	1.32
1	A	686	ALA	CA-C	-7.23	1.43	1.52
6	H	44	VAL	CA-C	7.23	1.61	1.52
1	A	363	GLN	CA-C	-7.23	1.43	1.52
1	A	575	LYS	N-CA	7.23	1.55	1.46
1	A	1239	ARG	CG-CD	7.23	1.74	1.52
2	B	554	ILE	C-O	-7.23	1.15	1.24
1	A	1359	ASP	CG-OD1	7.22	1.39	1.25
1	A	672	ASP	CA-C	7.22	1.62	1.52
1	A	966	ASN	C-O	-7.22	1.15	1.24
1	A	1361	SER	N-CA	7.22	1.54	1.45
2	B	1158	PHE	C-O	-7.22	1.15	1.23
1	A	85	ASP	N-CA	7.22	1.55	1.46
1	A	489	LEU	N-CA	-7.21	1.36	1.46
1	A	677	ARG	C-O	-7.21	1.15	1.24
1	A	1226	VAL	C-O	7.21	1.31	1.24
8	J	24	LEU	CA-C	-7.21	1.42	1.52
1	A	934	LYS	CG-CD	7.21	1.74	1.52
1	A	1272	THR	CB-CG2	7.21	1.76	1.52
1	A	379	VAL	CA-CB	-7.21	1.45	1.54
1	A	907	THR	CA-CB	7.21	1.64	1.53
4	E	153	HIS	C-O	-7.21	1.15	1.24
9	K	39	ASP	C-N	-7.21	1.24	1.33
1	A	826	ASP	C-O	-7.20	1.15	1.24
2	B	1212	ILE	N-CA	7.20	1.55	1.46
2	B	657	HIS	C-O	-7.20	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	709	ASP	C-O	-7.20	1.14	1.24
1	A	1330	ASN	CA-C	-7.20	1.42	1.52
1	A	1345	ARG	C-O	-7.20	1.15	1.24
1	A	706	HIS	CA-C	-7.20	1.43	1.52
1	A	969	GLN	CD-OE1	7.20	1.37	1.23
2	B	887	HIS	CA-CB	7.20	1.65	1.53
1	A	416	ARG	C-O	-7.18	1.14	1.24
1	A	479	ASN	C-O	-7.18	1.14	1.23
2	B	109	THR	N-CA	7.18	1.55	1.46
4	E	103	LYS	N-CA	7.18	1.54	1.46
2	B	23	ALA	CA-CB	-7.18	1.41	1.53
1	A	976	THR	N-CA	7.18	1.54	1.46
1	A	1232	ASN	CA-C	7.18	1.62	1.52
3	C	28	ALA	CA-CB	-7.18	1.42	1.53
2	B	231	PRO	CB-CG	7.18	1.85	1.49
2	B	767	ASN	N-CA	-7.18	1.37	1.46
10	L	62	LYS	CD-CE	7.18	1.74	1.52
1	A	1029	ARG	CB-CG	-7.17	1.30	1.52
3	C	180	TYR	CG-CD1	-7.17	1.24	1.39
5	F	145	ASP	C-O	7.17	1.32	1.24
2	B	831	SER	C-O	-7.17	1.15	1.24
2	B	117	ALA	CA-C	-7.17	1.42	1.52
3	C	75	MET	N-CA	7.17	1.54	1.46
7	I	1	MET	CB-CG	7.17	1.74	1.52
1	A	645	LEU	C-O	-7.17	1.15	1.24
2	B	950	ASP	C-N	-7.17	1.24	1.33
7	I	73	ARG	CA-CB	-7.17	1.42	1.53
1	A	15	LYS	C-O	-7.16	1.14	1.24
1	A	891	ALA	CA-C	-7.16	1.43	1.52
4	E	6	GLU	C-O	-7.16	1.15	1.24
2	B	1100	ASP	N-CA	7.16	1.55	1.46
2	B	645	SER	C-O	-7.16	1.15	1.24
5	F	87	LYS	CG-CD	7.16	1.74	1.52
9	K	94	ILE	CA-C	-7.16	1.44	1.52
3	C	128	ASN	CA-C	7.16	1.62	1.52
9	K	97	LYS	C-O	-7.16	1.14	1.24
1	A	541	ILE	C-O	7.15	1.31	1.24
7	I	30	ARG	CA-C	-7.15	1.42	1.52
2	B	937	ALA	CA-CB	7.15	1.65	1.53
10	L	58	LYS	C-O	-7.15	1.15	1.24
3	C	14	SER	C-O	-7.15	1.16	1.23
2	B	616	ILE	CA-C	-7.14	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	227	THR	CA-C	7.14	1.60	1.52
1	A	9	ALA	CA-C	-7.14	1.45	1.52
2	B	303	TYR	CG-CD2	-7.14	1.24	1.39
2	B	343	ILE	C-O	-7.14	1.17	1.24
2	B	700	SER	C-O	-7.14	1.14	1.24
6	H	58	THR	CA-C	7.14	1.61	1.52
2	B	366	GLN	N-CA	7.14	1.54	1.46
2	B	485	ARG	CG-CD	-7.14	1.31	1.52
10	L	63	ARG	N-CA	7.14	1.55	1.46
1	A	534	LEU	CA-C	-7.13	1.42	1.52
1	A	1116	LEU	CB-CG	-7.13	1.39	1.53
3	C	184	ASN	N-CA	7.13	1.57	1.47
3	C	199	LYS	CG-CD	7.13	1.73	1.52
1	A	1269	GLU	N-CA	7.13	1.55	1.46
2	B	190	TYR	C-O	-7.13	1.15	1.24
2	B	239	GLU	CD-OE1	7.13	1.38	1.25
4	E	192	ARG	CZ-NH2	7.13	1.42	1.33
4	E	110	PHE	C-O	7.13	1.31	1.24
2	B	577	ALA	CA-CB	-7.12	1.42	1.53
1	A	404	TYR	CG-CD1	-7.12	1.24	1.39
5	F	97	ARG	CB-CG	-7.12	1.31	1.52
2	B	263	GLY	C-O	7.12	1.33	1.23
2	B	585	VAL	N-CA	7.12	1.54	1.46
2	B	794	ASN	N-CA	-7.12	1.37	1.46
2	B	1219	ASP	N-CA	7.12	1.54	1.46
3	C	14	SER	N-CA	-7.12	1.37	1.46
2	B	328	GLU	CD-OE1	7.12	1.38	1.25
1	A	832	ALA	CA-C	7.12	1.61	1.52
1	A	1068	ALA	CA-CB	-7.12	1.42	1.53
2	B	385	LEU	N-CA	-7.12	1.38	1.46
4	E	181	ALA	CA-CB	-7.12	1.43	1.53
1	A	1075	PRO	C-O	-7.11	1.15	1.24
2	B	783	THR	C-O	-7.11	1.14	1.24
1	A	1021	LEU	CA-C	-7.11	1.43	1.52
2	B	235	SER	CB-OG	-7.11	1.27	1.42
8	J	31	ASP	C-O	7.11	1.32	1.23
3	C	190	ASP	C-O	-7.11	1.16	1.24
4	E	155	ARG	CD-NE	7.11	1.56	1.46
5	F	75	PRO	C-O	7.11	1.31	1.23
1	A	980	ASP	CA-C	-7.11	1.43	1.52
3	C	196	ASP	CB-CG	7.11	1.69	1.52
7	I	86	PHE	C-O	-7.11	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1417	GLU	CG-CD	7.10	1.69	1.52
2	B	1198	TYR	CA-CB	7.10	1.64	1.53
9	K	1	MET	N-CA	7.10	1.59	1.46
1	A	719	VAL	CB-CG1	-7.10	1.29	1.52
1	A	941	LYS	CE-NZ	7.10	1.70	1.49
1	A	900	ASP	C-N	-7.09	1.24	1.33
1	A	492	PRO	CA-C	-7.09	1.43	1.52
3	C	253	LYS	CA-C	7.09	1.62	1.52
6	H	42	ILE	N-CA	-7.09	1.37	1.46
2	B	595	ARG	CG-CD	7.09	1.73	1.52
1	A	1079	MET	C-O	7.09	1.33	1.24
1	A	891	ALA	C-O	-7.09	1.16	1.24
2	B	1048	THR	CA-C	-7.09	1.43	1.53
1	A	439	ASN	CG-ND2	-7.08	1.18	1.33
2	B	266	ALA	CA-C	7.08	1.62	1.52
2	B	916	THR	CA-C	7.08	1.67	1.52
2	B	723	VAL	N-CA	7.08	1.54	1.46
4	E	164	LEU	CA-CB	-7.08	1.42	1.53
3	C	207	CYS	CA-C	7.08	1.61	1.52
2	B	448	ILE	CA-C	7.08	1.61	1.52
2	B	781	PHE	CB-CG	-7.08	1.34	1.50
3	C	160	LYS	CG-CD	7.08	1.73	1.52
2	B	1043	ASP	CG-OD2	7.08	1.38	1.25
1	A	1239	ARG	CZ-NH2	-7.07	1.24	1.33
2	B	710	LEU	C-O	-7.07	1.15	1.23
1	A	757	ASN	CA-C	-7.07	1.44	1.52
2	B	652	LYS	C-O	-7.07	1.15	1.24
1	A	722	LEU	CA-C	-7.07	1.42	1.52
1	A	1002	GLY	CA-C	7.07	1.61	1.51
2	B	661	LEU	C-O	-7.07	1.16	1.24
1	A	948	VAL	CB-CG1	-7.07	1.29	1.52
2	B	377	PHE	C-O	-7.07	1.15	1.24
1	A	507	VAL	CB-CG2	-7.06	1.29	1.52
6	H	134	ASN	CA-C	-7.06	1.43	1.52
1	A	94	GLY	CA-C	7.06	1.61	1.51
7	I	43	VAL	C-O	7.06	1.32	1.24
1	A	1029	ARG	CA-C	7.06	1.61	1.52
9	K	88	LYS	CG-CD	7.05	1.73	1.52
7	I	84	VAL	CB-CG1	-7.05	1.29	1.52
2	B	37	PHE	CA-CB	-7.05	1.42	1.53
6	H	22	LYS	C-O	7.05	1.33	1.24
1	A	700	ASN	CG-ND2	-7.05	1.18	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	353	LYS	CG-CD	7.05	1.73	1.52
6	H	3	ASN	CA-C	7.05	1.61	1.53
1	A	45	GLN	N-CA	7.05	1.55	1.46
1	A	1137	ALA	C-O	7.05	1.33	1.24
1	A	1077	THR	CA-C	7.04	1.62	1.52
1	A	1383	SER	CA-CB	-7.04	1.41	1.53
1	A	728	LYS	CE-NZ	7.04	1.70	1.49
2	B	418	LYS	CD-CE	7.04	1.73	1.52
2	B	690	VAL	CB-CG1	-7.04	1.29	1.52
4	E	79	TRP	N-CA	-7.04	1.37	1.46
1	A	566	ILE	CB-CG2	7.04	1.75	1.52
6	H	79	TRP	CA-C	-7.04	1.44	1.52
1	A	1060	PRO	CA-C	-7.04	1.43	1.52
2	B	1057	LYS	CD-CE	7.04	1.73	1.52
3	C	169	LYS	CA-C	-7.04	1.43	1.52
1	A	506	ALA	CA-C	-7.03	1.43	1.52
1	A	827	THR	C-O	-7.03	1.16	1.24
1	A	1230	GLU	CD-OE1	7.03	1.38	1.25
1	A	717	ASN	CG-OD1	7.03	1.36	1.23
4	E	156	LEU	CA-C	7.03	1.61	1.52
1	A	4	GLN	CB-CG	7.03	1.73	1.52
1	A	665	GLY	CA-C	-7.03	1.44	1.51
2	B	598	GLU	CD-OE2	7.03	1.38	1.25
2	B	870	ILE	CA-C	7.03	1.61	1.52
1	A	53	LEU	CA-C	7.03	1.62	1.53
1	A	899	VAL	CA-CB	-7.03	1.45	1.54
1	A	1428	VAL	CA-C	-7.03	1.44	1.52
4	E	169	ARG	C-O	7.03	1.33	1.23
1	A	346	ASP	CA-CB	7.02	1.67	1.53
3	C	206	ASN	C-O	-7.02	1.15	1.24
5	F	86	THR	C-O	-7.02	1.14	1.23
1	A	847	ASP	CG-OD2	7.02	1.38	1.25
3	C	79	GLN	CD-OE1	7.02	1.36	1.23
1	A	4	GLN	CA-C	7.02	1.62	1.52
1	A	1368	MET	SD-CE	-7.02	1.62	1.79
2	B	1130	PHE	C-O	-7.02	1.13	1.23
1	A	1359	ASP	CB-CG	7.01	1.69	1.52
2	B	613	VAL	CA-C	-7.01	1.44	1.52
2	B	233	PRO	C-O	-7.01	1.15	1.24
3	C	104	PHE	CA-C	-7.01	1.43	1.52
3	C	167	HIS	CA-CB	-7.01	1.42	1.53
2	B	1196	ILE	C-O	7.01	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	75	MET	CB-CG	-7.01	1.31	1.52
1	A	703	THR	C-O	-7.00	1.15	1.23
1	A	1142	THR	C-O	7.00	1.33	1.23
6	H	92	ASP	CA-CB	7.00	1.62	1.53
2	B	623	GLU	CA-C	-7.00	1.44	1.52
7	I	107	SER	CA-CB	-7.00	1.42	1.53
2	B	296	GLU	CD-OE1	7.00	1.38	1.25
2	B	608	ASP	CG-OD2	7.00	1.38	1.25
2	B	977	GLY	C-O	-7.00	1.14	1.24
3	C	48	SER	C-O	-7.00	1.14	1.23
1	A	612	ILE	CA-CB	-6.99	1.45	1.54
2	B	228	LYS	CB-CG	6.99	1.73	1.52
2	B	937	ALA	N-CA	6.99	1.55	1.46
1	A	23	SER	C-O	6.98	1.33	1.24
1	A	677	ARG	CZ-NH1	6.98	1.42	1.32
1	A	453	MET	SD-CE	6.98	1.97	1.79
2	B	119	LEU	N-CA	-6.98	1.38	1.46
4	E	52	ARG	CA-C	6.97	1.60	1.53
1	A	4	GLN	C-N	6.97	1.42	1.33
1	A	459	ARG	CA-CB	-6.97	1.43	1.53
2	B	404	LYS	CE-NZ	-6.97	1.28	1.49
3	C	50	GLU	CD-OE2	6.97	1.38	1.25
3	C	219	PHE	C-O	6.97	1.31	1.23
3	C	223	ALA	CA-CB	-6.97	1.41	1.53
1	A	346	ASP	CG-OD1	6.96	1.38	1.25
3	C	184	ASN	CA-C	-6.96	1.42	1.53
3	C	38	ILE	C-O	6.96	1.32	1.24
7	I	3	THR	CB-CG2	6.96	1.75	1.52
2	B	106	ASP	CA-CB	6.96	1.65	1.53
3	C	13	ALA	C-N	-6.95	1.24	1.33
2	B	1186	ASP	CA-CB	6.95	1.63	1.53
9	K	22	ASP	CB-CG	6.95	1.69	1.52
2	B	25	ILE	CA-C	-6.95	1.44	1.52
2	B	115	GLN	CA-C	6.95	1.62	1.52
2	B	945	GLU	C-O	6.95	1.32	1.23
1	A	412	ARG	N-CA	-6.94	1.37	1.46
4	E	66	GLU	CA-CB	6.94	1.64	1.53
1	A	826	ASP	CA-C	-6.94	1.43	1.52
1	A	704	ALA	C-O	6.94	1.32	1.23
9	K	46	ILE	C-N	-6.93	1.25	1.33
1	A	393	ARG	NE-CZ	6.93	1.40	1.33
1	A	1291	VAL	CB-CG1	-6.93	1.29	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1429	ILE	CA-C	-6.93	1.43	1.52
6	H	88	SER	CA-CB	6.93	1.65	1.53
1	A	1385	THR	CB-CG2	6.92	1.75	1.52
3	C	123	ASN	C-O	-6.92	1.15	1.24
2	B	668	ASP	CB-CG	6.92	1.69	1.52
3	C	103	ALA	CA-C	-6.92	1.43	1.52
2	B	236	HIS	CA-C	-6.92	1.44	1.52
1	A	514	PRO	CA-C	-6.92	1.40	1.52
1	A	1344	GLY	C-O	-6.92	1.15	1.23
7	I	57	GLY	C-O	-6.92	1.14	1.24
1	A	590	ARG	N-CA	-6.91	1.37	1.46
1	A	1312	ASN	C-O	-6.91	1.15	1.23
1	A	979	SER	C-O	-6.91	1.14	1.23
2	B	57	TYR	CA-CB	6.91	1.65	1.53
2	B	852	ARG	C-O	-6.91	1.15	1.23
1	A	536	LEU	C-O	6.91	1.33	1.23
2	B	1041	GLU	CD-OE1	6.91	1.38	1.25
9	K	63	VAL	CB-CG1	-6.90	1.29	1.52
7	I	119	THR	CA-CB	6.90	1.64	1.53
9	K	21	ILE	CA-CB	-6.90	1.46	1.54
10	L	26	THR	CB-CG2	6.90	1.75	1.52
1	A	65	LEU	CA-CB	6.90	1.65	1.53
1	A	971	PHE	CA-C	6.90	1.62	1.52
2	B	622	LYS	CE-NZ	6.90	1.70	1.49
1	A	74	MET	CA-CB	6.90	1.65	1.53
1	A	708	MET	N-CA	-6.89	1.38	1.46
2	B	204	ILE	C-O	-6.89	1.16	1.24
3	C	138	GLU	C-N	6.89	1.40	1.33
2	B	55	VAL	C-O	6.89	1.30	1.24
3	C	220	ASP	N-CA	-6.89	1.38	1.46
2	B	178	ASN	CG-OD1	6.89	1.36	1.23
2	B	227	LYS	CE-NZ	6.89	1.70	1.49
2	B	1202	LEU	N-CA	6.89	1.54	1.46
7	I	30	ARG	C-O	-6.89	1.14	1.24
1	A	1020	CYS	C-O	6.88	1.32	1.24
10	L	61	THR	CB-CG2	6.88	1.75	1.52
1	A	946	VAL	C-O	-6.88	1.16	1.24
5	F	106	PRO	C-O	-6.88	1.16	1.23
1	A	1164	PRO	CG-CD	6.88	1.74	1.50
2	B	430	ARG	NE-CZ	6.88	1.40	1.33
2	B	1102	LYS	CA-CB	6.88	1.66	1.54
3	C	7	GLN	CD-OE1	6.88	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	198	ILE	CA-CB	-6.88	1.45	1.54
2	B	387	LEU	CB-CG	-6.88	1.39	1.53
2	B	510	LYS	N-CA	6.88	1.55	1.46
2	B	967	ARG	CA-C	-6.88	1.44	1.52
2	B	459	TYR	CE2-CZ	6.88	1.54	1.38
9	K	92	ASN	C-O	-6.88	1.15	1.24
1	A	607	ILE	CB-CG1	-6.88	1.39	1.53
2	B	702	LEU	CG-CD2	-6.88	1.29	1.52
4	E	179	GLN	CG-CD	-6.88	1.34	1.52
1	A	434	ARG	CD-NE	-6.88	1.36	1.46
2	B	327	ARG	NE-CZ	-6.87	1.25	1.33
2	B	1041	GLU	CD-OE2	6.87	1.38	1.25
4	E	212	ARG	CZ-NH1	-6.87	1.23	1.32
6	H	35	GLN	CA-C	6.87	1.60	1.52
1	A	879	GLU	CD-OE1	6.87	1.38	1.25
1	A	670	ILE	C-O	-6.87	1.16	1.24
1	A	1212	VAL	CA-CB	-6.87	1.46	1.54
1	A	1223	ASP	CG-OD1	6.87	1.38	1.25
2	B	1058	LEU	C-O	6.87	1.32	1.24
2	B	986	GLN	CB-CG	6.86	1.73	1.52
4	E	77	SER	C-O	-6.86	1.15	1.24
1	A	1132	LYS	CD-CE	6.86	1.73	1.52
8	J	48	ARG	CG-CD	-6.86	1.31	1.52
1	A	973	ILE	CB-CG2	6.86	1.75	1.52
3	C	64	ALA	CA-CB	-6.86	1.42	1.53
1	A	361	LEU	N-CA	6.86	1.55	1.46
1	A	422	GLY	C-O	-6.86	1.16	1.23
1	A	532	ARG	C-O	-6.86	1.16	1.24
3	C	222	LYS	CG-CD	6.86	1.73	1.52
2	B	317	CYS	C-O	-6.86	1.16	1.24
3	C	192	TRP	CE3-CZ3	-6.86	1.18	1.38
1	A	451	HIS	N-CA	-6.85	1.37	1.45
1	A	443	LEU	CA-C	-6.85	1.44	1.52
1	A	777	PHE	CD1-CE1	6.85	1.59	1.38
2	B	18	PHE	CA-CB	6.85	1.67	1.53
2	B	963	PHE	CD2-CE2	6.85	1.59	1.38
4	E	114	ASN	CA-C	-6.85	1.44	1.52
7	I	109	ILE	CA-CB	6.85	1.63	1.54
1	A	920	LEU	CA-CB	-6.85	1.42	1.53
1	A	1143	LEU	C-O	6.85	1.32	1.24
1	A	720	ARG	CA-CB	6.85	1.64	1.53
1	A	825	ILE	C-O	-6.85	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	95	CYS	CA-C	6.85	1.61	1.52
1	A	570	PRO	CA-C	6.85	1.62	1.52
2	B	390	LEU	CA-C	6.84	1.62	1.52
2	B	1176	ASN	N-CA	6.84	1.54	1.46
3	C	148	ARG	N-CA	-6.84	1.37	1.45
6	H	126	GLU	N-CA	6.84	1.54	1.45
8	J	6	ARG	N-CA	6.84	1.54	1.45
2	B	198	ASP	C-O	-6.83	1.15	1.23
2	B	662	MET	CG-SD	-6.83	1.63	1.80
4	E	34	GLU	C-O	-6.83	1.16	1.24
6	H	17	PRO	C-O	-6.83	1.16	1.23
2	B	325	GLN	CA-CB	-6.83	1.43	1.53
2	B	1097	HIS	CE1-NE2	6.83	1.39	1.32
6	H	63	LEU	C-O	6.82	1.37	1.23
1	A	1143	LEU	N-CA	6.82	1.54	1.46
2	B	406	LEU	CA-C	6.82	1.60	1.52
6	H	77	ARG	NE-CZ	6.82	1.40	1.33
1	A	462	VAL	C-O	6.82	1.31	1.24
1	A	894	GLU	C-N	6.82	1.42	1.33
3	C	122	SER	CB-OG	6.82	1.55	1.42
1	A	714	PHE	CD2-CE2	-6.82	1.18	1.38
4	E	5	ASN	CA-C	-6.82	1.43	1.52
2	B	413	LEU	C-O	-6.81	1.13	1.24
2	B	1215	ARG	CG-CD	6.81	1.72	1.52
3	C	149	LYS	C-N	6.81	1.41	1.33
3	C	250	THR	CA-C	6.81	1.61	1.52
1	A	1154	TYR	CE2-CZ	6.81	1.54	1.38
1	A	1258	HIS	CA-C	-6.81	1.43	1.52
1	A	1269	GLU	C-N	-6.81	1.25	1.33
2	B	523	CYS	C-O	-6.81	1.14	1.24
4	E	128	PRO	CA-CB	6.81	1.63	1.54
1	A	671	ALA	CA-C	6.80	1.61	1.52
4	E	69	ILE	N-CA	6.80	1.55	1.46
6	H	141	TYR	CE1-CZ	-6.80	1.22	1.38
1	A	496	GLU	CG-CD	6.79	1.69	1.52
1	A	1277	GLU	N-CA	6.79	1.54	1.46
1	A	681	GLU	CG-CD	6.79	1.69	1.52
1	A	829	VAL	CA-C	6.79	1.61	1.52
1	A	1212	VAL	C-O	-6.79	1.16	1.24
2	B	188	ASP	N-CA	-6.79	1.37	1.46
2	B	604	ARG	CD-NE	-6.79	1.36	1.46
2	B	883	LEU	CA-C	6.79	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	763	GLN	C-N	-6.79	1.24	1.33
4	E	58	MET	CA-C	6.79	1.61	1.52
7	I	40	SER	CA-C	-6.79	1.44	1.52
4	E	162	ARG	CD-NE	6.79	1.55	1.46
7	I	51	ASN	C-O	-6.79	1.14	1.23
1	A	833	GLU	CG-CD	6.79	1.69	1.52
1	A	1414	ALA	N-CA	-6.79	1.37	1.46
2	B	329	THR	N-CA	-6.79	1.37	1.46
7	I	21	GLU	C-N	-6.79	1.24	1.33
2	B	274	PRO	CA-CB	6.78	1.62	1.53
3	C	95	CYS	C-O	-6.78	1.14	1.24
1	A	1029	ARG	CA-CB	-6.78	1.42	1.53
9	K	6	ARG	CB-CG	-6.78	1.32	1.52
1	A	1141	THR	CB-CG2	-6.78	1.30	1.52
1	A	905	ASP	CA-CB	-6.78	1.42	1.53
2	B	635	ARG	C-O	-6.78	1.17	1.24
1	A	1157	ASP	CB-CG	6.78	1.69	1.52
2	B	880	THR	N-CA	6.78	1.54	1.46
6	H	141	TYR	CA-C	-6.78	1.43	1.53
2	B	1100	ASP	CA-C	6.77	1.62	1.52
2	B	1157	ALA	CA-CB	6.77	1.63	1.52
7	I	20	LYS	CD-CE	6.77	1.72	1.52
7	I	108	HIS	N-CA	-6.77	1.37	1.46
1	A	386	ASP	CG-OD1	6.77	1.38	1.25
5	F	125	LEU	CA-C	-6.77	1.43	1.52
1	A	993	LEU	CA-C	-6.77	1.44	1.52
1	A	292	ALA	CA-C	-6.76	1.44	1.52
2	B	310	MET	SD-CE	-6.76	1.62	1.79
2	B	1069	PHE	CE2-CZ	-6.76	1.18	1.38
7	I	93	LYS	C-O	6.76	1.32	1.24
6	H	5	LEU	CA-C	-6.76	1.43	1.52
4	E	146	HIS	CA-C	-6.76	1.43	1.52
7	I	60	GLN	C-N	-6.76	1.24	1.33
9	K	110	ASN	CB-CG	6.76	1.69	1.52
6	H	113	ALA	N-CA	6.75	1.54	1.46
1	A	1366	ARG	N-CA	-6.75	1.37	1.46
2	B	704	ALA	CA-CB	-6.75	1.43	1.53
4	E	14	ARG	CZ-NH2	-6.75	1.24	1.33
2	B	138	GLU	N-CA	6.75	1.59	1.46
2	B	832	GLY	CA-C	-6.75	1.42	1.51
2	B	833	TYR	CE1-CZ	-6.75	1.22	1.38
2	B	989	THR	CA-CB	-6.75	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	49	SER	N-CA	6.75	1.55	1.46
1	A	676	MET	N-CA	-6.75	1.37	1.46
7	I	17	ARG	C-O	-6.75	1.16	1.23
1	A	1366	ARG	CD-NE	-6.75	1.36	1.46
1	A	396	PRO	CA-C	-6.75	1.40	1.52
1	A	726	ARG	N-CA	-6.75	1.38	1.46
4	E	67	GLU	C-O	6.75	1.32	1.24
7	I	15	TYR	CA-C	6.74	1.61	1.52
1	A	24	PRO	CG-CD	-6.74	1.27	1.50
1	A	659	HIS	CA-CB	-6.74	1.43	1.53
1	A	874	ASP	C-O	-6.74	1.16	1.23
5	F	109	VAL	N-CA	-6.74	1.37	1.46
9	K	39	ASP	CA-CB	-6.74	1.48	1.54
1	A	1070	GLN	N-CA	-6.74	1.37	1.46
2	B	212	LEU	CA-CB	-6.73	1.43	1.53
1	A	945	GLU	CD-OE2	6.73	1.38	1.25
5	F	91	ALA	CA-C	-6.73	1.43	1.52
2	B	535	LEU	CG-CD1	-6.73	1.30	1.52
2	B	279	ASP	CG-OD1	6.73	1.38	1.25
4	E	148	GLU	CA-C	-6.73	1.43	1.52
2	B	52	ASN	CA-CB	-6.73	1.42	1.53
7	I	18	GLU	CA-C	6.73	1.61	1.52
1	A	763	ALA	CA-C	-6.72	1.47	1.52
1	A	709	THR	CB-CG2	-6.72	1.30	1.52
2	B	955	THR	CA-C	-6.72	1.44	1.53
9	K	28	PRO	C-O	-6.72	1.16	1.23
1	A	688	LYS	C-O	-6.72	1.15	1.24
3	C	189	THR	C-O	-6.72	1.15	1.23
1	A	756	ILE	CB-CG2	-6.72	1.30	1.52
2	B	853	SER	CB-OG	6.72	1.55	1.42
1	A	237	THR	CA-CB	-6.72	1.42	1.53
1	A	1155	ASP	CA-CB	-6.72	1.44	1.53
1	A	1235	LYS	CE-NZ	6.72	1.69	1.49
10	L	46	VAL	C-O	-6.72	1.16	1.24
2	B	1000	PRO	N-CA	-6.71	1.39	1.46
7	I	3	THR	CA-C	-6.71	1.44	1.53
10	L	42	ARG	CA-C	6.71	1.60	1.52
2	B	1208	MET	CA-C	6.71	1.61	1.52
5	F	116	ASP	N-CA	6.71	1.55	1.46
1	A	607	ILE	C-O	6.71	1.31	1.23
1	A	1215	ARG	CA-C	-6.71	1.44	1.52
1	A	986	ILE	CA-C	-6.71	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	961	LEU	CA-C	6.71	1.61	1.52
2	B	22	SER	C-O	-6.71	1.14	1.24
2	B	993	THR	N-CA	6.71	1.53	1.45
2	B	1034	VAL	C-O	-6.70	1.16	1.24
2	B	1130	PHE	N-CA	-6.70	1.35	1.46
1	A	302	THR	CA-CB	6.70	1.64	1.53
2	B	854	LEU	C-O	-6.70	1.16	1.23
4	E	70	SER	C-N	6.70	1.42	1.33
1	A	23	SER	CA-C	6.70	1.61	1.52
2	B	453	ILE	CA-CB	6.69	1.63	1.54
7	I	13	MET	N-CA	-6.69	1.37	1.45
1	A	71	GLN	CG-CD	6.69	1.68	1.52
2	B	568	ASP	C-O	-6.69	1.15	1.24
4	E	66	GLU	CD-OE1	6.69	1.38	1.25
1	A	1268	LEU	CA-CB	-6.69	1.42	1.53
2	B	622	LYS	CA-C	6.69	1.61	1.53
4	E	136	ASN	CG-ND2	6.69	1.47	1.33
1	A	926	GLN	CD-OE1	6.69	1.36	1.23
1	A	1036	ARG	CZ-NH1	6.69	1.42	1.32
1	A	1419	ASP	CA-C	-6.69	1.44	1.52
2	B	1171	VAL	CA-C	6.69	1.60	1.52
4	E	92	THR	N-CA	6.69	1.54	1.46
5	F	135	ARG	CA-C	6.69	1.61	1.52
1	A	1009	ASN	C-O	6.68	1.31	1.24
7	I	8	ARG	CZ-NH1	6.68	1.42	1.32
9	K	100	ALA	CA-C	-6.68	1.44	1.52
1	A	1171	GLN	CA-CB	6.68	1.64	1.53
2	B	599	THR	CA-CB	-6.68	1.43	1.53
2	B	1163	CYS	CA-C	6.68	1.61	1.52
7	I	30	ARG	CA-CB	-6.68	1.42	1.53
1	A	1315	GLU	CA-C	-6.68	1.43	1.52
2	B	667	GLN	CD-OE1	6.68	1.36	1.23
3	C	39	ALA	C-O	6.68	1.32	1.23
6	H	3	ASN	CB-CG	6.67	1.68	1.52
1	A	654	ASN	C-O	-6.67	1.16	1.24
2	B	347	LYS	N-CA	-6.67	1.38	1.46
2	B	486	TYR	C-O	-6.67	1.16	1.24
4	E	83	CYS	CA-C	-6.67	1.44	1.52
5	F	85	MET	C-O	-6.67	1.15	1.23
2	B	169	ARG	CA-C	6.67	1.60	1.52
1	A	386	ASP	CB-CG	6.67	1.68	1.52
1	A	652	VAL	N-CA	-6.67	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1450	LEU	CA-CB	6.67	1.66	1.53
2	B	566	LEU	C-O	-6.67	1.16	1.24
4	E	92	THR	CA-CB	6.67	1.63	1.53
10	L	49	LYS	N-CA	6.67	1.54	1.46
3	C	82	TYR	N-CA	6.67	1.54	1.46
1	A	843	LYS	CA-CB	6.66	1.63	1.53
1	A	1036	ARG	CA-C	-6.66	1.44	1.53
5	F	137	TYR	CA-CB	-6.66	1.43	1.53
3	C	40	GLU	CD-OE2	6.66	1.38	1.25
3	C	210	GLU	C-O	-6.66	1.15	1.23
2	B	702	LEU	C-O	6.66	1.31	1.23
3	C	22	LEU	CA-C	-6.66	1.44	1.52
7	I	45	ARG	CA-C	6.66	1.60	1.52
7	I	86	PHE	N-CA	-6.66	1.37	1.45
1	A	688	LYS	CD-CE	6.66	1.72	1.52
1	A	1277	GLU	CA-CB	6.66	1.64	1.53
10	L	63	ARG	NE-CZ	6.66	1.40	1.33
3	C	230	MET	C-O	-6.65	1.15	1.23
9	K	107	THR	CA-C	-6.65	1.44	1.52
1	A	1316	VAL	CB-CG2	-6.65	1.30	1.52
1	A	389	THR	C-O	6.65	1.31	1.24
1	A	1233	ASP	C-O	-6.65	1.15	1.24
4	E	26	ARG	N-CA	6.65	1.54	1.46
1	A	735	VAL	C-O	-6.64	1.16	1.24
2	B	49	ASP	C-N	-6.64	1.24	1.33
1	A	820	GLY	CA-C	-6.64	1.44	1.52
1	A	1136	SER	N-CA	-6.64	1.37	1.46
2	B	57	TYR	CA-C	6.64	1.61	1.52
2	B	417	PHE	CA-C	6.63	1.62	1.52
5	F	94	LEU	CA-C	-6.63	1.43	1.52
6	H	52	GLN	C-O	-6.63	1.15	1.24
1	A	720	ARG	CD-NE	6.63	1.55	1.46
1	A	737	LEU	CA-C	-6.63	1.44	1.52
1	A	982	THR	CB-OG1	-6.63	1.33	1.43
1	A	1035	TYR	CA-CB	6.63	1.64	1.53
2	B	820	GLY	N-CA	-6.63	1.38	1.45
2	B	370	PHE	CD2-CE2	6.63	1.58	1.38
3	C	142	VAL	N-CA	-6.63	1.38	1.46
7	I	82	GLU	CG-CD	6.63	1.68	1.52
7	I	94	ASP	CA-CB	6.62	1.63	1.53
1	A	969	GLN	CG-CD	6.62	1.68	1.52
4	E	17	ARG	CZ-NH2	6.62	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	408	ASP	N-CA	-6.62	1.37	1.46
4	E	203	GLU	CA-CB	-6.62	1.42	1.53
4	E	207	ARG	NE-CZ	6.62	1.40	1.33
6	H	128	ASN	CA-C	6.62	1.61	1.52
1	A	387	ARG	CD-NE	6.62	1.55	1.46
4	E	37	LEU	CG-CD2	6.62	1.74	1.52
2	B	327	ARG	CB-CG	-6.61	1.32	1.52
2	B	1035	ALA	N-CA	-6.61	1.38	1.46
2	B	1141	HIS	CA-C	6.61	1.61	1.52
3	C	10	ILE	N-CA	-6.60	1.38	1.46
3	C	154	LYS	CB-CG	6.60	1.72	1.52
7	I	48	LEU	CG-CD2	-6.60	1.30	1.52
2	B	198	ASP	CA-C	-6.60	1.44	1.52
2	B	1218	THR	CA-CB	-6.60	1.42	1.53
2	B	47	GLN	CA-C	6.60	1.61	1.52
2	B	325	GLN	CB-CG	-6.60	1.32	1.52
2	B	626	ILE	N-CA	-6.60	1.38	1.46
2	B	654	ARG	CA-CB	-6.60	1.42	1.53
2	B	1090	THR	N-CA	-6.60	1.37	1.45
1	A	402	ALA	N-CA	6.60	1.54	1.46
2	B	497	ARG	C-O	-6.60	1.15	1.23
1	A	700	ASN	CA-C	-6.60	1.43	1.53
1	A	18	GLN	CA-C	-6.59	1.44	1.52
1	A	745	GLN	C-O	-6.59	1.15	1.24
2	B	114	PRO	CG-CD	-6.59	1.28	1.50
2	B	581	PHE	CG-CD1	-6.59	1.25	1.38
2	B	608	ASP	CA-C	-6.59	1.43	1.52
2	B	638	PHE	CA-C	-6.59	1.44	1.52
2	B	909	ASP	C-O	-6.59	1.15	1.24
4	E	20	LYS	CD-CE	6.59	1.72	1.52
1	A	1269	GLU	C-O	-6.59	1.15	1.23
6	H	80	ARG	C-O	-6.59	1.18	1.24
7	I	13	MET	C-O	-6.59	1.15	1.23
1	A	1373	ASP	CG-OD2	6.59	1.37	1.25
1	A	1450	LEU	CA-C	6.59	1.66	1.52
9	K	90	ALA	CA-CB	-6.59	1.43	1.53
3	C	4	GLU	CA-C	-6.58	1.44	1.52
1	A	1064	VAL	CA-C	-6.58	1.42	1.52
1	A	49	LYS	CA-C	6.58	1.61	1.52
1	A	471	ASN	C-N	-6.58	1.25	1.33
1	A	839	ARG	CG-CD	6.58	1.72	1.52
1	A	914	GLU	CD-OE1	6.58	1.37	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1064	VAL	CB-CG1	-6.58	1.30	1.52
1	A	1209	MET	CA-CB	-6.58	1.43	1.53
2	B	762	ASN	C-O	-6.58	1.15	1.24
3	C	238	ILE	C-O	-6.58	1.16	1.24
3	C	138	GLU	C-O	6.58	1.32	1.24
1	A	941	LYS	CB-CG	-6.58	1.32	1.52
9	K	55	LYS	CB-CG	6.58	1.72	1.52
1	A	91	PHE	CG-CD1	-6.58	1.25	1.38
1	A	393	ARG	CD-NE	6.58	1.55	1.46
2	B	137	TYR	CG-CD1	6.58	1.53	1.39
2	B	350	GLN	CA-CB	-6.58	1.42	1.53
2	B	761	HIS	CA-C	-6.57	1.44	1.52
6	H	118	PHE	CD2-CE2	6.57	1.58	1.38
7	I	25	LEU	CA-CB	6.57	1.62	1.53
2	B	850	LEU	C-O	-6.57	1.16	1.23
3	C	214	ASN	CA-C	6.57	1.60	1.52
7	I	55	THR	CA-CB	-6.57	1.42	1.53
1	A	741	ASN	C-O	-6.57	1.16	1.24
2	B	115	GLN	C-O	-6.57	1.16	1.24
2	B	352	ALA	CA-C	-6.57	1.44	1.52
5	F	121	ALA	C-O	-6.57	1.16	1.24
1	A	53	LEU	CG-CD1	6.57	1.74	1.52
1	A	943	LEU	N-CA	-6.57	1.38	1.46
8	J	29	GLU	CA-C	6.57	1.62	1.53
3	C	3	GLU	CD-OE1	6.56	1.37	1.25
7	I	109	ILE	N-CA	-6.56	1.38	1.46
1	A	513	SER	C-O	-6.56	1.17	1.24
1	A	962	ARG	C-O	-6.56	1.15	1.24
1	A	1193	LEU	CA-CB	6.56	1.62	1.53
2	B	1044	ALA	CA-C	6.56	1.61	1.52
2	B	329	THR	CB-OG1	-6.56	1.33	1.43
1	A	49	LYS	CD-CE	6.56	1.72	1.52
2	B	684	LEU	C-N	-6.56	1.25	1.33
9	K	14	GLU	CA-C	6.56	1.61	1.52
3	C	196	ASP	CG-OD1	6.56	1.37	1.25
1	A	87	ALA	C-O	-6.55	1.16	1.24
2	B	658	ILE	CA-C	-6.55	1.43	1.52
2	B	898	LEU	CA-C	-6.55	1.44	1.52
1	A	1187	GLN	C-O	6.55	1.36	1.23
6	H	57	VAL	CA-C	6.55	1.61	1.52
1	A	1133	LEU	CA-C	-6.55	1.44	1.52
5	F	100	GLN	CG-CD	6.55	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	624	SER	CA-CB	6.55	1.62	1.53
1	A	881	GLN	N-CA	-6.55	1.37	1.45
7	I	10	CYS	CA-C	-6.55	1.43	1.52
1	A	479	ASN	CA-CB	-6.55	1.43	1.53
1	A	1159	ARG	C-O	-6.55	1.15	1.24
1	A	1092	LYS	CB-CG	6.54	1.72	1.52
1	A	598	LEU	CA-C	6.54	1.61	1.53
2	B	216	GLU	C-O	-6.54	1.16	1.24
2	B	103	ASN	C-O	6.54	1.32	1.24
6	H	3	ASN	CA-CB	6.54	1.62	1.53
3	C	54	ASN	CA-C	-6.54	1.46	1.53
1	A	1340	GLY	CA-C	-6.53	1.44	1.52
9	K	96	ASN	CA-C	-6.53	1.44	1.52
4	E	82	PHE	C-O	-6.53	1.15	1.23
9	K	21	ILE	N-CA	6.53	1.53	1.46
1	A	244	PRO	C-N	6.53	1.43	1.33
5	F	96	THR	N-CA	-6.53	1.38	1.46
8	J	37	SER	CA-CB	-6.53	1.41	1.53
1	A	788	SER	CA-CB	6.53	1.63	1.53
2	B	538	ASN	CA-CB	-6.53	1.41	1.53
2	B	916	THR	CB-CG2	6.53	1.74	1.52
1	A	32	VAL	C-O	6.53	1.31	1.24
3	C	68	GLY	N-CA	6.53	1.54	1.45
4	E	34	GLU	CD-OE1	6.53	1.37	1.25
1	A	819	GLY	C-O	-6.52	1.16	1.23
1	A	1112	LYS	CG-CD	6.52	1.72	1.52
1	A	1267	MET	CA-C	-6.51	1.44	1.52
2	B	698	GLU	C-N	-6.51	1.25	1.33
2	B	1103	ILE	N-CA	6.51	1.54	1.46
2	B	1033	LYS	CA-C	6.51	1.61	1.52
6	H	119	GLY	C-O	6.51	1.32	1.23
2	B	200	GLY	C-N	-6.51	1.24	1.33
2	B	740	HIS	C-O	-6.51	1.15	1.23
7	I	25	LEU	CG-CD2	-6.51	1.31	1.52
3	C	260	LEU	CG-CD2	6.51	1.74	1.52
4	E	69	ILE	CA-CB	-6.51	1.45	1.54
2	B	246	LYS	CA-CB	6.50	1.63	1.53
6	H	116	TYR	C-O	6.50	1.32	1.24
2	B	384	ARG	CB-CG	6.50	1.72	1.52
3	C	209	TYR	C-O	-6.50	1.15	1.24
2	B	50	SER	CB-OG	-6.50	1.29	1.42
3	C	94	LYS	CB-CG	6.50	1.72	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	66	GLN	CD-OE1	6.50	1.35	1.23
1	A	291	GLU	CD-OE1	6.50	1.37	1.25
2	B	965	LYS	CA-C	-6.50	1.44	1.52
3	C	13	ALA	CA-CB	-6.50	1.43	1.53
3	C	161	LYS	CD-CE	-6.49	1.32	1.52
1	A	1307	GLU	N-CA	-6.49	1.37	1.46
2	B	447	ALA	C-N	6.49	1.41	1.33
2	B	540	SER	C-O	-6.49	1.15	1.24
1	A	1235	LYS	CD-CE	6.49	1.72	1.52
1	A	434	ARG	C-O	-6.49	1.15	1.23
1	A	608	ILE	CA-CB	6.49	1.64	1.54
2	B	823	ALA	CA-CB	-6.49	1.43	1.53
2	B	285	ILE	CA-C	6.49	1.61	1.52
3	C	137	LYS	CD-CE	6.49	1.72	1.52
2	B	1047	PHE	CA-CB	-6.49	1.43	1.53
3	C	243	VAL	CA-C	-6.49	1.44	1.52
4	E	205	SER	N-CA	6.48	1.55	1.45
1	A	432	VAL	N-CA	-6.48	1.38	1.46
1	A	1014	ALA	CA-C	6.48	1.61	1.52
2	B	836	GLU	C-N	6.48	1.43	1.33
3	C	9	LYS	CD-CE	6.48	1.71	1.52
9	K	50	LEU	CG-CD2	-6.48	1.31	1.52
9	K	56	VAL	CA-C	6.48	1.60	1.53
6	H	97	MET	CA-CB	-6.48	1.44	1.53
1	A	787	PHE	CG-CD1	-6.48	1.25	1.38
2	B	189	LEU	N-CA	6.48	1.54	1.46
1	A	661	GLY	C-O	6.47	1.31	1.23
1	A	1221	LYS	CA-CB	6.47	1.64	1.53
2	B	434	ARG	CA-C	6.47	1.61	1.52
2	B	987	LYS	CA-CB	-6.47	1.43	1.53
2	B	1215	ARG	NE-CZ	-6.47	1.25	1.33
1	A	800	VAL	CA-CB	-6.47	1.46	1.53
2	B	336	ARG	CA-C	-6.47	1.43	1.52
2	B	1106	ARG	N-CA	6.47	1.55	1.46
1	A	367	PRO	N-CA	-6.47	1.39	1.47
2	B	661	LEU	CA-C	-6.47	1.44	1.52
2	B	848	ARG	CA-CB	-6.47	1.43	1.53
2	B	711	GLU	C-O	6.46	1.32	1.24
3	C	12	GLU	CD-OE1	6.46	1.37	1.25
2	B	1062	HIS	C-O	6.46	1.32	1.24
2	B	226	PHE	CG-CD2	6.46	1.52	1.38
2	B	249	ARG	C-N	6.46	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1085	ILE	CB-CG2	-6.46	1.31	1.52
1	A	745	GLN	CD-OE1	6.46	1.35	1.23
2	B	699	GLU	N-CA	-6.46	1.37	1.46
1	A	845	LEU	N-CA	6.46	1.54	1.46
7	I	28	GLU	N-CA	-6.46	1.38	1.45
6	H	101	ALA	CA-C	-6.46	1.44	1.52
1	A	372	LYS	C-O	-6.45	1.15	1.24
5	F	116	ASP	CA-C	-6.45	1.45	1.52
1	A	608	ILE	CB-CG2	-6.45	1.31	1.52
2	B	595	ARG	CA-C	-6.45	1.44	1.52
2	B	1060	ARG	N-CA	6.45	1.54	1.46
1	A	417	TYR	C-O	-6.45	1.15	1.24
7	I	93	LYS	CD-CE	6.45	1.71	1.52
1	A	421	ALA	N-CA	-6.45	1.38	1.46
2	B	734	HIS	C-O	6.45	1.34	1.23
2	B	986	GLN	C-O	6.45	1.31	1.24
3	C	208	GLU	CD-OE2	6.45	1.37	1.25
2	B	1151	LEU	CA-C	6.44	1.61	1.52
1	A	1030	ARG	CZ-NH2	-6.44	1.25	1.33
2	B	621	GLU	N-CA	-6.44	1.37	1.46
1	A	651	LYS	CA-C	6.44	1.61	1.52
1	A	580	VAL	CA-CB	-6.43	1.46	1.54
2	B	785	TYR	CE1-CZ	-6.43	1.22	1.38
8	J	62	ARG	C-O	-6.43	1.14	1.24
1	A	796	SER	N-CA	-6.43	1.38	1.46
2	B	344	LYS	C-O	6.43	1.31	1.23
2	B	911	ILE	CA-CB	6.43	1.63	1.54
9	K	95	ILE	C-O	6.43	1.32	1.24
1	A	517	ASN	CA-C	-6.43	1.44	1.53
1	A	986	ILE	CA-CB	-6.43	1.47	1.54
2	B	609	ILE	N-CA	6.43	1.54	1.46
3	C	57	VAL	C-O	-6.43	1.17	1.24
5	F	131	PRO	CA-CB	6.43	1.61	1.53
2	B	191	LYS	CA-C	-6.43	1.44	1.52
1	A	1167	GLU	CA-CB	6.42	1.63	1.53
6	H	124	ARG	CB-CG	-6.42	1.33	1.52
2	B	288	ALA	C-O	6.42	1.32	1.24
1	A	1217	LYS	N-CA	-6.42	1.38	1.46
2	B	935	ARG	NE-CZ	6.42	1.40	1.33
2	B	1050	ILE	C-N	-6.42	1.23	1.33
7	I	98	VAL	CA-CB	-6.42	1.48	1.54
9	K	81	TYR	CD2-CE2	-6.42	1.19	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	567	LYS	CD-CE	6.42	1.71	1.52
4	E	178	ILE	CA-C	6.42	1.60	1.52
1	A	1427	ASN	C-O	6.42	1.32	1.24
2	B	328	GLU	C-N	-6.42	1.24	1.33
2	B	1223	ASP	C-N	6.42	1.42	1.33
4	E	108	GLY	C-N	-6.42	1.24	1.33
1	A	590	ARG	CZ-NH2	-6.42	1.25	1.33
2	B	594	ALA	CA-C	-6.42	1.44	1.52
3	C	91	HIS	C-N	-6.42	1.25	1.33
10	L	26	THR	CA-C	6.41	1.61	1.52
1	A	773	LYS	CB-CG	-6.41	1.33	1.52
2	B	375	ALA	CA-CB	-6.41	1.43	1.53
1	A	718	VAL	C-O	-6.41	1.15	1.24
2	B	1178	ASN	CB-CG	-6.41	1.36	1.52
1	A	742	ASN	CA-C	6.41	1.61	1.52
1	A	944	ARG	N-CA	-6.41	1.37	1.46
1	A	1127	ASP	CG-OD2	6.41	1.37	1.25
2	B	657	HIS	CA-CB	-6.41	1.43	1.53
2	B	182	SER	CA-C	-6.40	1.44	1.52
2	B	610	ASN	CG-ND2	-6.40	1.19	1.33
2	B	449	ASN	CA-C	6.40	1.60	1.52
3	C	249	ASP	CA-CB	6.40	1.64	1.53
5	F	95	GLY	C-O	-6.40	1.15	1.23
1	A	840	ARG	C-O	-6.40	1.16	1.24
1	A	1341	ILE	CA-C	-6.40	1.44	1.52
2	B	91	SER	N-CA	6.40	1.54	1.46
2	B	499	ASN	CG-ND2	6.40	1.46	1.33
2	B	340	ALA	N-CA	-6.40	1.37	1.45
1	A	668	ASP	CA-C	6.40	1.61	1.52
1	A	1438	THR	CA-CB	-6.40	1.41	1.53
1	A	938	LYS	CA-C	-6.40	1.44	1.52
1	A	1036	ARG	C-N	-6.40	1.25	1.33
1	A	1266	THR	CA-C	6.39	1.61	1.52
1	A	1066	VAL	CA-CB	-6.39	1.47	1.54
2	B	866	TYR	N-CA	6.39	1.54	1.46
7	I	120	GLN	C-O	6.39	1.29	1.23
1	A	36	ARG	CA-C	-6.39	1.44	1.52
1	A	987	VAL	CB-CG1	-6.39	1.31	1.52
2	B	537	LYS	C-O	-6.39	1.15	1.23
4	E	73	PRO	CA-C	6.39	1.61	1.52
4	E	134	THR	C-O	-6.38	1.16	1.24
1	A	1148	ILE	C-O	-6.38	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1222	ASN	CA-C	6.38	1.61	1.52
2	B	632	ARG	NE-CZ	-6.38	1.26	1.33
3	C	119	VAL	N-CA	-6.38	1.38	1.46
1	A	1160	SER	CA-C	6.38	1.60	1.52
2	B	1002	THR	CB-OG1	-6.38	1.33	1.43
9	K	59	ALA	CA-C	-6.38	1.44	1.52
9	K	61	TYR	CE1-CZ	-6.38	1.23	1.38
2	B	436	VAL	N-CA	6.38	1.54	1.46
3	C	83	SER	N-CA	-6.38	1.38	1.46
1	A	1002	GLY	C-O	6.38	1.32	1.23
2	B	964	VAL	CA-CB	-6.38	1.44	1.55
2	B	634	TYR	CA-C	-6.38	1.44	1.52
2	B	959	ASP	CA-C	6.37	1.61	1.52
10	L	27	LEU	CG-CD1	6.37	1.73	1.52
1	A	969	GLN	CD-NE2	6.37	1.46	1.33
2	B	529	GLU	C-N	-6.37	1.24	1.33
7	I	89	GLN	C-O	-6.37	1.15	1.24
2	B	418	LYS	C-O	-6.37	1.16	1.24
2	B	394	ASP	CB-CG	6.37	1.68	1.52
2	B	449	ASN	C-O	6.37	1.31	1.24
2	B	536	VAL	C-O	6.37	1.31	1.24
3	C	15	LYS	CD-CE	6.37	1.71	1.52
1	A	789	LYS	CG-CD	-6.37	1.33	1.52
1	A	670	ILE	CA-C	6.37	1.60	1.52
2	B	706	GLN	CA-C	-6.37	1.45	1.52
1	A	539	THR	CA-CB	6.36	1.61	1.53
1	A	765	VAL	C-O	-6.36	1.16	1.23
1	A	1103	GLU	CD-OE2	6.36	1.37	1.25
2	B	195	CYS	C-O	-6.36	1.16	1.24
1	A	987	VAL	CA-CB	-6.36	1.47	1.54
4	E	191	LYS	CD-CE	6.36	1.71	1.52
2	B	553	PRO	C-N	6.36	1.42	1.33
2	B	893	LEU	CG-CD2	-6.36	1.31	1.52
1	A	1039	LYS	N-CA	6.36	1.54	1.46
2	B	42	GLY	C-O	6.36	1.32	1.23
3	C	70	ILE	C-N	-6.36	1.25	1.33
10	L	34	CYS	N-CA	6.36	1.54	1.46
1	A	1239	ARG	C-O	-6.36	1.16	1.24
2	B	635	ARG	CA-C	-6.35	1.45	1.52
2	B	598	GLU	N-CA	6.35	1.54	1.46
2	B	660	LYS	CG-CD	6.35	1.71	1.52
2	B	753	ALA	C-O	-6.35	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	245	GLU	CA-CB	6.35	1.64	1.53
2	B	1135	ARG	CD-NE	-6.35	1.37	1.46
7	I	50	THR	C-O	-6.35	1.16	1.23
10	L	50	ASP	CA-CB	6.35	1.64	1.53
2	B	284	ILE	CA-C	6.35	1.60	1.52
2	B	422	LYS	CB-CG	6.35	1.71	1.52
2	B	659	ALA	C-O	-6.35	1.16	1.24
2	B	685	LEU	CG-CD1	-6.35	1.31	1.52
7	I	97	MET	CA-CB	-6.35	1.44	1.53
1	A	290	GLU	CD-OE1	6.35	1.37	1.25
1	A	838	GLN	N-CA	-6.34	1.38	1.46
5	F	103	MET	CA-CB	-6.34	1.44	1.52
9	K	10	PHE	C-O	-6.34	1.15	1.24
2	B	869	SER	C-N	6.34	1.42	1.33
1	A	838	GLN	CD-OE1	6.34	1.35	1.23
5	F	130	ILE	CA-CB	-6.34	1.47	1.53
7	I	84	VAL	CB-CG2	-6.34	1.31	1.52
2	B	265	SER	CA-CB	6.34	1.63	1.53
2	B	638	PHE	C-O	-6.34	1.15	1.23
3	C	65	HIS	N-CA	-6.34	1.38	1.46
3	C	91	HIS	C-O	-6.34	1.15	1.23
5	F	119	ARG	N-CA	-6.34	1.38	1.46
2	B	1030	LEU	N-CA	-6.33	1.38	1.46
5	F	110	ASP	CG-OD1	6.33	1.37	1.25
6	H	6	PHE	CA-CB	-6.33	1.43	1.53
6	H	37	LYS	N-CA	6.33	1.53	1.45
6	H	12	VAL	CA-C	6.33	1.60	1.52
1	A	1383	SER	C-O	-6.33	1.15	1.23
2	B	230	ALA	C-N	6.33	1.41	1.34
2	B	1001	PHE	CA-C	-6.33	1.44	1.52
2	B	123	THR	CA-C	-6.33	1.46	1.53
3	C	240	VAL	CA-CB	6.33	1.61	1.54
2	B	328	GLU	CD-OE2	6.33	1.37	1.25
3	C	139	GLY	CA-C	6.33	1.58	1.51
4	E	121	MET	CA-C	6.33	1.61	1.52
9	K	93	SER	N-CA	6.33	1.54	1.46
10	L	63	ARG	CD-NE	6.33	1.55	1.46
10	L	69	ALA	CA-C	-6.33	1.44	1.53
2	B	70	ILE	CA-CB	6.33	1.71	1.54
2	B	685	LEU	N-CA	6.33	1.54	1.46
2	B	787	VAL	CA-C	-6.33	1.43	1.52
1	A	705	LYS	CA-C	-6.32	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	873	THR	CA-CB	6.32	1.64	1.53
4	E	201	LYS	CB-CG	6.32	1.71	1.52
6	H	56	THR	C-O	6.32	1.31	1.24
1	A	1141	THR	N-CA	6.32	1.54	1.46
2	B	1074	ASN	N-CA	-6.32	1.38	1.46
3	C	30	ALA	CA-CB	-6.32	1.43	1.53
3	C	102	GLN	CA-C	-6.32	1.44	1.52
3	C	201	TRP	CD2-CE3	-6.32	1.30	1.40
3	C	243	VAL	CA-CB	-6.32	1.46	1.54
8	J	6	ARG	C-O	-6.32	1.15	1.23
2	B	796	LEU	C-O	-6.32	1.16	1.23
2	B	205	ILE	CA-CB	-6.32	1.45	1.53
3	C	7	GLN	CA-CB	6.32	1.62	1.53
8	J	50	ILE	CA-C	-6.32	1.44	1.52
1	A	411	ASP	CG-OD1	6.32	1.37	1.25
1	A	806	ARG	CZ-NH2	6.32	1.41	1.33
2	B	1100	ASP	CB-CG	6.32	1.67	1.52
1	A	677	ARG	CD-NE	6.31	1.55	1.46
1	A	1255	GLU	N-CA	6.31	1.54	1.46
1	A	549	MET	CA-C	-6.31	1.44	1.52
1	A	1193	LEU	C-O	-6.31	1.16	1.24
1	A	1198	ASP	N-CA	6.31	1.53	1.46
2	B	1153	GLU	CD-OE2	6.31	1.37	1.25
1	A	568	PRO	CB-CG	-6.31	1.18	1.49
1	A	1194	ARG	CD-NE	-6.31	1.37	1.46
2	B	978	ASP	CB-CG	6.31	1.67	1.52
4	E	25	ASP	CA-C	-6.31	1.44	1.52
1	A	661	GLY	C-N	6.30	1.41	1.33
6	H	137	GLN	CB-CG	6.30	1.71	1.52
7	I	32	CYS	CB-SG	-6.30	1.60	1.81
7	I	111	THR	CB-OG1	-6.30	1.33	1.43
1	A	439	ASN	CA-CB	-6.30	1.45	1.54
1	A	1255	GLU	CA-C	6.30	1.61	1.52
5	F	110	ASP	CA-CB	6.30	1.61	1.53
7	I	100	PHE	CE1-CZ	-6.30	1.19	1.38
5	F	149	GLU	CA-CB	6.30	1.63	1.53
10	L	42	ARG	CD-NE	6.30	1.55	1.46
1	A	905	ASP	CG-OD2	6.29	1.37	1.25
2	B	827	ILE	CA-CB	-6.29	1.46	1.53
2	B	486	TYR	CG-CD1	6.29	1.52	1.39
3	C	16	ASP	C-O	-6.29	1.15	1.23
1	A	703	THR	CA-C	-6.29	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1040	GLN	CD-OE1	6.29	1.35	1.23
1	A	1427	ASN	CA-CB	-6.29	1.43	1.53
2	B	218	SER	C-N	-6.29	1.24	1.33
4	E	59	SER	N-CA	-6.29	1.38	1.46
2	B	191	LYS	CD-CE	6.29	1.71	1.52
2	B	91	SER	C-N	6.29	1.42	1.33
9	K	66	PRO	N-CD	-6.29	1.39	1.47
1	A	795	GLU	C-N	-6.29	1.25	1.34
3	C	40	GLU	CD-OE1	6.29	1.37	1.25
10	L	47	ARG	NE-CZ	6.29	1.40	1.33
4	E	79	TRP	CD2-CE3	6.28	1.50	1.40
1	A	420	ARG	CB-CG	-6.28	1.33	1.52
1	A	1144	LYS	C-O	-6.28	1.16	1.24
2	B	112	LEU	N-CA	6.28	1.53	1.46
2	B	643	ASP	CA-C	-6.28	1.39	1.52
2	B	880	THR	C-O	6.28	1.31	1.24
3	C	181	ASP	CA-CB	6.28	1.58	1.52
2	B	250	PHE	CA-CB	6.28	1.62	1.53
2	B	815	ARG	CD-NE	-6.28	1.37	1.46
6	H	26	ILE	CA-CB	-6.28	1.46	1.53
10	L	43	THR	N-CA	6.28	1.53	1.46
1	A	37	PHE	CD2-CE2	6.27	1.57	1.38
3	C	232	VAL	CA-CB	-6.27	1.46	1.54
1	A	1035	TYR	CG-CD1	-6.27	1.26	1.39
6	H	43	ASN	C-O	-6.27	1.16	1.23
1	A	1109	LYS	CD-CE	6.27	1.71	1.52
1	A	1196	GLU	C-O	-6.27	1.16	1.24
1	A	1377	THR	C-O	-6.27	1.15	1.24
2	B	21	GLU	C-O	-6.27	1.16	1.24
1	A	1078	GLN	CB-CG	6.27	1.71	1.52
2	B	763	GLN	CA-C	-6.27	1.45	1.52
9	K	54	ARG	CG-CD	6.27	1.71	1.52
1	A	411	ASP	N-CA	6.27	1.54	1.46
1	A	561	PRO	CA-CB	6.27	1.62	1.53
1	A	711	ARG	CB-CG	6.26	1.71	1.52
1	A	902	LEU	N-CA	-6.26	1.39	1.46
1	A	548	ASN	CA-C	6.26	1.61	1.52
2	B	862	GLN	CD-OE1	6.26	1.35	1.23
1	A	441	PRO	CA-CB	-6.26	1.45	1.53
2	B	422	LYS	CG-CD	6.26	1.71	1.52
1	A	5	GLN	CA-CB	6.26	1.63	1.53
1	A	709	THR	CA-C	-6.26	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	848	ILE	C-O	-6.26	1.17	1.24
7	I	11	ASN	CB-CG	-6.25	1.36	1.52
1	A	1140	HIS	CA-C	-6.25	1.44	1.52
1	A	1159	ARG	CA-CB	6.25	1.64	1.53
2	B	231	PRO	N-CA	6.25	1.55	1.47
1	A	847	ASP	C-O	-6.25	1.15	1.24
3	C	259	LEU	CA-CB	-6.25	1.43	1.53
1	A	347	PHE	C-O	-6.24	1.15	1.23
4	E	118	PRO	CA-CB	6.24	1.62	1.53
2	B	1169	MET	N-CA	-6.24	1.38	1.46
2	B	394	ASP	CG-OD2	6.24	1.37	1.25
2	B	1097	HIS	CG-ND1	6.24	1.45	1.38
2	B	49	ASP	CG-OD2	6.24	1.37	1.25
2	B	814	PHE	CA-C	-6.24	1.44	1.52
4	E	207	ARG	CG-CD	6.24	1.71	1.52
1	A	1289	ARG	CZ-NH2	-6.24	1.25	1.33
4	E	52	ARG	CB-CG	6.24	1.71	1.52
1	A	1019	CYS	CA-C	-6.24	1.44	1.52
4	E	170	LEU	N-CA	6.24	1.53	1.45
6	H	144	ILE	N-CA	6.24	1.53	1.46
5	F	127	GLU	CD-OE1	6.23	1.37	1.25
9	K	29	ASN	CG-ND2	6.23	1.46	1.33
3	C	192	TRP	C-O	-6.23	1.16	1.23
8	J	22	LEU	N-CA	-6.23	1.38	1.46
2	B	1035	ALA	C-O	6.23	1.31	1.24
1	A	438	ASP	C-O	-6.23	1.16	1.23
9	K	70	ARG	CA-C	-6.23	1.44	1.52
1	A	280	GLU	C-O	-6.23	1.16	1.24
1	A	1196	GLU	CA-CB	-6.23	1.44	1.53
1	A	1277	GLU	CD-OE1	6.23	1.37	1.25
4	E	103	LYS	CD-CE	6.23	1.71	1.52
2	B	797	TYR	N-CA	-6.22	1.39	1.46
1	A	787	PHE	CD1-CE1	6.22	1.57	1.38
1	A	1362	TYR	CG-CD2	-6.22	1.26	1.39
3	C	34	ARG	N-CA	6.22	1.53	1.46
2	B	961	LEU	CB-CG	6.22	1.65	1.53
1	A	821	ARG	NE-CZ	-6.22	1.26	1.33
2	B	1190	ASP	C-O	-6.22	1.16	1.24
3	C	129	ILE	N-CA	-6.22	1.39	1.46
8	J	31	ASP	CG-OD1	6.22	1.37	1.25
1	A	486	GLU	C-O	-6.22	1.16	1.23
2	B	323	VAL	CA-CB	-6.22	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	639	ILE	C-N	-6.22	1.25	1.33
6	H	19	ARG	CB-CG	6.22	1.71	1.52
1	A	1288	ASP	N-CA	6.21	1.54	1.46
7	I	72	ASP	C-O	-6.21	1.16	1.24
1	A	1202	MET	CG-SD	-6.21	1.65	1.80
5	F	79	ARG	CD-NE	-6.21	1.37	1.46
7	I	8	ARG	CA-C	6.21	1.60	1.52
3	C	181	ASP	N-CA	-6.21	1.40	1.46
1	A	724	GLU	CD-OE2	6.21	1.37	1.25
1	A	734	GLU	CG-CD	6.21	1.67	1.52
2	B	513	GLN	C-O	-6.21	1.15	1.23
1	A	858	ASN	C-O	-6.21	1.16	1.23
2	B	699	GLU	CA-C	-6.21	1.44	1.52
6	H	85	GLY	CA-C	6.21	1.60	1.51
1	A	1280	GLU	CG-CD	6.21	1.67	1.52
2	B	1133	MET	CA-CB	-6.21	1.43	1.53
2	B	340	ALA	CA-C	6.20	1.61	1.53
2	B	370	PHE	CA-CB	6.20	1.64	1.53
6	H	14	GLU	CA-C	-6.20	1.44	1.52
2	B	268	THR	N-CA	-6.20	1.38	1.45
2	B	602	THR	CB-CG2	-6.20	1.32	1.52
6	H	89	LEU	CA-C	6.20	1.61	1.52
1	A	1056	SER	CA-CB	-6.20	1.42	1.53
5	F	111	LEU	N-CA	-6.20	1.39	1.46
7	I	113	ASP	CA-C	-6.20	1.45	1.52
1	A	923	LEU	CA-C	-6.20	1.44	1.52
3	C	177	GLU	C-O	-6.20	1.16	1.23
9	K	20	LYS	CD-CE	6.20	1.71	1.52
5	F	76	LYS	C-O	-6.19	1.16	1.24
1	A	965	GLN	CD-OE1	6.19	1.35	1.23
2	B	265	SER	C-O	6.19	1.31	1.23
3	C	154	LYS	CA-C	-6.19	1.45	1.52
2	B	55	VAL	CA-CB	-6.19	1.47	1.54
2	B	830	TYR	CA-CB	6.19	1.62	1.52
3	C	178	PHE	CG-CD2	-6.19	1.25	1.38
4	E	44	ALA	CA-CB	6.19	1.64	1.53
2	B	963	PHE	CA-C	-6.19	1.45	1.52
2	B	1041	GLU	N-CA	6.18	1.54	1.46
1	A	676	MET	CA-C	-6.18	1.44	1.52
4	E	153	HIS	CA-CB	-6.18	1.44	1.53
5	F	77	ASP	CG-OD1	6.18	1.37	1.25
8	J	1	MET	CG-SD	-6.18	1.65	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	13	SER	CA-CB	6.18	1.63	1.53
1	A	959	ASN	CA-CB	-6.18	1.44	1.52
1	A	1093	LYS	CA-C	6.18	1.61	1.52
1	A	939	ASP	CB-CG	6.17	1.67	1.52
4	E	200	ARG	CB-CG	-6.17	1.33	1.52
1	A	786	HIS	CA-CB	-6.17	1.42	1.53
1	A	1037	LEU	CA-C	-6.17	1.44	1.52
3	C	26	ASP	CA-C	6.17	1.61	1.52
9	K	34	THR	C-N	-6.17	1.24	1.33
1	A	951	GLU	CA-C	-6.17	1.44	1.52
2	B	60	GLN	CA-C	-6.17	1.44	1.52
2	B	234	ILE	CA-CB	-6.17	1.46	1.54
1	A	1060	PRO	C-O	-6.17	1.16	1.23
2	B	883	LEU	CG-CD2	6.17	1.73	1.52
8	J	54	VAL	CA-CB	-6.17	1.46	1.54
2	B	132	VAL	CA-C	6.17	1.60	1.52
2	B	646	LEU	CA-C	6.17	1.61	1.52
1	A	1222	ASN	C-N	6.16	1.42	1.33
2	B	839	MET	CG-SD	6.16	1.96	1.80
3	C	99	LEU	C-O	-6.16	1.16	1.23
1	A	777	PHE	CD2-CE2	6.16	1.57	1.38
2	B	770	GLN	C-O	-6.16	1.16	1.24
2	B	814	PHE	C-O	6.16	1.32	1.24
2	B	1051	THR	C-N	-6.16	1.26	1.34
6	H	110	ASP	N-CA	6.16	1.53	1.46
1	A	1262	LYS	CA-CB	6.16	1.63	1.53
2	B	167	ILE	C-O	6.16	1.31	1.24
6	H	31	THR	CA-C	6.16	1.60	1.52
1	A	664	THR	CA-C	-6.16	1.45	1.52
2	B	972	LYS	CA-C	-6.16	1.45	1.52
2	B	1094	ARG	NE-CZ	-6.16	1.26	1.33
6	H	109	LYS	CA-CB	6.16	1.63	1.53
1	A	591	PHE	CA-CB	6.15	1.62	1.53
2	B	400	HIS	C-O	6.15	1.31	1.24
1	A	1126	ALA	CA-CB	-6.15	1.44	1.53
2	B	839	MET	C-O	-6.15	1.16	1.23
4	E	99	HIS	CA-CB	6.15	1.63	1.53
10	L	29	TYR	N-CA	6.15	1.53	1.45
1	A	995	GLU	CD-OE1	6.15	1.37	1.25
2	B	738	PHE	N-CA	-6.15	1.38	1.46
2	B	934	LYS	CA-CB	6.15	1.62	1.53
6	H	127	GLY	CA-C	6.15	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	289	ILE	CA-CB	6.15	1.61	1.54
2	B	694	ASP	CG-OD2	6.15	1.37	1.25
4	E	166	LYS	C-O	6.15	1.31	1.24
9	K	114	LEU	CB-CG	6.15	1.65	1.53
1	A	22	PHE	N-CA	-6.14	1.38	1.46
1	A	662	PHE	CE1-CZ	-6.14	1.20	1.38
3	C	152	GLU	C-O	-6.14	1.16	1.23
2	B	680	THR	CB-CG2	-6.14	1.32	1.52
1	A	873	MET	C-O	-6.14	1.16	1.23
1	A	1171	GLN	CB-CG	6.14	1.70	1.52
3	C	211	ASP	CG-OD1	6.14	1.37	1.25
9	K	56	VAL	CA-CB	6.14	1.60	1.53
2	B	249	ARG	CD-NE	6.14	1.54	1.46
4	E	23	VAL	CA-CB	-6.14	1.47	1.54
1	A	438	ASP	CA-C	-6.14	1.44	1.52
1	A	893	PHE	CG-CD1	-6.14	1.25	1.38
1	A	1450	LEU	N-CA	6.14	1.57	1.46
4	E	174	GLN	CD-NE2	-6.14	1.20	1.33
1	A	34	LYS	C-O	-6.13	1.16	1.24
2	B	135	ARG	CA-C	6.13	1.60	1.52
2	B	452	THR	CA-C	6.13	1.60	1.52
2	B	995	ARG	NE-CZ	-6.13	1.26	1.33
3	C	117	ASP	CG-OD1	6.13	1.37	1.25
1	A	467	THR	CA-C	-6.13	1.44	1.52
1	A	956	LEU	CA-C	-6.13	1.46	1.52
2	B	106	ASP	CG-OD2	6.13	1.37	1.25
1	A	1023	ARG	CA-CB	-6.13	1.43	1.53
2	B	1021	MET	C-O	6.13	1.31	1.23
1	A	606	LEU	N-CA	-6.13	1.38	1.46
3	C	23	SER	CA-CB	6.13	1.63	1.53
7	I	104	LEU	CA-C	-6.13	1.44	1.52
2	B	96	TYR	CE1-CZ	6.12	1.52	1.38
2	B	227	LYS	CD-CE	6.12	1.70	1.52
2	B	749	LEU	CA-CB	-6.12	1.43	1.53
3	C	3	GLU	CD-OE2	6.12	1.36	1.25
4	E	198	ILE	C-N	-6.12	1.25	1.33
1	A	814	PHE	C-O	-6.12	1.16	1.24
2	B	1043	ASP	CA-CB	6.12	1.60	1.52
4	E	212	ARG	CD-NE	-6.12	1.37	1.46
5	F	108	PHE	CA-CB	-6.12	1.44	1.53
1	A	963	ILE	C-O	-6.12	1.17	1.24
1	A	1101	LEU	CA-C	-6.12	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	89	GLU	C-O	6.12	1.35	1.23
1	A	238	CYS	CA-C	-6.12	1.45	1.52
1	A	580	VAL	CB-CG2	-6.12	1.32	1.52
1	A	84	ILE	CA-CB	6.11	1.62	1.54
1	A	971	PHE	CE2-CZ	-6.11	1.20	1.38
2	B	934	LYS	CA-C	6.11	1.59	1.53
3	C	256	ALA	C-O	6.11	1.32	1.24
2	B	1067	ARG	C-O	-6.11	1.15	1.24
4	E	142	VAL	CA-C	6.11	1.59	1.52
1	A	901	LEU	CA-C	6.11	1.61	1.52
6	H	33	GLN	C-O	-6.11	1.16	1.24
9	K	2	ASN	C-N	6.11	1.43	1.33
9	K	26	LYS	CB-CG	6.11	1.70	1.52
1	A	503	GLN	C-O	-6.11	1.15	1.24
1	A	612	ILE	C-O	-6.11	1.16	1.24
3	C	94	LYS	CE-NZ	6.11	1.67	1.49
3	C	166	GLU	N-CA	-6.11	1.38	1.46
1	A	387	ARG	NE-CZ	6.10	1.39	1.33
1	A	845	LEU	CA-C	6.10	1.60	1.52
1	A	645	LEU	C-N	-6.10	1.25	1.33
1	A	818	MET	C-N	-6.10	1.26	1.33
3	C	50	GLU	CD-OE1	6.10	1.36	1.25
7	I	1	MET	CA-CB	6.10	1.65	1.53
4	E	57	MET	CG-SD	6.10	1.96	1.80
2	B	1011	ILE	N-CA	6.10	1.55	1.46
1	A	348	SER	CA-CB	-6.10	1.43	1.53
1	A	368	LYS	CA-C	-6.10	1.44	1.52
1	A	659	HIS	CG-CD2	6.10	1.42	1.35
2	B	1081	LEU	C-N	-6.10	1.25	1.33
1	A	1022	LEU	C-O	6.10	1.31	1.24
2	B	237	VAL	CB-CG1	-6.09	1.32	1.52
2	B	761	HIS	CA-CB	6.09	1.62	1.53
2	B	870	ILE	CB-CG1	6.09	1.65	1.53
8	J	29	GLU	CD-OE1	6.09	1.36	1.25
2	B	652	LYS	CD-CE	6.09	1.70	1.52
1	A	708	MET	C-N	-6.09	1.25	1.33
2	B	345	LYS	CA-CB	-6.09	1.44	1.53
2	B	486	TYR	CA-C	-6.09	1.45	1.52
7	I	107	SER	CB-OG	-6.09	1.29	1.42
1	A	654	ASN	N-CA	-6.09	1.38	1.46
1	A	1444	MET	C-O	6.09	1.31	1.23
1	A	55	ASP	N-CA	6.09	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	821	GLN	C-O	-6.09	1.16	1.23
3	C	148	ARG	CZ-NH1	6.08	1.41	1.32
1	A	491	VAL	N-CA	-6.08	1.41	1.46
1	A	972	HIS	CA-CB	6.08	1.61	1.53
1	A	1024	SER	C-O	-6.08	1.16	1.24
2	B	112	LEU	CA-C	-6.08	1.45	1.52
2	B	807	ARG	NE-CZ	-6.08	1.26	1.33
1	A	1421	CYS	C-O	-6.08	1.15	1.23
7	I	24	ARG	N-CA	6.08	1.53	1.45
7	I	105	SER	N-CA	6.08	1.53	1.46
1	A	425	GLN	C-O	6.08	1.31	1.24
1	A	1267	MET	C-N	-6.08	1.25	1.33
2	B	336	ARG	CZ-NH1	6.08	1.41	1.32
2	B	1222	ARG	CA-CB	6.07	1.63	1.53
1	A	1112	LYS	CD-CE	6.07	1.70	1.52
1	A	1015	VAL	CA-C	6.07	1.60	1.52
7	I	79	HIS	CA-C	6.07	1.60	1.52
2	B	630	ALA	CA-CB	-6.07	1.43	1.53
2	B	1201	LYS	CA-CB	-6.07	1.44	1.53
5	F	123	LYS	CE-NZ	6.07	1.67	1.49
7	I	67	THR	CA-CB	-6.07	1.43	1.53
2	B	585	VAL	C-O	-6.06	1.17	1.24
2	B	707	PRO	CA-CB	-6.06	1.45	1.53
8	J	38	ARG	CB-CG	6.06	1.70	1.52
1	A	968	GLN	CA-C	-6.06	1.44	1.52
1	A	704	ALA	CA-C	-6.06	1.44	1.53
2	B	370	PHE	N-CA	6.06	1.54	1.46
2	B	982	SER	C-O	-6.06	1.15	1.23
2	B	1178	ASN	N-CA	6.06	1.55	1.46
5	F	72	LYS	CG-CD	6.06	1.70	1.52
9	K	95	ILE	C-N	6.06	1.42	1.33
2	B	529	GLU	CG-CD	6.05	1.67	1.52
2	B	605	ARG	NE-CZ	-6.05	1.26	1.33
1	A	1314	SER	CA-C	-6.05	1.44	1.52
1	A	1277	GLU	CA-C	-6.05	1.45	1.52
3	C	57	VAL	CB-CG2	-6.05	1.32	1.52
1	A	626	ASN	CG-OD1	6.05	1.35	1.23
2	B	405	ARG	C-O	-6.04	1.16	1.23
1	A	98	LYS	CD-CE	6.04	1.70	1.52
1	A	393	ARG	CZ-NH2	6.04	1.41	1.33
2	B	173	MET	CA-C	-6.04	1.44	1.52
2	B	250	PHE	CB-CG	6.04	1.64	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	981	ALA	CA-CB	-6.04	1.43	1.53
3	C	121	VAL	C-O	-6.04	1.16	1.24
1	A	55	ASP	CA-C	-6.03	1.45	1.52
1	A	459	ARG	CD-NE	-6.03	1.37	1.46
1	A	1325	THR	CB-CG2	-6.03	1.32	1.52
2	B	275	TYR	CA-C	-6.03	1.45	1.52
1	A	953	ASN	CG-OD1	6.03	1.35	1.23
2	B	278	GLN	CB-CG	-6.03	1.34	1.52
2	B	1149	GLU	C-N	-6.03	1.25	1.34
7	I	65	ASP	C-O	6.03	1.31	1.24
1	A	945	GLU	CD-OE1	6.03	1.36	1.25
2	B	356	LEU	C-O	-6.03	1.16	1.24
2	B	694	ASP	CB-CG	6.03	1.67	1.52
2	B	804	GLY	N-CA	6.03	1.54	1.45
2	B	974	PRO	CA-C	-6.03	1.45	1.52
4	E	188	LEU	C-O	6.03	1.32	1.24
3	C	238	ILE	CB-CG1	-6.02	1.41	1.53
1	A	1429	ILE	CA-CB	6.02	1.61	1.54
3	C	180	TYR	C-N	-6.02	1.25	1.33
1	A	885	THR	CA-C	6.02	1.60	1.52
1	A	678	GLU	CD-OE2	6.02	1.36	1.25
1	A	1026	LEU	C-N	-6.02	1.25	1.33
9	K	3	ALA	CA-C	6.02	1.59	1.52
2	B	217	ARG	CD-NE	-6.02	1.37	1.46
1	A	788	SER	N-CA	-6.01	1.39	1.45
4	E	149	LEU	CA-CB	-6.01	1.43	1.53
1	A	274	ILE	CB-CG2	6.01	1.72	1.52
1	A	599	SER	CA-CB	6.01	1.62	1.53
1	A	1331	SER	C-O	6.01	1.31	1.23
2	B	665	GLU	CG-CD	6.01	1.67	1.52
6	H	104	PHE	CA-CB	6.01	1.63	1.53
1	A	1078	GLN	N-CA	6.01	1.53	1.46
7	I	93	LYS	CG-CD	6.01	1.70	1.52
2	B	96	TYR	CE2-CZ	6.01	1.52	1.38
2	B	456	GLY	N-CA	6.01	1.53	1.45
2	B	745	PRO	C-O	-6.01	1.16	1.24
3	C	170	TRP	CZ3-CH2	-6.01	1.25	1.40
2	B	1109	GLY	CA-C	6.01	1.60	1.51
4	E	159	ASP	CA-CB	6.01	1.62	1.53
1	A	514	PRO	C-N	-6.00	1.25	1.33
2	B	955	THR	CA-CB	6.00	1.61	1.53
6	H	126	GLU	CD-OE1	6.00	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	183	GLU	CD-OE1	6.00	1.36	1.25
1	A	977	LYS	C-O	-6.00	1.15	1.25
2	B	915	THR	CA-CB	6.00	1.65	1.54
4	E	157	SER	C-O	6.00	1.31	1.24
4	E	131	THR	CA-C	-6.00	1.45	1.52
1	A	385	ILE	CA-CB	-6.00	1.45	1.54
1	A	893	PHE	CA-C	-6.00	1.45	1.52
1	A	268	ASP	CB-CG	6.00	1.67	1.52
2	B	233	PRO	CA-C	6.00	1.61	1.52
4	E	198	ILE	CB-CG2	-6.00	1.32	1.52
5	F	114	GLU	CA-C	6.00	1.60	1.52
7	I	47	GLU	CG-CD	6.00	1.67	1.52
8	J	55	ASP	CA-C	-6.00	1.46	1.53
1	A	687	LYS	CE-NZ	6.00	1.67	1.49
9	K	65	HIS	CA-C	-6.00	1.45	1.52
10	L	27	LEU	CG-CD2	6.00	1.72	1.52
2	B	165	VAL	CA-C	5.99	1.60	1.52
1	A	698	GLN	CA-C	-5.99	1.44	1.52
2	B	1005	GLY	C-O	5.99	1.32	1.23
3	C	110	THR	N-CA	5.99	1.53	1.46
1	A	764	CYS	C-N	-5.99	1.25	1.33
3	C	54	ASN	C-N	-5.99	1.25	1.33
8	J	1	MET	CA-CB	-5.99	1.41	1.53
9	K	85	ASP	C-O	-5.99	1.16	1.24
2	B	1013	ASN	C-N	-5.99	1.26	1.33
2	B	641	GLU	C-O	-5.99	1.16	1.23
2	B	979	LYS	C-N	-5.99	1.26	1.33
1	A	1236	LEU	CB-CG	5.98	1.65	1.53
1	A	1291	VAL	CB-CG2	5.98	1.72	1.52
2	B	743	ILE	CA-C	-5.98	1.45	1.52
1	A	1285	MET	CB-CG	5.98	1.70	1.52
7	I	47	GLU	CD-OE2	5.98	1.36	1.25
1	A	1147	THR	CA-C	-5.98	1.45	1.52
1	A	1221	LYS	CB-CG	5.98	1.70	1.52
1	A	950	GLY	C-O	-5.98	1.15	1.24
1	A	1283	VAL	C-O	-5.98	1.18	1.24
2	B	333	PHE	CA-C	-5.98	1.45	1.52
2	B	1172	ILE	C-O	5.98	1.30	1.23
9	K	99	GLY	C-O	5.98	1.31	1.23
1	A	1377	THR	CB-OG1	-5.97	1.34	1.43
1	A	1424	VAL	CA-CB	-5.97	1.46	1.54
4	E	96	PHE	CA-CB	5.97	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	174	LEU	CG-CD1	5.97	1.72	1.52
9	K	66	PRO	CB-CG	-5.97	1.19	1.49
4	E	104	ASN	CA-C	5.97	1.60	1.53
7	I	30	ARG	CG-CD	5.97	1.70	1.52
1	A	1346	ALA	CA-C	5.97	1.60	1.52
2	B	137	TYR	N-CA	5.97	1.53	1.46
2	B	226	PHE	CA-C	-5.97	1.45	1.52
2	B	393	LYS	CA-C	-5.97	1.45	1.52
2	B	875	GLU	CA-C	-5.96	1.44	1.52
2	B	958	GLN	CD-NE2	5.96	1.45	1.33
2	B	1072	MET	C-O	5.96	1.32	1.23
3	C	6	PRO	N-CA	-5.96	1.40	1.47
4	E	208	TYR	C-O	5.96	1.31	1.23
7	I	104	LEU	C-O	-5.96	1.16	1.24
9	K	61	TYR	CE2-CZ	-5.96	1.24	1.38
1	A	1223	ASP	N-CA	5.96	1.53	1.46
2	B	34	ILE	CB-CG2	-5.96	1.32	1.52
1	A	1111	MET	CA-C	-5.96	1.44	1.53
3	C	12	GLU	N-CA	-5.96	1.38	1.46
1	A	1035	TYR	CE2-CZ	-5.96	1.24	1.38
3	C	125	MET	CG-SD	5.96	1.95	1.80
6	H	27	GLU	C-O	-5.96	1.16	1.23
2	B	946	ASN	C-O	-5.96	1.16	1.23
4	E	93	MET	CA-CB	5.96	1.62	1.53
1	A	762	SER	C-O	-5.95	1.15	1.23
1	A	1239	ARG	CB-CG	-5.95	1.34	1.52
2	B	728	ARG	CZ-NH1	-5.95	1.24	1.32
3	C	76	ASP	CA-CB	5.95	1.61	1.52
4	E	176	PRO	N-CD	-5.95	1.39	1.47
5	F	150	GLU	C-N	5.95	1.41	1.33
3	C	183	TRP	CE2-CZ2	-5.95	1.27	1.39
1	A	593	GLU	C-N	5.95	1.42	1.33
1	A	1121	GLU	C-O	5.95	1.31	1.24
2	B	102	VAL	CA-C	5.95	1.60	1.52
2	B	1168	LEU	C-O	-5.95	1.16	1.23
7	I	7	CYS	CA-C	-5.95	1.45	1.52
1	A	890	ASP	C-O	-5.95	1.16	1.24
2	B	808	ALA	CA-C	-5.95	1.44	1.52
4	E	122	LYS	CA-C	5.95	1.60	1.52
7	I	111	THR	CA-C	-5.94	1.45	1.52
1	A	441	PRO	C-O	-5.94	1.17	1.23
8	J	24	LEU	CG-CD2	-5.94	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	650	GLN	CA-CB	-5.94	1.44	1.53
1	A	827	THR	CA-CB	5.94	1.62	1.53
4	E	45	LYS	CD-CE	5.94	1.70	1.52
6	H	45	GLU	CD-OE2	5.93	1.36	1.25
1	A	505	CYS	C-N	-5.93	1.25	1.33
2	B	273	LEU	CA-C	5.93	1.60	1.53
2	B	434	ARG	CA-CB	5.93	1.61	1.53
1	A	516	SER	C-O	-5.93	1.15	1.24
1	A	1222	ASN	C-O	5.93	1.31	1.24
2	B	327	ARG	CA-C	-5.93	1.44	1.52
4	E	48	ASP	C-O	5.93	1.31	1.24
1	A	442	VAL	C-O	-5.93	1.16	1.23
2	B	785	TYR	N-CA	5.92	1.53	1.46
2	B	833	TYR	CG-CD2	-5.92	1.26	1.39
3	C	238	ILE	CA-CB	-5.92	1.46	1.54
4	E	180	ARG	CD-NE	5.92	1.54	1.46
2	B	60	GLN	CB-CG	-5.92	1.34	1.52
2	B	395	GLN	C-O	-5.92	1.16	1.23
1	A	109	HIS	CB-CG	5.92	1.58	1.50
1	A	1337	GLU	CG-CD	5.92	1.66	1.52
2	B	791	THR	CA-C	-5.92	1.45	1.52
2	B	967	ARG	C-O	-5.92	1.16	1.24
2	B	1222	ARG	CA-C	5.92	1.60	1.52
1	A	1001	ARG	CD-NE	-5.92	1.38	1.46
2	B	30	SER	CB-OG	-5.92	1.30	1.42
1	A	713	SER	N-CA	-5.92	1.38	1.46
1	A	1208	THR	CA-CB	5.91	1.62	1.53
1	A	709	THR	CA-CB	-5.91	1.43	1.53
1	A	499	ALA	CA-C	-5.91	1.45	1.52
1	A	1231	ASP	N-CA	5.91	1.53	1.46
1	A	1350	LYS	CD-CE	5.91	1.70	1.52
1	A	596	THR	C-O	-5.91	1.16	1.24
1	A	864	ILE	C-O	5.91	1.29	1.23
3	C	56	THR	CB-CG2	-5.91	1.33	1.52
7	I	70	ARG	CZ-NH2	-5.91	1.25	1.33
1	A	69	THR	N-CA	5.91	1.53	1.46
1	A	713	SER	CA-C	-5.91	1.44	1.52
1	A	726	ARG	CA-C	-5.91	1.45	1.52
1	A	1223	ASP	C-O	-5.91	1.16	1.24
4	E	57	MET	CA-CB	5.91	1.63	1.53
1	A	1036	ARG	NE-CZ	-5.90	1.26	1.33
2	B	652	LYS	CE-NZ	5.90	1.67	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	94	ASP	CB-CG	5.90	1.66	1.52
1	A	66	LYS	CA-CB	5.90	1.65	1.53
1	A	624	SER	N-CA	5.90	1.54	1.46
1	A	348	SER	N-CA	-5.90	1.38	1.45
1	A	1103	GLU	C-O	5.90	1.31	1.24
2	B	615	MET	CA-C	-5.90	1.45	1.52
3	C	54	ASN	N-CA	5.90	1.54	1.46
2	B	46	GLN	CG-CD	-5.90	1.37	1.52
1	A	621	THR	C-O	5.90	1.31	1.24
5	F	149	GLU	N-CA	5.90	1.53	1.46
1	A	691	LEU	C-O	-5.89	1.16	1.24
1	A	805	LEU	CG-CD1	-5.89	1.33	1.52
4	E	164	LEU	N-CA	-5.89	1.39	1.46
1	A	348	SER	C-O	-5.89	1.16	1.23
1	A	521	MET	C-O	-5.89	1.17	1.24
2	B	296	GLU	CA-C	-5.89	1.45	1.52
2	B	335	GLY	C-N	-5.89	1.26	1.34
2	B	939	THR	C-O	-5.89	1.16	1.24
2	B	1215	ARG	N-CA	5.89	1.53	1.46
3	C	43	THR	N-CA	-5.89	1.39	1.46
1	A	490	HIS	N-CA	-5.89	1.38	1.46
1	A	1114	PRO	CA-CB	-5.89	1.45	1.53
1	A	1172	LEU	N-CA	5.89	1.54	1.46
3	C	183	TRP	N-CA	5.89	1.53	1.45
1	A	1107	VAL	C-O	5.89	1.31	1.24
1	A	433	GLU	N-CA	-5.89	1.39	1.46
2	B	164	LYS	CA-C	5.89	1.65	1.52
1	A	1143	LEU	CA-CB	-5.88	1.44	1.53
10	L	64	LEU	CG-CD1	5.88	1.72	1.52
1	A	944	ARG	CA-CB	-5.88	1.43	1.53
1	A	280	GLU	N-CA	-5.88	1.39	1.46
2	B	31	TRP	CG-CD1	-5.88	1.22	1.36
1	A	714	PHE	CA-C	-5.88	1.45	1.52
6	H	109	LYS	N-CA	5.88	1.53	1.46
1	A	699	ALA	CA-CB	-5.88	1.43	1.53
2	B	1140	ALA	N-CA	-5.88	1.39	1.46
10	L	53	HIS	C-O	-5.88	1.16	1.24
1	A	1418	LEU	CG-CD1	5.88	1.72	1.52
2	B	1135	ARG	C-O	-5.88	1.17	1.24
1	A	1113	THR	C-O	-5.87	1.18	1.24
5	F	124	GLU	N-CA	-5.87	1.38	1.46
6	H	22	LYS	CE-NZ	5.87	1.67	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	102	LYS	C-O	5.87	1.31	1.24
2	B	282	ILE	CA-C	-5.87	1.44	1.52
2	B	376	PHE	CE2-CZ	-5.87	1.21	1.38
2	B	479	VAL	CB-CG1	-5.87	1.33	1.52
1	A	41	MET	CG-SD	5.87	1.95	1.80
1	A	846	GLU	CD-OE1	5.87	1.36	1.25
2	B	181	LEU	CA-CB	-5.87	1.43	1.53
2	B	1134	GLU	CD-OE1	5.87	1.36	1.25
5	F	99	LEU	CB-CG	-5.87	1.41	1.53
7	I	22	ASN	C-O	5.87	1.32	1.24
1	A	359	LEU	CG-CD2	-5.87	1.33	1.52
1	A	1151	GLU	C-O	5.87	1.31	1.23
4	E	59	SER	CB-OG	5.87	1.53	1.42
4	E	96	PHE	CA-C	5.87	1.60	1.52
9	K	60	ALA	N-CA	5.87	1.53	1.46
1	A	1144	LYS	CD-CE	5.87	1.70	1.52
1	A	691	LEU	CA-CB	-5.86	1.43	1.53
1	A	1164	PRO	N-CA	5.86	1.54	1.47
1	A	1339	LEU	CB-CG	-5.86	1.41	1.53
1	A	87	ALA	CA-C	-5.86	1.45	1.52
1	A	542	GLU	CD-OE1	5.86	1.36	1.25
4	E	75	MET	N-CA	-5.86	1.39	1.46
2	B	1008	PRO	N-CA	-5.86	1.40	1.47
8	J	26	GLN	CB-CG	5.86	1.70	1.52
1	A	523	ILE	N-CA	-5.86	1.39	1.46
1	A	896	ARG	N-CA	-5.86	1.39	1.46
1	A	1110	ASN	CG-OD1	5.86	1.34	1.23
2	B	895	ASP	N-CA	5.86	1.53	1.46
2	B	1155	SER	CA-C	5.86	1.60	1.52
2	B	605	ARG	CZ-NH1	-5.86	1.24	1.32
2	B	987	LYS	N-CA	-5.86	1.39	1.45
1	A	1074	GLU	CG-CD	5.85	1.66	1.52
1	A	858	ASN	CB-CG	-5.85	1.37	1.52
2	B	344	LYS	CD-CE	5.85	1.70	1.52
5	F	118	LEU	C-O	-5.85	1.17	1.24
1	A	852	TYR	C-O	5.85	1.31	1.24
5	F	79	ARG	CZ-NH2	-5.85	1.25	1.33
1	A	1142	THR	CA-CB	-5.85	1.45	1.53
2	B	252	SER	CA-CB	5.85	1.62	1.53
1	A	505	CYS	CA-C	-5.84	1.44	1.52
1	A	520	CYS	C-O	-5.84	1.16	1.24
2	B	753	ALA	CA-CB	-5.84	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	999	MET	CA-C	-5.84	1.45	1.53
6	H	19	ARG	C-O	-5.84	1.16	1.24
1	A	659	HIS	C-N	-5.84	1.25	1.33
1	A	922	ASP	C-N	-5.84	1.25	1.33
2	B	183	GLU	CA-C	5.84	1.60	1.52
5	F	76	LYS	CD-CE	5.84	1.70	1.52
2	B	287	ARG	N-CA	5.84	1.53	1.46
1	A	353	ILE	CB-CG1	-5.84	1.41	1.53
2	B	614	SER	N-CA	5.84	1.53	1.46
4	E	48	ASP	CA-C	5.84	1.60	1.52
1	A	894	GLU	C-O	5.83	1.31	1.24
1	A	1381	LEU	CA-C	-5.83	1.45	1.52
2	B	452	THR	N-CA	5.83	1.53	1.46
2	B	592	ASN	CB-CG	5.83	1.66	1.52
2	B	1205	GLN	CA-CB	-5.83	1.44	1.53
3	C	79	GLN	C-O	-5.83	1.16	1.24
1	A	568	PRO	CA-C	-5.83	1.44	1.52
6	H	24	CYS	C-O	-5.83	1.16	1.23
1	A	737	LEU	CG-CD2	5.83	1.71	1.52
2	B	957	ASN	C-O	5.83	1.31	1.24
1	A	1080	THR	C-N	5.83	1.41	1.33
3	C	87	PHE	C-O	5.83	1.31	1.24
2	B	972	LYS	C-O	-5.83	1.17	1.24
9	K	26	LYS	CE-NZ	5.83	1.66	1.49
1	A	1077	THR	CB-CG2	5.83	1.71	1.52
1	A	1202	MET	SD-CE	5.83	1.94	1.79
2	B	343	ILE	CB-CG2	-5.83	1.33	1.52
2	B	324	ILE	N-CA	-5.82	1.39	1.46
2	B	635	ARG	CZ-NH2	-5.82	1.25	1.33
2	B	641	GLU	CD-OE1	5.82	1.36	1.25
1	A	680	THR	C-O	-5.82	1.16	1.24
2	B	734	HIS	CA-CB	5.82	1.60	1.52
2	B	1165	ILE	CB-CG1	5.82	1.65	1.53
3	C	58	LEU	CG-CD2	-5.82	1.33	1.52
8	J	36	LEU	CA-C	-5.82	1.45	1.52
1	A	757	ASN	C-O	-5.82	1.17	1.24
1	A	420	ARG	CZ-NH2	-5.82	1.25	1.33
1	A	851	HIS	CA-C	-5.82	1.45	1.52
1	A	1236	LEU	CG-CD2	5.82	1.71	1.52
4	E	26	ARG	CG-CD	-5.82	1.34	1.52
1	A	1290	LYS	CD-CE	5.81	1.69	1.52
1	A	913	LEU	CA-C	5.81	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	977	LYS	CG-CD	5.81	1.69	1.52
3	C	193	TYR	C-N	-5.81	1.25	1.33
6	H	146	ARG	NE-CZ	5.81	1.39	1.33
2	B	780	VAL	C-N	-5.81	1.25	1.34
2	B	979	LYS	CA-C	-5.81	1.45	1.52
8	J	42	LYS	CG-CD	5.81	1.69	1.52
9	K	49	GLU	C-O	-5.81	1.17	1.24
2	B	348	ARG	C-N	-5.81	1.26	1.33
1	A	1301	GLU	CD-OE1	5.81	1.36	1.25
1	A	860	LEU	N-CA	5.80	1.53	1.46
2	B	513	GLN	CD-NE2	5.80	1.45	1.33
2	B	523	CYS	CA-C	-5.80	1.47	1.53
2	B	597	MET	N-CA	-5.80	1.39	1.46
2	B	847	ASP	CG-OD2	5.80	1.36	1.25
3	C	12	GLU	C-O	5.80	1.30	1.23
6	H	120	GLY	C-O	5.80	1.32	1.24
4	E	60	PHE	CA-C	5.80	1.59	1.52
1	A	820	GLY	C-N	-5.80	1.26	1.33
1	A	1234	GLU	N-CA	5.80	1.53	1.46
2	B	245	GLU	C-O	5.80	1.31	1.24
2	B	454	THR	N-CA	5.79	1.53	1.46
5	F	93	ILE	CA-CB	-5.79	1.46	1.54
2	B	1031	LEU	C-O	-5.79	1.16	1.24
2	B	1080	LYS	CD-CE	5.79	1.69	1.52
3	C	256	ALA	C-N	5.79	1.41	1.33
4	E	211	TYR	CE1-CZ	-5.79	1.24	1.38
2	B	46	GLN	CA-C	5.79	1.60	1.52
2	B	519	TRP	CB-CG	5.79	1.68	1.50
3	C	180	TYR	N-CA	-5.79	1.38	1.46
4	E	40	GLU	N-CA	5.79	1.53	1.46
1	A	93	VAL	C-O	5.79	1.30	1.24
1	A	683	ILE	CA-C	-5.79	1.45	1.52
2	B	370	PHE	CE2-CZ	5.79	1.56	1.38
1	A	771	GLU	C-O	-5.79	1.16	1.23
2	B	726	ALA	C-O	-5.79	1.16	1.24
4	E	62	ALA	CA-C	-5.79	1.45	1.52
1	A	1262	LYS	CB-CG	5.78	1.69	1.52
2	B	169	ARG	CZ-NH2	5.78	1.41	1.33
2	B	358	LYS	CA-C	-5.78	1.45	1.52
6	H	129	TYR	CE1-CZ	5.78	1.52	1.38
7	I	44	TYR	N-CA	5.78	1.52	1.46
1	A	921	GLY	C-N	-5.78	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1176	ASN	CG-OD1	5.78	1.34	1.23
1	A	1238	ILE	N-CA	-5.78	1.39	1.46
6	H	20	TYR	C-O	5.78	1.31	1.23
2	B	41	LYS	CD-CE	5.78	1.69	1.52
2	B	409	ALA	CA-CB	-5.78	1.44	1.53
4	E	142	VAL	C-N	5.78	1.41	1.33
1	A	481	ASP	CG-OD1	5.78	1.36	1.25
1	A	589	GLN	CD-OE1	5.78	1.34	1.23
2	B	636	PRO	N-CA	-5.78	1.40	1.47
2	B	1018	PRO	N-CA	-5.78	1.40	1.47
3	C	151	GLN	CA-C	-5.78	1.46	1.52
4	E	42	PHE	CD1-CE1	5.78	1.55	1.38
6	H	36	CYS	CA-C	5.78	1.60	1.52
2	B	314	LEU	C-O	5.77	1.31	1.24
2	B	704	ALA	CA-C	-5.77	1.45	1.52
7	I	41	PRO	CA-CB	-5.77	1.43	1.54
1	A	811	GLN	CD-OE1	5.77	1.34	1.23
2	B	395	GLN	N-CA	5.77	1.53	1.46
7	I	11	ASN	CG-ND2	-5.77	1.21	1.33
1	A	613	ILE	CA-C	-5.77	1.44	1.53
6	H	105	GLU	CA-CB	5.77	1.63	1.53
2	B	197	PHE	C-O	-5.77	1.16	1.24
1	A	839	ARG	CZ-NH1	5.77	1.40	1.32
2	B	1080	LYS	CA-C	5.77	1.59	1.52
3	C	166	GLU	CD-OE1	5.77	1.36	1.25
1	A	288	ALA	C-O	-5.76	1.17	1.24
1	A	611	GLN	CD-NE2	5.76	1.45	1.33
7	I	112	SER	CA-CB	-5.76	1.44	1.53
1	A	794	PRO	C-O	-5.76	1.16	1.24
2	B	119	LEU	CA-C	-5.76	1.45	1.52
10	L	47	ARG	CD-NE	5.76	1.54	1.46
2	B	344	LYS	CG-CD	5.76	1.69	1.52
2	B	546	SER	CA-C	-5.76	1.45	1.52
2	B	679	TYR	CA-CB	-5.76	1.44	1.53
2	B	723	VAL	CB-CG2	5.76	1.71	1.52
3	C	195	GLN	CD-OE1	5.76	1.34	1.23
3	C	211	ASP	CA-C	5.76	1.60	1.52
9	K	3	ALA	C-N	5.76	1.41	1.33
9	K	105	PHE	CA-CB	5.76	1.62	1.53
1	A	705	LYS	C-O	5.76	1.30	1.23
1	A	1098	VAL	CA-C	-5.76	1.46	1.52
3	C	122	SER	CA-C	-5.76	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	GLN	C-O	-5.76	1.16	1.24
2	B	94	LYS	CA-C	5.76	1.60	1.53
2	B	362	PRO	N-CA	-5.76	1.40	1.47
2	B	367	LEU	CG-CD2	5.76	1.71	1.52
2	B	778	MET	CA-C	-5.76	1.45	1.52
2	B	1089	PRO	C-O	-5.76	1.17	1.23
4	E	9	ILE	CA-CB	5.76	1.62	1.54
2	B	308	TRP	N-CA	-5.75	1.38	1.46
1	A	884	ASP	CG-OD1	5.75	1.36	1.25
2	B	658	ILE	CA-CB	-5.75	1.46	1.54
1	A	1199	ARG	N-CA	5.75	1.53	1.46
2	B	808	ALA	CA-CB	-5.75	1.43	1.53
4	E	40	GLU	CD-OE1	5.75	1.36	1.25
6	H	6	PHE	C-O	-5.75	1.17	1.23
1	A	567	LYS	CA-C	-5.75	1.45	1.52
1	A	805	LEU	CA-C	-5.75	1.45	1.52
7	I	117	LYS	C-O	-5.75	1.16	1.24
9	K	24	ASP	CA-CB	-5.75	1.45	1.53
1	A	351	THR	C-O	-5.75	1.17	1.23
1	A	1154	TYR	C-N	5.75	1.40	1.33
4	E	206	GLY	C-O	-5.75	1.18	1.23
7	I	41	PRO	CA-C	5.75	1.59	1.52
9	K	6	ARG	CD-NE	-5.75	1.38	1.46
2	B	451	LYS	CG-CD	5.75	1.69	1.52
3	C	20	PHE	CB-CG	-5.75	1.37	1.50
1	A	1357	ALA	CA-CB	-5.74	1.43	1.53
2	B	237	VAL	CA-CB	-5.74	1.45	1.55
2	B	791	THR	CA-CB	-5.74	1.44	1.53
2	B	1141	HIS	CA-CB	-5.74	1.43	1.53
2	B	1150	ARG	CD-NE	-5.74	1.38	1.46
1	A	740	LEU	N-CA	-5.74	1.38	1.46
1	A	1193	LEU	CA-C	-5.74	1.45	1.52
2	B	46	GLN	N-CA	5.74	1.53	1.46
2	B	589	VAL	N-CA	-5.74	1.39	1.46
3	C	50	GLU	C-O	-5.74	1.17	1.24
7	I	25	LEU	C-O	-5.74	1.17	1.24
7	I	30	ARG	C-N	-5.74	1.23	1.33
8	J	1	MET	CB-CG	-5.74	1.35	1.52
2	B	175	ARG	C-O	-5.74	1.15	1.24
4	E	3	GLN	N-CA	5.74	1.53	1.46
7	I	14	LEU	CA-C	-5.74	1.45	1.52
1	A	1003	LYS	CA-C	5.74	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1287	TYR	CG-CD1	5.74	1.51	1.39
1	A	1008	GLN	CB-CG	5.74	1.69	1.52
2	B	602	THR	N-CA	5.74	1.53	1.46
2	B	1188	LYS	CD-CE	5.74	1.69	1.52
5	F	136	ARG	CA-CB	-5.74	1.45	1.53
2	B	665	GLU	CD-OE2	5.73	1.36	1.25
4	E	133	GLU	CD-OE1	5.73	1.36	1.25
1	A	772	GLY	C-O	-5.73	1.16	1.23
1	A	1092	LYS	C-N	5.73	1.42	1.33
2	B	1064	TYR	CA-CB	-5.73	1.44	1.53
2	B	465	ASN	CB-CG	5.73	1.66	1.52
2	B	1003	ALA	N-CA	-5.73	1.39	1.46
1	A	427	GLN	CG-CD	5.73	1.66	1.52
1	A	589	GLN	N-CA	-5.73	1.38	1.45
1	A	656	TRP	CG-CD2	-5.73	1.33	1.43
1	A	1230	GLU	CD-OE2	5.73	1.36	1.25
6	H	3	ASN	N-CA	5.73	1.54	1.46
7	I	56	ALA	CA-C	-5.73	1.45	1.52
8	J	18	TRP	CE2-CZ2	-5.73	1.27	1.39
1	A	829	VAL	C-N	5.72	1.41	1.33
1	A	1378	GLN	C-O	-5.72	1.15	1.24
2	B	811	TYR	N-CA	-5.72	1.38	1.46
3	C	6	PRO	CA-C	-5.72	1.47	1.52
4	E	21	GLU	N-CA	5.72	1.53	1.46
1	A	602	ASP	CA-C	5.72	1.60	1.53
2	B	855	PHE	CG-CD2	-5.72	1.26	1.38
2	B	895	ASP	CA-CB	5.72	1.63	1.53
3	C	64	ALA	C-O	-5.72	1.17	1.24
7	I	20	LYS	CG-CD	5.72	1.69	1.52
2	B	209	GLU	CA-CB	-5.72	1.44	1.53
2	B	1224	PHE	CA-C	5.72	1.65	1.52
5	F	108	PHE	C-N	-5.72	1.26	1.33
1	A	868	TYR	CA-C	-5.72	1.45	1.52
1	A	1317	MET	SD-CE	-5.72	1.65	1.79
2	B	1188	LYS	CG-CD	5.72	1.69	1.52
4	E	26	ARG	CA-C	5.72	1.60	1.52
9	K	55	LYS	N-CA	5.72	1.53	1.46
1	A	748	MET	SD-CE	5.71	1.93	1.79
7	I	101	PHE	CB-CG	-5.71	1.37	1.50
2	B	358	LYS	CB-CG	5.71	1.69	1.52
2	B	691	GLU	C-O	5.71	1.30	1.23
5	F	100	GLN	N-CA	-5.71	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	711	ARG	C-N	-5.71	1.26	1.34
6	H	19	ARG	CA-CB	5.71	1.63	1.53
1	A	560	ILE	C-N	-5.71	1.26	1.33
1	A	761	MET	N-CA	-5.71	1.39	1.46
2	B	289	LEU	N-CA	-5.71	1.38	1.46
2	B	311	LEU	CG-CD1	-5.71	1.33	1.52
3	C	152	GLU	C-N	-5.71	1.26	1.33
2	B	882	THR	CB-CG2	5.70	1.71	1.52
4	E	18	THR	CA-C	-5.70	1.45	1.52
2	B	496	ARG	NE-CZ	5.70	1.39	1.33
1	A	978	PRO	CB-CG	5.70	1.78	1.49
2	B	330	ALA	N-CA	-5.70	1.39	1.46
2	B	818	PRO	CG-CD	-5.70	1.31	1.50
4	E	11	ARG	NE-CZ	-5.70	1.26	1.33
4	E	65	THR	CB-OG1	5.70	1.52	1.43
1	A	571	LEU	C-O	5.70	1.30	1.24
1	A	1223	ASP	CA-CB	5.70	1.63	1.53
2	B	775	LYS	N-CA	-5.70	1.38	1.46
4	E	79	TRP	CA-C	-5.69	1.45	1.52
1	A	592	ASP	N-CA	5.69	1.53	1.46
2	B	296	GLU	CA-CB	-5.69	1.44	1.53
3	C	254	LYS	N-CA	5.69	1.53	1.46
10	L	26	THR	C-O	5.69	1.31	1.24
2	B	368	GLU	CA-C	5.69	1.60	1.52
1	A	644	LYS	CD-CE	5.69	1.69	1.52
1	A	405	VAL	CA-CB	-5.69	1.47	1.54
1	A	564	ALA	C-O	-5.69	1.16	1.24
1	A	1416	ALA	CA-CB	-5.69	1.45	1.53
2	B	859	TYR	C-O	-5.69	1.17	1.24
2	B	1010	LEU	CG-CD2	-5.69	1.33	1.52
1	A	598	LEU	CG-CD1	5.69	1.71	1.52
1	A	1056	SER	C-O	-5.69	1.16	1.24
2	B	38	PHE	C-O	-5.69	1.16	1.24
1	A	236	LEU	N-CA	-5.68	1.39	1.45
1	A	554	PRO	N-CD	-5.68	1.39	1.47
2	B	595	ARG	CD-NE	5.68	1.54	1.46
2	B	875	GLU	C-O	-5.68	1.16	1.23
3	C	47	ASP	CG-OD1	5.68	1.36	1.25
1	A	838	GLN	CG-CD	5.68	1.66	1.52
2	B	249	ARG	CB-CG	5.68	1.69	1.52
2	B	1086	PHE	CG-CD1	-5.68	1.26	1.38
1	A	248	PRO	CB-CG	5.68	1.78	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	618	GLU	CA-C	5.68	1.59	1.53
3	C	81	GLU	CA-C	5.68	1.60	1.52
1	A	1220	PHE	CG-CD1	-5.68	1.26	1.38
1	A	445	ASN	CA-C	5.68	1.59	1.52
2	B	291	ILE	CA-CB	-5.68	1.47	1.53
2	B	373	ARG	C-O	-5.68	1.17	1.24
3	C	36	VAL	N-CA	5.68	1.53	1.46
4	E	168	TYR	C-N	-5.68	1.26	1.33
2	B	435	THR	CA-C	5.67	1.59	1.53
9	K	36	GLU	CD-OE1	5.67	1.36	1.25
2	B	29	ASP	CA-C	5.67	1.60	1.52
2	B	118	ARG	CG-CD	5.67	1.69	1.52
2	B	689	LEU	C-O	5.67	1.31	1.24
6	H	139	ASN	CG-OD1	5.67	1.34	1.23
7	I	78	CYS	C-O	-5.67	1.16	1.24
1	A	398	GLU	CG-CD	5.67	1.66	1.52
4	E	127	ILE	C-O	5.67	1.31	1.24
6	H	63	LEU	CA-C	5.67	1.64	1.52
2	B	640	VAL	CA-CB	-5.67	1.47	1.54
2	B	1071	VAL	CA-CB	-5.67	1.47	1.54
1	A	56	PRO	C-N	5.66	1.41	1.33
1	A	492	PRO	C-O	-5.66	1.17	1.23
1	A	514	PRO	CA-CB	-5.66	1.44	1.53
1	A	650	GLN	CD-NE2	-5.66	1.21	1.33
3	C	205	LYS	CG-CD	5.66	1.69	1.52
7	I	2	THR	CA-C	5.66	1.59	1.52
1	A	1159	ARG	CD-NE	5.66	1.54	1.46
1	A	242	PRO	CA-C	5.66	1.54	1.51
2	B	296	GLU	C-N	5.66	1.41	1.33
3	C	66	ARG	CA-CB	-5.66	1.44	1.53
6	H	43	ASN	CB-CG	5.66	1.66	1.52
1	A	843	LYS	C-N	-5.66	1.26	1.33
1	A	931	GLU	CD-OE1	5.66	1.36	1.25
2	B	109	THR	C-O	-5.66	1.16	1.24
4	E	20	LYS	N-CA	-5.66	1.39	1.46
1	A	518	LYS	CE-NZ	-5.66	1.32	1.49
1	A	748	MET	CA-C	-5.66	1.45	1.52
2	B	425	THR	CB-CG2	5.66	1.71	1.52
2	B	944	THR	N-CA	5.66	1.53	1.46
4	E	43	LYS	C-O	5.66	1.31	1.24
9	K	50	LEU	CA-C	-5.66	1.45	1.52
2	B	1034	VAL	C-N	-5.65	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	58	PHE	CB-CG	5.65	1.63	1.50
1	A	802	ASN	CB-CG	5.65	1.66	1.52
6	H	128	ASN	N-CA	5.65	1.53	1.46
1	A	1448	GLU	CA-CB	5.65	1.63	1.53
2	B	39	ARG	CD-NE	5.65	1.54	1.46
1	A	1129	GLU	CA-C	5.65	1.60	1.52
2	B	948	ILE	CA-C	-5.64	1.45	1.52
2	B	1085	ILE	C-N	-5.64	1.25	1.33
7	I	82	GLU	CD-OE1	5.64	1.36	1.25
1	A	872	GLY	CA-C	-5.64	1.43	1.51
2	B	828	ALA	CA-CB	-5.64	1.44	1.53
4	E	178	ILE	C-O	-5.64	1.18	1.24
9	K	45	LEU	N-CA	5.64	1.53	1.46
4	E	8	ASN	CG-OD1	5.64	1.34	1.23
5	F	101	ILE	CA-C	5.64	1.59	1.52
6	H	79	TRP	CA-CB	-5.64	1.42	1.54
1	A	1309	ASP	CA-CB	-5.64	1.45	1.53
3	C	21	ILE	CA-CB	-5.64	1.47	1.54
10	L	56	LEU	C-O	-5.64	1.17	1.23
1	A	364	VAL	C-N	-5.64	1.27	1.33
4	E	90	VAL	CB-CG1	5.64	1.71	1.52
4	E	169	ARG	N-CA	-5.64	1.38	1.46
9	K	70	ARG	CZ-NH1	-5.64	1.24	1.32
4	E	207	ARG	N-CA	-5.63	1.39	1.45
5	F	74	ILE	CA-C	-5.63	1.48	1.52
4	E	186	LEU	N-CA	-5.63	1.39	1.46
2	B	1148	LYS	CG-CD	5.63	1.69	1.52
1	A	1012	ARG	CG-CD	5.63	1.69	1.52
2	B	225	VAL	C-O	-5.63	1.17	1.24
2	B	406	LEU	CG-CD2	-5.63	1.33	1.52
2	B	1008	PRO	CG-CD	-5.63	1.31	1.50
5	F	104	ASN	CG-OD1	5.63	1.34	1.23
9	K	97	LYS	CA-C	-5.63	1.45	1.52
1	A	692	ASP	CA-C	-5.63	1.44	1.52
1	A	840	ARG	NE-CZ	5.63	1.39	1.33
2	B	1019	SER	C-N	-5.63	1.25	1.33
2	B	1060	ARG	CZ-NH2	-5.63	1.26	1.33
5	F	93	ILE	C-N	-5.63	1.25	1.33
9	K	26	LYS	CD-CE	5.63	1.69	1.52
2	B	574	SER	CA-C	5.62	1.59	1.52
2	B	865	LYS	CB-CG	5.62	1.69	1.52
2	B	1106	ARG	C-O	5.62	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	32	CYS	CA-CB	5.62	1.61	1.53
2	B	199	MET	CG-SD	5.62	1.94	1.80
2	B	751	VAL	C-O	-5.62	1.17	1.24
6	H	2	SER	N-CA	5.62	1.56	1.46
9	K	97	LYS	C-N	-5.62	1.25	1.33
1	A	12	ARG	CZ-NH1	5.62	1.40	1.32
1	A	1005	GLU	C-O	-5.62	1.17	1.24
2	B	18	PHE	C-N	5.62	1.41	1.33
2	B	137	TYR	CA-CB	5.62	1.62	1.53
2	B	535	LEU	CA-C	-5.62	1.44	1.52
1	A	891	ALA	N-CA	5.62	1.53	1.46
1	A	1044	TRP	C-N	5.62	1.40	1.33
2	B	236	HIS	C-O	-5.62	1.17	1.23
1	A	692	ASP	CG-OD1	5.62	1.36	1.25
3	C	87	PHE	CB-CG	-5.62	1.37	1.50
1	A	630	ILE	CB-CG2	-5.61	1.34	1.52
1	A	1447	GLU	C-O	5.61	1.30	1.24
4	E	179	GLN	C-O	-5.61	1.16	1.23
4	E	185	ALA	CA-C	5.61	1.60	1.52
7	I	90	GLN	CA-C	-5.61	1.45	1.53
2	B	695	ALA	CA-C	-5.61	1.45	1.52
4	E	20	LYS	CA-C	5.61	1.60	1.52
1	A	781	ASP	CG-OD1	5.61	1.36	1.25
1	A	1233	ASP	CA-C	-5.61	1.44	1.52
1	A	1318	THR	CB-OG1	-5.61	1.34	1.43
2	B	337	ARG	CZ-NH2	-5.61	1.26	1.33
3	C	251	LEU	CG-CD2	-5.61	1.34	1.52
1	A	836	TYR	N-CA	-5.61	1.39	1.46
2	B	320	ASP	CG-OD1	5.61	1.36	1.25
4	E	155	ARG	CZ-NH1	5.61	1.40	1.32
7	I	43	VAL	CB-CG1	-5.61	1.34	1.52
2	B	975	GLN	CD-OE1	5.60	1.34	1.23
7	I	45	ARG	C-O	5.60	1.30	1.23
2	B	283	VAL	C-O	-5.60	1.17	1.24
3	C	122	SER	CA-CB	5.60	1.64	1.53
2	B	478	GLY	C-O	-5.60	1.16	1.24
2	B	906	SER	CA-C	-5.60	1.45	1.52
2	B	1079	LYS	CE-NZ	-5.60	1.32	1.49
6	H	140	ALA	C-O	-5.60	1.17	1.24
9	K	96	ASN	CG-ND2	5.60	1.45	1.33
4	E	75	MET	SD-CE	5.60	1.93	1.79
1	A	15	LYS	CB-CG	5.59	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	ALA	N-CA	5.59	1.53	1.46
2	B	64	CYS	C-O	-5.59	1.16	1.24
1	A	827	THR	C-N	-5.59	1.26	1.33
1	A	994	GLN	CD-OE1	-5.59	1.12	1.23
1	A	1214	GLU	CG-CD	5.59	1.66	1.52
2	B	109	THR	CB-OG1	5.59	1.52	1.43
1	A	1238	ILE	CA-C	5.59	1.59	1.52
2	B	446	LEU	CA-C	5.59	1.64	1.52
4	E	74	ASP	CB-CG	-5.59	1.38	1.52
2	B	409	ALA	C-O	-5.59	1.17	1.24
4	E	197	LYS	N-CA	-5.58	1.39	1.46
1	A	303	TYR	C-O	-5.58	1.17	1.24
1	A	273	ASN	CG-ND2	5.58	1.45	1.33
6	H	21	ASN	N-CA	5.58	1.53	1.46
10	L	27	LEU	CA-CB	5.58	1.68	1.54
2	B	699	GLU	C-N	-5.58	1.26	1.33
4	E	2	ASP	CA-C	5.58	1.60	1.52
1	A	716	ASP	CG-OD1	5.57	1.35	1.25
1	A	1322	ILE	CB-CG2	-5.57	1.34	1.52
2	B	235	SER	CA-C	-5.57	1.45	1.52
2	B	649	LYS	CA-C	-5.57	1.45	1.52
2	B	1037	LEU	C-O	-5.57	1.17	1.24
1	A	852	TYR	CA-C	-5.57	1.45	1.52
6	H	109	LYS	CA-C	5.57	1.60	1.52
6	H	13	SER	N-CA	5.57	1.53	1.46
1	A	236	LEU	CA-C	-5.57	1.45	1.52
1	A	440	ASP	CG-OD2	-5.57	1.14	1.25
2	B	48	LEU	N-CA	-5.57	1.39	1.46
6	H	85	GLY	C-O	5.57	1.31	1.23
1	A	525	GLN	CD-OE1	5.57	1.34	1.23
1	A	854	ASN	CB-CG	5.57	1.66	1.52
2	B	514	LEU	N-CA	-5.57	1.39	1.46
6	H	141	TYR	CZ-OH	-5.57	1.26	1.38
8	J	30	LEU	CA-CB	-5.57	1.44	1.53
1	A	469	ARG	CA-C	5.56	1.59	1.52
1	A	1305	VAL	CB-CG1	-5.56	1.34	1.52
8	J	58	GLU	CG-CD	5.56	1.66	1.52
1	A	325	ILE	C-O	-5.56	1.18	1.24
2	B	660	LYS	CA-C	5.56	1.60	1.52
3	C	224	GLN	CD-NE2	5.56	1.45	1.33
2	B	224	GLN	CB-CG	5.56	1.69	1.52
2	B	805	THR	C-N	-5.56	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1075	GLY	CA-C	5.56	1.58	1.51
5	F	106	PRO	CA-CB	-5.56	1.46	1.53
1	A	1291	VAL	CA-CB	-5.56	1.47	1.54
1	A	1341	ILE	CA-CB	-5.56	1.47	1.54
2	B	686	ASN	CG-OD1	5.56	1.34	1.23
7	I	44	TYR	CA-C	-5.56	1.45	1.52
1	A	517	ASN	CB-CG	5.55	1.66	1.52
1	A	27	VAL	CA-CB	-5.55	1.48	1.54
1	A	572	TRP	CE2-CZ2	-5.55	1.28	1.39
1	A	1286	LYS	CA-CB	5.55	1.60	1.53
1	A	1290	LYS	C-N	-5.55	1.27	1.33
2	B	114	PRO	C-O	5.55	1.31	1.24
7	I	96	SER	CA-CB	-5.55	1.44	1.53
1	A	484	GLY	C-O	-5.55	1.17	1.24
1	A	634	THR	CA-C	-5.55	1.45	1.52
2	B	275	TYR	CG-CD1	-5.55	1.27	1.39
4	E	119	SER	C-O	5.55	1.30	1.24
1	A	5	GLN	N-CA	5.55	1.53	1.45
2	B	127	GLY	C-O	-5.55	1.16	1.23
1	A	37	PHE	CE1-CZ	5.54	1.55	1.38
9	K	18	LYS	CA-CB	5.54	1.61	1.53
1	A	529	CYS	CA-C	-5.54	1.45	1.52
1	A	1139	GLU	CA-C	-5.54	1.44	1.52
2	B	272	THR	N-CA	-5.54	1.39	1.46
2	B	384	ARG	CD-NE	5.54	1.54	1.46
4	E	75	MET	C-O	5.54	1.30	1.24
4	E	214	CYS	C-O	-5.54	1.17	1.23
9	K	69	ALA	CA-C	-5.54	1.45	1.52
1	A	830	LYS	CE-NZ	5.54	1.66	1.49
1	A	1207	LEU	CA-C	5.54	1.59	1.52
3	C	159	ALA	CA-C	-5.54	1.45	1.53
1	A	65	LEU	C-O	5.54	1.30	1.24
1	A	781	ASP	C-O	5.54	1.32	1.24
1	A	944	ARG	CZ-NH2	-5.54	1.26	1.33
2	B	686	ASN	C-O	5.54	1.31	1.24
2	B	960	GLY	CA-C	5.54	1.59	1.51
1	A	72	GLU	N-CA	5.53	1.53	1.46
1	A	294	SER	C-O	-5.53	1.16	1.24
1	A	445	ASN	N-CA	-5.53	1.39	1.46
1	A	1163	ILE	CA-C	-5.53	1.48	1.53
2	B	697	GLU	CD-OE2	5.53	1.35	1.25
3	C	244	VAL	CA-C	5.53	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	202	SER	CA-C	-5.53	1.45	1.52
2	B	763	GLN	CB-CG	-5.53	1.35	1.52
1	A	264	PHE	CG-CD2	5.53	1.50	1.38
1	A	285	PRO	CB-CG	-5.53	1.22	1.49
1	A	689	LYS	C-O	-5.53	1.17	1.24
1	A	1446	ASP	CG-OD2	5.53	1.35	1.25
2	B	274	PRO	C-O	5.53	1.29	1.23
2	B	372	SER	C-N	-5.53	1.26	1.33
1	A	400	PRO	C-O	-5.53	1.12	1.23
2	B	241	ARG	CD-NE	5.53	1.53	1.46
1	A	990	VAL	N-CA	-5.53	1.39	1.46
2	B	100	PRO	CB-CG	-5.53	1.22	1.49
2	B	464	GLY	CA-C	5.53	1.59	1.51
1	A	1078	GLN	CA-C	5.53	1.60	1.52
2	B	810	GLU	N-CA	-5.53	1.39	1.46
2	B	935	ARG	CA-CB	5.53	1.59	1.52
5	F	118	LEU	CG-CD1	-5.53	1.34	1.52
1	A	402	ALA	C-O	-5.52	1.17	1.23
2	B	841	MET	C-O	5.52	1.30	1.23
3	C	36	VAL	CA-CB	-5.52	1.47	1.54
1	A	781	ASP	CA-C	-5.52	1.44	1.52
1	A	1057	VAL	C-O	-5.52	1.18	1.24
2	B	542	MET	CA-CB	5.52	1.61	1.53
1	A	602	ASP	C-O	-5.52	1.16	1.23
1	A	1025	ARG	N-CA	-5.52	1.39	1.46
3	C	92	CYS	C-O	-5.52	1.18	1.24
1	A	9	ALA	N-CA	5.52	1.54	1.46
1	A	1066	VAL	CA-C	-5.52	1.46	1.52
9	K	67	PHE	C-O	-5.52	1.16	1.24
10	L	37	LYS	CA-C	-5.52	1.45	1.52
1	A	487	MET	C-O	-5.52	1.16	1.23
1	A	1207	LEU	C-O	-5.52	1.17	1.24
6	H	145	ARG	N-CA	5.52	1.52	1.45
1	A	1095	THR	CA-C	-5.51	1.45	1.52
2	B	310	MET	CA-CB	-5.51	1.44	1.53
2	B	871	THR	CA-CB	5.51	1.62	1.53
2	B	354	ASP	N-CA	-5.51	1.39	1.46
2	B	817	LEU	N-CA	-5.51	1.41	1.46
2	B	1109	GLY	C-O	5.51	1.31	1.24
3	C	128	ASN	CG-OD1	5.51	1.34	1.23
1	A	556	TRP	C-O	5.51	1.30	1.24
1	A	811	GLN	C-O	5.51	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	918	GLU	N-CA	-5.51	1.38	1.46
1	A	1113	THR	CB-OG1	-5.51	1.34	1.43
2	B	599	THR	CA-C	-5.51	1.46	1.52
1	A	1061	GLY	N-CA	-5.51	1.35	1.44
2	B	124	TYR	CA-CB	-5.51	1.44	1.53
2	B	605	ARG	C-O	-5.51	1.17	1.24
6	H	89	LEU	CA-CB	5.51	1.62	1.53
8	J	15	GLY	C-O	5.51	1.30	1.23
1	A	552	TRP	CG-CD1	-5.50	1.23	1.36
2	B	216	GLU	CD-OE2	5.50	1.35	1.25
2	B	1077	THR	C-N	-5.50	1.26	1.33
10	L	36	SER	CA-C	-5.50	1.46	1.52
1	A	1040	GLN	C-O	-5.50	1.17	1.24
2	B	99	LYS	CD-CE	5.50	1.69	1.52
2	B	1219	ASP	CA-CB	5.50	1.63	1.53
3	C	60	ASP	CA-CB	-5.50	1.44	1.53
4	E	28	TYR	N-CA	-5.50	1.38	1.45
6	H	86	ASP	CA-C	5.50	1.60	1.52
7	I	78	CYS	CA-CB	5.50	1.63	1.53
9	K	62	LYS	CA-CB	-5.50	1.44	1.53
2	B	216	GLU	CD-OE1	5.50	1.35	1.25
5	F	109	VAL	CA-CB	-5.50	1.46	1.54
1	A	709	THR	C-N	-5.50	1.27	1.33
1	A	804	TYR	N-CA	-5.50	1.39	1.46
2	B	118	ARG	CA-CB	5.50	1.62	1.53
2	B	203	PHE	N-CA	5.50	1.52	1.45
3	C	90	ASP	CG-OD1	5.50	1.35	1.25
7	I	98	VAL	CB-CG2	-5.50	1.34	1.52
9	K	35	PHE	CE1-CZ	-5.50	1.22	1.38
1	A	834	THR	C-O	-5.50	1.17	1.24
1	A	912	LEU	C-O	-5.50	1.17	1.24
4	E	186	LEU	C-O	-5.50	1.17	1.24
7	I	70	ARG	C-O	-5.50	1.16	1.23
1	A	458	HIS	C-N	5.49	1.41	1.33
4	E	40	GLU	CA-C	5.49	1.59	1.52
2	B	633	VAL	C-N	5.49	1.40	1.33
1	A	277	GLU	CA-C	5.49	1.59	1.52
2	B	1045	SER	CA-C	-5.49	1.45	1.53
6	H	139	ASN	C-O	5.49	1.30	1.24
1	A	1129	GLU	CG-CD	5.49	1.65	1.52
7	I	12	ASN	CG-ND2	-5.49	1.21	1.33
7	I	39	GLY	C-O	-5.49	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	699	ALA	CA-C	5.49	1.60	1.52
2	B	793	ALA	CA-CB	-5.49	1.44	1.53
1	A	1170	ILE	CA-C	-5.49	1.45	1.52
2	B	556	THR	CA-C	5.49	1.59	1.52
2	B	852	ARG	N-CA	-5.49	1.39	1.45
1	A	871	ASP	CG-OD2	5.48	1.35	1.25
1	A	1013	ASP	C-O	5.48	1.30	1.24
2	B	272	THR	CA-CB	-5.48	1.46	1.53
1	A	639	PRO	CA-C	5.48	1.60	1.52
3	C	80	LEU	CA-C	5.48	1.59	1.52
3	C	145	CYS	CA-C	-5.48	1.46	1.52
3	C	198	ALA	CA-C	-5.48	1.45	1.52
9	K	87	LEU	C-O	5.48	1.31	1.24
1	A	1442	ASP	CA-CB	-5.48	1.44	1.53
2	B	1060	ARG	CB-CG	-5.48	1.36	1.52
3	C	146	LYS	C-O	-5.48	1.17	1.23
8	J	10	CYS	CA-C	5.48	1.59	1.52
4	E	3	GLN	CA-CB	5.48	1.62	1.53
1	A	468	PHE	CE2-CZ	-5.47	1.22	1.38
1	A	983	ILE	C-O	-5.47	1.17	1.24
2	B	96	TYR	CG-CD2	5.47	1.50	1.39
9	K	105	PHE	CD1-CE1	-5.47	1.22	1.38
1	A	779	PHE	C-N	-5.47	1.28	1.33
2	B	122	LEU	C-O	-5.47	1.16	1.23
2	B	347	LYS	CA-C	5.47	1.59	1.52
4	E	88	VAL	CA-C	5.47	1.59	1.52
1	A	386	ASP	CA-CB	5.47	1.62	1.53
1	A	581	ALA	CA-CB	5.47	1.62	1.53
1	A	1411	GLU	C-O	5.47	1.30	1.24
3	C	249	ASP	CG-OD1	5.47	1.35	1.25
4	E	212	ARG	NE-CZ	-5.47	1.27	1.33
4	E	196	VAL	CB-CG1	-5.47	1.34	1.52
1	A	46	THR	CA-C	5.47	1.58	1.53
1	A	284	ALA	CA-CB	5.47	1.62	1.53
2	B	319	GLU	CD-OE1	5.47	1.35	1.25
2	B	461	LEU	CG-CD1	-5.47	1.34	1.52
2	B	578	THR	CB-CG2	-5.47	1.34	1.52
2	B	965	LYS	CG-CD	5.47	1.68	1.52
3	C	18	VAL	CB-CG2	-5.47	1.34	1.52
1	A	743	VAL	CA-CB	-5.46	1.47	1.54
1	A	925	LEU	CA-C	-5.46	1.45	1.52
2	B	1103	ILE	C-O	5.46	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	609	ILE	CA-CB	-5.46	1.47	1.54
1	A	916	GLY	CA-C	5.46	1.58	1.52
2	B	314	LEU	N-CA	-5.46	1.38	1.46
4	E	154	ILE	C-O	5.46	1.30	1.24
5	F	78	GLN	N-CA	5.46	1.53	1.46
2	B	359	GLU	CD-OE1	5.46	1.35	1.25
8	J	37	SER	C-O	-5.46	1.17	1.24
1	A	69	THR	C-O	5.46	1.30	1.24
1	A	683	ILE	C-O	-5.46	1.18	1.24
1	A	957	PRO	CA-CB	-5.46	1.45	1.53
1	A	1191	TRP	CE2-CZ2	-5.46	1.28	1.39
2	B	409	ALA	CA-C	-5.46	1.45	1.52
3	C	89	GLU	CD-OE2	5.46	1.35	1.25
3	C	101	LEU	C-O	-5.46	1.17	1.23
2	B	597	MET	CB-CG	-5.46	1.36	1.52
2	B	238	ALA	CA-CB	5.45	1.66	1.53
1	A	16	GLU	CG-CD	5.45	1.65	1.52
1	A	493	GLN	CA-CB	-5.45	1.45	1.53
1	A	698	GLN	C-O	-5.45	1.17	1.24
3	C	117	ASP	C-O	5.45	1.38	1.24
1	A	831	THR	CB-OG1	5.45	1.52	1.43
2	B	1149	GLU	CD-OE1	5.45	1.35	1.25
1	A	1327	ILE	CA-CB	5.45	1.59	1.54
2	B	580	VAL	CA-CB	-5.45	1.47	1.54
2	B	703	ILE	N-CA	-5.45	1.40	1.46
2	B	741	CYS	CA-C	5.45	1.59	1.52
2	B	1023	VAL	N-CA	-5.45	1.40	1.46
2	B	1129	ARG	CZ-NH1	5.45	1.40	1.32
3	C	44	LEU	N-CA	5.45	1.52	1.46
9	K	19	LEU	CA-CB	-5.45	1.41	1.53
1	A	388	LEU	CB-CG	-5.44	1.42	1.53
1	A	1138	ILE	CA-CB	-5.44	1.48	1.54
2	B	406	LEU	C-O	5.44	1.30	1.24
5	F	91	ALA	CA-CB	-5.44	1.44	1.53
1	A	515	GLN	CD-OE1	5.44	1.33	1.23
2	B	509	ALA	CA-C	5.44	1.64	1.52
1	A	669	THR	N-CA	-5.44	1.38	1.46
2	B	112	LEU	CB-CG	-5.44	1.42	1.53
4	E	74	ASP	CG-OD1	-5.44	1.15	1.25
7	I	29	CYS	CA-CB	-5.44	1.44	1.53
7	I	120	GLN	N-CA	5.44	1.54	1.47
4	E	67	GLU	CD-OE1	5.44	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	96	ASN	CB-CG	5.44	1.65	1.52
1	A	737	LEU	C-O	5.44	1.30	1.23
2	B	953	LEU	N-CA	-5.44	1.39	1.46
10	L	70	ARG	NE-CZ	5.44	1.39	1.33
1	A	1214	GLU	CD-OE2	5.44	1.35	1.25
9	K	47	ARG	CD-NE	5.44	1.53	1.46
1	A	54	ASN	CA-C	5.43	1.60	1.52
1	A	559	VAL	C-N	-5.43	1.27	1.33
2	B	603	LEU	CG-CD2	-5.43	1.34	1.52
2	B	887	HIS	CB-CG	5.43	1.57	1.50
6	H	146	ARG	CZ-NH1	5.43	1.40	1.32
1	A	53	LEU	CB-CG	5.43	1.64	1.53
1	A	687	LYS	C-O	-5.43	1.17	1.24
9	K	87	LEU	C-N	5.43	1.40	1.33
1	A	1017	LEU	CG-CD1	-5.43	1.34	1.52
2	B	539	LEU	C-O	-5.43	1.17	1.23
2	B	1198	TYR	C-O	5.43	1.30	1.24
3	C	244	VAL	C-O	5.43	1.30	1.24
7	I	110	PHE	CD1-CE1	5.43	1.54	1.38
1	A	382	PRO	C-O	-5.43	1.17	1.24
9	K	103	THR	CA-CB	5.43	1.62	1.53
1	A	346	ASP	C-O	-5.43	1.12	1.23
2	B	173	MET	CB-CG	5.43	1.68	1.52
2	B	569	TYR	C-O	-5.43	1.17	1.23
3	C	228	PHE	N-CA	-5.43	1.40	1.46
1	A	468	PHE	CG-CD1	-5.42	1.27	1.38
1	A	1156	PRO	CA-C	5.42	1.60	1.52
2	B	108	VAL	CB-CG2	5.42	1.70	1.52
2	B	538	ASN	CA-C	-5.42	1.46	1.52
3	C	24	ASN	C-O	5.42	1.31	1.23
2	B	542	MET	C-N	-5.42	1.26	1.33
1	A	642	CYS	CA-C	5.42	1.59	1.52
8	J	52	THR	C-O	5.42	1.31	1.24
2	B	70	ILE	CB-CG2	5.42	1.70	1.52
2	B	620	ARG	C-N	-5.42	1.25	1.33
3	C	215	GLU	N-CA	5.42	1.53	1.46
1	A	678	GLU	CG-CD	5.42	1.65	1.52
1	A	1228	TRP	CE2-CZ2	-5.42	1.28	1.39
2	B	254	LEU	C-O	5.42	1.30	1.24
2	B	736	THR	CB-OG1	-5.42	1.35	1.43
3	C	232	VAL	C-N	-5.42	1.25	1.33
6	H	123	MET	CA-C	-5.42	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	LEU	C-O	-5.42	1.17	1.24
2	B	1098	MET	N-CA	5.42	1.53	1.45
6	H	109	LYS	CB-CG	5.42	1.68	1.52
7	I	84	VAL	CA-CB	-5.42	1.46	1.55
8	J	39	LEU	CA-C	-5.42	1.43	1.52
9	K	106	GLU	CA-C	5.42	1.60	1.52
1	A	1033	GLN	CA-CB	5.42	1.62	1.53
2	B	463	THR	CA-CB	5.42	1.62	1.53
7	I	62	ILE	C-N	-5.42	1.25	1.33
1	A	721	PHE	N-CA	-5.41	1.39	1.46
5	F	109	VAL	C-O	-5.41	1.17	1.23
6	H	118	PHE	CG-CD1	5.41	1.50	1.38
7	I	108	HIS	CA-CB	5.41	1.61	1.53
9	K	72	LYS	N-CA	-5.41	1.39	1.46
2	B	336	ARG	N-CA	-5.41	1.39	1.46
1	A	238	CYS	C-N	-5.41	1.27	1.33
1	A	839	ARG	CZ-NH2	5.41	1.40	1.33
1	A	1001	ARG	CZ-NH2	5.41	1.40	1.33
2	B	250	PHE	CD2-CE2	5.41	1.54	1.38
2	B	732	SER	CA-CB	5.41	1.62	1.53
3	C	41	ILE	CA-C	5.41	1.58	1.52
5	F	148	VAL	N-CA	-5.41	1.40	1.46
9	K	110	ASN	C-O	-5.41	1.17	1.24
1	A	898	ARG	C-O	5.41	1.30	1.24
1	A	1110	ASN	CG-ND2	5.41	1.44	1.33
1	A	1445	ILE	C-N	5.41	1.40	1.33
3	C	206	ASN	C-N	-5.41	1.26	1.33
3	C	241	ASP	N-CA	5.41	1.53	1.46
7	I	101	PHE	CD1-CE1	5.41	1.54	1.38
8	J	20	SER	N-CA	5.41	1.53	1.46
2	B	351	TYR	CA-C	5.41	1.59	1.52
6	H	104	PHE	CG-CD1	5.41	1.50	1.38
1	A	1159	ARG	CB-CG	5.41	1.68	1.52
2	B	46	GLN	C-O	5.41	1.30	1.24
2	B	827	ILE	C-O	-5.41	1.18	1.24
4	E	159	ASP	CG-OD1	5.41	1.35	1.25
2	B	1094	ARG	CA-CB	-5.40	1.45	1.53
4	E	78	LEU	CB-CG	5.40	1.64	1.53
7	I	91	ARG	N-CA	-5.40	1.38	1.47
1	A	787	PHE	CA-CB	-5.40	1.45	1.53
1	A	1071	SER	CA-CB	-5.40	1.44	1.53
2	B	250	PHE	CG-CD2	5.40	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	193	TYR	CA-C	-5.40	1.46	1.52
2	B	817	LEU	CA-CB	-5.40	1.47	1.53
1	A	802	ASN	CA-CB	-5.40	1.44	1.53
1	A	932	GLU	CD-OE2	5.40	1.35	1.25
2	B	1055	ILE	C-N	-5.40	1.26	1.33
3	C	205	LYS	CB-CG	5.40	1.68	1.52
2	B	639	ILE	C-O	-5.40	1.17	1.24
2	B	835	GLN	CB-CG	5.40	1.68	1.52
4	E	58	MET	N-CA	5.40	1.52	1.46
1	A	738	LYS	CG-CD	5.39	1.68	1.52
1	A	1445	ILE	CA-C	-5.39	1.46	1.52
7	I	99	LEU	CB-CG	-5.39	1.42	1.53
2	B	348	ARG	CD-NE	-5.39	1.38	1.46
2	B	608	ASP	CB-CG	5.39	1.65	1.52
3	C	174	ALA	C-N	-5.39	1.26	1.33
1	A	771	GLU	CD-OE1	5.39	1.35	1.25
2	B	336	ARG	NE-CZ	-5.39	1.27	1.33
2	B	1026	LEU	CB-CG	-5.39	1.42	1.53
3	C	67	LEU	CG-CD1	-5.39	1.34	1.52
4	E	68	SER	C-O	5.39	1.30	1.24
1	A	1074	GLU	C-O	-5.39	1.17	1.24
2	B	65	GLU	CG-CD	5.39	1.65	1.52
5	F	146	TRP	CB-CG	-5.39	1.33	1.50
1	A	813	PHE	CE1-CZ	-5.39	1.22	1.38
2	B	1047	PHE	C-O	-5.39	1.16	1.23
4	E	197	LYS	CG-CD	5.39	1.68	1.52
1	A	12	ARG	C-O	-5.38	1.17	1.23
1	A	1450	LEU	CB-CG	5.38	1.64	1.53
2	B	852	ARG	CZ-NH2	-5.38	1.26	1.33
2	B	44	VAL	CA-CB	-5.38	1.47	1.54
1	A	767	GLN	C-O	-5.38	1.17	1.24
1	A	1342	GLU	CD-OE1	5.38	1.35	1.25
1	A	1363	VAL	CB-CG1	5.38	1.70	1.52
2	B	233	PRO	CB-CG	5.38	1.76	1.49
2	B	288	ALA	CA-CB	5.38	1.62	1.53
2	B	1152	MET	SD-CE	5.38	1.93	1.79
3	C	222	LYS	CB-CG	5.38	1.68	1.52
6	H	129	TYR	CG-CD2	5.38	1.50	1.39
1	A	534	LEU	CA-CB	-5.38	1.44	1.53
2	B	53	GLN	CD-NE2	-5.38	1.22	1.33
3	C	169	LYS	CA-CB	-5.38	1.44	1.53
1	A	942	PHE	C-N	-5.38	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	57	TYR	CE2-CZ	-5.38	1.25	1.38
2	B	664	THR	N-CA	-5.38	1.39	1.46
6	H	22	LYS	CB-CG	5.38	1.68	1.52
7	I	35	VAL	CB-CG2	-5.38	1.34	1.52
1	A	876	ALA	CA-CB	-5.37	1.44	1.53
1	A	937	VAL	CA-C	-5.37	1.45	1.52
2	B	449	ASN	N-CA	5.37	1.52	1.46
2	B	565	PRO	CA-CB	-5.37	1.47	1.53
2	B	579	ARG	CA-CB	-5.37	1.45	1.53
1	A	1379	GLY	C-O	-5.37	1.16	1.24
2	B	242	SER	C-O	-5.37	1.17	1.23
2	B	447	ALA	CA-CB	-5.37	1.44	1.53
2	B	875	GLU	CG-CD	5.37	1.65	1.52
6	H	85	GLY	N-CA	5.37	1.53	1.45
9	K	6	ARG	C-O	5.37	1.30	1.24
1	A	1153	TYR	C-O	5.37	1.30	1.23
1	A	1164	PRO	CA-CB	5.37	1.61	1.53
2	B	1103	ILE	CA-CB	5.37	1.61	1.54
2	B	131	ASP	CA-CB	5.37	1.62	1.53
1	A	84	ILE	CA-C	-5.37	1.46	1.52
1	A	474	VAL	CA-CB	-5.37	1.47	1.54
2	B	120	ARG	CZ-NH2	5.37	1.40	1.33
2	B	336	ARG	CA-CB	-5.37	1.44	1.53
2	B	684	LEU	CA-CB	-5.37	1.45	1.53
9	K	67	PHE	N-CA	-5.37	1.39	1.46
2	B	732	SER	C-N	5.36	1.41	1.33
2	B	844	SER	C-O	-5.36	1.18	1.24
2	B	1180	PHE	C-O	5.36	1.30	1.24
2	B	296	GLU	CG-CD	5.36	1.65	1.52
2	B	915	THR	N-CA	5.36	1.52	1.45
4	E	99	HIS	CB-CG	5.36	1.57	1.50
9	K	25	THR	CB-CG2	5.36	1.70	1.52
2	B	35	SER	CA-CB	-5.36	1.45	1.53
4	E	154	ILE	CB-CG2	-5.36	1.34	1.52
2	B	758	PHE	CG-CD2	-5.36	1.27	1.38
4	E	122	LYS	N-CA	5.36	1.53	1.46
1	A	51	GLY	C-O	-5.35	1.16	1.23
2	B	52	ASN	N-CA	-5.35	1.39	1.46
2	B	208	SER	N-CA	5.35	1.52	1.46
2	B	633	VAL	CA-CB	-5.35	1.47	1.54
5	F	146	TRP	CA-CB	-5.35	1.43	1.53
6	H	146	ARG	CZ-NH2	5.35	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	58	VAL	C-O	-5.35	1.18	1.24
2	B	115	GLN	CD-NE2	5.35	1.44	1.33
2	B	889	THR	CA-C	-5.35	1.45	1.52
1	A	653	VAL	CA-C	5.35	1.59	1.52
1	A	1208	THR	CA-C	5.35	1.59	1.52
1	A	1432	GLN	N-CA	-5.35	1.39	1.45
1	A	589	GLN	CD-NE2	5.35	1.44	1.33
1	A	865	GLN	CA-C	5.34	1.59	1.52
1	A	962	ARG	C-N	-5.34	1.27	1.34
1	A	1005	GLU	CG-CD	5.34	1.65	1.52
1	A	1337	GLU	CD-OE1	5.34	1.35	1.25
2	B	569	TYR	CG-CD2	-5.34	1.28	1.39
2	B	1092	TYR	CG-CD1	-5.34	1.28	1.39
4	E	162	ARG	C-N	-5.34	1.26	1.33
1	A	5	GLN	CA-C	-5.34	1.46	1.53
2	B	405	ARG	N-CA	-5.34	1.39	1.46
9	K	50	LEU	CB-CG	-5.34	1.42	1.53
1	A	404	TYR	CA-C	-5.34	1.46	1.52
1	A	1092	LYS	CG-CD	5.34	1.68	1.52
2	B	221	ASN	CA-C	5.34	1.60	1.52
1	A	53	LEU	C-O	5.34	1.31	1.23
1	A	553	VAL	CB-CG1	-5.34	1.34	1.52
1	A	406	ILE	CA-C	-5.34	1.46	1.52
1	A	1013	ASP	CG-OD1	5.34	1.35	1.25
2	B	478	GLY	CA-C	5.34	1.58	1.51
2	B	773	MET	C-N	-5.34	1.25	1.33
4	E	203	GLU	C-O	-5.34	1.16	1.24
5	F	123	LYS	CG-CD	5.33	1.68	1.52
9	K	55	LYS	CD-CE	5.33	1.68	1.52
1	A	1032	LEU	C-N	-5.33	1.25	1.33
1	A	1194	ARG	N-CA	-5.33	1.39	1.46
2	B	249	ARG	CG-CD	5.33	1.68	1.52
2	B	1021	MET	CG-SD	-5.33	1.67	1.80
2	B	1204	PHE	CA-C	-5.33	1.46	1.52
1	A	884	ASP	N-CA	5.33	1.52	1.46
1	A	1072	ILE	CA-C	5.33	1.58	1.52
1	A	1264	GLU	CA-CB	-5.33	1.45	1.53
1	A	1217	LYS	C-O	5.33	1.30	1.24
8	J	29	GLU	C-O	5.33	1.31	1.23
1	A	423	ASP	C-O	5.33	1.29	1.23
1	A	731	ARG	CZ-NH1	5.33	1.40	1.32
1	A	1025	ARG	CG-CD	-5.33	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	486	TYR	CE1-CZ	5.33	1.51	1.38
2	B	554	ILE	CA-C	-5.33	1.46	1.52
2	B	956	THR	CA-CB	-5.33	1.44	1.53
3	C	15	LYS	CB-CG	5.33	1.68	1.52
1	A	577	ILE	CA-CB	-5.33	1.47	1.54
1	A	982	THR	CA-CB	-5.33	1.45	1.53
2	B	654	ARG	CZ-NH1	-5.33	1.25	1.32
2	B	1017	ILE	C-O	-5.33	1.17	1.24
2	B	297	ILE	C-O	-5.33	1.17	1.24
4	E	66	GLU	CG-CD	5.33	1.65	1.52
6	H	120	GLY	CA-C	5.33	1.59	1.51
1	A	701	LEU	CA-CB	-5.32	1.45	1.53
2	B	1152	MET	CA-CB	5.32	1.61	1.53
1	A	1230	GLU	N-CA	5.32	1.52	1.45
1	A	700	ASN	C-O	-5.32	1.16	1.23
1	A	940	ARG	CZ-NH2	-5.32	1.26	1.33
5	F	72	LYS	CA-C	5.32	1.64	1.52
1	A	567	LYS	CA-CB	-5.32	1.45	1.53
2	B	887	HIS	C-N	5.32	1.39	1.33
2	B	971	THR	CA-CB	-5.32	1.45	1.53
5	F	131	PRO	CA-C	-5.32	1.48	1.53
2	B	279	ASP	CG-OD2	5.32	1.35	1.25
7	I	34	TYR	CG-CD2	-5.32	1.28	1.39
1	A	1059	HIS	C-O	-5.31	1.17	1.24
2	B	879	ARG	N-CA	5.31	1.53	1.46
10	L	47	ARG	CB-CG	5.31	1.68	1.52
2	B	534	GLY	C-O	5.31	1.31	1.24
2	B	781	PHE	N-CA	-5.31	1.39	1.46
2	B	898	LEU	C-O	-5.31	1.17	1.23
4	E	92	THR	CA-C	5.31	1.59	1.52
2	B	652	LYS	CG-CD	5.31	1.68	1.52
3	C	58	LEU	C-O	-5.31	1.17	1.23
7	I	97	MET	SD-CE	5.31	1.92	1.79
10	L	31	CYS	CA-C	-5.31	1.46	1.52
2	B	259	TYR	CA-C	-5.31	1.46	1.52
2	B	731	VAL	CB-CG2	5.31	1.70	1.52
2	B	896	ASP	C-O	-5.31	1.17	1.24
6	H	104	PHE	N-CA	5.31	1.53	1.46
1	A	1289	ARG	CB-CG	-5.31	1.36	1.52
2	B	321	GLY	C-O	-5.31	1.17	1.23
2	B	519	TRP	CZ3-CH2	-5.30	1.27	1.40
10	L	25	ALA	CA-CB	5.30	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	270	LYS	CA-C	-5.30	1.46	1.52
2	B	790	ASP	CA-CB	5.30	1.62	1.53
2	B	1193	GLN	C-O	-5.30	1.17	1.23
2	B	1216	LEU	C-O	5.30	1.30	1.24
3	C	51	VAL	CB-CG1	-5.30	1.35	1.52
1	A	757	ASN	CG-ND2	-5.30	1.22	1.33
1	A	266	LEU	C-O	-5.30	1.17	1.24
1	A	464	PRO	N-CA	-5.30	1.40	1.47
1	A	700	ASN	CG-OD1	-5.30	1.13	1.23
1	A	786	HIS	CB-CG	-5.30	1.42	1.50
2	B	341	LEU	CA-CB	-5.30	1.44	1.53
2	B	874	PHE	CA-CB	5.30	1.59	1.53
1	A	1049	ILE	C-N	-5.30	1.27	1.33
1	A	1130	GLN	C-O	5.30	1.31	1.24
2	B	912	ILE	N-CA	-5.30	1.39	1.46
6	H	83	GLN	N-CA	5.30	1.53	1.46
3	C	85	ASP	C-O	-5.29	1.17	1.24
1	A	657	LEU	CG-CD1	-5.29	1.35	1.52
4	E	103	LYS	C-O	5.29	1.32	1.24
9	K	74	ARG	C-O	5.29	1.30	1.24
1	A	927	VAL	CA-CB	-5.29	1.47	1.54
2	B	354	ASP	CG-OD2	5.29	1.35	1.25
7	I	56	ALA	C-N	-5.29	1.25	1.33
1	A	447	GLN	CA-C	-5.29	1.46	1.53
2	B	838	SER	C-O	-5.29	1.17	1.23
4	E	14	ARG	CA-C	-5.29	1.46	1.52
8	J	6	ARG	CB-CG	5.29	1.68	1.52
2	B	188	ASP	C-N	5.29	1.41	1.33
6	H	87	ARG	CD-NE	5.29	1.53	1.46
2	B	614	SER	CA-C	5.28	1.58	1.52
2	B	644	GLU	N-CA	-5.28	1.39	1.46
3	C	173	ALA	N-CA	5.28	1.52	1.45
8	J	51	LEU	CA-CB	-5.28	1.44	1.53
2	B	296	GLU	CD-OE2	5.28	1.35	1.25
1	A	268	ASP	CA-C	5.28	1.59	1.52
1	A	631	HIS	CA-C	-5.28	1.46	1.52
2	B	874	PHE	CD2-CE2	-5.28	1.22	1.38
1	A	1003	LYS	CD-CE	5.28	1.68	1.52
2	B	327	ARG	C-O	-5.28	1.17	1.24
7	I	14	LEU	CG-CD1	-5.28	1.35	1.52
1	A	833	GLU	CD-OE1	5.28	1.35	1.25
1	A	1111	MET	N-CA	-5.28	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	124	GLU	C-O	5.28	1.30	1.24
1	A	1221	LYS	N-CA	5.27	1.52	1.46
1	A	608	ILE	CB-CG1	5.27	1.64	1.53
1	A	961	ARG	CD-NE	5.27	1.53	1.46
4	E	164	LEU	C-N	-5.27	1.26	1.34
1	A	623	GLY	CA-C	-5.27	1.44	1.52
1	A	1308	THR	CB-CG2	-5.27	1.35	1.52
1	A	1315	GLU	CD-OE2	5.27	1.35	1.25
1	A	1064	VAL	C-O	-5.27	1.17	1.24
2	B	1050	ILE	CA-CB	5.27	1.61	1.54
1	A	351	THR	CB-CG2	-5.27	1.35	1.52
2	B	786	ASN	CG-ND2	5.27	1.44	1.33
3	C	153	LEU	C-O	-5.27	1.18	1.23
3	C	238	ILE	CA-C	-5.27	1.47	1.52
6	H	121	LEU	CA-CB	-5.27	1.45	1.53
8	J	18	TRP	CA-C	5.27	1.59	1.52
8	J	20	SER	C-O	-5.27	1.17	1.24
1	A	1058	VAL	CA-CB	5.26	1.60	1.54
2	B	172	ILE	N-CA	-5.26	1.40	1.46
2	B	797	TYR	CG-CD1	-5.26	1.28	1.39
2	B	987	LYS	C-O	-5.26	1.17	1.23
7	I	47	GLU	CA-CB	-5.26	1.46	1.53
1	A	919	ILE	C-O	-5.26	1.18	1.24
2	B	1014	PRO	C-O	5.26	1.30	1.24
7	I	68	LEU	CA-C	-5.26	1.45	1.52
7	I	120	GLN	CG-CD	5.26	1.65	1.52
1	A	800	VAL	N-CA	-5.26	1.40	1.46
2	B	208	SER	CA-CB	-5.26	1.45	1.53
2	B	710	LEU	CA-CB	-5.26	1.45	1.53
5	F	119	ARG	C-O	5.26	1.30	1.24
6	H	9	ILE	N-CA	5.26	1.52	1.46
1	A	269	ILE	C-N	-5.26	1.26	1.34
1	A	453	MET	CG-SD	5.26	1.93	1.80
8	J	64	ASN	CA-C	5.26	1.64	1.52
1	A	563	PRO	CG-CD	5.26	1.68	1.50
1	A	1003	LYS	CE-NZ	5.26	1.65	1.49
1	A	1176	LEU	CA-CB	5.26	1.64	1.53
2	B	1109	GLY	N-CA	5.25	1.51	1.44
1	A	1297	GLU	CD-OE1	-5.25	1.15	1.25
3	C	218	PRO	CA-C	5.25	1.59	1.52
1	A	455	MET	CB-CG	-5.25	1.36	1.52
6	H	19	ARG	CZ-NH2	5.25	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	103	CYS	CA-C	-5.25	1.45	1.52
1	A	523	ILE	CA-C	-5.25	1.46	1.52
2	B	1211	ASN	CB-CG	-5.25	1.39	1.52
2	B	970	THR	C-N	-5.25	1.25	1.33
3	C	189	THR	CA-C	-5.25	1.46	1.52
4	E	83	CYS	N-CA	-5.25	1.39	1.46
1	A	430	TRP	CA-C	-5.25	1.46	1.53
7	I	36	GLU	CG-CD	5.25	1.65	1.52
1	A	275	SER	CA-C	5.24	1.59	1.52
4	E	198	ILE	C-O	-5.24	1.18	1.24
2	B	21	GLU	CD-OE2	5.24	1.35	1.25
3	C	109	SER	CA-CB	5.24	1.60	1.53
1	A	975	HIS	CB-CG	5.24	1.57	1.50
2	B	248	SER	N-CA	5.24	1.52	1.46
1	A	248	PRO	N-CD	5.24	1.55	1.47
1	A	897	TYR	CG-CD2	-5.24	1.28	1.39
2	B	451	LYS	CA-C	5.24	1.59	1.52
4	E	111	VAL	CA-CB	-5.24	1.48	1.54
4	E	130	ALA	CA-CB	5.24	1.61	1.53
9	K	54	ARG	CZ-NH1	5.24	1.40	1.32
4	E	215	MET	CG-SD	5.24	1.93	1.80
8	J	41	LEU	CG-CD2	-5.24	1.35	1.52
2	B	250	PHE	CD1-CE1	5.24	1.54	1.38
2	B	646	LEU	CA-CB	5.24	1.62	1.53
2	B	1049	ASP	CG-OD1	5.24	1.35	1.25
1	A	739	ASP	CB-CG	5.23	1.65	1.52
1	A	379	VAL	CB-CG1	-5.23	1.35	1.52
1	A	411	ASP	CG-OD2	5.23	1.35	1.25
1	A	438	ASP	CG-OD1	-5.23	1.15	1.25
2	B	968	VAL	C-O	5.23	1.30	1.24
3	C	209	TYR	CE2-CZ	5.23	1.50	1.38
9	K	5	ASP	CA-CB	-5.23	1.44	1.53
9	K	53	ASP	C-O	-5.23	1.18	1.24
1	A	862	ASN	CA-CB	-5.23	1.45	1.53
1	A	972	HIS	C-O	-5.23	1.15	1.23
2	B	279	ASP	CB-CG	5.23	1.65	1.52
2	B	314	LEU	CG-CD2	-5.23	1.35	1.52
2	B	433	GLN	N-CA	5.23	1.52	1.46
2	B	829	CYS	CA-CB	5.23	1.60	1.53
2	B	1021	MET	CB-CG	5.23	1.68	1.52
1	A	884	ASP	CA-C	5.23	1.59	1.52
2	B	879	ARG	NE-CZ	5.23	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	84	LYS	CG-CD	5.23	1.68	1.52
1	A	689	LYS	CD-CE	5.22	1.68	1.52
1	A	949	ASP	CA-C	-5.22	1.45	1.52
1	A	1299	VAL	C-O	5.22	1.29	1.23
2	B	245	GLU	CG-CD	5.22	1.65	1.52
1	A	1426	GLU	CD-OE2	5.22	1.35	1.25
2	B	170	LEU	CA-C	-5.22	1.46	1.52
2	B	242	SER	CB-OG	5.22	1.52	1.42
2	B	266	ALA	N-CA	5.22	1.52	1.46
2	B	1136	ASP	CG-OD1	5.22	1.35	1.25
3	C	180	TYR	C-O	-5.22	1.17	1.23
9	K	101	LEU	CA-C	5.22	1.59	1.52
1	A	1415	SER	C-O	-5.22	1.17	1.24
1	A	487	MET	N-CA	-5.22	1.39	1.45
1	A	717	ASN	N-CA	-5.22	1.40	1.46
1	A	1012	ARG	CD-NE	5.22	1.53	1.46
2	B	1018	PRO	C-O	-5.22	1.18	1.24
3	C	195	GLN	CD-NE2	5.22	1.44	1.33
1	A	681	GLU	C-O	5.22	1.30	1.24
2	B	568	ASP	CA-CB	5.22	1.63	1.53
5	F	108	PHE	C-O	-5.22	1.16	1.24
1	A	595	THR	C-O	-5.22	1.17	1.23
1	A	1158	PRO	C-O	-5.22	1.17	1.24
2	B	588	GLY	C-O	5.22	1.30	1.23
2	B	739	THR	CA-C	-5.22	1.45	1.52
6	H	36	CYS	CA-CB	5.22	1.60	1.53
1	A	726	ARG	CZ-NH2	5.21	1.40	1.33
1	A	1305	VAL	CA-CB	-5.21	1.47	1.54
2	B	601	ARG	CA-CB	5.21	1.61	1.53
2	B	1143	ALA	N-CA	-5.21	1.40	1.46
2	B	1012	ILE	C-O	-5.21	1.17	1.24
3	C	168	ALA	C-O	-5.21	1.17	1.24
2	B	185	THR	CA-C	-5.21	1.46	1.53
9	K	91	CYS	CA-CB	-5.21	1.45	1.53
1	A	1211	GLN	CD-OE1	5.21	1.33	1.23
1	A	1357	ALA	N-CA	5.21	1.52	1.46
2	B	800	GLN	C-O	-5.21	1.17	1.23
9	K	19	LEU	C-O	-5.21	1.17	1.23
1	A	705	LYS	CG-CD	5.21	1.68	1.52
1	A	1449	SER	C-N	5.21	1.40	1.33
2	B	206	ASN	CG-OD1	5.21	1.33	1.23
10	L	29	TYR	CE1-CZ	-5.21	1.25	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1116	LEU	C-O	-5.21	1.17	1.24
2	B	390	LEU	CA-CB	5.21	1.62	1.53
2	B	708	GLU	CD-OE2	5.21	1.35	1.25
2	B	994	TYR	CG-CD2	-5.21	1.28	1.39
1	A	1013	ASP	CA-C	5.21	1.59	1.52
6	H	44	VAL	C-O	5.21	1.30	1.24
1	A	578	LEU	CG-CD1	-5.20	1.35	1.52
1	A	620	LYS	CA-CB	5.20	1.61	1.53
1	A	1121	GLU	CD-OE1	5.20	1.35	1.25
4	E	182	ASP	C-O	-5.20	1.18	1.24
6	H	81	PRO	CA-C	5.20	1.56	1.52
1	A	791	ASP	C-N	5.20	1.40	1.33
1	A	1242	VAL	N-CA	-5.20	1.39	1.46
1	A	859	SER	C-O	5.20	1.30	1.24
2	B	1027	ILE	CA-C	-5.20	1.44	1.52
2	B	1030	LEU	CA-CB	-5.20	1.45	1.53
3	C	177	GLU	CG-CD	5.20	1.65	1.52
2	B	95	ILE	C-O	-5.20	1.18	1.24
2	B	695	ALA	C-O	-5.20	1.17	1.24
5	F	129	LYS	CG-CD	5.20	1.68	1.52
5	F	144	GLU	N-CA	-5.20	1.39	1.45
1	A	376	TYR	CG-CD1	-5.20	1.28	1.39
1	A	792	TYR	CE1-CZ	-5.20	1.25	1.38
1	A	963	ILE	CA-C	5.20	1.59	1.52
1	A	1223	ASP	CG-OD2	5.20	1.35	1.25
2	B	518	HIS	CG-ND1	-5.20	1.32	1.38
2	B	690	VAL	N-CA	-5.20	1.40	1.46
3	C	44	LEU	C-O	5.20	1.30	1.24
7	I	72	ASP	CA-CB	5.20	1.60	1.53
9	K	29	ASN	CG-OD1	5.20	1.33	1.23
1	A	407	ARG	C-O	5.19	1.30	1.23
2	B	370	PHE	C-N	5.19	1.40	1.33
2	B	373	ARG	C-N	-5.19	1.26	1.33
2	B	914	LYS	CA-CB	-5.19	1.45	1.53
2	B	1199	ALA	CA-C	-5.19	1.45	1.52
6	H	2	SER	CA-CB	5.19	1.63	1.53
9	K	100	ALA	N-CA	5.19	1.52	1.46
1	A	237	THR	C-N	5.19	1.40	1.33
1	A	787	PHE	N-CA	-5.19	1.39	1.45
2	B	901	PRO	CG-CD	5.19	1.68	1.50
3	C	220	ASP	CG-OD1	5.19	1.35	1.25
5	F	90	ARG	CZ-NH2	-5.19	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	LEU	CA-C	5.19	1.59	1.52
1	A	913	LEU	N-CA	5.19	1.52	1.46
2	B	215	GLN	N-CA	-5.19	1.39	1.46
2	B	338	GLY	C-O	-5.19	1.17	1.23
2	B	961	LEU	CG-CD1	5.19	1.69	1.52
3	C	156	THR	CA-C	-5.19	1.46	1.52
2	B	851	PHE	CB-CG	5.19	1.62	1.50
1	A	950	GLY	CA-C	5.19	1.59	1.51
2	B	420	LEU	CG-CD1	5.19	1.69	1.52
2	B	831	SER	C-N	5.19	1.40	1.33
2	B	1181	GLU	C-O	5.19	1.29	1.24
6	H	12	VAL	CA-CB	5.19	1.59	1.53
1	A	1139	GLU	C-O	5.19	1.30	1.24
1	A	349	ALA	CA-C	-5.18	1.46	1.52
1	A	518	LYS	CB-CG	-5.18	1.36	1.52
2	B	315	LYS	CB-CG	-5.18	1.36	1.52
2	B	1180	PHE	N-CA	-5.18	1.40	1.46
3	C	209	TYR	CA-C	-5.18	1.45	1.52
3	C	231	ASN	CB-CG	5.18	1.65	1.52
1	A	45	GLN	CA-CB	5.18	1.62	1.53
2	B	632	ARG	CA-CB	-5.18	1.45	1.53
3	C	242	GLN	C-O	-5.18	1.17	1.24
4	E	43	LYS	CA-C	5.18	1.59	1.52
7	I	6	PHE	CE1-CZ	-5.18	1.23	1.38
1	A	745	GLN	N-CA	5.18	1.52	1.46
1	A	1290	LYS	CB-CG	5.18	1.68	1.52
1	A	295	LEU	C-N	5.18	1.40	1.33
1	A	1162	VAL	N-CA	-5.18	1.39	1.46
9	K	17	SER	C-N	-5.18	1.27	1.33
1	A	791	ASP	N-CA	-5.18	1.39	1.46
4	E	102	GLU	CA-C	-5.18	1.45	1.52
4	E	135	PHE	C-O	-5.18	1.18	1.24
1	A	963	ILE	C-N	-5.17	1.27	1.33
2	B	738	PHE	CG-CD1	-5.17	1.27	1.38
2	B	807	ARG	C-O	-5.17	1.17	1.24
3	C	46	ILE	CA-CB	-5.17	1.48	1.54
6	H	25	ARG	CA-C	5.17	1.59	1.52
1	A	711	ARG	CD-NE	-5.17	1.39	1.46
1	A	591	PHE	CB-CG	5.17	1.62	1.50
2	B	491	THR	N-CA	-5.17	1.40	1.46
8	J	10	CYS	CA-CB	-5.17	1.46	1.54
1	A	664	THR	CB-CG2	-5.17	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	805	THR	C-O	-5.17	1.16	1.23
6	H	30	SER	N-CA	5.17	1.52	1.46
9	K	66	PRO	CA-C	-5.17	1.43	1.52
9	K	111	LEU	CG-CD2	5.17	1.69	1.52
1	A	269	ILE	C-O	-5.17	1.18	1.24
1	A	449	SER	C-N	-5.17	1.26	1.33
1	A	620	LYS	C-O	-5.17	1.17	1.24
1	A	852	TYR	CZ-OH	-5.17	1.27	1.38
1	A	1269	GLU	CA-C	5.17	1.59	1.53
2	B	461	LEU	CA-C	-5.17	1.45	1.52
2	B	962	LYS	CE-NZ	5.17	1.64	1.49
4	E	106	GLN	CD-OE1	5.17	1.33	1.23
9	K	113	THR	CB-CG2	5.17	1.69	1.52
10	L	41	SER	C-O	5.17	1.30	1.24
1	A	731	ARG	CA-C	-5.17	1.45	1.52
1	A	759	ALA	CA-C	-5.17	1.46	1.52
1	A	247	ARG	CA-C	5.16	1.58	1.52
1	A	997	LEU	CA-C	-5.16	1.46	1.53
2	B	380	TYR	C-O	-5.16	1.18	1.24
4	E	3	GLN	CA-C	5.16	1.59	1.52
4	E	13	TRP	CG-CD1	5.16	1.49	1.36
1	A	890	ASP	CA-CB	-5.16	1.44	1.53
1	A	1119	TYR	CG-CD1	-5.16	1.28	1.39
2	B	367	LEU	CB-CG	5.16	1.63	1.53
2	B	538	ASN	C-O	-5.16	1.18	1.24
2	B	1132	GLU	CG-CD	5.16	1.65	1.52
3	C	99	LEU	CG-CD1	-5.16	1.35	1.52
1	A	398	GLU	CD-OE2	5.16	1.35	1.25
1	A	514	PRO	N-CA	-5.16	1.40	1.47
2	B	377	PHE	CB-CG	-5.16	1.38	1.50
2	B	901	PRO	C-N	-5.16	1.25	1.33
3	C	99	LEU	CG-CD2	-5.16	1.35	1.52
3	C	209	TYR	CD2-CE2	5.16	1.54	1.38
2	B	980	PHE	CG-CD1	-5.16	1.28	1.38
2	B	1181	GLU	CA-C	5.16	1.58	1.52
2	B	1192	TYR	N-CA	-5.16	1.39	1.45
1	A	656	TRP	NE1-CE2	-5.16	1.31	1.37
1	A	1281	ARG	CD-NE	5.16	1.53	1.46
2	B	767	ASN	CG-OD1	5.16	1.33	1.23
5	F	107	VAL	CA-C	5.15	1.59	1.52
7	I	58	VAL	C-N	-5.15	1.27	1.33
2	B	234	ILE	C-O	-5.15	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	839	MET	CA-CB	-5.15	1.45	1.53
5	F	104	ASN	N-CA	5.15	1.54	1.46
7	I	28	GLU	CG-CD	5.15	1.65	1.52
1	A	63	ARG	CB-CG	5.15	1.67	1.52
2	B	666	TYR	CE1-CZ	5.15	1.50	1.38
1	A	994	GLN	CG-CD	-5.15	1.39	1.52
2	B	1130	PHE	CE1-CZ	-5.15	1.23	1.38
4	E	63	ASN	CG-OD1	5.15	1.33	1.23
1	A	61	ILE	CB-CG2	5.14	1.69	1.52
1	A	1026	LEU	CA-CB	-5.14	1.46	1.53
1	A	1267	MET	C-O	-5.14	1.17	1.24
3	C	143	LEU	C-N	-5.14	1.27	1.33
5	F	77	ASP	CG-OD2	5.14	1.35	1.25
2	B	364	ILE	N-CA	-5.14	1.40	1.46
2	B	629	ASP	CG-OD2	5.14	1.35	1.25
9	K	112	GLN	CB-CG	5.14	1.67	1.52
3	C	147	LEU	CA-CB	-5.14	1.44	1.53
2	B	385	LEU	CA-C	-5.14	1.46	1.52
9	K	53	ASP	CA-CB	5.14	1.59	1.53
1	A	189	ARG	N-CA	5.14	1.52	1.46
1	A	1337	GLU	CD-OE2	5.14	1.35	1.25
1	A	659	HIS	CA-C	-5.14	1.45	1.52
2	B	20	ASP	CG-OD1	5.14	1.35	1.25
2	B	348	ARG	CZ-NH2	-5.14	1.26	1.33
2	B	643	ASP	C-O	-5.14	1.13	1.23
2	B	942	ARG	CZ-NH2	5.14	1.40	1.33
3	C	93	ASP	CA-C	-5.14	1.45	1.52
5	F	76	LYS	CG-CD	5.14	1.67	1.52
8	J	47	ARG	NE-CZ	-5.14	1.27	1.33
10	L	49	LYS	CG-CD	5.13	1.67	1.52
1	A	787	PHE	CA-C	5.13	1.58	1.52
3	C	215	GLU	CA-C	5.13	1.59	1.52
4	E	33	GLU	CD-OE1	5.13	1.35	1.25
10	L	66	GLN	CA-C	5.13	1.58	1.52
1	A	1232	ASN	N-CA	5.13	1.53	1.46
1	A	62	ASP	CA-CB	5.13	1.62	1.53
1	A	779	PHE	CA-CB	-5.13	1.45	1.53
2	B	889	THR	C-O	-5.13	1.17	1.23
2	B	1043	ASP	C-O	-5.13	1.17	1.23
5	F	87	LYS	CE-NZ	5.13	1.64	1.49
1	A	290	GLU	CA-CB	-5.13	1.45	1.53
2	B	20	ASP	N-CA	5.13	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	463	THR	N-CA	5.13	1.52	1.46
2	B	533	CYS	CA-CB	-5.13	1.44	1.53
1	A	1147	THR	C-O	-5.12	1.17	1.24
1	A	621	THR	CB-CG2	-5.12	1.35	1.52
1	A	920	LEU	CG-CD2	-5.12	1.35	1.52
2	B	416	LEU	CA-CB	-5.12	1.45	1.53
3	C	260	LEU	C-O	5.12	1.30	1.24
9	K	20	LYS	CA-C	-5.12	1.46	1.52
1	A	780	VAL	CA-C	-5.12	1.47	1.53
1	A	837	ILE	N-CA	-5.12	1.40	1.46
2	B	812	LEU	CA-C	-5.12	1.45	1.52
1	A	1255	GLU	CA-CB	5.12	1.62	1.53
2	B	569	TYR	CA-CB	5.12	1.61	1.53
2	B	908	GLU	CB-CG	5.12	1.67	1.52
4	E	207	ARG	C-O	-5.12	1.17	1.23
6	H	123	MET	CG-SD	5.12	1.93	1.80
8	J	26	GLN	CG-CD	5.12	1.64	1.52
1	A	777	PHE	C-N	-5.11	1.27	1.34
1	A	787	PHE	CB-CG	-5.11	1.38	1.50
1	A	1166	ASP	CG-OD2	5.11	1.35	1.25
2	B	186	GLU	CD-OE2	5.11	1.35	1.25
3	C	134	ILE	CA-C	-5.11	1.46	1.52
1	A	35	ILE	C-N	5.11	1.40	1.33
1	A	48	ALA	N-CA	5.11	1.52	1.46
1	A	774	ARG	CZ-NH1	-5.11	1.25	1.32
2	B	935	ARG	N-CA	5.11	1.53	1.46
2	B	1033	LYS	CB-CG	-5.11	1.37	1.52
1	A	426	LEU	C-O	-5.11	1.17	1.23
2	B	1132	GLU	C-O	5.11	1.30	1.24
1	A	376	TYR	C-O	-5.11	1.18	1.24
1	A	1411	GLU	CD-OE1	5.11	1.35	1.25
2	B	578	THR	C-O	-5.11	1.17	1.24
2	B	641	GLU	CB-CG	5.11	1.67	1.52
2	B	681	TRP	C-O	5.11	1.30	1.24
1	A	464	PRO	CA-CB	-5.11	1.46	1.53
2	B	364	ILE	CA-CB	-5.11	1.47	1.54
2	B	851	PHE	N-CA	-5.11	1.39	1.46
3	C	81	GLU	N-CA	-5.10	1.39	1.45
1	A	1110	ASN	C-N	-5.10	1.25	1.33
2	B	319	GLU	C-O	-5.10	1.17	1.24
2	B	798	TYR	C-O	-5.10	1.18	1.24
7	I	45	ARG	CZ-NH2	-5.10	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	999	VAL	CA-C	5.10	1.57	1.52
9	K	9	LEU	C-O	5.10	1.30	1.24
1	A	520	CYS	CA-C	5.10	1.59	1.52
5	F	106	PRO	CG-CD	-5.10	1.33	1.50
2	B	463	THR	C-O	5.09	1.30	1.24
7	I	48	LEU	CA-CB	-5.09	1.45	1.53
1	A	714	PHE	CD1-CE1	-5.09	1.23	1.38
9	K	77	THR	C-O	5.09	1.30	1.23
1	A	404	TYR	N-CA	-5.09	1.39	1.45
2	B	619	ILE	CA-C	-5.09	1.46	1.52
6	H	144	ILE	CA-C	5.09	1.58	1.52
1	A	72	GLU	CA-C	5.09	1.59	1.52
1	A	931	GLU	CA-CB	-5.09	1.45	1.53
2	B	516	ASN	C-O	-5.09	1.18	1.24
9	K	49	GLU	CA-C	-5.09	1.46	1.52
1	A	1414	ALA	CA-CB	-5.08	1.45	1.53
2	B	746	SER	C-O	5.08	1.30	1.24
4	E	43	LYS	N-CA	5.08	1.52	1.46
1	A	350	ARG	NE-CZ	-5.08	1.27	1.33
1	A	840	ARG	CD-NE	5.08	1.53	1.46
2	B	268	THR	CB-OG1	-5.08	1.35	1.43
2	B	353	LYS	N-CA	5.08	1.52	1.46
2	B	360	PHE	CE2-CZ	-5.08	1.23	1.38
4	E	183	PRO	C-N	-5.08	1.27	1.33
8	J	31	ASP	C-N	5.08	1.40	1.33
10	L	56	LEU	CG-CD2	-5.08	1.35	1.52
1	A	719	VAL	C-O	-5.08	1.17	1.24
1	A	1032	LEU	C-O	-5.08	1.17	1.23
2	B	1041	GLU	C-O	5.08	1.30	1.23
2	B	1091	TYR	CA-C	-5.08	1.46	1.52
1	A	1202	MET	CB-CG	-5.08	1.37	1.52
2	B	176	SER	C-O	-5.08	1.15	1.23
2	B	234	ILE	N-CA	-5.08	1.40	1.46
7	I	10	CYS	N-CA	5.08	1.52	1.46
1	A	368	LYS	CE-NZ	5.08	1.64	1.49
1	A	1033	GLN	CA-C	-5.08	1.45	1.52
3	C	60	ASP	CG-OD2	5.08	1.34	1.25
7	I	87	GLN	CB-CG	5.08	1.67	1.52
1	A	1079	MET	C-N	5.07	1.40	1.33
1	A	1080	THR	C-O	5.07	1.30	1.24
1	A	377	PRO	N-CA	-5.07	1.42	1.47
2	B	641	GLU	CD-OE2	5.07	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	26	ARG	CZ-NH2	-5.07	1.26	1.33
1	A	889	SER	N-CA	5.07	1.52	1.45
2	B	28	GLU	CG-CD	5.07	1.64	1.52
2	B	70	ILE	CB-CG1	5.07	1.63	1.53
2	B	451	LYS	N-CA	-5.07	1.39	1.46
3	C	180	TYR	CD2-CE2	5.07	1.53	1.38
1	A	988	LEU	C-O	-5.07	1.17	1.24
2	B	830	TYR	N-CA	-5.07	1.40	1.47
1	A	813	PHE	N-CA	-5.07	1.40	1.46
1	A	976	THR	C-O	-5.07	1.16	1.24
1	A	1280	GLU	CD-OE1	5.07	1.34	1.25
2	B	107	GLY	CA-C	5.07	1.59	1.51
2	B	903	VAL	CA-C	-5.07	1.47	1.52
3	C	108	GLU	CG-CD	5.07	1.64	1.52
4	E	91	LYS	CB-CG	5.07	1.67	1.52
7	I	18	GLU	CA-CB	5.07	1.60	1.53
1	A	1232	ASN	C-N	5.07	1.41	1.33
2	B	788	ARG	C-O	-5.07	1.17	1.23
1	A	1116	LEU	CA-CB	-5.06	1.42	1.53
3	C	132	PRO	C-O	-5.06	1.17	1.24
1	A	300	VAL	C-O	-5.06	1.18	1.24
1	A	412	ARG	CA-C	-5.06	1.46	1.52
1	A	756	ILE	CA-CB	5.06	1.60	1.54
1	A	1359	ASP	C-O	-5.06	1.17	1.24
2	B	483	LEU	C-N	-5.06	1.26	1.33
6	H	25	ARG	NE-CZ	-5.06	1.27	1.33
1	A	880	LYS	CB-CG	5.06	1.67	1.52
1	A	1277	GLU	C-N	-5.06	1.26	1.33
2	B	1169	MET	CA-C	-5.06	1.47	1.53
4	E	186	LEU	CA-C	-5.06	1.46	1.52
7	I	93	LYS	C-N	5.06	1.40	1.33
2	B	982	SER	CA-C	-5.06	1.46	1.53
2	B	1150	ARG	CG-CD	-5.06	1.37	1.52
1	A	1079	MET	CG-SD	5.06	1.93	1.80
2	B	31	TRP	N-CA	-5.06	1.40	1.46
4	E	29	PHE	CA-CB	5.06	1.59	1.53
1	A	14	VAL	CA-C	-5.06	1.46	1.52
2	B	563	MET	C-O	-5.06	1.17	1.23
7	I	19	ASP	N-CA	5.06	1.53	1.46
2	B	64	CYS	CA-C	-5.05	1.45	1.52
3	C	191	TYR	CA-C	-5.05	1.46	1.52
1	A	1027	ALA	CA-CB	5.05	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	62	ILE	CA-C	5.05	1.59	1.52
4	E	37	LEU	CA-C	-5.05	1.46	1.52
1	A	754	SER	N-CA	-5.05	1.39	1.45
1	A	1037	LEU	C-O	-5.05	1.17	1.23
1	A	1329	THR	N-CA	-5.05	1.39	1.45
2	B	49	ASP	CB-CG	5.05	1.64	1.52
2	B	228	LYS	CA-C	-5.05	1.46	1.52
2	B	384	ARG	CG-CD	5.05	1.67	1.52
8	J	26	GLN	CA-C	5.05	1.59	1.52
2	B	176	SER	CB-OG	-5.05	1.32	1.42
9	K	79	GLU	CG-CD	5.05	1.64	1.52
1	A	569	LYS	N-CA	5.05	1.53	1.46
2	B	579	ARG	CG-CD	5.05	1.67	1.52
1	A	744	LYS	CG-CD	5.05	1.67	1.52
6	H	11	GLN	CA-CB	5.05	1.61	1.53
2	B	993	THR	CB-OG1	-5.04	1.35	1.43
1	A	469	ARG	CG-CD	5.04	1.67	1.52
1	A	548	ASN	N-CA	-5.04	1.39	1.46
1	A	1124	HIS	CA-CB	5.04	1.60	1.53
1	A	1140	HIS	C-O	-5.04	1.17	1.23
2	B	962	LYS	C-O	5.04	1.30	1.23
10	L	62	LYS	CE-NZ	5.04	1.64	1.49
1	A	326	ARG	C-N	-5.04	1.27	1.33
2	B	347	LYS	C-N	-5.04	1.27	1.33
3	C	106	GLU	CD-OE1	5.04	1.34	1.25
1	A	1234	GLU	CG-CD	5.04	1.64	1.52
2	B	1026	LEU	C-O	-5.04	1.18	1.24
2	B	1072	MET	CA-CB	-5.04	1.46	1.53
3	C	3	GLU	CA-CB	-5.04	1.43	1.53
1	A	1199	ARG	C-O	5.04	1.29	1.24
8	J	3	VAL	C-O	-5.04	1.19	1.25
2	B	758	PHE	CA-CB	-5.04	1.45	1.53
3	C	127	ARG	CG-CD	-5.04	1.37	1.52
4	E	145	THR	C-O	-5.04	1.16	1.24
1	A	36	ARG	C-O	-5.03	1.17	1.24
1	A	552	TRP	NE1-CE2	-5.03	1.31	1.37
1	A	1023	ARG	CZ-NH1	-5.03	1.25	1.32
1	A	1103	GLU	CD-OE1	5.03	1.34	1.25
2	B	1157	ALA	N-CA	-5.03	1.40	1.46
7	I	83	ASN	CA-C	5.03	1.58	1.52
2	B	202	TYR	CE1-CZ	-5.03	1.26	1.38
10	L	45	ALA	C-O	5.03	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	155	LEU	CG-CD1	-5.03	1.35	1.52
4	E	53	PRO	CB-CG	5.03	1.74	1.49
4	E	106	GLN	CD-NE2	5.03	1.43	1.33
9	K	114	LEU	CA-C	5.03	1.63	1.52
1	A	868	TYR	C-O	5.03	1.29	1.23
2	B	54	PHE	CA-C	5.03	1.59	1.52
1	A	715	GLU	CA-C	-5.03	1.46	1.52
1	A	1425	SER	N-CA	5.03	1.52	1.46
3	C	159	ALA	CA-CB	5.03	1.61	1.53
4	E	40	GLU	CA-CB	5.03	1.61	1.53
4	E	129	PRO	CB-CG	5.03	1.70	1.51
1	A	565	ILE	CB-CG2	-5.02	1.35	1.52
4	E	113	GLN	CG-CD	5.02	1.64	1.52
1	A	498	ARG	CD-NE	5.02	1.53	1.46
2	B	846	ILE	N-CA	5.02	1.52	1.46
7	I	66	PRO	C-O	5.02	1.30	1.24
1	A	1307	GLU	CA-C	5.02	1.58	1.52
1	A	1408	ILE	C-O	-5.02	1.17	1.24
2	B	319	GLU	CD-OE2	5.02	1.34	1.25
2	B	381	MET	CG-SD	5.02	1.93	1.80
2	B	828	ALA	C-O	-5.02	1.17	1.23
6	H	126	GLU	CG-CD	5.02	1.64	1.52
1	A	611	GLN	N-CA	5.02	1.52	1.46
2	B	418	LYS	CA-C	-5.02	1.46	1.52
2	B	1098	MET	SD-CE	5.02	1.92	1.79
6	H	95	TYR	C-N	-5.02	1.27	1.33
10	L	47	ARG	CG-CD	5.02	1.67	1.52
1	A	350	ARG	C-N	-5.02	1.27	1.33
1	A	821	ARG	N-CA	-5.02	1.40	1.46
1	A	857	ARG	CZ-NH2	5.01	1.40	1.33
1	A	863	VAL	N-CA	-5.01	1.40	1.46
1	A	1057	VAL	C-N	-5.01	1.27	1.33
2	B	557	PHE	CG-CD2	5.01	1.49	1.38
5	F	135	ARG	C-O	-5.01	1.17	1.24
2	B	365	THR	C-O	5.01	1.29	1.23
9	K	47	ARG	N-CA	-5.01	1.40	1.46
1	A	405	VAL	CA-C	-5.01	1.46	1.52
1	A	746	MET	CG-SD	-5.01	1.68	1.80
1	A	946	VAL	C-N	-5.01	1.27	1.33
7	I	22	ASN	C-N	5.01	1.40	1.33
1	A	1101	LEU	C-N	-5.01	1.27	1.33
7	I	15	TYR	N-CA	-5.01	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1264	GLU	N-CA	-5.01	1.40	1.46
2	B	569	TYR	CA-C	-5.00	1.46	1.52
3	C	79	GLN	CA-C	-5.00	1.46	1.52
3	C	138	GLU	CA-C	-5.00	1.45	1.52
8	J	49	MET	CG-SD	5.00	1.93	1.80
5	F	137	TYR	C-O	-5.00	1.17	1.23
6	H	39	THR	CA-C	-5.00	1.46	1.52

All (2492) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1366	ARG	NE-CZ-NH2	-17.80	103.18	119.20
5	F	81	THR	N-CA-CB	-17.55	86.34	110.38
1	A	61	ILE	N-CA-C	-17.24	91.26	110.05
3	C	34	ARG	NE-CZ-NH2	-16.31	104.53	119.20
2	B	1097	HIS	CB-CG-ND1	-15.75	99.07	122.70
2	B	995	ARG	NE-CZ-NH2	-15.70	105.07	119.20
3	C	240	VAL	N-CA-C	15.68	125.51	110.30
1	A	93	VAL	CB-CA-C	-15.68	90.97	112.14
8	J	3	VAL	CB-CA-C	-15.00	93.43	110.68
1	A	774	ARG	NE-CZ-NH1	14.89	136.39	121.50
1	A	172	PRO	CA-N-CD	-14.77	91.33	112.00
1	A	1004	ASN	N-CA-C	14.51	129.05	110.33
10	L	48	CYS	N-CA-C	14.47	126.85	108.19
3	C	183	TRP	CA-C-N	-14.26	101.28	123.24
3	C	183	TRP	C-N-CA	-14.26	101.28	123.24
9	K	47	ARG	NE-CZ-NH2	-14.16	106.45	119.20
7	I	43	VAL	N-CA-CB	-13.93	90.90	112.07
1	A	469	ARG	NE-CZ-NH2	-13.75	106.82	119.20
1	A	724	GLU	N-CA-C	-13.74	94.92	112.23
1	A	1336	MET	CG-SD-CE	13.71	131.07	100.90
1	A	153	PRO	CA-N-CD	-13.42	93.21	112.00
1	A	1259	MET	N-CA-C	-13.38	96.38	110.97
1	A	538	ASP	CB-CA-C	-13.31	84.83	110.11
1	A	1366	ARG	NE-CZ-NH1	13.27	134.77	121.50
1	A	1062	GLU	CB-CA-C	-13.21	87.05	109.65
2	B	642	ASP	N-CA-C	-13.02	87.45	108.41
3	C	124	LEU	N-CA-C	12.75	128.31	113.01
2	B	1160	VAL	CB-CA-C	-12.51	92.53	111.80
9	K	94	ILE	N-CA-C	-12.50	98.67	110.42
1	A	1170	ILE	N-CA-C	-12.41	97.47	111.00
1	A	999	VAL	N-CA-C	-12.32	101.77	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1077	THR	N-CA-CB	-12.28	94.57	110.90
3	C	35	ARG	NE-CZ-NH2	-12.25	108.17	119.20
2	B	839	MET	CG-SD-CE	-12.15	74.18	100.90
2	B	501	PRO	CA-C-O	-12.10	107.24	121.03
2	B	620	ARG	NH1-CZ-NH2	12.09	135.02	119.30
2	B	1019	SER	CB-CA-C	-11.96	84.99	109.99
4	E	212	ARG	CD-NE-CZ	11.92	141.09	124.40
1	A	949	ASP	N-CA-CB	-11.80	91.16	110.40
3	C	163	ILE	CA-CB-CG2	11.79	130.54	110.50
1	A	1376	THR	N-CA-CB	-11.74	91.78	111.27
1	A	1146	VAL	N-CA-CB	-11.68	99.36	112.21
2	B	368	GLU	N-CA-C	11.65	123.72	111.14
3	C	66	ARG	NE-CZ-NH2	11.58	129.62	119.20
1	A	50	ILE	CB-CA-C	-11.49	95.21	110.84
4	E	93	MET	N-CA-C	11.49	123.36	111.07
1	A	466	SER	CB-CA-C	-11.45	91.38	110.72
2	B	1135	ARG	NE-CZ-NH2	-11.45	108.90	119.20
2	B	709	ASP	N-CA-C	-11.41	99.02	113.16
2	B	620	ARG	NE-CZ-NH1	-11.39	110.11	121.50
2	B	559	SER	CA-CB-OG	-11.38	88.35	111.10
6	H	106	GLU	N-CA-C	-11.37	99.66	113.19
1	A	1136	SER	N-CA-C	-11.36	99.53	113.50
10	L	57	LEU	N-CA-C	11.35	127.61	108.20
1	A	446	ARG	NE-CZ-NH2	-11.34	109.00	119.20
1	A	466	SER	N-CA-C	11.33	127.49	112.88
1	A	974	ASP	N-CA-CB	11.30	128.19	110.21
1	A	197	PRO	CA-N-CD	-11.30	96.18	112.00
2	B	102	VAL	N-CA-C	11.19	124.24	108.12
2	B	463	THR	N-CA-C	11.19	125.45	111.69
3	C	18	VAL	CB-CA-C	-11.19	92.94	111.29
2	B	960	GLY	N-CA-C	11.17	130.21	115.36
3	C	40	GLU	N-CA-C	11.17	126.93	112.41
1	A	1228	TRP	CB-CA-C	-11.16	90.86	110.95
1	A	596	THR	CA-C-O	-11.16	109.02	121.40
2	B	416	LEU	CB-CA-C	-11.15	93.67	110.95
3	C	66	ARG	NE-CZ-NH1	-11.12	110.38	121.50
10	L	68	GLU	CB-CG-CD	11.02	131.34	112.60
4	E	204	THR	CA-CB-CG2	10.95	129.12	110.50
1	A	459	ARG	NE-CZ-NH2	-10.95	109.35	119.20
5	F	82	THR	CB-CA-C	-10.94	92.24	109.42
3	C	256	ALA	N-CA-C	-10.90	98.63	112.90
4	E	5	ASN	N-CA-C	-10.89	100.12	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	593	GLU	N-CA-C	10.83	124.17	111.71
1	A	982	THR	N-CA-CB	-10.82	92.78	110.41
1	A	1172	LEU	CB-CA-C	-10.82	97.81	111.22
2	B	496	ARG	NE-CZ-NH1	10.81	132.31	121.50
1	A	739	ASP	N-CA-C	10.80	125.56	112.38
3	C	20	PHE	N-CA-C	10.79	124.07	108.86
1	A	826	ASP	N-CA-C	-10.79	99.52	111.28
6	H	57	VAL	N-CA-C	10.76	123.29	107.37
2	B	168	GLY	N-CA-C	10.74	123.75	110.96
1	A	940	ARG	NE-CZ-NH1	10.72	132.22	121.50
1	A	1014	ALA	CA-C-O	10.69	132.17	120.20
2	B	567	GLU	O-C-N	-10.69	108.37	122.59
2	B	593	PRO	N-CA-C	-10.68	100.89	114.03
4	E	77	SER	N-CA-C	-10.66	93.82	108.86
10	L	68	GLU	CG-CD-OE1	10.66	142.93	118.40
2	B	484	ASN	CB-CA-C	-10.63	92.58	109.70
1	A	1368	MET	N-CA-C	-10.63	99.71	112.89
1	A	469	ARG	NE-CZ-NH1	10.62	132.12	121.50
7	I	31	THR	N-CA-CB	-10.61	95.10	110.81
2	B	680	THR	N-CA-CB	-10.52	93.39	111.69
2	B	56	ASP	N-CA-C	10.49	125.97	112.34
1	A	377	PRO	CB-CA-C	-10.48	103.07	111.87
2	B	608	ASP	N-CA-C	-10.47	99.04	112.23
7	I	10	CYS	N-CA-C	10.47	126.21	113.23
3	C	239	PRO	CA-C-O	10.46	135.47	122.08
4	E	63	ASN	N-CA-C	10.46	126.10	110.10
1	A	289	ILE	N-CA-C	-10.46	100.70	110.53
2	B	653	VAL	CB-CA-C	-10.45	96.86	111.28
2	B	1097	HIS	CB-CA-C	10.45	131.21	110.42
8	J	3	VAL	N-CA-CB	10.43	121.75	110.17
1	A	159	THR	N-CA-C	-10.35	98.96	111.69
1	A	446	ARG	NH1-CZ-NH2	10.34	132.74	119.30
2	B	995	ARG	NE-CZ-NH1	10.33	131.83	121.50
1	A	859	SER	N-CA-C	-10.33	100.08	112.89
1	A	295	LEU	N-CA-C	-10.31	99.01	111.69
1	A	962	ARG	N-CA-C	-10.29	98.14	112.45
1	A	389	THR	OG1-CB-CG2	-10.27	88.76	109.30
2	B	791	THR	OG1-CB-CG2	-10.27	88.76	109.30
1	A	789	LYS	N-CA-C	10.26	123.87	110.43
2	B	1150	ARG	NH1-CZ-NH2	10.23	132.61	119.30
2	B	802	PRO	CA-C-O	-10.22	109.01	120.97
1	A	566	ILE	CB-CA-C	-10.15	99.15	111.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	49	MET	CG-SD-CE	-10.14	78.58	100.90
1	A	659	HIS	CB-CG-ND1	-10.12	107.52	122.70
2	B	648	HIS	N-CA-C	10.11	125.07	109.60
1	A	481	ASP	CA-C-O	-10.10	110.20	120.80
1	A	495	GLU	N-CA-CB	-10.07	95.26	110.16
5	F	119	ARG	N-CA-C	10.03	123.24	111.71
7	I	118	ARG	N-CA-C	10.02	125.33	110.30
3	C	172	PRO	N-CD-CG	9.98	118.17	103.20
10	L	48	CYS	N-CA-CB	-9.95	94.44	110.55
2	B	996	ARG	NE-CZ-NH1	-9.94	111.56	121.50
3	C	23	SER	N-CA-C	-9.93	93.46	108.46
3	C	150	GLY	CA-C-O	9.92	129.47	118.86
1	A	160	GLN	OE1-CD-NE2	-9.91	112.69	122.60
1	A	802	ASN	N-CA-C	9.89	123.80	110.35
5	F	150	GLU	N-CA-CB	-9.89	95.08	110.30
1	A	969	GLN	N-CA-C	-9.85	99.58	112.68
2	B	55	VAL	N-CA-C	-9.84	101.78	110.74
2	B	496	ARG	NE-CZ-NH2	-9.84	110.35	119.20
2	B	604	ARG	NE-CZ-NH1	9.79	131.29	121.50
5	F	81	THR	N-CA-C	9.79	122.45	110.41
6	H	102	TYR	CA-C-O	9.77	130.06	119.03
1	A	124	GLN	OE1-CD-NE2	-9.76	112.84	122.60
2	B	598	GLU	N-CA-CB	9.76	124.46	110.12
2	B	24	PRO	N-CD-CG	-9.74	88.59	103.20
2	B	414	ALA	N-CA-C	-9.71	102.00	114.04
1	A	894	GLU	CA-C-O	-9.71	108.80	119.97
1	A	1135	ARG	NE-CZ-NH1	-9.70	111.80	121.50
1	A	566	ILE	N-CA-C	9.70	121.86	111.58
1	A	830	LYS	CB-CA-C	-9.68	95.32	110.81
2	B	337	ARG	CG-CD-NE	-9.68	90.72	112.00
8	J	21	TYR	N-CA-C	-9.67	98.11	112.04
1	A	1006	ILE	CG1-CB-CG2	-9.63	81.80	110.70
5	F	125	LEU	N-CA-C	-9.63	99.06	112.45
1	A	922	ASP	N-CA-C	9.59	123.92	109.25
1	A	171	GLN	OE1-CD-NE2	-9.58	113.02	122.60
6	H	91	ASP	CA-C-O	9.57	130.85	120.32
2	B	137	TYR	CA-CB-CG	9.56	131.12	113.90
8	J	6	ARG	NE-CZ-NH2	9.53	127.77	119.20
3	C	183	TRP	N-CA-C	-9.52	94.99	109.94
2	B	1165	ILE	N-CA-C	-9.51	102.64	111.67
2	B	336	ARG	CB-CA-C	-9.50	93.05	110.63
1	A	244	PRO	CA-C-O	-9.50	106.79	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	16	ASP	CB-CA-C	-9.49	99.03	109.85
10	L	40	LEU	CA-C-O	-9.49	111.35	120.56
8	J	22	LEU	N-CA-CB	-9.44	96.38	110.07
9	K	52	ASN	N-CA-C	-9.44	101.53	113.23
2	B	297	ILE	CA-CB-CG1	9.43	126.42	110.40
2	B	807	ARG	NE-CZ-NH2	-9.40	110.74	119.20
1	A	1366	ARG	CD-NE-CZ	9.40	137.55	124.40
10	L	34	CYS	CA-CB-SG	-9.40	92.79	114.40
1	A	895	LYS	N-CA-CB	9.38	123.91	110.12
2	B	1135	ARG	NH1-CZ-NH2	9.36	131.47	119.30
1	A	916	GLY	CA-C-N	9.34	132.58	120.44
1	A	916	GLY	C-N-CA	9.34	132.58	120.44
1	A	1226	VAL	CB-CA-C	-9.33	95.55	110.28
2	B	1150	ARG	NE-CZ-NH1	-9.32	112.17	121.50
1	A	744	LYS	N-CA-C	-9.30	99.53	112.45
1	A	1072	ILE	N-CA-C	-9.28	103.83	111.81
3	C	35	ARG	NE-CZ-NH1	9.25	130.75	121.50
2	B	399	ASP	N-CA-C	9.24	124.29	112.92
1	A	725	ALA	N-CA-C	9.24	121.35	111.28
5	F	72	LYS	CA-C-N	9.22	139.15	121.54
5	F	72	LYS	C-N-CA	9.22	139.15	121.54
3	C	84	ARG	NE-CZ-NH2	9.22	127.50	119.20
1	A	856	THR	OG1-CB-CG2	-9.21	90.89	109.30
1	A	1284	MET	CA-CB-CG	-9.21	95.69	114.10
9	K	64	GLU	N-CA-C	9.21	122.30	111.71
3	C	34	ARG	NE-CZ-NH1	9.20	130.70	121.50
2	B	498	THR	N-CA-CB	-9.20	95.68	111.69
2	B	501	PRO	O-C-N	9.19	133.40	123.10
1	A	1154	TYR	N-CA-C	-9.19	93.75	108.73
1	A	231	PRO	CA-N-CD	-9.17	99.17	112.00
5	F	73	ALA	CA-C-N	-9.16	114.88	122.85
5	F	73	ALA	C-N-CA	-9.16	114.88	122.85
3	C	229	TYR	N-CA-C	9.14	124.42	108.52
1	A	607	ILE	N-CA-C	-9.10	96.34	108.35
2	B	513	GLN	CA-CB-CG	9.10	132.29	114.10
2	B	1018	PRO	CA-C-O	-9.09	106.55	119.74
3	C	24	ASN	N-CA-C	9.08	123.78	111.24
1	A	557	ASP	O-C-N	-9.07	111.22	122.82
2	B	1158	PHE	N-CA-C	9.06	123.04	110.35
1	A	771	GLU	CG-CD-OE1	-9.05	97.58	118.40
1	A	1055	ARG	CG-CD-NE	-9.05	92.09	112.00
7	I	111	THR	CB-CA-C	-9.05	92.82	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	434	ARG	NE-CZ-NH2	-9.04	111.06	119.20
1	A	795	GLU	CB-CG-CD	9.03	127.96	112.60
1	A	896	ARG	NE-CZ-NH2	-9.03	111.07	119.20
4	E	20	LYS	CA-CB-CG	9.03	132.16	114.10
2	B	90	ILE	CB-CA-C	-9.03	96.48	111.29
2	B	46	GLN	CA-CB-CG	-9.02	96.06	114.10
1	A	1016	THR	N-CA-C	9.02	120.72	111.07
4	E	98	ILE	N-CA-C	-9.02	103.06	111.45
2	B	1131	GLY	N-CA-C	9.02	125.93	112.41
8	J	43	ARG	NE-CZ-NH2	9.02	127.31	119.20
5	F	77	ASP	CA-C-N	-9.01	104.34	121.54
5	F	77	ASP	C-N-CA	-9.01	104.34	121.54
1	A	1239	ARG	CB-CA-C	9.01	126.00	109.70
1	A	1222	ASN	CA-C-O	-8.99	110.89	120.42
1	A	1385	THR	N-CA-CB	-8.99	96.22	111.50
1	A	1161	THR	OG1-CB-CG2	-8.98	91.33	109.30
7	I	38	ALA	CA-C-N	8.98	129.91	119.94
7	I	38	ALA	C-N-CA	8.98	129.91	119.94
1	A	590	ARG	NE-CZ-NH2	-8.96	111.13	119.20
1	A	932	GLU	CB-CG-CD	8.95	127.81	112.60
7	I	32	CYS	CB-CA-C	-8.94	93.94	112.44
3	C	181	ASP	CA-C-O	-8.93	114.31	120.47
1	A	982	THR	CA-CB-CG2	8.93	125.68	110.50
1	A	244	PRO	N-CA-C	8.92	121.58	110.70
4	E	204	THR	N-CA-CB	-8.91	98.73	110.59
1	A	1064	VAL	N-CA-CB	-8.91	92.34	111.05
10	L	55	ILE	CB-CA-C	-8.91	98.12	110.77
2	B	316	PRO	N-CD-CG	-8.90	89.85	103.20
3	C	230	MET	N-CA-C	8.90	122.63	110.35
2	B	46	GLN	N-CA-C	-8.87	100.46	111.11
8	J	43	ARG	NE-CZ-NH1	-8.86	112.64	121.50
10	L	25	ALA	CA-C-N	8.83	138.40	121.54
10	L	25	ALA	C-N-CA	8.83	138.40	121.54
1	A	493	GLN	CB-CG-CD	8.82	127.59	112.60
7	I	93	LYS	N-CA-C	-8.81	101.60	111.82
1	A	649	ILE	N-CA-C	-8.80	99.64	111.44
1	A	1166	ASP	N-CA-C	-8.80	102.69	112.72
1	A	283	GLY	N-CA-C	-8.79	92.34	113.18
3	C	86	CYS	CA-CB-SG	8.79	134.61	114.40
2	B	1198	TYR	N-CA-C	-8.77	101.72	111.28
1	A	1318	THR	N-CA-CB	-8.75	97.53	110.49
4	E	96	PHE	N-CA-C	-8.74	101.70	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	709	THR	N-CA-CB	-8.72	95.75	110.49
2	B	354	ASP	N-CA-C	-8.71	101.87	111.36
5	F	153	VAL	CA-C-O	-8.68	110.64	120.97
1	A	821	ARG	NE-CZ-NH2	-8.67	111.39	119.20
1	A	1130	GLN	N-CA-C	-8.67	102.70	113.28
1	A	1136	SER	CB-CA-C	8.65	125.03	109.29
2	B	122	LEU	N-CA-C	8.64	122.27	110.35
2	B	734	HIS	N-CA-C	-8.64	100.97	112.72
1	A	1284	MET	CA-C-O	-8.63	111.21	121.05
2	B	1166	CYS	O-C-N	-8.63	111.12	122.59
7	I	75	CYS	CB-CA-C	-8.63	96.06	109.09
1	A	907	THR	CB-CA-C	-8.62	92.62	113.15
2	B	41	LYS	N-CA-C	-8.62	102.89	113.50
9	K	4	PRO	CA-C-O	-8.62	111.13	121.48
3	C	33	LEU	N-CA-C	-8.61	101.10	111.69
2	B	589	VAL	O-C-N	-8.60	113.50	123.05
1	A	821	ARG	CG-CD-NE	-8.59	93.11	112.00
7	I	18	GLU	N-CA-C	-8.58	95.54	109.96
1	A	419	LYS	N-CA-C	-8.58	102.07	112.54
2	B	368	GLU	CA-C-N	-8.58	104.60	121.41
2	B	368	GLU	C-N-CA	-8.58	104.60	121.41
1	A	537	ARG	CB-CG-CD	8.57	131.02	111.30
3	C	89	GLU	N-CA-C	-8.57	95.33	108.96
1	A	1176	LEU	N-CA-C	-8.57	87.00	111.00
2	B	212	LEU	N-CA-C	8.55	123.66	109.46
2	B	1097	HIS	CA-CB-CG	-8.55	105.25	113.80
1	A	694	THR	N-CA-C	8.55	120.29	110.97
1	A	1417	GLU	N-CA-C	-8.55	97.14	109.96
2	B	552	MET	O-C-N	-8.54	112.68	120.71
2	B	747	MET	CG-SD-CE	-8.53	82.12	100.90
4	E	136	ASN	CA-C-O	-8.53	112.26	121.56
1	A	464	PRO	O-C-N	-8.50	111.16	122.64
1	A	829	VAL	CA-C-N	8.50	132.02	120.54
1	A	829	VAL	C-N-CA	8.50	132.02	120.54
3	C	11	ARG	CB-CA-C	-8.50	95.33	109.27
2	B	1064	TYR	CA-C-N	-8.50	107.60	120.94
2	B	1064	TYR	C-N-CA	-8.50	107.60	120.94
2	B	889	THR	CB-CA-C	-8.49	95.52	109.53
2	B	753	ALA	N-CA-C	-8.48	102.92	113.18
2	B	622	LYS	CA-CB-CG	8.47	131.04	114.10
3	C	241	ASP	N-CA-C	-8.47	100.91	111.75
6	H	81	PRO	CB-CA-C	8.46	121.24	110.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1280	GLU	CB-CG-CD	8.45	126.96	112.60
2	B	448	ILE	N-CA-C	8.45	120.00	108.17
1	A	1014	ALA	N-CA-C	8.44	122.56	111.75
2	B	484	ASN	N-CA-C	8.44	122.14	110.24
9	K	26	LYS	CG-CD-CE	8.44	130.71	111.30
9	K	95	ILE	CA-C-N	8.43	131.91	120.44
9	K	95	ILE	C-N-CA	8.43	131.91	120.44
1	A	961	ARG	NE-CZ-NH1	-8.43	113.07	121.50
1	A	518	LYS	CD-CE-NZ	-8.42	84.96	111.90
1	A	1162	VAL	N-CA-C	-8.41	101.55	113.07
1	A	1445	ILE	O-C-N	8.41	132.54	122.95
2	B	120	ARG	N-CA-C	8.40	123.15	113.15
3	C	77	ILE	N-CA-C	-8.39	101.58	113.07
2	B	329	THR	OG1-CB-CG2	-8.38	92.53	109.30
1	A	1438	THR	N-CA-CB	-8.38	95.07	110.32
1	A	567	LYS	CA-C-O	-8.38	108.69	120.16
1	A	1158	PRO	CA-C-O	-8.37	107.94	118.99
2	B	963	PHE	CB-CA-C	-8.37	92.84	109.33
1	A	461	LYS	CB-CA-C	-8.37	97.98	110.62
10	L	58	LYS	N-CA-C	8.36	128.61	110.80
3	C	245	VAL	N-CA-C	-8.35	101.90	111.00
2	B	399	ASP	N-CA-CB	-8.35	98.37	110.56
1	A	531	ILE	N-CA-C	-8.34	100.26	111.44
2	B	997	GLU	CA-CB-CG	-8.34	97.42	114.10
6	H	125	LEU	CA-C-O	-8.34	111.87	120.54
1	A	1425	SER	N-CA-C	8.33	119.98	111.07
1	A	288	ALA	CA-C-N	8.33	131.22	120.56
1	A	288	ALA	C-N-CA	8.33	131.22	120.56
1	A	393	ARG	CA-C-O	-8.33	112.12	120.70
3	C	44	LEU	CA-C-O	-8.32	111.72	120.70
9	K	95	ILE	O-C-N	8.32	130.30	121.90
2	B	1167	GLY	N-CA-C	8.31	132.88	113.18
2	B	996	ARG	NH1-CZ-NH2	8.31	130.11	119.30
1	A	1116	LEU	N-CA-C	-8.30	95.87	109.40
1	A	708	MET	N-CA-CB	-8.29	96.64	110.32
1	A	659	HIS	CB-CG-CD2	8.28	141.96	131.20
2	B	732	SER	CA-C-O	-8.27	112.78	121.55
1	A	394	ASN	N-CA-C	8.26	122.32	111.75
4	E	24	LYS	CD-CE-NZ	-8.25	85.49	111.90
1	A	918	GLU	N-CA-C	8.25	123.00	113.19
5	F	148	VAL	O-C-N	8.24	129.96	121.89
7	I	107	SER	N-CA-C	8.24	122.91	112.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	HIS	C-N-CD	-8.22	102.51	120.60
2	B	983	ARG	NE-CZ-NH2	-8.22	111.80	119.20
3	C	185	LYS	N-CA-C	-8.22	103.38	113.41
1	A	830	LYS	N-CA-CB	8.21	122.18	109.94
1	A	554	PRO	CA-C-N	-8.20	110.62	122.67
1	A	554	PRO	C-N-CA	-8.20	110.62	122.67
1	A	589	GLN	CA-C-O	-8.17	111.58	121.06
1	A	932	GLU	N-CA-C	-8.16	101.44	111.40
1	A	970	THR	N-CA-C	8.16	121.09	111.71
1	A	1357	ALA	N-CA-C	8.16	122.33	112.38
1	A	1384	VAL	N-CA-C	8.15	119.03	111.45
9	K	114	LEU	CB-CG-CD2	8.14	135.12	110.70
1	A	704	ALA	CA-C-N	-8.14	109.50	122.76
1	A	704	ALA	C-N-CA	-8.14	109.50	122.76
1	A	1008	GLN	N-CA-C	8.13	120.15	111.28
7	I	57	GLY	CA-C-N	-8.13	112.20	122.37
7	I	57	GLY	C-N-CA	-8.13	112.20	122.37
2	B	287	ARG	NE-CZ-NH2	-8.12	111.89	119.20
2	B	1108	ARG	N-CA-C	8.11	128.07	110.80
1	A	1370	LEU	CD1-CG-CD2	-8.10	92.98	110.80
2	B	531	GLN	N-CA-C	-8.10	102.42	111.82
1	A	241	VAL	O-C-N	8.09	126.47	121.37
1	A	1022	LEU	N-CA-C	8.09	119.73	111.07
6	H	12	VAL	N-CA-C	8.08	120.34	107.73
2	B	165	VAL	CB-CA-C	-8.07	98.05	111.29
1	A	649	ILE	CA-CB-CG1	8.06	124.11	110.40
1	A	9	ALA	O-C-N	8.06	128.16	121.31
1	A	728	LYS	CD-CE-NZ	8.06	137.69	111.90
6	H	27	GLU	N-CA-C	8.06	122.09	108.23
1	A	377	PRO	CA-C-O	-8.05	112.42	121.11
1	A	1280	GLU	O-C-N	-8.04	111.89	122.59
1	A	50	ILE	N-CA-C	8.04	119.86	108.36
1	A	925	LEU	N-CA-C	-8.04	102.52	111.28
4	E	167	ARG	N-CA-C	8.03	122.18	112.38
4	E	66	GLU	N-CA-C	-8.03	102.61	111.36
3	C	240	VAL	CB-CA-C	-8.02	101.78	111.81
2	B	118	ARG	CD-NE-CZ	8.02	135.63	124.40
2	B	828	ALA	N-CA-C	8.02	121.42	108.76
9	K	4	PRO	N-CA-C	-8.01	97.62	111.32
1	A	898	ARG	CB-CA-C	-8.01	98.25	110.26
2	B	20	ASP	CA-C-O	-8.01	111.71	120.92
2	B	190	TYR	CA-C-O	-8.01	112.33	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1015	VAL	N-CA-CB	-7.99	101.65	112.28
1	A	916	GLY	N-CA-C	7.99	122.32	112.73
8	J	38	ARG	N-CA-C	-7.98	102.17	112.23
4	E	28	TYR	N-CA-C	-7.98	97.15	109.52
1	A	706	HIS	N-CA-CB	7.98	123.97	110.49
1	A	1100	ARG	NE-CZ-NH2	-7.97	112.02	119.20
1	A	372	LYS	CD-CE-NZ	-7.97	86.40	111.90
1	A	603	ASN	N-CA-CB	-7.97	98.13	110.56
1	A	1269	GLU	N-CA-C	7.96	123.50	112.04
1	A	514	PRO	CA-C-O	7.96	129.84	118.86
2	B	990	ILE	CB-CA-C	-7.96	100.81	111.15
4	E	102	GLU	CA-C-N	-7.95	109.70	122.66
4	E	102	GLU	C-N-CA	-7.95	109.70	122.66
1	A	1137	ALA	CA-C-N	-7.95	114.95	122.66
1	A	1137	ALA	C-N-CA	-7.95	114.95	122.66
7	I	98	VAL	N-CA-C	7.95	122.33	109.78
2	B	412	LEU	N-CA-C	-7.94	102.71	111.36
1	A	1138	ILE	O-C-N	7.94	130.32	122.07
1	A	242	PRO	CA-C-O	-7.93	115.19	120.90
2	B	1007	VAL	N-CA-CB	-7.93	100.11	111.21
2	B	362	PRO	CA-C-O	-7.92	107.93	118.86
1	A	1019	CYS	CA-C-O	-7.92	111.15	120.10
1	A	411	ASP	N-CA-C	7.91	121.89	110.10
2	B	455	SER	N-CA-C	-7.91	103.78	113.50
3	C	64	ALA	CA-C-O	7.89	128.92	120.55
2	B	354	ASP	CA-C-O	-7.87	112.08	120.42
1	A	1238	ILE	CA-C-O	-7.87	111.75	120.72
2	B	512	ARG	N-CA-C	7.86	122.13	112.54
3	C	62	PHE	N-CA-C	-7.86	102.65	111.14
1	A	1067	LEU	N-CA-C	7.85	120.53	111.11
4	E	162	ARG	CB-CG-CD	7.85	129.35	111.30
6	H	82	PRO	N-CA-C	-7.85	96.30	112.47
7	I	119	THR	CB-CA-C	-7.84	98.51	110.90
1	A	1299	VAL	CB-CA-C	7.84	123.55	110.30
3	C	14	SER	N-CA-C	-7.84	96.23	108.14
2	B	787	VAL	N-CA-CB	-7.83	100.16	112.07
2	B	642	ASP	CA-C-N	-7.83	107.60	121.70
2	B	642	ASP	C-N-CA	-7.83	107.60	121.70
1	A	1416	ALA	CA-C-N	7.83	131.91	120.95
1	A	1416	ALA	C-N-CA	7.83	131.91	120.95
4	E	176	PRO	CB-CA-C	-7.82	101.03	111.12
1	A	605	MET	CG-SD-CE	-7.82	83.70	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1208	THR	CB-CA-C	-7.82	96.14	109.51
2	B	848	ARG	N-CA-C	7.82	122.45	113.15
9	K	114	LEU	CA-CB-CG	7.81	143.65	116.30
1	A	561	PRO	CA-C-O	-7.81	112.19	121.95
2	B	731	VAL	N-CA-C	-7.81	96.48	107.80
1	A	704	ALA	CA-C-O	-7.81	112.51	121.72
1	A	158	PRO	CA-N-CD	-7.80	101.07	112.00
4	E	103	LYS	N-CA-CB	7.80	121.73	110.65
5	F	87	LYS	N-CA-C	-7.80	102.74	111.71
7	I	55	THR	N-CA-CB	-7.79	98.96	110.49
4	E	11	ARG	NE-CZ-NH1	-7.79	113.71	121.50
2	B	89	GLU	N-CA-C	7.79	132.80	111.00
1	A	1241	ARG	NE-CZ-NH2	-7.79	112.19	119.20
6	H	6	PHE	N-CA-C	-7.79	96.88	108.79
1	A	705	LYS	N-CA-C	7.78	123.48	107.37
1	A	938	LYS	CB-CA-C	-7.78	97.62	110.85
1	A	475	THR	N-CA-CB	-7.78	98.22	110.28
6	H	116	TYR	N-CA-C	7.77	127.35	110.80
9	K	17	SER	N-CA-C	7.77	122.47	110.42
3	C	68	GLY	N-CA-C	-7.77	104.05	113.99
3	C	163	ILE	CB-CA-C	7.76	122.77	110.82
6	H	55	LEU	N-CA-C	7.76	121.14	108.26
1	A	351	THR	CB-CA-C	-7.75	93.50	111.95
1	A	475	THR	CA-CB-CG2	7.75	123.67	110.50
2	B	607	GLY	N-CA-C	-7.74	103.86	115.00
5	F	79	ARG	CB-CG-CD	-7.72	93.54	111.30
8	J	1	MET	CG-SD-CE	-7.72	83.91	100.90
2	B	117	ALA	CA-C-N	-7.72	109.94	120.44
2	B	117	ALA	C-N-CA	-7.72	109.94	120.44
2	B	903	VAL	CB-CA-C	-7.72	101.12	111.15
2	B	642	ASP	N-CA-CB	7.71	122.47	110.21
1	A	1434	ALA	N-CA-C	7.71	119.48	109.93
2	B	252	SER	N-CA-CB	7.70	121.32	109.85
1	A	1358	SER	N-CA-C	-7.69	102.83	111.14
1	A	173	THR	N-CA-C	-7.69	95.98	108.52
2	B	883	LEU	CA-CB-CG	7.69	143.20	116.30
1	A	722	LEU	N-CA-C	-7.68	102.84	112.90
1	A	1425	SER	CA-CB-OG	-7.68	95.75	111.10
2	B	1220	ARG	NE-CZ-NH2	7.68	126.11	119.20
3	C	221	TYR	N-CA-C	7.68	121.75	112.38
1	A	941	LYS	CD-CE-NZ	-7.67	87.34	111.90
1	A	944	ARG	NE-CZ-NH2	7.67	126.11	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	68	SER	N-CA-C	7.67	119.28	111.07
3	C	252	GLN	CA-CB-CG	7.67	129.44	114.10
4	E	39	LEU	N-CA-C	-7.67	100.99	112.04
1	A	832	ALA	CA-C-N	7.67	131.44	120.79
1	A	832	ALA	C-N-CA	7.67	131.44	120.79
1	A	806	ARG	N-CA-C	7.66	120.71	111.82
2	B	598	GLU	CB-CG-CD	7.66	125.62	112.60
1	A	235	ILE	CB-CG1-CD1	7.66	129.88	113.80
1	A	410	GLY	N-CA-C	-7.66	104.96	114.92
7	I	45	ARG	CD-NE-CZ	-7.66	113.68	124.40
1	A	1171	GLN	N-CA-CB	7.65	122.00	110.22
2	B	589	VAL	N-CA-CB	-7.65	98.91	111.45
2	B	351	TYR	N-CA-C	-7.64	103.03	111.36
3	C	233	GLU	CA-C-O	-7.64	111.88	120.66
3	C	100	THR	OG1-CB-CG2	-7.63	94.03	109.30
7	I	119	THR	O-C-N	7.63	130.34	122.09
1	A	782	ARG	CA-C-O	-7.63	112.44	120.99
2	B	836	GLU	O-C-N	7.63	132.24	122.86
1	A	352	VAL	CG1-CB-CG2	-7.62	94.02	110.80
1	A	748	MET	CG-SD-CE	7.62	117.66	100.90
1	A	806	ARG	NE-CZ-NH1	-7.62	113.88	121.50
1	A	944	ARG	NH1-CZ-NH2	-7.62	109.40	119.30
9	K	2	ASN	N-CA-C	7.62	122.61	113.16
2	B	452	THR	CA-C-N	7.62	135.68	121.97
2	B	452	THR	C-N-CA	7.62	135.68	121.97
9	K	93	SER	N-CA-C	7.62	120.54	111.33
3	C	53	THR	OG1-CB-CG2	-7.61	94.08	109.30
5	F	107	VAL	CA-C-N	-7.61	110.73	122.60
5	F	107	VAL	C-N-CA	-7.61	110.73	122.60
2	B	254	LEU	N-CA-C	-7.61	96.83	109.46
5	F	149	GLU	N-CA-CB	7.61	121.28	109.94
7	I	110	PHE	CA-C-O	-7.60	113.12	121.33
1	A	919	ILE	N-CA-C	-7.60	105.14	113.43
1	A	455	MET	CG-SD-CE	-7.60	84.18	100.90
1	A	843	LYS	CB-CA-C	7.60	122.91	110.90
1	A	1006	ILE	CA-CB-CG1	7.59	123.31	110.40
8	J	48	ARG	CA-CB-CG	7.59	129.29	114.10
1	A	1172	LEU	N-CA-C	7.59	123.52	113.20
2	B	336	ARG	N-CA-C	7.59	120.44	111.71
1	A	962	ARG	NE-CZ-NH2	-7.58	112.38	119.20
9	K	111	LEU	CD1-CG-CD2	7.58	127.47	110.80
2	B	769	TYR	N-CA-C	-7.57	102.69	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	GLY	N-CA-C	7.57	131.12	113.18
2	B	435	THR	OG1-CB-CG2	-7.57	94.17	109.30
4	E	65	THR	CA-C-N	-7.56	109.55	120.29
4	E	65	THR	C-N-CA	-7.56	109.55	120.29
1	A	1319	VAL	CB-CA-C	7.55	119.04	110.89
3	C	39	ALA	N-CA-C	7.54	123.16	113.88
2	B	447	ALA	CA-C-N	7.53	132.53	123.19
2	B	447	ALA	C-N-CA	7.53	132.53	123.19
2	B	604	ARG	NE-CZ-NH2	-7.53	112.42	119.20
9	K	23	PRO	CA-C-N	-7.53	110.95	122.09
9	K	23	PRO	C-N-CA	-7.53	110.95	122.09
1	A	1012	ARG	CG-CD-NE	-7.53	95.44	112.00
2	B	620	ARG	CG-CD-NE	-7.52	95.45	112.00
2	B	706	GLN	O-C-N	-7.52	116.59	121.85
2	B	1103	ILE	CB-CA-C	-7.51	98.97	111.29
4	E	49	SER	N-CA-C	7.51	122.10	107.98
2	B	552	MET	CG-SD-CE	7.51	117.41	100.90
2	B	1212	ILE	N-CA-C	7.51	119.39	108.58
2	B	525	ALA	N-CA-C	7.50	122.50	113.12
6	H	54	SER	N-CA-C	7.50	120.57	109.24
6	H	128	ASN	N-CA-C	7.50	126.78	110.80
2	B	983	ARG	CA-CB-CG	7.50	129.09	114.10
8	J	7	CYS	CB-CA-C	-7.49	98.60	109.84
1	A	1077	THR	N-CA-C	7.49	121.34	111.75
2	B	1019	SER	CA-C-N	-7.49	106.98	121.58
2	B	1019	SER	C-N-CA	-7.49	106.98	121.58
2	B	1019	SER	CA-CB-OG	-7.49	96.13	111.10
6	H	140	ALA	N-CA-C	7.48	120.75	107.80
2	B	1097	HIS	CB-CG-CD2	7.48	140.92	131.20
4	E	149	LEU	CA-C-N	-7.48	114.33	122.85
4	E	149	LEU	C-N-CA	-7.48	114.33	122.85
1	A	600	PRO	N-CD-CG	-7.47	91.99	103.20
9	K	16	GLU	CA-C-O	-7.47	112.39	121.36
2	B	56	ASP	O-C-N	-7.47	112.62	122.33
2	B	1178	ASN	N-CA-C	7.47	121.76	111.90
3	C	90	ASP	N-CA-C	7.46	126.68	110.80
3	C	252	GLN	N-CA-C	-7.46	103.15	111.28
1	A	1203	ASN	CB-CA-C	7.45	123.52	110.85
2	B	764	SER	N-CA-CB	-7.45	98.88	110.43
2	B	1048	THR	CA-C-O	-7.44	112.16	121.46
2	B	90	ILE	N-CA-C	7.44	124.81	109.34
1	A	948	VAL	CA-C-N	7.43	134.15	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	948	VAL	C-N-CA	7.43	134.15	121.14
1	A	876	ALA	N-CA-C	7.43	121.61	112.54
9	K	94	ILE	O-C-N	7.42	129.88	121.94
2	B	398	ARG	CB-CA-C	-7.42	93.96	110.21
1	A	979	SER	N-CA-C	-7.42	99.48	110.46
2	B	115	GLN	N-CA-C	7.42	121.24	111.75
2	B	612	GLU	CB-CG-CD	7.42	125.21	112.60
2	B	964	VAL	CA-CB-CG2	-7.42	97.79	110.40
2	B	106	ASP	CB-CG-OD2	7.42	135.46	118.40
2	B	167	ILE	CB-CA-C	-7.41	99.15	111.29
6	H	120	GLY	N-CA-C	7.40	125.53	115.32
1	A	557	ASP	CA-C-N	-7.40	106.91	121.41
1	A	557	ASP	C-N-CA	-7.40	106.91	121.41
3	C	27	LEU	CA-C-N	-7.40	110.25	120.38
3	C	27	LEU	C-N-CA	-7.40	110.25	120.38
3	C	155	LEU	CB-CA-C	-7.39	93.15	109.56
10	L	68	GLU	OE1-CD-OE2	-7.39	105.17	122.90
2	B	836	GLU	CA-C-O	-7.38	112.98	122.14
3	C	254	LYS	N-CA-CB	7.38	120.77	110.07
2	B	735	ALA	O-C-N	7.38	132.73	123.28
3	C	28	ALA	N-CA-C	7.38	120.26	111.33
6	H	103	LYS	CB-CG-CD	7.38	128.26	111.30
7	I	111	THR	OG1-CB-CG2	-7.37	94.56	109.30
8	J	17	LYS	CA-C-N	-7.37	109.82	120.29
8	J	17	LYS	C-N-CA	-7.37	109.82	120.29
1	A	380	VAL	N-CA-C	7.37	118.51	109.30
3	C	50	GLU	CB-CG-CD	7.37	125.13	112.60
4	E	46	TYR	CA-C-N	-7.37	112.60	122.99
4	E	46	TYR	C-N-CA	-7.37	112.60	122.99
1	A	1231	ASP	N-CA-C	7.36	119.39	111.36
1	A	1271	ILE	N-CA-CB	7.36	121.21	111.64
1	A	940	ARG	NE-CZ-NH2	-7.36	112.57	119.20
2	B	1006	ILE	CG1-CB-CG2	-7.35	88.65	110.70
1	A	367	PRO	CB-CA-C	-7.35	101.98	111.39
1	A	829	VAL	CA-C-O	-7.35	113.63	121.27
1	A	1325	THR	N-CA-CB	-7.35	98.42	110.40
1	A	1415	SER	CB-CA-C	-7.35	95.61	109.72
1	A	1406	VAL	O-C-N	7.34	129.54	121.90
4	E	100	ILE	CB-CA-C	-7.34	102.41	112.02
1	A	884	ASP	CA-C-O	-7.33	112.70	120.55
1	A	1284	MET	O-C-N	7.33	131.66	123.01
7	I	88	SER	CB-CA-C	-7.33	98.84	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1278	ASN	CA-C-N	-7.33	113.33	122.93
1	A	1278	ASN	C-N-CA	-7.33	113.33	122.93
2	B	315	LYS	CB-CA-C	-7.33	99.14	112.76
7	I	80	SER	N-CA-C	7.33	120.31	110.35
2	B	633	VAL	CB-CA-C	-7.32	101.18	111.21
9	K	75	ILE	CA-CB-CG1	7.32	122.84	110.40
1	A	1318	THR	CA-CB-CG2	7.32	122.94	110.50
1	A	627	GLY	N-CA-C	7.31	125.47	115.30
1	A	850	VAL	N-CA-C	7.31	119.16	109.21
1	A	81	PHE	CA-C-O	7.31	128.40	120.43
2	B	1083	ALA	CA-C-N	-7.30	110.04	122.67
2	B	1083	ALA	C-N-CA	-7.30	110.04	122.67
1	A	586	ILE	N-CA-C	-7.30	97.89	108.11
9	K	101	LEU	N-CA-C	7.30	121.09	111.75
2	B	129	PHE	N-CA-C	7.30	122.00	107.62
4	E	46	TYR	CA-C-O	7.29	126.59	119.08
2	B	559	SER	N-CA-C	-7.29	104.19	113.23
7	I	94	ASP	N-CA-C	7.28	122.28	112.88
1	A	982	THR	N-CA-C	7.28	121.90	110.32
1	A	468	PHE	N-CA-C	-7.28	98.70	110.20
3	C	81	GLU	N-CA-C	-7.28	98.75	110.32
2	B	993	THR	OG1-CB-CG2	-7.27	94.75	109.30
4	E	98	ILE	CB-CA-C	7.27	121.44	111.92
8	J	1	MET	N-CA-CB	-7.27	98.14	110.50
3	C	7	GLN	N-CA-C	7.26	122.16	109.96
2	B	228	LYS	CA-C-O	-7.26	112.91	121.11
4	E	200	ARG	NE-CZ-NH1	-7.26	114.24	121.50
1	A	774	ARG	NE-CZ-NH2	-7.26	112.67	119.20
8	J	34	THR	N-CA-C	-7.26	102.36	112.45
5	F	115	THR	OG1-CB-CG2	-7.25	94.79	109.30
10	L	63	ARG	N-CA-CB	7.25	121.23	109.69
2	B	691	GLU	CA-CB-CG	7.25	128.61	114.10
1	A	469	ARG	CG-CD-NE	-7.24	96.06	112.00
3	C	97	VAL	CA-C-O	-7.24	112.53	120.71
3	C	32	SER	N-CA-C	7.24	121.02	111.75
2	B	268	THR	N-CA-CB	-7.24	99.47	111.20
6	H	9	ILE	N-CA-CB	7.24	123.30	111.58
1	A	84	ILE	CA-C-O	-7.23	111.74	120.78
2	B	595	ARG	N-CA-CB	7.23	120.75	110.12
2	B	246	LYS	N-CA-C	7.23	122.11	109.96
2	B	1042	GLY	CA-C-O	-7.23	114.62	120.91
2	B	652	LYS	CD-CE-NZ	7.23	135.03	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	GLU	CA-CB-CG	7.22	128.55	114.10
6	H	130	ARG	CA-C-N	7.22	130.55	120.29
6	H	130	ARG	C-N-CA	7.22	130.55	120.29
1	A	27	VAL	CB-CA-C	-7.22	102.72	111.97
2	B	646	LEU	N-CA-C	7.22	126.18	110.80
4	E	132	ILE	N-CA-C	7.22	118.51	108.12
7	I	4	PHE	N-CA-C	7.22	126.17	110.80
8	J	62	ARG	CG-CD-NE	-7.22	96.12	112.00
2	B	547	VAL	CG1-CB-CG2	7.21	126.67	110.80
4	E	153	HIS	CA-CB-CG	7.21	121.02	113.80
9	K	36	GLU	N-CA-C	7.21	121.20	110.52
2	B	678	GLU	CB-CG-CD	7.21	124.86	112.60
1	A	1161	THR	N-CA-C	7.21	120.22	108.55
2	B	942	ARG	CB-CA-C	-7.20	96.08	110.42
6	H	56	THR	N-CA-C	-7.20	95.88	108.20
6	H	94	ASP	N-CA-C	7.20	120.18	111.82
1	A	454	SER	N-CA-C	-7.20	104.23	113.16
8	J	36	LEU	N-CA-C	-7.20	103.52	111.36
2	B	497	ARG	NE-CZ-NH2	-7.19	112.73	119.20
2	B	130	VAL	N-CA-C	7.19	124.29	109.34
2	B	518	HIS	CA-CB-CG	7.19	120.99	113.80
2	B	477	ALA	N-CA-CB	7.18	121.18	110.40
3	C	252	GLN	CB-CA-C	7.18	122.71	110.79
2	B	120	ARG	NE-CZ-NH1	-7.17	114.33	121.50
1	A	462	VAL	O-C-N	7.17	130.49	122.67
3	C	183	TRP	O-C-N	-7.17	112.96	122.14
6	H	126	GLU	CA-C-O	-7.17	113.69	121.94
2	B	1129	ARG	CG-CD-NE	-7.17	96.23	112.00
8	J	56	LEU	CD1-CG-CD2	-7.17	95.03	110.80
1	A	12	ARG	CG-CD-NE	-7.17	96.23	112.00
3	C	10	ILE	N-CA-C	7.17	124.24	109.34
1	A	434	ARG	NE-CZ-NH1	7.16	128.66	121.50
7	I	60	GLN	CA-C-O	7.16	128.22	120.20
2	B	452	THR	OG1-CB-CG2	-7.16	94.98	109.30
2	B	990	ILE	CA-CB-CG1	7.16	122.57	110.40
3	C	206	ASN	O-C-N	-7.16	113.07	122.59
6	H	117	SER	CB-CA-C	-7.16	99.12	110.14
3	C	253	LYS	N-CA-C	7.15	120.11	111.82
1	A	608	ILE	CA-CB-CG1	7.14	122.54	110.40
2	B	852	ARG	N-CA-CB	-7.14	99.89	110.17
1	A	56	PRO	O-C-N	7.13	132.27	122.64
1	A	478	TYR	N-CA-C	-7.13	104.58	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	14	GLU	CB-CA-C	7.13	121.56	109.72
2	B	629	ASP	N-CA-C	7.13	120.55	110.50
1	A	1385	THR	N-CA-C	7.13	130.96	111.00
1	A	728	LYS	CB-CG-CD	7.13	127.70	111.30
1	A	728	LYS	N-CA-CB	7.13	121.19	110.22
3	C	238	ILE	CA-CB-CG2	7.12	122.60	110.50
2	B	781	PHE	N-CA-C	7.12	120.07	111.82
5	F	114	GLU	CA-C-O	-7.12	114.01	121.55
6	H	86	ASP	CB-CA-C	7.12	124.58	110.42
2	B	396	ASP	O-C-N	7.11	131.25	122.86
2	B	1026	LEU	CA-C-O	-7.11	112.88	120.42
1	A	858	ASN	CA-C-O	-7.11	112.62	121.50
4	E	128	PRO	N-CD-CG	7.11	113.86	103.20
1	A	346	ASP	CA-CB-CG	7.10	119.70	112.60
1	A	1036	ARG	NE-CZ-NH2	-7.10	112.81	119.20
3	C	172	PRO	CB-CA-C	-7.10	99.85	111.56
4	E	119	SER	CA-C-O	7.10	126.86	118.69
1	A	27	VAL	N-CA-C	7.10	117.23	110.42
3	C	160	LYS	CD-CE-NZ	7.10	134.61	111.90
4	E	50	MET	CG-SD-CE	7.10	116.52	100.90
2	B	312	GLU	N-CA-CB	-7.10	99.28	110.28
2	B	969	ARG	N-CA-C	7.09	121.01	109.59
7	I	84	VAL	N-CA-CB	-7.09	97.23	111.91
2	B	552	MET	CA-CB-CG	7.09	128.28	114.10
1	A	399	HIS	CA-C-N	7.09	144.01	127.00
1	A	399	HIS	C-N-CA	7.09	144.01	127.00
1	A	857	ARG	NE-CZ-NH2	7.09	125.58	119.20
2	B	412	LEU	N-CA-CB	7.09	120.65	110.16
1	A	1420	ASP	N-CA-C	7.08	121.37	112.87
1	A	96	ILE	CA-CB-CG1	7.08	122.44	110.40
1	A	367	PRO	CA-C-O	7.08	129.36	121.43
2	B	253	THR	N-CA-C	7.08	120.27	108.73
1	A	670	ILE	CB-CA-C	-7.08	102.40	110.96
2	B	1085	ILE	N-CA-C	7.07	118.01	108.11
4	E	87	SER	CB-CA-C	7.07	121.78	110.19
2	B	391	ASP	OD1-CG-OD2	-7.07	105.94	122.90
2	B	547	VAL	N-CA-CB	-7.06	104.44	112.21
1	A	1103	GLU	CB-CA-C	7.06	122.85	110.85
8	J	43	ARG	CG-CD-NE	-7.06	96.47	112.00
5	F	143	PHE	O-C-N	-7.06	115.20	123.25
1	A	1445	ILE	CA-C-O	-7.06	112.74	120.71
2	B	165	VAL	N-CA-CB	7.05	122.87	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	381	MET	CB-CA-C	-7.05	98.86	110.85
1	A	620	LYS	CD-CE-NZ	7.05	134.47	111.90
2	B	1078	GLY	CA-C-O	7.05	125.93	118.95
2	B	798	TYR	CA-C-N	7.05	127.09	119.90
2	B	798	TYR	C-N-CA	7.05	127.09	119.90
1	A	1021	LEU	N-CA-C	-7.04	103.03	111.69
2	B	272	THR	OG1-CB-CG2	-7.04	95.22	109.30
8	J	14	VAL	O-C-N	-7.04	113.77	122.57
2	B	1017	ILE	CA-CB-CG1	-7.04	98.44	110.40
6	H	135	LEU	CA-CB-CG	7.04	140.92	116.30
3	C	16	ASP	CB-CG-OD2	7.03	134.57	118.40
1	A	44	THR	N-CA-CB	7.03	122.37	110.49
7	I	53	GLY	N-CA-C	7.03	125.17	115.27
1	A	1405	THR	OG1-CB-CG2	-7.02	95.26	109.30
2	B	297	ILE	N-CA-C	-7.02	103.63	110.72
1	A	4	GLN	CA-C-N	7.02	133.74	120.97
1	A	4	GLN	C-N-CA	7.02	133.74	120.97
2	B	607	GLY	O-C-N	-7.01	114.12	122.33
3	C	207	CYS	CB-CA-C	-7.01	99.82	110.90
2	B	425	THR	CA-C-N	7.01	130.24	120.29
2	B	425	THR	C-N-CA	7.01	130.24	120.29
4	E	204	THR	CA-CB-OG1	7.00	120.09	109.60
8	J	20	SER	N-CA-C	7.00	119.75	111.71
2	B	1002	THR	O-C-N	-6.99	115.23	123.06
1	A	914	GLU	CG-CD-OE2	-6.98	102.34	118.40
1	A	934	LYS	N-CA-CB	6.98	120.50	110.16
1	A	980	ASP	CB-CA-C	-6.98	98.92	110.72
2	B	297	ILE	CA-CB-CG2	-6.98	98.63	110.50
2	B	597	MET	CA-C-O	-6.98	113.49	120.82
4	E	21	GLU	CB-CG-CD	6.98	124.46	112.60
1	A	124	GLN	CG-CD-NE2	6.97	126.86	116.40
6	H	19	ARG	CD-NE-CZ	6.97	134.16	124.40
3	C	132	PRO	CA-C-O	-6.97	107.91	120.60
2	B	1194	ILE	CA-C-O	-6.97	114.73	121.63
1	A	890	ASP	N-CA-C	-6.97	103.74	111.82
6	H	60	ALA	CA-C-N	-6.96	108.24	121.54
6	H	60	ALA	C-N-CA	-6.96	108.24	121.54
3	C	147	LEU	N-CA-C	6.96	121.02	109.95
6	H	130	ARG	NE-CZ-NH1	-6.96	114.54	121.50
4	E	161	LYS	CA-CB-CG	6.96	128.01	114.10
1	A	476	SER	CA-CB-OG	-6.95	97.20	111.10
3	C	79	GLN	N-CA-C	-6.95	103.14	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	895	LYS	O-C-N	-6.95	114.76	122.12
1	A	917	SER	CB-CA-C	-6.95	99.98	110.88
7	I	113	ASP	OD1-CG-OD2	-6.95	106.23	122.90
1	A	1384	VAL	CA-C-O	-6.94	112.36	120.83
1	A	1046	LEU	N-CA-C	6.94	118.92	111.36
1	A	961	ARG	NE-CZ-NH2	6.93	125.44	119.20
3	C	38	ILE	N-CA-C	6.93	117.64	110.36
2	B	694	ASP	N-CA-C	6.93	120.63	110.17
6	H	107	VAL	N-CA-C	-6.92	94.94	109.34
1	A	596	THR	CB-CA-C	-6.92	95.04	111.65
1	A	664	THR	CB-CA-C	-6.92	95.20	109.94
2	B	289	LEU	O-C-N	-6.92	113.47	122.39
1	A	291	GLU	N-CA-C	-6.91	103.19	111.69
6	H	91	ASP	N-CA-C	6.91	119.79	108.52
1	A	39	GLU	N-CA-C	6.91	119.67	109.24
7	I	75	CYS	N-CA-CB	6.91	119.69	109.88
2	B	48	LEU	CA-C-O	-6.90	113.48	121.07
1	A	548	ASN	N-CA-C	-6.89	103.55	112.23
3	C	84	ARG	CA-C-O	-6.89	111.54	119.60
1	A	292	ALA	O-C-N	6.89	129.16	122.07
2	B	273	LEU	N-CA-C	6.88	120.29	110.24
1	A	472	LEU	N-CA-C	6.88	119.66	111.33
3	C	248	ILE	CB-CA-C	-6.88	102.85	112.14
1	A	72	GLU	N-CA-C	6.88	125.46	110.80
7	I	119	THR	CA-C-N	6.88	131.28	121.71
7	I	119	THR	C-N-CA	6.88	131.28	121.71
1	A	1143	LEU	N-CA-C	-6.88	103.78	111.28
2	B	284	ILE	N-CA-C	-6.88	103.61	110.62
2	B	522	VAL	N-CA-CB	-6.88	99.21	111.93
7	I	55	THR	CA-CB-OG1	-6.87	99.29	109.60
7	I	5	ARG	CB-CG-CD	6.87	127.10	111.30
1	A	557	ASP	OD1-CG-OD2	-6.87	106.41	122.90
1	A	857	ARG	NE-CZ-NH1	-6.87	114.63	121.50
2	B	589	VAL	CB-CA-C	6.87	122.59	110.71
2	B	405	ARG	NE-CZ-NH1	6.87	128.37	121.50
1	A	79	GLY	N-CA-C	-6.86	96.91	113.18
1	A	76	GLU	CA-C-N	6.86	130.80	121.20
1	A	76	GLU	C-N-CA	6.86	130.80	121.20
1	A	641	VAL	N-CA-C	-6.86	103.80	110.72
1	A	85	ASP	N-CA-CB	6.85	120.41	110.06
2	B	97	VAL	N-CA-C	-6.85	97.63	107.77
1	A	612	ILE	CA-C-O	-6.85	112.96	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	941	LYS	N-CA-CB	6.84	120.00	110.07
1	A	575	LYS	N-CA-C	6.84	119.61	111.33
1	A	1005	GLU	CG-CD-OE1	6.84	134.13	118.40
1	A	1138	ILE	N-CA-C	6.84	117.44	111.90
1	A	1154	TYR	CA-C-O	-6.84	113.04	120.36
2	B	1183	LYS	CA-CB-CG	6.84	127.78	114.10
2	B	712	PRO	N-CD-CG	-6.83	92.95	103.20
2	B	177	LYS	N-CA-C	-6.83	103.62	112.23
1	A	1226	VAL	N-CA-C	6.83	118.14	108.17
1	A	1049	ILE	N-CA-C	-6.83	102.84	110.62
2	B	285	ILE	CA-C-O	6.82	128.05	120.95
4	E	168	TYR	CA-C-O	6.82	126.92	119.15
1	A	403	LYS	N-CA-C	-6.82	105.59	114.04
1	A	1377	THR	N-CA-CB	6.82	121.51	110.40
2	B	400	HIS	N-CA-C	-6.82	99.57	109.59
1	A	1009	ASN	O-C-N	6.82	129.34	122.12
1	A	1165	GLU	CA-C-N	-6.81	111.76	122.73
1	A	1165	GLU	C-N-CA	-6.81	111.76	122.73
2	B	436	VAL	CB-CA-C	6.81	122.46	111.29
10	L	41	SER	N-CA-C	6.80	125.29	110.80
1	A	1031	VAL	CB-CA-C	-6.80	102.96	112.14
4	E	33	GLU	N-CA-C	-6.80	104.98	113.28
2	B	795	ILE	CB-CA-C	-6.80	100.03	110.50
4	E	162	ARG	CB-CA-C	6.80	122.07	110.79
2	B	992	ILE	CA-C-O	-6.79	115.52	121.09
6	H	21	ASN	N-CA-C	6.79	122.24	113.88
1	A	883	LEU	N-CA-C	-6.79	96.59	108.20
1	A	938	LYS	CG-CD-CE	-6.79	95.69	111.30
1	A	1005	GLU	CG-CD-OE2	-6.79	102.79	118.40
3	C	18	VAL	N-CA-C	-6.79	95.23	109.34
9	K	110	ASN	N-CA-C	-6.79	103.02	112.45
1	A	1195	LEU	CA-C-O	6.78	127.90	120.71
2	B	662	MET	CA-CB-CG	-6.78	100.53	114.10
1	A	470	LEU	CA-C-O	6.78	128.93	121.06
1	A	1077	THR	O-C-N	-6.78	114.47	122.20
2	B	68	THR	OG1-CB-CG2	-6.78	95.74	109.30
2	B	365	THR	OG1-CB-CG2	-6.78	95.75	109.30
2	B	419	THR	OG1-CB-CG2	-6.78	95.74	109.30
1	A	1196	GLU	CG-CD-OE2	-6.78	102.81	118.40
1	A	1111	MET	N-CA-CB	-6.77	99.63	110.46
10	L	57	LEU	CB-CA-C	-6.77	99.95	110.78
2	B	735	ALA	CA-C-O	-6.77	111.94	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	59	ILE	CB-CA-C	-6.77	101.94	111.28
6	H	110	ASP	CA-C-N	6.76	134.14	122.64
6	H	110	ASP	C-N-CA	6.76	134.14	122.64
7	I	45	ARG	NE-CZ-NH1	-6.76	114.74	121.50
1	A	1139	GLU	CB-CA-C	-6.75	100.44	110.16
2	B	957	ASN	N-CA-C	6.75	125.17	110.80
9	K	4	PRO	CB-CA-C	6.74	120.35	110.85
7	I	109	ILE	CG1-CB-CG2	-6.74	90.49	110.70
1	A	828	ALA	N-CA-C	6.73	118.28	111.07
1	A	982	THR	CA-CB-OG1	-6.73	99.50	109.60
1	A	1349	TYR	N-CA-C	-6.73	104.02	111.36
4	E	66	GLU	N-CA-CB	6.73	120.12	110.16
7	I	27	PHE	N-CA-C	6.73	119.71	108.73
2	B	1078	GLY	N-CA-C	6.73	124.47	115.59
4	E	25	ASP	OD1-CG-OD2	-6.73	106.75	122.90
5	F	94	LEU	CA-C-N	-6.73	108.22	121.41
5	F	94	LEU	C-N-CA	-6.73	108.22	121.41
2	B	789	MET	CB-CA-C	-6.73	101.68	111.23
3	C	239	PRO	O-C-N	-6.73	114.79	123.00
1	A	602	ASP	CA-C-N	6.72	134.98	122.74
1	A	602	ASP	C-N-CA	6.72	134.98	122.74
2	B	264	SER	N-CA-C	-6.72	99.44	109.86
2	B	982	SER	CA-C-O	-6.72	114.95	122.01
1	A	1062	GLU	CB-CG-CD	6.72	124.02	112.60
2	B	706	GLN	CG-CD-NE2	6.72	126.48	116.40
5	F	72	LYS	N-CA-C	6.72	129.80	111.00
1	A	788	SER	CA-CB-OG	-6.71	97.67	111.10
1	A	940	ARG	CG-CD-NE	-6.71	97.25	112.00
2	B	266	ALA	CA-C-N	-6.71	111.56	120.95
2	B	266	ALA	C-N-CA	-6.71	111.56	120.95
2	B	1047	PHE	CA-C-O	-6.71	113.81	121.65
1	A	917	SER	CA-CB-OG	-6.70	97.70	111.10
1	A	387	ARG	CA-C-N	-6.70	111.31	120.28
1	A	387	ARG	C-N-CA	-6.70	111.31	120.28
6	H	52	GLN	O-C-N	-6.69	113.69	122.59
9	K	93	SER	CB-CA-C	-6.69	99.30	110.68
1	A	1442	ASP	O-C-N	6.69	131.59	123.16
2	B	954	VAL	CB-CA-C	-6.69	100.19	110.50
2	B	732	SER	N-CA-C	6.68	119.44	110.35
1	A	885	THR	OG1-CB-CG2	-6.68	95.94	109.30
1	A	509	LEU	N-CA-C	6.68	121.14	113.19
4	E	187	TYR	CA-C-O	-6.67	112.56	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	563	MET	CG-SD-CE	6.67	115.57	100.90
3	C	204	SER	N-CA-CB	-6.67	100.57	110.17
2	B	1106	ARG	N-CA-C	6.67	120.51	107.98
9	K	6	ARG	CG-CD-NE	-6.66	97.34	112.00
1	A	963	ILE	N-CA-C	6.66	118.21	110.62
2	B	858	SER	CA-CB-OG	-6.66	97.78	111.10
7	I	6	PHE	CA-C-N	6.66	130.58	121.05
7	I	6	PHE	C-N-CA	6.66	130.58	121.05
4	E	201	LYS	CD-CE-NZ	-6.66	90.59	111.90
9	K	26	LYS	O-C-N	-6.66	115.07	122.12
1	A	598	LEU	N-CA-C	6.65	121.04	112.26
2	B	106	ASP	CA-CB-CG	6.65	119.25	112.60
2	B	66	ASP	CA-C-N	6.65	129.08	120.44
2	B	66	ASP	C-N-CA	6.65	129.08	120.44
2	B	1053	GLU	N-CA-CB	6.65	119.71	110.07
2	B	258	LEU	CA-C-N	6.64	130.31	120.87
2	B	258	LEU	C-N-CA	6.64	130.31	120.87
2	B	579	ARG	NE-CZ-NH1	-6.64	114.86	121.50
1	A	934	LYS	CA-C-O	-6.64	113.39	120.42
2	B	549	THR	N-CA-C	-6.64	98.28	108.76
5	F	113	GLY	N-CA-C	6.64	121.56	113.79
9	K	26	LYS	CA-C-O	6.63	127.80	120.63
1	A	923	LEU	CB-CA-C	-6.63	98.57	110.70
2	B	365	THR	N-CA-C	-6.63	98.58	108.99
3	C	15	LYS	N-CA-C	-6.63	104.67	112.89
7	I	33	SER	N-CA-C	-6.63	104.50	112.59
1	A	465	TYR	O-C-N	-6.62	113.78	122.59
3	C	192	TRP	O-C-N	-6.62	114.81	122.89
2	B	395	GLN	N-CA-CB	6.62	119.77	110.04
3	C	55	THR	OG1-CB-CG2	-6.62	96.06	109.30
1	A	14	VAL	CA-C-O	-6.62	113.49	120.57
1	A	968	GLN	CA-CB-CG	-6.62	100.87	114.10
1	A	1273	LEU	N-CA-C	6.62	119.78	111.24
1	A	404	TYR	CA-C-O	-6.62	113.92	121.40
1	A	547	LEU	N-CA-C	-6.62	104.47	112.54
1	A	1299	VAL	N-CA-CB	-6.61	100.14	112.36
2	B	249	ARG	NE-CZ-NH1	6.61	128.11	121.50
2	B	950	ASP	N-CA-CB	-6.61	101.03	110.81
4	E	38	PRO	O-C-N	6.61	131.56	122.64
1	A	32	VAL	N-CA-CB	-6.61	100.33	111.23
2	B	386	LEU	N-CA-C	6.61	119.48	111.82
2	B	181	LEU	N-CA-C	-6.60	105.22	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	939	THR	N-CA-C	6.60	117.97	109.72
4	E	76	GLY	N-CA-C	-6.60	100.03	112.64
3	C	78	GLU	CB-CG-CD	6.60	123.82	112.60
8	J	25	LEU	N-CA-C	6.59	119.80	111.69
10	L	55	ILE	N-CA-C	6.59	117.38	107.75
6	H	80	ARG	N-CA-C	-6.59	98.27	108.55
2	B	393	LYS	N-CA-CB	6.59	122.92	111.13
1	A	166	GLY	N-CA-C	6.58	123.32	111.34
3	C	248	ILE	CA-C-O	6.58	127.80	120.95
1	A	1217	LYS	N-CA-C	6.58	119.29	111.33
6	H	11	GLN	CB-CA-C	-6.58	98.33	109.72
2	B	373	ARG	NE-CZ-NH2	-6.58	113.28	119.20
1	A	1280	GLU	CG-CD-OE2	6.58	133.52	118.40
3	C	147	LEU	CD1-CG-CD2	-6.58	96.33	110.80
4	E	61	GLN	N-CA-C	-6.58	99.42	109.41
2	B	944	THR	N-CA-C	6.57	121.31	113.16
2	B	240	ILE	CA-C-O	-6.57	114.32	121.28
4	E	121	MET	CB-CG-SD	6.57	132.40	112.70
2	B	304	ASP	N-CA-CB	6.56	121.57	110.49
1	A	275	SER	CA-CB-OG	-6.56	97.98	111.10
7	I	55	THR	CA-CB-CG2	6.56	121.65	110.50
1	A	1062	GLU	CA-CB-CG	6.55	127.21	114.10
7	I	35	VAL	CA-CB-CG2	-6.55	99.26	110.40
2	B	567	GLU	CB-CG-CD	6.55	123.74	112.60
2	B	895	ASP	N-CA-C	-6.55	104.55	112.54
4	E	150	VAL	CA-C-O	6.55	124.23	119.25
3	C	4	GLU	O-C-N	6.55	131.30	122.59
1	A	912	LEU	N-CA-CB	6.54	120.48	110.14
1	A	948	VAL	N-CA-CB	-6.54	99.46	110.65
2	B	59	LEU	N-CA-C	-6.54	102.80	111.24
2	B	767	ASN	N-CA-C	-6.54	104.23	111.82
3	C	107	SER	N-CA-C	6.54	119.00	110.43
3	C	263	THR	CA-CB-CG2	6.54	121.62	110.50
8	J	64	ASN	CB-CA-C	6.53	122.51	110.10
1	A	1100	ARG	NE-CZ-NH1	6.53	128.03	121.50
2	B	527	THR	CB-CA-C	6.53	118.92	109.45
3	C	263	THR	N-CA-CB	-6.53	99.45	110.49
2	B	888	GLY	CA-C-O	-6.53	111.79	122.56
1	A	474	VAL	N-CA-C	-6.53	105.29	112.80
1	A	1321	GLY	CA-C-N	-6.53	115.28	122.27
1	A	1321	GLY	C-N-CA	-6.53	115.28	122.27
1	A	720	ARG	CB-CG-CD	6.53	126.31	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	415	GLN	N-CA-C	-6.53	103.28	111.11
1	A	171	GLN	CG-CD-NE2	6.52	126.17	116.40
1	A	519	PRO	N-CD-CG	6.52	112.98	103.20
1	A	680	THR	OG1-CB-CG2	-6.52	96.27	109.30
2	B	909	ASP	CB-CG-OD2	6.52	133.39	118.40
1	A	1376	THR	CA-CB-OG1	6.51	119.37	109.60
1	A	1036	ARG	NH1-CZ-NH2	6.51	127.77	119.30
6	H	26	ILE	CB-CA-C	-6.51	102.61	111.33
7	I	31	THR	CA-C-N	6.51	135.72	123.09
7	I	31	THR	C-N-CA	6.51	135.72	123.09
1	A	160	GLN	CG-CD-NE2	6.51	126.16	116.40
1	A	717	ASN	CB-CG-ND2	-6.51	106.63	116.40
1	A	1003	LYS	CA-CB-CG	-6.51	101.08	114.10
1	A	549	MET	CG-SD-CE	6.51	115.22	100.90
2	B	95	ILE	CB-CA-C	-6.51	100.93	110.62
10	L	58	LYS	O-C-N	-6.51	113.94	122.59
5	F	97	ARG	CB-CG-CD	6.50	126.26	111.30
2	B	35	SER	CB-CA-C	-6.50	99.99	110.79
2	B	344	LYS	N-CA-C	6.50	119.41	110.24
9	K	78	THR	N-CA-CB	6.50	120.33	109.92
3	C	121	VAL	CA-CB-CG1	6.50	121.45	110.40
2	B	184	ALA	N-CA-C	6.50	119.40	110.24
1	A	941	LYS	CB-CA-C	-6.50	100.64	110.90
4	E	80	VAL	CB-CA-C	-6.50	100.67	110.55
2	B	498	THR	CA-CB-OG1	6.50	119.34	109.60
2	B	53	GLN	CA-C-N	-6.49	111.58	120.28
2	B	53	GLN	C-N-CA	-6.49	111.58	120.28
1	A	774	ARG	NH1-CZ-NH2	-6.49	110.86	119.30
3	C	267	GLN	N-CA-C	6.49	124.63	110.80
1	A	715	GLU	N-CA-C	6.49	118.01	111.07
1	A	1281	ARG	CB-CA-C	-6.49	97.60	109.54
1	A	808	LEU	O-C-N	-6.49	115.79	123.06
1	A	1265	ASN	O-C-N	-6.49	115.34	122.09
2	B	49	ASP	CA-C-O	6.49	127.47	120.20
1	A	25	GLU	CB-CG-CD	6.49	123.63	112.60
9	K	88	LYS	N-CA-C	-6.49	104.13	111.07
2	B	759	PRO	CA-CB-CG	-6.48	92.18	104.50
9	K	79	GLU	N-CA-C	-6.48	100.06	109.59
1	A	1285	MET	CG-SD-CE	6.48	115.15	100.90
2	B	125	SER	CB-CA-C	6.48	123.07	109.79
2	B	249	ARG	CD-NE-CZ	6.48	133.47	124.40
1	A	766	GLY	N-CA-C	6.46	122.45	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	205	ILE	CB-CA-C	-6.45	102.60	110.99
6	H	117	SER	O-C-N	6.45	131.54	123.28
7	I	98	VAL	CA-C-O	-6.45	115.13	121.58
1	A	893	PHE	N-CA-C	-6.45	103.76	111.69
9	K	49	GLU	CA-C-O	-6.45	114.05	120.82
1	A	1309	ASP	CB-CA-C	-6.44	100.47	110.78
2	B	942	ARG	CA-CB-CG	6.44	126.98	114.10
2	B	1050	ILE	CG1-CB-CG2	-6.44	91.38	110.70
2	B	289	LEU	CA-C-N	-6.44	110.40	122.05
2	B	289	LEU	C-N-CA	-6.44	110.40	122.05
3	C	4	GLU	N-CA-C	6.43	124.50	110.80
3	C	15	LYS	CG-CD-CE	6.43	126.10	111.30
1	A	779	PHE	N-CA-C	-6.43	101.47	110.35
1	A	992	ASP	N-CA-CB	-6.43	100.64	110.16
1	A	1422	ARG	NE-CZ-NH1	6.43	127.93	121.50
2	B	1135	ARG	CG-CD-NE	-6.43	97.85	112.00
10	L	65	VAL	O-C-N	6.42	130.20	123.26
3	C	184	ASN	CA-C-N	-6.42	110.60	122.09
3	C	184	ASN	C-N-CA	-6.42	110.60	122.09
1	A	292	ALA	CA-C-O	-6.42	114.08	120.82
1	A	1004	ASN	N-CA-CB	-6.42	101.56	110.29
7	I	18	GLU	CB-CA-C	6.41	120.11	109.53
1	A	622	VAL	N-CA-CB	-6.41	104.03	112.36
1	A	819	GLY	N-CA-C	6.41	120.39	112.64
2	B	277	LYS	N-CA-CB	-6.41	100.80	110.73
2	B	108	VAL	CB-CA-C	6.41	121.80	111.29
1	A	53	LEU	CA-CB-CG	6.41	138.72	116.30
2	B	856	PHE	CA-C-O	-6.41	113.78	120.70
9	K	6	ARG	N-CA-CB	-6.40	100.36	110.28
10	L	70	ARG	NE-CZ-NH1	6.40	127.90	121.50
1	A	740	LEU	CB-CG-CD1	6.40	129.90	110.70
6	H	139	ASN	CA-C-N	-6.40	113.16	122.44
6	H	139	ASN	C-N-CA	-6.40	113.16	122.44
9	K	62	LYS	N-CA-C	6.40	118.92	108.55
1	A	1310	GLY	CA-C-O	-6.40	118.06	122.22
8	J	42	LYS	CA-C-N	-6.40	110.77	121.39
8	J	42	LYS	C-N-CA	-6.40	110.77	121.39
1	A	96	ILE	N-CA-C	-6.39	103.33	110.62
2	B	387	LEU	N-CA-C	-6.39	104.40	111.82
5	F	73	ALA	N-CA-C	6.39	124.42	110.80
7	I	13	MET	CG-SD-CE	-6.39	86.83	100.90
2	B	990	ILE	N-CA-C	-6.39	100.46	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	773	MET	O-C-N	-6.39	115.35	122.12
1	A	497	THR	N-CA-CB	-6.38	100.48	110.06
2	B	851	PHE	N-CA-C	6.38	120.39	112.47
1	A	610	GLY	O-C-N	6.38	129.05	122.54
2	B	170	LEU	CB-CA-C	-6.38	102.81	110.15
1	A	472	LEU	CA-CB-CG	-6.38	93.98	116.30
1	A	726	ARG	CG-CD-NE	-6.38	97.97	112.00
2	B	759	PRO	N-CD-CG	-6.37	93.64	103.20
2	B	1162	ILE	N-CA-CB	-6.37	102.56	111.99
2	B	213	ILE	N-CA-C	-6.37	99.25	108.36
1	A	33	ALA	N-CA-C	6.37	119.46	110.23
2	B	446	LEU	CB-CA-C	6.36	122.19	110.10
2	B	1196	ILE	N-CA-C	6.36	114.41	109.19
3	C	165	LYS	CD-CE-NZ	6.36	132.26	111.90
1	A	1047	SER	N-CA-C	-6.36	104.44	111.82
2	B	1047	PHE	N-CA-C	6.36	120.42	111.52
8	J	13	VAL	N-CA-C	-6.36	101.38	109.58
2	B	104	GLU	N-CA-C	6.36	119.89	110.48
2	B	236	HIS	CA-C-O	-6.36	114.47	121.33
2	B	772	ALA	N-CA-C	6.36	117.87	111.07
3	C	235	VAL	CA-C-O	6.36	126.54	119.42
2	B	644	GLU	CB-CG-CD	-6.35	101.81	112.60
3	C	3	GLU	CA-C-N	6.35	133.66	121.54
3	C	3	GLU	C-N-CA	6.35	133.66	121.54
2	B	1019	SER	N-CA-CB	6.35	120.74	110.40
10	L	28	LYS	N-CA-C	6.35	124.32	110.80
10	L	63	ARG	O-C-N	-6.35	115.23	122.97
1	A	1234	GLU	CA-CB-CG	6.34	126.79	114.10
9	K	17	SER	CB-CA-C	-6.34	99.33	109.80
2	B	1099	VAL	CB-CA-C	-6.34	100.89	111.29
3	C	75	MET	N-CA-C	-6.34	104.28	111.07
9	K	42	LEU	CB-CG-CD1	-6.34	91.68	110.70
1	A	1271	ILE	CA-C-O	6.34	126.98	120.39
1	A	827	THR	N-CA-C	6.33	117.84	111.07
1	A	596	THR	CA-CB-CG2	-6.33	99.74	110.50
2	B	684	LEU	N-CA-C	6.33	118.18	111.28
1	A	37	PHE	CA-C-O	-6.32	113.54	120.69
1	A	843	LYS	O-C-N	-6.32	115.26	122.09
1	A	1167	GLU	N-CA-C	-6.32	104.31	111.07
1	A	495	GLU	CB-CG-CD	6.32	123.34	112.60
1	A	913	LEU	N-CA-CB	-6.32	99.69	111.13
2	B	1223	ASP	CA-C-N	6.32	133.07	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1223	ASP	C-N-CA	6.32	133.07	121.70
3	C	164	ALA	CA-C-O	-6.31	112.97	120.10
9	K	70	ARG	CB-CA-C	6.31	121.22	109.86
2	B	201	GLY	CA-C-O	6.31	126.32	119.06
1	A	407	ARG	NE-CZ-NH2	-6.31	113.52	119.20
2	B	273	LEU	CB-CA-C	-6.31	99.65	109.11
4	E	148	GLU	CG-CD-OE2	6.31	132.90	118.40
7	I	118	ARG	CA-CB-CG	6.31	126.71	114.10
2	B	889	THR	N-CA-CB	6.30	120.44	110.23
4	E	17	ARG	CG-CD-NE	-6.30	98.13	112.00
2	B	542	MET	CG-SD-CE	-6.30	87.04	100.90
8	J	28	ASP	O-C-N	6.30	130.14	122.20
1	A	918	GLU	CA-CB-CG	6.30	126.69	114.10
2	B	999	MET	CA-C-O	-6.30	113.94	120.87
6	H	139	ASN	N-CA-C	-6.30	97.39	110.80
7	I	15	TYR	O-C-N	-6.30	115.46	121.57
3	C	165	LYS	N-CA-CB	6.29	121.13	110.49
1	A	1296	GLY	N-CA-C	6.29	120.31	113.58
3	C	108	GLU	N-CA-C	-6.28	103.73	111.40
2	B	904	ARG	N-CA-C	6.28	119.34	110.23
1	A	1003	LYS	N-CA-C	6.28	118.12	111.28
2	B	699	GLU	CB-CA-C	-6.28	97.18	110.31
1	A	1188	GLN	N-CA-C	6.28	118.94	108.96
1	A	1202	MET	N-CA-C	-6.28	104.36	111.14
9	K	46	ILE	CA-C-O	6.28	127.94	121.41
2	B	166	PHE	N-CA-CB	-6.28	100.74	109.97
2	B	250	PHE	CA-C-N	6.27	133.26	121.97
2	B	250	PHE	C-N-CA	6.27	133.26	121.97
2	B	224	GLN	CA-CB-CG	-6.27	101.55	114.10
5	F	148	VAL	CA-C-O	-6.27	114.53	121.05
7	I	14	LEU	CA-C-O	-6.27	113.84	120.80
1	A	1040	GLN	N-CA-C	-6.26	103.99	111.69
2	B	639	ILE	CA-CB-CG1	6.26	121.04	110.40
2	B	1202	LEU	N-CA-C	6.26	118.65	111.02
2	B	357	GLN	N-CA-C	-6.25	105.47	113.23
1	A	1001	ARG	CG-CD-NE	-6.25	98.25	112.00
1	A	1069	ALA	N-CA-C	6.25	118.09	111.28
1	A	1241	ARG	NE-CZ-NH1	6.25	127.75	121.50
2	B	582	VAL	CG1-CB-CG2	-6.25	97.05	110.80
2	B	182	SER	N-CA-C	-6.25	104.36	112.23
2	B	1086	PHE	N-CA-C	-6.25	99.83	109.76
7	I	92	ARG	O-C-N	6.25	131.48	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	983	ARG	NE-CZ-NH1	6.25	127.75	121.50
2	B	217	ARG	CG-CD-NE	-6.24	98.26	112.00
2	B	1062	HIS	CB-CA-C	-6.24	100.64	110.94
1	A	151	ASP	CA-CB-CG	-6.24	106.36	112.60
2	B	426	LYS	N-CA-C	6.24	118.16	111.36
2	B	667	GLN	N-CA-C	6.24	119.30	109.39
2	B	531	GLN	CA-C-N	-6.23	111.10	122.38
2	B	531	GLN	C-N-CA	-6.23	111.10	122.38
1	A	866	PHE	N-CA-C	-6.22	105.17	112.89
9	K	47	ARG	NE-CZ-NH1	6.22	127.72	121.50
3	C	35	ARG	CG-CD-NE	-6.22	98.31	112.00
4	E	149	LEU	N-CA-C	-6.22	105.69	113.28
1	A	764	CYS	N-CA-CB	-6.22	100.44	110.77
7	I	95	THR	N-CA-CB	-6.22	100.89	110.04
2	B	1181	GLU	CA-CB-CG	6.22	126.54	114.10
6	H	36	CYS	N-CA-C	6.22	118.73	109.59
2	B	974	PRO	CB-CA-C	-6.22	103.66	111.56
2	B	1071	VAL	N-CA-C	-6.22	101.56	109.58
3	C	125	MET	CG-SD-CE	6.22	114.58	100.90
7	I	114	GLN	N-CA-C	6.22	120.47	113.01
2	B	39	ARG	NE-CZ-NH1	6.21	127.71	121.50
2	B	217	ARG	CB-CG-CD	6.21	125.59	111.30
1	A	613	ILE	N-CA-C	-6.21	105.64	111.48
5	F	135	ARG	CA-C-O	-6.21	113.93	120.58
1	A	651	LYS	CB-CA-C	6.21	120.75	110.81
2	B	1083	ALA	N-CA-CB	-6.21	100.87	110.56
1	A	383	TYR	CA-C-O	6.21	127.01	119.31
9	K	37	LYS	N-CA-C	6.21	119.74	111.30
1	A	1293	SER	N-CA-C	6.20	119.70	110.39
2	B	60	GLN	CA-C-O	-6.20	113.97	120.55
4	E	179	GLN	CB-CG-CD	-6.20	102.06	112.60
1	A	833	GLU	CB-CG-CD	6.20	123.14	112.60
2	B	276	ILE	N-CA-C	-6.20	99.43	108.11
1	A	706	HIS	O-C-N	6.20	130.83	122.59
2	B	497	ARG	N-CA-C	6.20	118.92	110.55
2	B	95	ILE	CG1-CB-CG2	-6.20	92.11	110.70
7	I	83	ASN	CB-CA-C	-6.19	97.64	109.66
6	H	122	LEU	N-CA-C	6.19	120.14	110.17
1	A	1163	ILE	O-C-N	6.19	125.27	121.37
2	B	287	ARG	NE-CZ-NH1	6.19	127.69	121.50
1	A	294	SER	N-CA-C	6.19	120.09	112.54
3	C	210	GLU	CG-CD-OE2	-6.19	104.17	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	96	ASN	N-CA-CB	6.18	119.04	110.07
1	A	598	LEU	CB-CA-C	-6.18	101.18	111.13
1	A	705	LYS	N-CA-CB	6.18	122.73	111.11
3	C	87	PHE	N-CA-C	-6.18	105.60	113.02
2	B	601	ARG	NH1-CZ-NH2	6.18	127.34	119.30
2	B	1075	GLY	N-CA-C	6.18	121.49	113.27
9	K	78	THR	CA-CB-CG2	-6.18	99.99	110.50
6	H	87	ARG	CA-CB-CG	6.18	126.46	114.10
4	E	51	GLY	CA-C-N	6.18	129.26	120.49
4	E	51	GLY	C-N-CA	6.18	129.26	120.49
6	H	116	TYR	CA-C-O	6.18	129.34	120.51
2	B	205	ILE	CA-C-N	6.17	130.90	122.19
2	B	205	ILE	C-N-CA	6.17	130.90	122.19
7	I	17	ARG	CB-CG-CD	6.17	125.50	111.30
2	B	260	GLY	N-CA-C	-6.17	98.55	113.18
1	A	452	LYS	CB-CG-CD	-6.17	97.10	111.30
2	B	529	GLU	CA-C-O	6.17	128.57	121.47
4	E	53	PRO	CA-C-N	-6.17	114.27	122.85
4	E	53	PRO	C-N-CA	-6.17	114.27	122.85
4	E	81	GLU	N-CA-CB	-6.17	100.53	110.77
7	I	41	PRO	CA-C-O	6.17	127.41	118.78
7	I	23	ASN	CB-CA-C	6.16	121.11	112.11
1	A	985	ASP	CB-CG-OD1	-6.16	104.23	118.40
1	A	878	ILE	N-CA-CB	-6.16	100.68	111.39
2	B	605	ARG	NE-CZ-NH1	-6.16	115.34	121.50
2	B	620	ARG	CA-C-O	6.16	126.50	119.18
7	I	17	ARG	N-CA-CB	6.16	120.93	110.71
1	A	1271	ILE	CG1-CB-CG2	-6.15	92.25	110.70
1	A	1278	ASN	N-CA-C	6.15	122.94	113.28
2	B	962	LYS	N-CA-C	-6.15	101.18	110.28
1	A	909	ASP	CA-C-O	6.15	125.98	120.02
7	I	28	GLU	CA-C-O	-6.15	114.12	121.56
2	B	1151	LEU	O-C-N	-6.15	114.80	122.24
6	H	131	ASN	N-CA-CB	6.15	119.26	110.16
1	A	757	ASN	CA-C-O	-6.14	114.37	120.70
6	H	139	ASN	CA-CB-CG	6.14	118.75	112.60
1	A	347	PHE	N-CA-C	6.14	120.15	111.92
1	A	1069	ALA	CA-C-N	6.14	131.09	120.58
1	A	1069	ALA	C-N-CA	6.14	131.09	120.58
1	A	1219	THR	N-CA-C	6.14	118.94	111.82
2	B	764	SER	O-C-N	-6.14	114.94	120.71
2	B	806	THR	N-CA-CB	-6.14	100.58	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	ARG	CA-C-N	-6.14	114.11	122.95
1	A	326	ARG	C-N-CA	-6.14	114.11	122.95
1	A	645	LEU	O-C-N	-6.14	115.03	122.22
1	A	1163	ILE	N-CA-C	6.14	113.63	107.55
1	A	1377	THR	CA-CB-CG2	6.14	120.94	110.50
9	K	17	SER	O-C-N	-6.14	116.09	123.03
1	A	241	VAL	CA-C-O	-6.14	114.58	119.25
1	A	1445	ILE	CA-C-N	6.14	131.37	122.16
1	A	1445	ILE	C-N-CA	6.14	131.37	122.16
3	C	9	LYS	CD-CE-NZ	6.14	131.54	111.90
1	A	1057	VAL	CA-CB-CG2	-6.14	99.97	110.40
2	B	463	THR	CB-CA-C	-6.14	99.47	110.70
2	B	784	ASN	CA-C-N	-6.14	110.86	121.66
2	B	784	ASN	C-N-CA	-6.14	110.86	121.66
1	A	1233	ASP	N-CA-CB	6.13	120.36	110.42
2	B	798	TYR	CB-CA-C	-6.13	101.57	111.14
2	B	394	ASP	CB-CG-OD2	6.13	132.51	118.40
2	B	332	ASP	N-CA-C	6.13	117.62	111.07
2	B	239	GLU	CB-CA-C	6.12	121.80	109.68
6	H	127	GLY	N-CA-C	6.12	127.69	113.18
6	H	55	LEU	CA-C-N	-6.12	114.88	122.84
6	H	55	LEU	C-N-CA	-6.12	114.88	122.84
2	B	1077	THR	CA-C-O	6.12	125.56	118.77
1	A	949	ASP	CB-CG-OD2	6.11	132.46	118.40
2	B	312	GLU	N-CA-C	-6.11	104.73	111.82
2	B	644	GLU	N-CA-CB	-6.11	100.16	110.49
7	I	109	ILE	CA-CB-CG1	6.11	120.79	110.40
8	J	64	ASN	N-CA-CB	-6.11	100.11	110.50
3	C	10	ILE	CB-CA-C	-6.11	101.27	111.29
1	A	966	ASN	CA-C-O	-6.11	114.61	120.90
2	B	957	ASN	N-CA-CB	-6.11	100.17	110.49
9	K	93	SER	N-CA-CB	6.11	119.22	110.06
1	A	644	LYS	CB-CA-C	-6.11	100.30	110.68
1	A	795	GLU	CA-CB-CG	-6.11	101.89	114.10
1	A	1313	LEU	N-CA-C	-6.11	103.96	112.45
5	F	97	ARG	CG-CD-NE	-6.11	98.57	112.00
7	I	35	VAL	CB-CA-C	-6.10	99.49	110.48
1	A	29	ALA	N-CA-C	6.10	123.80	110.80
1	A	299	HIS	N-CA-C	-6.10	103.97	112.45
2	B	194	GLU	CB-CA-C	6.10	120.20	110.19
2	B	1161	HIS	CB-CA-C	6.10	120.50	109.83
1	A	37	PHE	CA-CB-CG	6.10	119.90	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	42	LEU	CB-CA-C	-6.10	100.48	110.85
1	A	808	LEU	N-CA-C	6.10	120.01	110.32
1	A	1194	ARG	CB-CA-C	-6.10	100.75	110.14
1	A	964	ILE	CA-C-O	-6.09	114.29	121.05
1	A	420	ARG	NE-CZ-NH1	6.09	127.59	121.50
1	A	764	CYS	O-C-N	-6.09	116.82	123.52
2	B	204	ILE	CA-C-N	6.09	131.29	123.13
2	B	204	ILE	C-N-CA	6.09	131.29	123.13
1	A	1102	LYS	N-CA-CB	-6.09	101.17	110.12
8	J	34	THR	OG1-CB-CG2	-6.09	97.12	109.30
9	K	26	LYS	N-CA-C	6.09	118.70	111.33
10	L	60	ARG	CA-C-O	-6.09	114.11	121.05
1	A	1003	LYS	CB-CG-CD	6.09	125.30	111.30
2	B	1096	ARG	O-C-N	-6.08	115.92	122.85
8	J	28	ASP	CB-CA-C	-6.08	100.22	110.44
1	A	396	PRO	CA-C-N	-6.08	113.06	122.49
1	A	396	PRO	C-N-CA	-6.08	113.06	122.49
7	I	40	SER	CA-CB-OG	6.08	123.26	111.10
1	A	1345	ARG	O-C-N	-6.08	115.68	122.12
3	C	248	ILE	O-C-N	-6.08	115.97	121.87
9	K	18	LYS	N-CA-CB	6.08	118.82	110.01
1	A	1427	ASN	N-CA-C	6.07	118.69	111.71
2	B	1160	VAL	N-CA-C	6.07	115.83	108.06
1	A	815	PHE	N-CA-C	-6.07	104.75	111.36
1	A	1033	GLN	CA-C-O	-6.07	112.50	119.60
1	A	61	ILE	CB-CA-C	6.07	118.26	111.59
4	E	94	LYS	N-CA-C	6.07	118.68	111.71
2	B	1103	ILE	N-CA-CB	6.06	121.23	111.23
2	B	1212	ILE	CA-CB-CG1	-6.06	100.09	110.40
1	A	1377	THR	CB-CA-C	-6.06	97.32	109.99
1	A	287	HIS	N-CA-C	6.06	120.22	112.34
1	A	586	ILE	O-C-N	6.06	129.80	123.26
2	B	39	ARG	NH1-CZ-NH2	-6.06	111.42	119.30
1	A	1187	GLN	CA-C-N	6.06	130.48	122.30
1	A	1187	GLN	C-N-CA	6.06	130.48	122.30
3	C	149	LYS	CD-CE-NZ	-6.06	92.52	111.90
1	A	652	VAL	CG1-CB-CG2	-6.05	97.48	110.80
3	C	235	VAL	CG1-CB-CG2	-6.05	97.48	110.80
3	C	60	ASP	N-CA-C	6.05	117.54	111.07
6	H	132	LEU	N-CA-C	-6.05	101.33	110.70
2	B	457	LEU	N-CA-C	-6.05	101.67	111.04
2	B	1141	HIS	CA-CB-CG	6.05	119.85	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	84	ARG	N-CA-C	-6.05	104.98	112.90
3	C	254	LYS	CA-C-O	-6.04	114.47	120.70
1	A	416	ARG	CA-CB-CG	6.04	126.19	114.10
1	A	11	LEU	O-C-N	-6.04	115.38	123.23
1	A	1121	GLU	O-C-N	6.04	127.52	121.30
2	B	343	ILE	CB-CA-C	6.04	119.42	111.33
1	A	973	ILE	N-CA-C	-6.04	99.73	108.36
1	A	782	ARG	N-CA-C	6.04	118.47	108.99
1	A	1044	TRP	CA-C-O	-6.04	113.54	120.24
1	A	1269	GLU	OE1-CD-OE2	6.04	137.38	122.90
1	A	1440	ALA	N-CA-CB	-6.03	102.24	110.56
5	F	151	LEU	CA-C-O	-6.03	114.05	120.92
9	K	113	THR	CA-C-N	6.03	132.56	121.70
9	K	113	THR	C-N-CA	6.03	132.56	121.70
1	A	165	GLY	CA-C-N	6.03	129.78	120.07
1	A	165	GLY	C-N-CA	6.03	129.78	120.07
3	C	138	GLU	CB-CG-CD	-6.03	102.35	112.60
4	E	14	ARG	CA-C-N	-6.03	111.15	120.31
4	E	14	ARG	C-N-CA	-6.03	111.15	120.31
1	A	419	LYS	CD-CE-NZ	-6.03	92.62	111.90
2	B	409	ALA	N-CA-C	6.03	121.25	111.37
1	A	595	THR	CA-C-O	-6.02	115.00	121.56
9	K	22	ASP	CB-CG-OD1	6.02	132.25	118.40
2	B	110	HIS	O-C-N	-6.02	116.03	123.44
2	B	20	ASP	N-CA-CB	6.02	119.98	110.23
2	B	346	GLU	CB-CG-CD	6.02	122.83	112.60
1	A	1171	GLN	N-CA-C	-6.02	104.79	111.71
6	H	115	TYR	N-CA-C	6.02	120.68	112.68
1	A	708	MET	O-C-N	-6.01	115.80	123.26
1	A	885	THR	CA-CB-CG2	6.01	120.73	110.50
1	A	935	GLN	CA-C-O	-6.01	113.05	119.97
1	A	1168	GLU	N-CA-C	6.01	118.61	111.33
1	A	985	ASP	CB-CA-C	-6.01	101.44	110.88
8	J	43	ARG	N-CA-C	6.01	119.38	110.48
2	B	711	GLU	CB-CA-C	-6.01	98.33	110.17
1	A	923	LEU	N-CA-CB	6.01	119.16	110.20
1	A	1222	ASN	O-C-N	6.01	129.00	122.15
1	A	686	ALA	O-C-N	-6.01	114.90	122.17
1	A	415	LEU	CA-C-N	-6.01	111.34	122.09
1	A	415	LEU	C-N-CA	-6.01	111.34	122.09
1	A	833	GLU	CG-CD-OE1	6.01	132.22	118.40
9	K	45	LEU	CA-C-O	-6.00	114.50	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	46	GLN	CA-C-O	-6.00	114.48	120.90
3	C	84	ARG	NH1-CZ-NH2	-6.00	111.50	119.30
2	B	814	PHE	N-CA-C	-6.00	104.67	112.23
1	A	864	ILE	N-CA-C	-6.00	106.65	111.81
2	B	242	SER	O-C-N	-6.00	115.93	123.01
2	B	41	LYS	CB-CA-C	6.00	120.20	109.29
2	B	119	LEU	O-C-N	6.00	128.48	122.12
8	J	6	ARG	CA-C-N	6.00	129.63	121.05
8	J	6	ARG	C-N-CA	6.00	129.63	121.05
9	K	103	THR	CA-C-O	-6.00	111.94	120.51
9	K	78	THR	N-CA-C	5.99	118.03	110.24
2	B	1022	THR	CB-CA-C	5.99	120.94	112.07
3	C	34	ARG	CD-NE-CZ	5.99	132.79	124.40
6	H	112	ILE	CB-CA-C	5.99	121.11	111.29
8	J	2	ILE	CB-CA-C	-5.99	102.98	111.19
1	A	720	ARG	CG-CD-NE	5.99	125.17	112.00
2	B	1176	ASN	N-CA-C	5.99	121.19	111.37
1	A	720	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	A	1074	GLU	CB-CG-CD	5.99	122.77	112.60
1	A	1158	PRO	N-CA-C	-5.99	107.02	114.20
9	K	85	ASP	N-CA-C	-5.99	104.88	111.82
10	L	70	ARG	NH1-CZ-NH2	-5.99	111.52	119.30
1	A	481	ASP	CB-CG-OD1	5.98	132.16	118.40
1	A	446	ARG	CG-CD-NE	5.98	125.16	112.00
10	L	70	ARG	N-CA-C	5.98	127.75	111.00
1	A	683	ILE	N-CA-C	-5.98	105.02	110.82
3	C	24	ASN	CB-CA-C	-5.98	102.89	112.09
1	A	1196	GLU	OE1-CD-OE2	5.98	137.24	122.90
2	B	101	MET	CG-SD-CE	5.98	114.05	100.90
4	E	1	MET	CG-SD-CE	5.98	114.05	100.90
1	A	1113	THR	OG1-CB-CG2	-5.97	97.35	109.30
1	A	1343	ALA	CA-C-O	-5.97	113.35	120.10
1	A	293	GLU	N-CA-CB	5.97	119.52	109.78
1	A	793	SER	N-CA-C	5.97	119.55	109.87
1	A	1031	VAL	N-CA-C	5.97	116.71	110.62
2	B	543	SER	CB-CA-C	-5.97	97.44	109.68
1	A	375	THR	N-CA-C	5.97	118.49	109.23
2	B	812	LEU	CA-C-O	-5.97	112.05	119.28
2	B	1098	MET	CG-SD-CE	5.97	114.04	100.90
2	B	116	GLU	N-CA-C	-5.97	105.08	112.90
2	B	1081	LEU	CA-C-O	5.97	126.93	120.43
2	B	461	LEU	N-CA-C	5.96	118.57	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1020	ARG	NE-CZ-NH2	5.96	124.56	119.20
5	F	84	TYR	N-CA-C	5.96	118.90	109.96
5	F	115	THR	N-CA-C	-5.96	106.62	114.31
1	A	901	LEU	N-CA-C	5.96	119.81	112.54
3	C	94	LYS	CA-CB-CG	5.96	126.02	114.10
8	J	6	ARG	NE-CZ-NH1	-5.96	115.54	121.50
7	I	107	SER	CA-C-O	5.95	127.35	120.32
9	K	63	VAL	CB-CA-C	5.95	119.65	111.31
2	B	267	ARG	O-C-N	-5.95	115.61	122.93
8	J	33	GLY	N-CA-C	5.95	121.36	114.16
1	A	119	ASN	CA-CB-CG	-5.95	106.65	112.60
2	B	1107	ALA	CA-C-N	5.95	132.90	121.54
2	B	1107	ALA	C-N-CA	5.95	132.90	121.54
4	E	121	MET	N-CA-C	-5.95	104.60	112.34
2	B	762	ASN	CA-C-O	5.95	127.12	120.70
2	B	775	LYS	CB-CG-CD	-5.95	97.62	111.30
2	B	730	ARG	NE-CZ-NH2	5.95	124.55	119.20
4	E	39	LEU	CD1-CG-CD2	-5.95	97.72	110.80
7	I	5	ARG	NE-CZ-NH2	5.95	124.55	119.20
2	B	63	ILE	N-CA-CB	-5.95	100.48	110.65
2	B	97	VAL	CB-CA-C	5.95	118.45	110.42
7	I	43	VAL	N-CA-C	5.94	120.53	113.22
1	A	416	ARG	CG-CD-NE	-5.94	98.93	112.00
1	A	934	LYS	N-CA-C	-5.94	104.88	111.36
2	B	230	ALA	N-CA-C	5.94	122.94	109.81
9	K	74	ARG	CG-CD-NE	-5.94	98.93	112.00
1	A	75	ASN	N-CA-C	5.94	123.45	110.80
1	A	857	ARG	CB-CA-C	-5.94	97.69	110.45
2	B	416	LEU	N-CA-C	5.93	117.62	111.03
4	E	120	ALA	N-CA-C	5.93	117.44	110.97
1	A	50	ILE	CA-C-O	-5.93	114.22	120.57
1	A	765	VAL	N-CA-C	-5.93	105.29	111.58
9	K	22	ASP	OD1-CG-OD2	-5.93	108.67	122.90
7	I	1	MET	CB-CG-SD	5.93	130.49	112.70
6	H	63	LEU	CB-CA-C	5.93	121.36	110.10
1	A	491	VAL	O-C-N	-5.92	116.84	121.46
3	C	123	ASN	O-C-N	-5.92	115.82	122.93
4	E	98	ILE	CA-CB-CG1	5.92	120.47	110.40
1	A	646	PHE	CA-C-N	-5.92	112.74	120.14
1	A	646	PHE	C-N-CA	-5.92	112.74	120.14
1	A	501	LEU	CB-CA-C	-5.92	100.79	110.85
3	C	68	GLY	CA-C-N	-5.92	111.67	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	68	GLY	C-N-CA	-5.92	111.67	122.38
2	B	1193	GLN	CB-CG-CD	-5.92	102.54	112.60
4	E	21	GLU	CB-CA-C	-5.92	100.97	110.79
2	B	434	ARG	CG-CD-NE	5.91	125.01	112.00
6	H	135	LEU	CA-C-N	5.91	132.84	121.54
6	H	135	LEU	C-N-CA	5.91	132.84	121.54
1	A	1171	GLN	CA-C-O	-5.91	113.42	120.10
2	B	239	GLU	N-CA-CB	-5.91	100.43	111.13
4	E	84	ASP	N-CA-C	5.91	119.68	112.23
1	A	1227	ILE	CA-CB-CG1	5.91	120.45	110.40
10	L	31	CYS	CB-CA-C	-5.91	100.35	110.22
1	A	400	PRO	N-CD-CG	5.91	110.89	103.80
2	B	249	ARG	CA-C-N	5.91	129.75	121.24
2	B	249	ARG	C-N-CA	5.91	129.75	121.24
5	F	78	GLN	N-CA-C	5.91	123.38	110.80
6	H	82	PRO	CA-C-O	-5.91	109.85	120.60
2	B	477	ALA	CB-CA-C	5.91	119.36	110.50
3	C	80	LEU	O-C-N	-5.90	116.32	123.29
2	B	103	ASN	CA-CB-CG	5.90	118.50	112.60
2	B	53	GLN	CB-CG-CD	-5.90	102.57	112.60
7	I	13	MET	N-CA-CB	-5.90	101.32	110.29
8	J	48	ARG	NE-CZ-NH1	5.90	127.40	121.50
2	B	511	PRO	N-CD-CG	-5.90	94.35	103.20
4	E	137	GLU	N-CA-C	-5.90	104.77	111.14
1	A	1053	PHE	N-CA-C	-5.89	104.94	111.36
7	I	30	ARG	CG-CD-NE	-5.89	99.03	112.00
1	A	977	LYS	CB-CA-C	5.89	118.00	110.16
9	K	1	MET	CG-SD-CE	5.89	113.86	100.90
4	E	200	ARG	N-CA-CB	5.89	121.15	111.08
1	A	1138	ILE	N-CA-CB	-5.89	101.99	111.82
2	B	633	VAL	CG1-CB-CG2	-5.89	97.85	110.80
5	F	108	PHE	CA-C-N	-5.89	114.44	122.92
5	F	108	PHE	C-N-CA	-5.89	114.44	122.92
6	H	96	VAL	N-CA-CB	-5.89	103.81	111.82
7	I	32	CYS	N-CA-C	-5.89	100.47	109.65
2	B	105	SER	CA-CB-OG	5.88	122.87	111.10
2	B	120	ARG	NE-CZ-NH2	5.88	124.50	119.20
2	B	586	TRP	CB-CA-C	5.88	120.60	110.77
3	C	263	THR	CA-CB-OG1	-5.88	100.77	109.60
7	I	45	ARG	N-CA-C	5.88	119.07	109.24
8	J	38	ARG	NE-CZ-NH1	5.88	127.39	121.50
1	A	516	SER	N-CA-CB	-5.88	101.72	111.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1135	ARG	CA-CB-CG	5.88	125.87	114.10
1	A	1054	LEU	CA-C-O	5.88	126.73	119.97
2	B	255	GLN	N-CA-C	5.88	118.99	109.40
2	B	895	ASP	N-CA-CB	5.88	120.16	110.39
3	C	87	PHE	CA-C-N	-5.88	111.06	121.29
3	C	87	PHE	C-N-CA	-5.88	111.06	121.29
1	A	921	GLY	CA-C-N	-5.87	113.20	121.72
1	A	921	GLY	C-N-CA	-5.87	113.20	121.72
3	C	248	ILE	N-CA-C	-5.87	104.63	110.62
2	B	49	ASP	O-C-N	-5.87	115.51	122.20
2	B	136	THR	CA-C-N	5.87	132.75	121.54
2	B	136	THR	C-N-CA	5.87	132.75	121.54
2	B	204	ILE	CA-CB-CG1	5.87	120.38	110.40
2	B	1104	HIS	N-CA-C	-5.87	100.64	108.74
1	A	726	ARG	NE-CZ-NH2	5.87	124.48	119.20
3	C	251	LEU	O-C-N	5.87	128.35	122.08
1	A	96	ILE	CG1-CB-CG2	-5.86	93.12	110.70
2	B	359	GLU	CB-CA-C	-5.86	99.80	109.99
4	E	198	ILE	O-C-N	-5.86	116.25	123.10
9	K	70	ARG	O-C-N	-5.86	116.80	123.48
1	A	14	VAL	N-CA-C	-5.85	99.99	108.36
2	B	1213	THR	CB-CA-C	-5.85	103.35	110.08
1	A	635	ARG	CA-C-O	-5.85	114.22	120.42
3	C	70	ILE	CA-CB-CG1	5.85	120.35	110.40
7	I	112	SER	N-CA-CB	-5.85	101.46	110.46
1	A	1328	TYR	N-CA-C	5.84	118.07	109.24
2	B	265	SER	CB-CA-C	5.84	119.30	109.48
2	B	723	VAL	N-CA-CB	5.84	120.72	110.49
6	H	14	GLU	CA-CB-CG	-5.84	102.41	114.10
2	B	884	ARG	CG-CD-NE	-5.84	99.15	112.00
1	A	1260	LEU	O-C-N	-5.84	115.93	122.12
2	B	346	GLU	CA-C-O	-5.84	113.50	120.10
1	A	775	ILE	CB-CG1-CD1	5.83	126.06	113.80
1	A	32	VAL	CG1-CB-CG2	-5.83	97.97	110.80
2	B	578	THR	CA-C-O	-5.83	113.90	120.43
1	A	481	ASP	N-CA-CB	-5.83	101.10	110.55
4	E	31	THR	N-CA-C	-5.83	100.17	109.96
4	E	175	LEU	N-CA-C	-5.83	102.81	110.39
8	J	9	SER	N-CA-C	5.83	120.55	112.45
3	C	220	ASP	CB-CG-OD1	5.83	131.80	118.40
1	A	1199	ARG	O-C-N	5.83	128.09	122.03
2	B	807	ARG	CG-CD-NE	-5.83	99.18	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	71	SER	N-CA-C	5.83	118.27	109.41
1	A	1241	ARG	CD-NE-CZ	5.82	132.55	124.40
2	B	626	ILE	N-CA-CB	-5.82	101.26	111.39
2	B	478	GLY	N-CA-C	-5.82	107.23	115.43
10	L	61	THR	N-CA-CB	5.82	118.58	110.26
2	B	245	GLU	CA-CB-CG	5.82	125.73	114.10
2	B	407	ASP	CA-C-O	5.82	126.58	120.36
1	A	1383	SER	CA-CB-OG	-5.82	99.47	111.10
2	B	63	ILE	O-C-N	-5.82	116.00	121.87
2	B	605	ARG	NE-CZ-NH2	5.82	124.43	119.20
7	I	106	CYS	CA-C-N	5.82	132.18	123.05
7	I	106	CYS	C-N-CA	5.82	132.18	123.05
6	H	131	ASN	CA-CB-CG	5.81	118.41	112.60
1	A	8	SER	CA-C-N	5.81	129.33	121.20
1	A	8	SER	C-N-CA	5.81	129.33	121.20
1	A	801	GLU	OE1-CD-OE2	5.81	136.84	122.90
1	A	1192	LEU	CB-CA-C	-5.81	99.67	109.72
2	B	710	LEU	CD1-CG-CD2	-5.81	98.02	110.80
4	E	212	ARG	NE-CZ-NH2	-5.81	113.97	119.20
9	K	5	ASP	CB-CG-OD1	-5.81	105.04	118.40
3	C	199	LYS	CA-C-O	-5.81	113.29	119.97
1	A	726	ARG	NE-CZ-NH1	-5.81	115.69	121.50
2	B	348	ARG	N-CA-C	5.80	118.08	111.11
2	B	606	LYS	CG-CD-CE	5.80	124.65	111.30
2	B	869	SER	CA-C-N	5.80	132.41	121.97
2	B	869	SER	C-N-CA	5.80	132.41	121.97
4	E	207	ARG	CB-CG-CD	5.80	124.64	111.30
9	K	110	ASN	CB-CA-C	5.80	121.07	110.11
2	B	404	LYS	CG-CD-CE	5.80	124.64	111.30
7	I	61	ASP	CB-CG-OD2	5.80	131.74	118.40
1	A	909	ASP	O-C-N	-5.80	115.65	121.27
2	B	186	GLU	CA-C-N	-5.80	112.44	120.38
2	B	186	GLU	C-N-CA	-5.80	112.44	120.38
3	C	168	ALA	N-CA-C	5.80	119.45	112.38
1	A	1080	THR	CA-CB-CG2	5.79	120.35	110.50
4	E	125	PRO	N-CA-C	-5.79	100.71	110.21
2	B	282	ILE	CA-CB-CG1	5.79	120.25	110.40
2	B	1054	GLY	O-C-N	5.79	127.75	122.19
1	A	93	VAL	N-CA-CB	5.79	118.41	110.54
2	B	942	ARG	CG-CD-NE	-5.79	99.27	112.00
2	B	1014	PRO	N-CA-C	5.79	121.46	113.65
2	B	1043	ASP	CB-CG-OD2	5.79	131.71	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	861	GLY	N-CA-C	-5.79	107.27	115.43
1	A	1114	PRO	CA-C-O	-5.79	114.37	121.31
4	E	12	LEU	N-CA-C	-5.79	105.06	111.71
4	E	18	THR	OG1-CB-CG2	-5.79	97.73	109.30
1	A	1068	ALA	N-CA-C	-5.78	104.88	111.07
2	B	653	VAL	CA-CB-CG1	5.78	120.23	110.40
1	A	7	SER	N-CA-C	5.78	117.82	108.34
2	B	178	ASN	N-CA-C	5.78	119.95	113.01
2	B	969	ARG	CD-NE-CZ	-5.78	116.31	124.40
4	E	98	ILE	CA-C-O	-5.78	113.78	120.83
6	H	45	GLU	N-CA-CB	-5.78	102.02	110.40
1	A	241	VAL	N-CA-C	5.78	113.27	107.55
4	E	47	CYS	N-CA-C	5.78	118.32	108.90
4	E	78	LEU	CD1-CG-CD2	-5.78	98.09	110.80
2	B	482	VAL	CB-CA-C	-5.77	102.73	111.33
3	C	3	GLU	CA-CB-CG	-5.77	102.56	114.10
4	E	14	ARG	NE-CZ-NH1	5.77	127.27	121.50
4	E	58	MET	CG-SD-CE	-5.77	88.20	100.90
8	J	28	ASP	N-CA-CB	5.77	120.85	111.27
10	L	26	THR	CA-CB-CG2	5.77	120.31	110.50
1	A	896	ARG	CD-NE-CZ	-5.77	116.32	124.40
2	B	690	VAL	N-CA-CB	-5.77	102.75	112.44
4	E	107	THR	N-CA-C	5.77	118.17	109.23
1	A	526	ASP	N-CA-C	-5.77	105.07	111.36
1	A	1010	ALA	CA-C-O	5.77	126.53	120.42
2	B	1210	MET	CB-CA-C	-5.77	102.34	111.17
6	H	116	TYR	CB-CA-C	-5.77	98.95	110.42
1	A	919	ILE	N-CA-CB	5.76	118.55	112.21
2	B	887	HIS	CA-CB-CG	5.76	119.56	113.80
1	A	1344	GLY	N-CA-C	5.76	119.64	112.73
2	B	699	GLU	N-CA-C	5.76	119.57	112.54
1	A	1170	ILE	O-C-N	5.76	129.44	121.84
4	E	11	ARG	NH1-CZ-NH2	5.75	126.78	119.30
1	A	1074	GLU	CA-C-O	-5.75	112.28	120.16
2	B	131	ASP	N-CA-C	-5.75	95.69	107.70
2	B	1179	GLN	CA-C-O	5.75	126.64	120.32
7	I	5	ARG	NH1-CZ-NH2	-5.75	111.83	119.30
1	A	581	ALA	N-CA-C	5.74	120.56	113.50
1	A	1272	THR	N-CA-C	-5.74	99.83	108.96
2	B	911	ILE	CA-CB-CG2	5.74	120.26	110.50
2	B	963	PHE	N-CA-C	-5.74	100.54	109.72
4	E	53	PRO	N-CD-CG	-5.74	94.59	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	142	VAL	N-CA-C	5.74	117.59	108.87
6	H	32	THR	N-CA-CB	5.74	120.19	110.49
6	H	89	LEU	O-C-N	-5.74	114.96	122.59
7	I	7	CYS	CA-C-N	5.74	127.97	120.28
7	I	7	CYS	C-N-CA	5.74	127.97	120.28
2	B	348	ARG	NE-CZ-NH2	-5.73	114.04	119.20
2	B	212	LEU	CD1-CG-CD2	-5.73	98.19	110.80
2	B	1166	CYS	N-CA-CB	-5.73	100.80	110.49
3	C	122	SER	N-CA-C	-5.73	100.42	108.96
1	A	1135	ARG	NE-CZ-NH2	5.73	124.36	119.20
1	A	1046	LEU	CA-C-O	5.73	126.49	120.42
4	E	73	PRO	CA-C-O	-5.73	110.18	120.60
1	A	559	VAL	N-CA-C	5.73	116.04	107.51
2	B	422	LYS	CA-C-O	-5.73	113.39	119.97
2	B	1048	THR	O-C-N	5.73	130.34	122.72
1	A	98	LYS	CG-CD-CE	-5.72	98.14	111.30
2	B	656	GLY	N-CA-C	-5.72	105.74	113.24
2	B	846	ILE	CB-CA-C	-5.72	102.99	112.26
2	B	650	GLU	CG-CD-OE1	-5.72	105.25	118.40
2	B	665	GLU	CA-CB-CG	5.72	125.54	114.10
6	H	20	TYR	N-CA-C	5.72	118.27	110.55
2	B	106	ASP	N-CA-CB	-5.72	100.83	110.49
4	E	146	HIS	CA-C-N	-5.72	112.29	122.07
4	E	146	HIS	C-N-CA	-5.72	112.29	122.07
4	E	156	LEU	CD1-CG-CD2	5.72	123.38	110.80
7	I	24	ARG	CG-CD-NE	-5.72	99.42	112.00
4	E	178	ILE	N-CA-C	-5.71	99.99	108.45
1	A	1207	LEU	CB-CG-CD1	-5.71	93.57	110.70
1	A	243	PRO	N-CD-CG	-5.71	94.64	103.20
2	B	616	ILE	CA-C-N	-5.71	114.84	122.72
2	B	616	ILE	C-N-CA	-5.71	114.84	122.72
10	L	47	ARG	NE-CZ-NH2	5.71	124.34	119.20
6	H	88	SER	CA-CB-OG	5.71	122.51	111.10
10	L	48	CYS	CA-C-N	5.71	132.44	121.54
10	L	48	CYS	C-N-CA	5.71	132.44	121.54
2	B	881	ASN	CA-C-N	5.71	132.44	121.54
2	B	881	ASN	C-N-CA	5.71	132.44	121.54
2	B	576	ASP	N-CA-C	-5.70	106.09	113.16
3	C	14	SER	O-C-N	-5.70	117.59	123.29
8	J	1	MET	CA-CB-CG	5.70	125.50	114.10
9	K	55	LYS	CG-CD-CE	5.70	124.41	111.30
1	A	1166	ASP	CA-CB-CG	5.70	118.30	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	PHE	CA-CB-CG	5.70	119.50	113.80
1	A	873	MET	N-CA-C	5.70	119.25	110.42
1	A	554	PRO	N-CA-C	5.69	121.24	113.84
1	A	844	ALA	CA-C-O	-5.69	114.48	120.63
1	A	1432	GLN	N-CA-C	5.69	118.34	109.52
7	I	93	LYS	CA-CB-CG	5.69	125.48	114.10
1	A	687	LYS	N-CA-C	5.68	119.02	111.75
1	A	1102	LYS	CA-C-O	5.68	126.57	120.55
2	B	1185	CYS	N-CA-C	-5.68	106.35	113.28
3	C	163	ILE	N-CA-CB	-5.68	100.16	111.91
5	F	81	THR	CA-CB-CG2	5.68	120.16	110.50
8	J	17	LYS	CD-CE-NZ	-5.68	93.72	111.90
1	A	52	GLY	CA-C-O	-5.68	110.69	120.57
1	A	1442	ASP	CA-C-O	-5.68	114.74	121.16
1	A	267	ALA	CA-C-N	5.68	128.45	120.28
1	A	267	ALA	C-N-CA	5.68	128.45	120.28
1	A	1417	GLU	CB-CG-CD	5.68	122.25	112.60
2	B	1107	ALA	N-CA-C	5.68	119.19	112.72
1	A	1147	THR	OG1-CB-CG2	-5.67	97.95	109.30
1	A	15	LYS	N-CA-C	-5.67	106.35	113.72
2	B	705	MET	CB-CG-SD	-5.67	95.69	112.70
7	I	83	ASN	CA-C-O	5.67	128.09	121.46
1	A	5	GLN	N-CA-CB	5.67	118.47	110.36
1	A	920	LEU	CA-C-O	5.67	127.38	120.92
1	A	922	ASP	CB-CA-C	-5.67	101.00	110.29
1	A	655	PHE	CA-C-N	-5.66	112.13	120.28
1	A	655	PHE	C-N-CA	-5.66	112.13	120.28
1	A	913	LEU	O-C-N	-5.66	116.78	123.41
5	F	143	PHE	N-CA-C	5.66	117.68	109.07
1	A	66	LYS	CA-CB-CG	5.66	125.42	114.10
1	A	1356	ILE	N-CA-C	5.66	115.85	110.53
2	B	956	THR	CB-CA-C	-5.66	99.20	109.38
2	B	1010	LEU	CB-CA-C	-5.66	99.68	109.86
3	C	11	ARG	N-CA-CB	5.66	118.45	110.98
2	B	487	THR	N-CA-CB	-5.65	102.22	111.66
1	A	724	GLU	CB-CG-CD	5.65	122.20	112.60
2	B	228	LYS	CB-CG-CD	5.65	124.29	111.30
5	F	85	MET	N-CA-C	5.65	118.54	110.24
1	A	93	VAL	N-CA-C	5.65	116.38	110.62
1	A	327	ALA	CA-C-O	5.65	128.37	120.52
1	A	512	VAL	CA-CB-CG1	5.65	120.00	110.40
1	A	917	SER	CA-C-O	-5.65	114.89	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1199	ARG	CA-C-O	-5.65	115.07	121.00
1	A	1026	LEU	O-C-N	-5.65	114.97	122.20
2	B	1018	PRO	CB-CA-C	-5.65	104.08	112.55
6	H	132	LEU	CA-CB-CG	5.65	136.06	116.30
1	A	302	THR	CA-C-O	5.64	126.48	120.10
1	A	366	VAL	N-CA-C	-5.64	96.69	108.88
2	B	1183	LYS	CB-CA-C	5.64	121.65	110.42
8	J	7	CYS	N-CA-CB	5.64	118.23	109.48
1	A	1318	THR	N-CA-C	-5.64	106.06	113.17
1	A	1442	ASP	CB-CG-OD2	5.64	131.38	118.40
1	A	64	ASN	CA-C-N	5.64	132.31	121.54
1	A	64	ASN	C-N-CA	5.64	132.31	121.54
7	I	30	ARG	N-CA-C	5.64	119.85	112.92
1	A	835	GLY	CA-C-O	-5.63	114.95	120.75
6	H	58	THR	N-CA-C	5.63	117.88	108.02
2	B	643	ASP	CA-CB-CG	5.63	118.23	112.60
4	E	91	LYS	CA-C-N	5.63	128.14	120.54
4	E	91	LYS	C-N-CA	5.63	128.14	120.54
7	I	21	GLU	O-C-N	-5.63	114.91	122.23
8	J	51	LEU	CB-CG-CD1	5.63	127.58	110.70
2	B	865	LYS	CA-C-N	5.62	131.65	122.65
2	B	865	LYS	C-N-CA	5.62	131.65	122.65
2	B	319	GLU	O-C-N	-5.62	115.64	122.22
7	I	98	VAL	CA-CB-CG2	-5.62	100.84	110.40
2	B	612	GLU	CA-C-O	5.62	126.14	119.56
1	A	495	GLU	CB-CA-C	5.62	120.40	110.85
1	A	843	LYS	CB-CG-CD	5.62	124.22	111.30
2	B	333	PHE	O-C-N	5.62	127.93	122.09
2	B	373	ARG	CB-CG-CD	5.62	124.22	111.30
2	B	1089	PRO	N-CD-CG	5.62	111.63	103.20
3	C	199	LYS	CA-CB-CG	-5.62	102.86	114.10
3	C	207	CYS	N-CA-C	5.62	117.21	111.14
2	B	196	PRO	CB-CA-C	-5.62	103.87	111.85
1	A	396	PRO	CB-CA-C	-5.62	103.48	111.68
6	H	15	VAL	O-C-N	5.62	128.48	123.03
1	A	1241	ARG	CG-CD-NE	-5.61	99.65	112.00
1	A	1167	GLU	CB-CA-C	5.61	119.69	110.88
10	L	27	LEU	CA-CB-CG	5.61	135.94	116.30
1	A	522	GLY	CA-C-O	-5.61	115.01	121.46
2	B	370	PHE	CB-CA-C	5.61	121.58	110.42
2	B	680	THR	CA-CB-OG1	-5.61	101.19	109.60
3	C	116	LYS	CA-C-O	-5.61	112.99	119.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	120	ILE	N-CA-C	-5.61	105.26	110.53
1	A	1316	VAL	CB-CA-C	-5.61	103.47	112.16
1	A	492	PRO	CA-C-O	-5.60	114.83	121.67
4	E	192	ARG	CB-CG-CD	5.60	124.19	111.30
3	C	5	GLY	CA-C-O	5.60	129.53	121.52
2	B	168	GLY	CA-C-O	5.60	127.65	122.05
2	B	244	LEU	N-CA-C	5.60	118.60	108.69
2	B	654	ARG	N-CA-CB	-5.60	101.86	111.21
6	H	40	LEU	CA-C-N	5.60	129.86	122.30
6	H	40	LEU	C-N-CA	5.60	129.86	122.30
1	A	413	ILE	CB-CA-C	-5.60	104.19	110.96
1	A	1371	LEU	CA-C-O	5.60	126.70	120.82
1	A	90	VAL	N-CA-CB	-5.60	101.58	111.93
8	J	14	VAL	N-CA-CB	-5.60	102.00	111.23
1	A	160	GLN	N-CA-C	5.59	119.21	110.32
4	E	115	ASN	N-CA-C	5.59	116.46	108.74
1	A	1019	CYS	N-CA-C	5.59	118.14	111.71
1	A	1103	GLU	N-CA-CB	-5.59	101.89	110.16
2	B	269	ILE	CB-CG1-CD1	5.59	125.54	113.80
2	B	644	GLU	N-CA-C	5.59	122.70	110.80
5	F	105	ALA	N-CA-C	-5.59	102.58	110.29
1	A	499	ALA	CA-C-N	-5.59	113.18	120.44
1	A	499	ALA	C-N-CA	-5.59	113.18	120.44
1	A	1198	ASP	CB-CA-C	-5.59	100.89	110.22
2	B	998	ASP	CB-CG-OD2	5.59	131.25	118.40
1	A	1208	THR	CA-CB-OG1	5.58	117.98	109.60
2	B	1165	ILE	CA-CB-CG1	5.58	119.89	110.40
3	C	205	LYS	CA-C-O	-5.58	114.96	120.82
4	E	99	HIS	N-CA-CB	5.58	118.88	109.78
7	I	76	PRO	N-CA-C	5.58	123.97	112.47
5	F	129	LYS	N-CA-C	5.58	118.88	112.57
2	B	186	GLU	N-CA-C	-5.58	105.11	111.14
2	B	511	PRO	CB-CA-C	-5.58	103.54	111.68
2	B	986	GLN	CG-CD-NE2	5.58	124.77	116.40
2	B	1055	ILE	CA-CB-CG1	5.58	119.88	110.40
1	A	1028	THR	OG1-CB-CG2	-5.57	98.15	109.30
2	B	91	SER	O-C-N	5.57	130.41	123.28
2	B	605	ARG	N-CA-C	5.57	119.56	112.87
2	B	348	ARG	CB-CA-C	-5.57	101.89	110.81
8	J	19	GLU	N-CA-C	-5.57	105.29	111.36
1	A	824	LEU	N-CA-C	-5.57	105.29	111.36
1	A	979	SER	CA-C-O	-5.57	114.81	121.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1095	THR	CB-CA-C	-5.57	101.48	109.84
2	B	326	ASP	CB-CG-OD2	5.57	131.20	118.40
2	B	938	SER	CB-CA-C	5.57	119.35	109.72
7	I	49	ILE	N-CA-CB	-5.57	105.41	112.15
9	K	1	MET	CB-CG-SD	-5.57	96.00	112.70
9	K	92	ASN	CA-C-O	-5.57	114.51	121.02
2	B	936	ASP	CA-C-O	-5.56	114.30	120.70
3	C	34	ARG	CG-CD-NE	-5.56	99.76	112.00
4	E	180	ARG	CD-NE-CZ	5.56	132.19	124.40
7	I	49	ILE	O-C-N	-5.56	115.87	122.66
1	A	158	PRO	N-CA-C	5.56	123.92	112.47
3	C	254	LYS	CD-CE-NZ	-5.56	94.11	111.90
1	A	538	ASP	CA-C-N	-5.56	114.80	122.30
1	A	538	ASP	C-N-CA	-5.56	114.80	122.30
2	B	940	PRO	N-CD-CG	-5.56	94.86	103.20
1	A	469	ARG	CA-CB-CG	5.55	125.21	114.10
2	B	1222	ARG	CA-C-N	5.55	132.15	121.54
2	B	1222	ARG	C-N-CA	5.55	132.15	121.54
1	A	441	PRO	N-CD-CG	-5.55	94.87	103.20
2	B	1020	ARG	CA-CB-CG	5.55	125.20	114.10
7	I	37	GLU	N-CA-C	-5.55	103.05	110.55
1	A	758	ILE	O-C-N	5.55	127.33	121.89
1	A	1036	ARG	N-CA-CB	-5.55	103.75	112.13
2	B	711	GLU	CB-CG-CD	-5.55	103.17	112.60
1	A	373	THR	N-CA-C	5.55	119.22	112.23
2	B	648	HIS	CA-CB-CG	5.55	119.35	113.80
2	B	403	LYS	CA-CB-CG	-5.54	103.01	114.10
2	B	592	ASN	N-CA-C	5.54	119.06	108.97
2	B	743	ILE	CA-CB-CG1	5.54	119.82	110.40
4	E	15	ALA	N-CA-C	5.54	118.25	111.82
5	F	92	ARG	NE-CZ-NH1	5.54	127.04	121.50
1	A	1291	VAL	N-CA-CB	-5.54	103.45	111.21
2	B	591	ARG	NE-CZ-NH1	5.54	127.04	121.50
2	B	727	LYS	N-CA-C	-5.54	102.28	110.48
2	B	1033	LYS	CA-C-O	-5.54	114.97	120.90
3	C	199	LYS	N-CA-C	-5.54	105.40	111.82
5	F	135	ARG	NE-CZ-NH1	-5.54	115.96	121.50
1	A	895	LYS	CA-C-O	5.53	126.42	120.55
1	A	1372	VAL	N-CA-CB	-5.53	102.28	110.58
1	A	412	ARG	CB-CG-CD	5.53	124.02	111.30
1	A	414	ASP	OD1-CG-OD2	-5.53	109.62	122.90
1	A	46	THR	CB-CA-C	-5.53	103.26	111.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	599	THR	CA-C-O	-5.53	115.19	121.00
3	C	138	GLU	CA-C-N	5.53	128.46	120.11
3	C	138	GLU	C-N-CA	5.53	128.46	120.11
1	A	1448	GLU	N-CA-C	5.53	122.58	110.80
2	B	434	ARG	CA-CB-CG	5.53	125.16	114.10
3	C	262	LEU	N-CA-C	5.53	117.76	111.02
7	I	25	LEU	N-CA-C	5.53	117.75	108.96
1	A	327	ALA	CA-C-N	5.53	132.09	121.54
1	A	327	ALA	C-N-CA	5.53	132.09	121.54
1	A	1289	ARG	NE-CZ-NH1	-5.53	115.97	121.50
1	A	267	ALA	O-C-N	5.52	127.99	122.08
1	A	412	ARG	N-CA-C	5.52	117.65	108.20
2	B	203	PHE	N-CA-CB	-5.52	102.01	110.85
4	E	82	PHE	N-CA-C	-5.52	101.58	110.14
3	C	88	CYS	CA-C-O	-5.52	116.21	122.01
7	I	59	VAL	O-C-N	-5.52	116.92	123.00
1	A	1001	ARG	CB-CG-CD	5.52	124.00	111.30
2	B	402	GLY	CA-C-O	5.52	126.19	119.01
3	C	225	ALA	O-C-N	5.52	129.62	123.05
1	A	149	GLU	N-CA-C	5.52	117.86	110.35
2	B	404	LYS	CD-CE-NZ	-5.52	94.24	111.90
2	B	1162	ILE	CA-CB-CG2	5.52	119.88	110.50
3	C	219	PHE	CA-C-O	-5.52	115.08	121.15
1	A	820	GLY	CA-C-N	-5.51	112.89	120.28
1	A	820	GLY	C-N-CA	-5.51	112.89	120.28
1	A	1271	ILE	CA-CB-CG2	-5.51	101.13	110.50
2	B	305	VAL	CG1-CB-CG2	5.51	122.93	110.80
2	B	583	ASN	CA-C-N	-5.51	112.07	122.05
2	B	583	ASN	C-N-CA	-5.51	112.07	122.05
1	A	672	ASP	CB-CA-C	-5.51	99.45	110.42
2	B	98	THR	CB-CA-C	-5.51	99.75	109.62
2	B	777	ALA	N-CA-C	-5.51	102.60	110.59
2	B	102	VAL	CB-CA-C	-5.51	102.29	110.33
1	A	416	ARG	CB-CA-C	5.51	118.88	109.24
1	A	1256	GLU	CB-CG-CD	5.51	121.96	112.60
2	B	272	THR	CA-C-O	-5.50	114.89	120.84
2	B	1183	LYS	CG-CD-CE	5.50	123.96	111.30
1	A	74	MET	CB-CG-SD	5.50	129.21	112.70
3	C	156	THR	N-CA-C	5.50	118.53	109.72
1	A	835	GLY	O-C-N	5.50	127.47	122.19
1	A	858	ASN	CB-CG-OD1	-5.50	109.80	120.80
1	A	1099	PRO	CB-CA-C	-5.50	103.65	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1228	TRP	CA-CB-CG	5.50	124.05	113.60
7	I	52	ILE	N-CA-CB	5.50	116.93	110.82
1	A	81	PHE	N-CA-C	5.50	118.20	109.24
1	A	487	MET	CG-SD-CE	-5.50	88.80	100.90
2	B	1101	ASP	CA-C-N	5.50	132.36	122.46
2	B	1101	ASP	C-N-CA	5.50	132.36	122.46
7	I	24	ARG	CB-CA-C	-5.50	97.97	110.07
2	B	958	GLN	N-CA-C	-5.50	104.93	111.69
2	B	587	HIS	CA-C-O	-5.49	113.17	119.60
3	C	26	ASP	CA-C-O	5.49	127.55	121.56
3	C	153	LEU	N-CA-CB	-5.49	101.82	110.77
4	E	75	MET	CB-CA-C	5.49	119.39	110.22
5	F	140	ASP	N-CA-C	5.49	119.69	113.15
10	L	50	ASP	N-CA-CB	5.49	119.77	110.49
7	I	54	GLU	N-CA-C	-5.49	105.29	111.28
2	B	175	ARG	N-CA-C	5.49	119.80	113.38
3	C	142	VAL	CB-CA-C	-5.49	103.69	111.21
7	I	16	PRO	N-CD-CG	-5.49	94.97	103.20
1	A	49	LYS	CB-CG-CD	5.49	123.92	111.30
1	A	1243	VAL	CA-CB-CG2	5.49	119.73	110.40
2	B	118	ARG	CB-CG-CD	5.49	123.92	111.30
2	B	686	ASN	O-C-N	5.49	129.02	122.27
1	A	1429	ILE	CA-C-O	-5.49	115.34	121.05
4	E	31	THR	CA-CB-CG2	5.49	119.83	110.50
6	H	115	TYR	CA-C-N	-5.49	111.06	121.54
6	H	115	TYR	C-N-CA	-5.49	111.06	121.54
9	K	28	PRO	CB-CA-C	5.49	118.83	110.21
2	B	132	VAL	N-CA-C	5.49	117.47	108.97
9	K	114	LEU	CD1-CG-CD2	-5.49	98.73	110.80
1	A	1038	THR	CA-C-O	-5.48	115.19	121.82
1	A	1444	MET	N-CA-CB	-5.48	102.15	111.69
1	A	407	ARG	NH1-CZ-NH2	5.48	126.42	119.30
1	A	470	LEU	CB-CA-C	-5.48	97.39	109.56
3	C	69	LEU	N-CA-C	5.48	119.96	113.16
4	E	113	GLN	CA-C-N	-5.48	111.16	121.63
4	E	113	GLN	C-N-CA	-5.48	111.16	121.63
3	C	108	GLU	O-C-N	5.48	128.80	122.17
2	B	408	LEU	CB-CG-CD2	-5.47	94.27	110.70
2	B	451	LYS	O-C-N	-5.47	115.31	122.59
1	A	665	GLY	CA-C-O	-5.47	115.86	121.61
1	A	962	ARG	CG-CD-NE	-5.47	99.96	112.00
1	A	1007	ILE	CA-C-N	-5.47	112.95	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1007	ILE	C-N-CA	-5.47	112.95	120.28
2	B	137	TYR	CA-C-N	5.47	131.55	121.70
2	B	137	TYR	C-N-CA	5.47	131.55	121.70
2	B	1011	ILE	CB-CA-C	-5.47	104.22	110.73
1	A	635	ARG	CG-CD-NE	-5.47	99.97	112.00
1	A	1190	PRO	N-CA-C	-5.47	106.89	114.27
1	A	458	HIS	CA-CB-CG	-5.47	108.33	113.80
1	A	927	VAL	N-CA-C	5.47	116.24	110.72
4	E	107	THR	O-C-N	-5.47	116.93	123.27
1	A	36	ARG	CA-C-O	-5.46	112.70	120.51
1	A	483	ASP	CB-CA-C	-5.46	102.60	111.06
1	A	182	VAL	N-CA-C	5.46	115.72	107.75
1	A	995	GLU	CA-C-O	-5.46	112.67	119.38
2	B	981	ALA	N-CA-C	5.46	118.08	108.75
5	F	86	THR	N-CA-C	5.46	117.92	110.55
8	J	48	ARG	CD-NE-CZ	5.46	132.04	124.40
2	B	979	LYS	N-CA-C	5.45	118.95	110.17
10	L	70	ARG	N-CA-CB	-5.45	101.23	110.50
1	A	293	GLU	CB-CA-C	-5.45	101.69	110.74
1	A	739	ASP	N-CA-CB	-5.45	101.06	110.32
1	A	1081	LEU	CB-CG-CD2	5.45	127.05	110.70
2	B	654	ARG	NE-CZ-NH2	5.45	124.10	119.20
7	I	111	THR	N-CA-C	5.45	118.61	109.95
1	A	1258	HIS	N-CA-CB	5.45	118.31	110.20
2	B	999	MET	CG-SD-CE	-5.45	88.92	100.90
4	E	198	ILE	CG1-CB-CG2	-5.45	94.37	110.70
1	A	894	GLU	CA-C-N	-5.44	112.99	120.28
1	A	894	GLU	C-N-CA	-5.44	112.99	120.28
6	H	77	ARG	NE-CZ-NH1	5.44	126.94	121.50
1	A	369	SER	CB-CA-C	-5.44	100.22	110.67
1	A	567	LYS	CD-CE-NZ	5.44	129.31	111.90
2	B	900	ALA	O-C-N	-5.44	116.23	121.94
2	B	1027	ILE	CB-CG1-CD1	-5.44	102.38	113.80
2	B	136	THR	O-C-N	5.44	129.47	123.16
3	C	49	VAL	CA-C-O	-5.44	114.50	120.43
4	E	142	VAL	CG1-CB-CG2	-5.44	98.84	110.80
2	B	239	GLU	CB-CG-CD	5.44	121.84	112.60
1	A	88	LYS	O-C-N	5.43	125.79	121.55
1	A	177	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	1236	LEU	N-CA-C	5.43	117.50	108.20
2	B	952	VAL	O-C-N	5.43	129.07	123.20
2	B	968	VAL	N-CA-C	5.43	117.15	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	603	ASN	CB-CA-C	-5.43	100.83	109.80
2	B	299	GLU	CA-CB-CG	5.43	124.96	114.10
6	H	17	PRO	CA-C-O	-5.43	112.49	118.68
2	B	766	ARG	NE-CZ-NH2	5.43	124.09	119.20
4	E	123	LEU	N-CA-C	5.43	120.86	113.37
5	F	74	ILE	CA-CB-CG1	5.43	119.63	110.40
1	A	439	ASN	O-C-N	-5.43	116.07	121.88
1	A	508	PRO	N-CA-C	-5.43	106.32	113.65
1	A	788	SER	CB-CA-C	5.43	118.76	109.80
2	B	512	ARG	CD-NE-CZ	-5.43	116.80	124.40
2	B	626	ILE	CA-C-O	-5.43	114.32	120.67
5	F	84	TYR	O-C-N	-5.43	116.25	122.93
1	A	375	THR	CA-CB-OG1	5.43	117.74	109.60
1	A	504	LEU	N-CA-CB	-5.43	101.32	110.49
3	C	105	GLY	N-CA-C	-5.43	100.32	113.18
4	E	110	PHE	CB-CA-C	-5.43	101.46	110.14
1	A	44	THR	CA-C-N	5.42	131.90	121.54
1	A	44	THR	C-N-CA	5.42	131.90	121.54
6	H	9	ILE	O-C-N	5.42	128.93	123.07
8	J	7	CYS	N-CA-C	-5.42	102.27	110.24
2	B	222	ILE	N-CA-CB	-5.42	103.88	111.25
2	B	267	ARG	N-CA-C	5.42	118.09	109.96
2	B	1183	LYS	N-CA-C	-5.42	99.26	110.80
4	E	17	ARG	NE-CZ-NH2	5.42	124.08	119.20
4	E	108	GLY	CA-C-O	5.42	130.00	120.57
2	B	567	GLU	CA-CB-CG	5.42	124.94	114.10
3	C	228	PHE	N-CA-C	5.42	117.50	108.02
4	E	199	ILE	N-CA-CB	-5.42	104.63	111.46
1	A	475	THR	CA-C-O	5.42	126.20	119.97
1	A	1012	ARG	CA-CB-CG	5.42	124.93	114.10
2	B	593	PRO	CB-CG-CD	-5.42	88.77	106.10
2	B	870	ILE	N-CA-CB	5.42	120.17	111.23
1	A	411	ASP	CA-CB-CG	-5.41	107.19	112.60
1	A	1221	LYS	N-CA-CB	5.41	119.64	110.49
2	B	107	GLY	CA-C-N	5.41	131.72	121.97
2	B	107	GLY	C-N-CA	5.41	131.72	121.97
3	C	195	GLN	N-CA-CB	5.41	119.96	110.27
8	J	50	ILE	CB-CA-C	5.41	118.76	111.94
4	E	32	GLN	CA-C-N	-5.41	111.99	122.06
4	E	32	GLN	C-N-CA	-5.41	111.99	122.06
2	B	311	LEU	O-C-N	-5.41	116.39	122.12
2	B	1040	ASN	CA-CB-CG	-5.41	107.19	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	75	CYS	N-CA-C	5.41	117.49	110.40
7	I	70	ARG	NE-CZ-NH2	-5.41	114.33	119.20
1	A	1432	GLN	CA-C-N	-5.41	113.69	121.42
1	A	1432	GLN	C-N-CA	-5.41	113.69	121.42
2	B	100	PRO	CA-N-CD	-5.41	104.43	112.00
2	B	964	VAL	N-CA-CB	-5.41	101.93	111.93
4	E	153	HIS	O-C-N	-5.41	116.91	123.29
7	I	7	CYS	CA-C-O	-5.41	115.07	120.96
1	A	372	LYS	N-CA-C	5.40	119.13	112.54
1	A	1326	ARG	NH1-CZ-NH2	-5.40	112.27	119.30
1	A	1242	VAL	N-CA-CB	-5.40	102.41	111.38
2	B	165	VAL	N-CA-C	5.40	120.58	109.34
1	A	15	LYS	CA-CB-CG	5.40	124.90	114.10
2	B	642	ASP	CA-CB-CG	5.40	118.00	112.60
3	C	55	THR	N-CA-C	-5.40	105.91	112.88
3	C	186	LEU	N-CA-C	5.40	119.35	112.87
6	H	93	TYR	N-CA-C	5.40	118.08	110.14
4	E	91	LYS	O-C-N	5.40	127.64	122.03
1	A	74	MET	CG-SD-CE	5.40	112.77	100.90
2	B	41	LYS	CB-CG-CD	5.40	123.71	111.30
6	H	115	TYR	CA-C-O	-5.40	112.58	120.13
1	A	919	ILE	CA-CB-CG1	5.39	119.57	110.40
6	H	23	VAL	CA-C-O	-5.39	114.63	120.67
6	H	106	GLU	CB-CA-C	5.39	120.73	110.27
1	A	227	VAL	CB-CA-C	-5.39	106.32	111.44
2	B	1005	GLY	N-CA-C	5.39	125.95	113.18
2	B	702	LEU	CD1-CG-CD2	-5.39	98.95	110.80
10	L	60	ARG	NE-CZ-NH1	-5.39	116.11	121.50
1	A	483	ASP	CB-CG-OD1	-5.38	106.01	118.40
1	A	790	ASP	CA-C-O	-5.38	115.29	121.54
1	A	1148	ILE	N-CA-C	5.38	115.59	110.53
2	B	746	SER	N-CA-C	-5.38	106.69	113.20
2	B	797	TYR	CB-CA-C	-5.38	102.39	110.90
4	E	181	ALA	N-CA-CB	-5.38	102.68	110.70
2	B	1197	PRO	CA-C-O	5.38	127.44	121.36
1	A	90	VAL	O-C-N	-5.38	117.24	123.00
1	A	1230	GLU	N-CA-CB	5.38	117.80	110.38
1	A	328	ARG	O-C-N	5.38	129.74	122.59
1	A	806	ARG	CB-CA-C	-5.38	100.34	110.67
2	B	541	LEU	N-CA-C	5.38	117.89	111.71
4	E	118	PRO	N-CD-CG	5.38	111.27	103.20
9	K	69	ALA	CA-C-O	-5.38	115.56	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	790	ASP	N-CA-C	5.38	118.85	111.54
1	A	972	HIS	N-CA-C	-5.38	104.30	111.02
2	B	499	ASN	CA-C-O	-5.38	114.15	120.60
2	B	910	VAL	CG1-CB-CG2	-5.38	98.97	110.80
7	I	74	GLU	N-CA-CB	-5.38	102.25	110.85
1	A	535	THR	N-CA-CB	-5.38	102.79	110.80
1	A	882	SER	CA-CB-OG	-5.38	100.35	111.10
1	A	1207	LEU	CD1-CG-CD2	5.37	122.62	110.80
2	B	206	ASN	N-CA-C	-5.37	104.48	111.74
4	E	102	GLU	CA-C-O	-5.37	113.31	119.60
8	J	50	ILE	N-CA-C	-5.37	105.88	111.58
1	A	709	THR	OG1-CB-CG2	-5.37	98.56	109.30
1	A	793	SER	N-CA-CB	-5.37	102.89	110.04
4	E	162	ARG	N-CA-C	-5.37	105.42	111.28
1	A	1009	ASN	CA-CB-CG	-5.37	107.23	112.60
8	J	6	ARG	CA-C-O	-5.37	115.18	121.46
2	B	595	ARG	NE-CZ-NH2	5.37	124.03	119.20
6	H	27	GLU	CA-C-O	5.37	126.78	120.98
6	H	56	THR	CB-CA-C	5.37	119.37	110.78
7	I	82	GLU	CB-CG-CD	5.37	121.73	112.60
7	I	95	THR	N-CA-C	5.37	117.65	110.35
1	A	32	VAL	CB-CA-C	5.37	120.09	111.29
1	A	960	ILE	CB-CG1-CD1	-5.37	102.53	113.80
1	A	351	THR	CA-CB-OG1	5.37	117.65	109.60
2	B	1183	LYS	O-C-N	-5.36	115.46	122.59
6	H	18	GLY	O-C-N	-5.36	115.73	122.70
9	K	30	ALA	CA-C-N	-5.36	115.07	122.69
9	K	30	ALA	C-N-CA	-5.36	115.07	122.69
1	A	351	THR	N-CA-C	5.36	116.14	108.74
3	C	93	ASP	CB-CG-OD2	5.36	130.73	118.40
1	A	731	ARG	NH1-CZ-NH2	5.36	126.27	119.30
1	A	856	THR	N-CA-CB	-5.36	102.16	110.57
9	K	47	ARG	CG-CD-NE	5.36	123.79	112.00
1	A	366	VAL	O-C-N	-5.36	114.99	121.10
1	A	443	LEU	N-CA-CB	-5.36	102.06	110.69
1	A	1311	VAL	CA-C-O	-5.36	114.68	120.36
3	C	238	ILE	N-CA-CB	-5.36	103.71	111.21
1	A	812	GLU	CA-C-O	5.36	126.13	119.97
7	I	84	VAL	CB-CA-C	5.36	119.07	110.82
1	A	771	GLU	OE1-CD-OE2	5.35	135.75	122.90
1	A	563	PRO	N-CA-C	5.35	119.89	111.38
1	A	975	HIS	N-CA-CB	-5.35	101.44	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	ASP	CA-C-N	-5.35	111.78	121.14
1	A	218	ASP	C-N-CA	-5.35	111.78	121.14
2	B	1099	VAL	N-CA-C	5.35	120.47	109.34
9	K	39	ASP	CA-C-O	5.35	124.04	120.19
1	A	434	ARG	CG-CD-NE	-5.35	100.24	112.00
1	A	1198	ASP	OD1-CG-OD2	-5.35	110.07	122.90
3	C	156	THR	CB-CA-C	-5.35	98.80	109.33
1	A	1037	LEU	CA-C-O	-5.34	115.73	121.56
1	A	984	LYS	CA-CB-CG	5.34	124.78	114.10
1	A	461	LYS	CB-CG-CD	5.34	123.58	111.30
1	A	1093	LYS	CB-CG-CD	5.34	123.58	111.30
2	B	707	PRO	N-CD-CG	-5.34	95.19	103.20
2	B	870	ILE	CA-CB-CG1	5.34	119.48	110.40
1	A	1113	THR	N-CA-C	5.34	118.69	108.97
2	B	745	PRO	CA-C-O	-5.34	111.53	119.00
10	L	55	ILE	CA-C-N	-5.34	114.09	122.73
10	L	55	ILE	C-N-CA	-5.34	114.09	122.73
1	A	290	GLU	N-CA-C	5.33	117.09	111.28
1	A	1196	GLU	N-CA-CB	-5.33	102.33	110.65
1	A	674	PRO	CA-C-N	-5.33	113.08	120.38
1	A	674	PRO	C-N-CA	-5.33	113.08	120.38
2	B	131	ASP	N-CA-CB	5.33	119.56	110.87
2	B	966	VAL	O-C-N	-5.33	117.58	123.18
1	A	1450	LEU	CA-C-O	-5.33	111.74	120.80
2	B	1003	ALA	O-C-N	-5.33	116.12	122.20
7	I	22	ASN	CB-CA-C	-5.33	101.16	110.17
1	A	458	HIS	CA-C-O	-5.33	115.09	121.11
1	A	978	PRO	CB-CG-CD	-5.33	89.05	106.10
2	B	460	ALA	CA-C-O	-5.33	114.77	120.42
4	E	198	ILE	CA-C-N	-5.33	116.19	123.12
4	E	198	ILE	C-N-CA	-5.33	116.19	123.12
3	C	161	LYS	O-C-N	-5.33	116.94	122.96
6	H	13	SER	CA-C-O	5.33	126.08	119.79
1	A	501	LEU	CA-C-N	-5.32	111.82	121.14
1	A	501	LEU	C-N-CA	-5.32	111.82	121.14
2	B	642	ASP	CB-CA-C	5.32	119.59	110.81
1	A	1111	MET	CG-SD-CE	-5.32	89.19	100.90
2	B	678	GLU	CA-CB-CG	-5.32	103.46	114.10
1	A	346	ASP	N-CA-CB	5.32	119.54	110.50
2	B	853	SER	CB-CA-C	-5.32	99.02	110.45
1	A	486	GLU	CG-CD-OE1	5.32	130.63	118.40
1	A	807	GLY	N-CA-C	5.32	118.92	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	109	THR	N-CA-C	5.32	122.13	110.80
2	B	799	PRO	CB-CA-C	-5.32	104.81	111.56
1	A	1112	LYS	N-CA-C	5.31	116.88	111.14
4	E	62	ALA	N-CA-CB	-5.31	101.58	110.99
1	A	483	ASP	CB-CG-OD2	5.31	130.62	118.40
1	A	555	ASP	OD1-CG-OD2	-5.31	110.15	122.90
1	A	926	GLN	N-CA-CB	5.31	119.21	110.39
4	E	104	ASN	CA-C-N	5.31	129.47	122.30
4	E	104	ASN	C-N-CA	5.31	129.47	122.30
1	A	994	GLN	CB-CA-C	-5.31	100.81	110.63
4	E	10	SER	CA-CB-OG	-5.31	100.48	111.10
1	A	844	ALA	N-CA-C	5.31	117.75	111.33
2	B	1127	GLY	N-CA-C	5.31	128.69	113.30
9	K	56	VAL	CA-C-O	5.31	127.29	120.76
10	L	58	LYS	CA-C-N	-5.31	111.41	121.54
10	L	58	LYS	C-N-CA	-5.31	111.41	121.54
1	A	861	GLY	CA-C-N	-5.30	111.31	120.97
1	A	861	GLY	C-N-CA	-5.30	111.31	120.97
1	A	1109	LYS	CB-CA-C	5.30	121.40	110.31
1	A	1165	GLU	CB-CG-CD	-5.30	103.59	112.60
1	A	155	GLU	CA-C-N	5.30	131.66	121.54
1	A	155	GLU	C-N-CA	5.30	131.66	121.54
1	A	1117	THR	CA-C-N	-5.30	116.20	123.14
1	A	1117	THR	C-N-CA	-5.30	116.20	123.14
4	E	72	PHE	O-C-N	5.30	126.23	121.04
8	J	10	CYS	CB-CA-C	5.30	118.45	109.55
6	H	110	ASP	O-C-N	5.30	128.78	122.21
8	J	44	TYR	N-CA-C	-5.29	106.08	112.54
1	A	54	ASN	O-C-N	-5.29	115.55	122.59
1	A	491	VAL	CA-C-O	5.29	123.06	119.20
3	C	250	THR	OG1-CB-CG2	-5.29	98.72	109.30
1	A	365	GLY	O-C-N	-5.29	117.57	122.96
2	B	636	PRO	N-CA-CB	-5.29	97.70	103.25
2	B	701	ILE	CB-CG1-CD1	5.29	124.91	113.80
1	A	721	PHE	CA-C-O	5.29	126.15	120.55
1	A	940	ARG	CB-CG-CD	5.29	123.46	111.30
5	F	141	GLY	N-CA-C	5.29	122.12	114.67
3	C	177	GLU	CA-C-O	-5.29	115.95	121.55
1	A	853	ASP	N-CA-C	5.28	119.59	113.20
1	A	1286	LYS	CD-CE-NZ	-5.28	94.99	111.90
2	B	283	VAL	O-C-N	-5.28	116.39	121.83
2	B	771	SER	N-CA-C	-5.28	105.69	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	11	LEU	CB-CA-C	-5.28	100.14	109.70
2	B	362	PRO	CB-CA-C	-5.28	103.47	111.44
3	C	17	ASN	N-CA-CB	-5.28	103.22	111.56
1	A	1360	GLY	N-CA-C	5.28	122.37	115.40
3	C	57	VAL	CG1-CB-CG2	5.28	122.42	110.80
1	A	1281	ARG	N-CA-C	5.28	117.94	110.50
8	J	14	VAL	CA-C-O	5.28	127.38	120.78
1	A	669	THR	CB-CA-C	-5.28	101.25	110.17
1	A	759	ALA	N-CA-C	5.28	116.84	111.14
4	E	87	SER	N-CA-C	-5.28	99.92	108.52
9	K	65	HIS	CA-C-N	5.28	125.36	119.87
9	K	65	HIS	C-N-CA	5.28	125.36	119.87
10	L	47	ARG	CB-CA-C	-5.28	108.84	116.54
3	C	250	THR	CA-C-O	5.28	126.01	120.42
1	A	483	ASP	CA-C-N	-5.27	117.17	123.08
1	A	483	ASP	C-N-CA	-5.27	117.17	123.08
6	H	92	ASP	N-CA-C	-5.27	107.38	112.97
1	A	749	ALA	N-CA-C	5.27	118.97	112.54
2	B	711	GLU	N-CA-C	5.27	121.46	109.81
3	C	202	PRO	N-CD-CG	-5.27	95.30	103.20
1	A	1106	ASN	N-CA-C	5.27	118.97	112.54
2	B	876	LYS	CA-C-O	-5.27	112.94	120.16
4	E	148	GLU	CB-CG-CD	5.27	121.56	112.60
1	A	280	GLU	N-CA-C	-5.27	105.54	111.28
1	A	770	VAL	CA-C-N	5.27	129.84	122.36
1	A	770	VAL	C-N-CA	5.27	129.84	122.36
1	A	576	GLN	CA-C-N	-5.26	112.94	120.42
1	A	576	GLN	C-N-CA	-5.26	112.94	120.42
2	B	418	LYS	N-CA-C	-5.26	104.45	111.24
2	B	106	ASP	N-CA-C	5.26	122.01	110.80
10	L	61	THR	CA-CB-CG2	5.26	119.45	110.50
1	A	523	ILE	CB-CG1-CD1	5.26	124.85	113.80
2	B	553	PRO	CA-C-O	-5.26	111.61	119.34
2	B	1109	GLY	N-CA-C	5.26	123.07	112.34
3	C	57	VAL	N-CA-CB	-5.26	100.03	111.81
1	A	825	ILE	CB-CA-C	-5.26	104.96	112.22
2	B	1185	CYS	CA-CB-SG	5.26	126.50	114.40
7	I	48	LEU	O-C-N	-5.26	116.15	122.15
1	A	466	SER	N-CA-CB	5.26	118.88	110.73
1	A	1350	LYS	N-CA-CB	-5.26	101.83	110.40
2	B	1168	LEU	CA-C-N	-5.26	114.27	122.05
2	B	1168	LEU	C-N-CA	-5.26	114.27	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	78	THR	O-C-N	5.26	129.55	122.82
2	B	367	LEU	CB-CG-CD2	5.25	126.47	110.70
3	C	5	GLY	N-CA-C	5.25	123.06	112.34
6	H	89	LEU	CA-CB-CG	5.25	134.69	116.30
7	I	45	ARG	CA-CB-CG	5.25	124.61	114.10
1	A	414	ASP	O-C-N	-5.25	116.63	122.93
1	A	1230	GLU	N-CA-C	-5.25	103.10	110.35
2	B	542	MET	N-CA-C	5.25	119.66	112.88
3	C	210	GLU	CG-CD-OE1	5.25	130.48	118.40
1	A	1025	ARG	N-CA-C	-5.25	105.15	112.45
2	B	868	MET	N-CA-C	5.25	117.65	108.52
6	H	37	LYS	N-CA-C	5.25	118.14	109.85
2	B	654	ARG	NE-CZ-NH1	-5.25	116.25	121.50
2	B	773	MET	CA-CB-CG	-5.25	103.61	114.10
2	B	884	ARG	CB-CG-CD	5.25	123.37	111.30
6	H	47	PHE	CA-C-N	-5.25	115.17	120.21
6	H	47	PHE	C-N-CA	-5.25	115.17	120.21
7	I	28	GLU	CA-CB-CG	5.25	124.59	114.10
1	A	1376	THR	CA-CB-CG2	5.25	119.42	110.50
2	B	900	ALA	CA-C-O	5.24	125.69	120.03
2	B	1002	THR	N-CA-CB	-5.24	101.86	110.41
2	B	114	PRO	N-CD-CG	5.24	111.06	103.20
6	H	32	THR	OG1-CB-CG2	-5.24	98.81	109.30
2	B	796	LEU	N-CA-CB	-5.24	101.87	110.41
2	B	1038	SER	N-CA-C	5.24	119.67	113.28
3	C	19	ASP	N-CA-CB	-5.24	101.89	110.43
3	C	209	TYR	N-CA-C	5.24	121.96	110.80
6	H	61	SER	CA-C-O	-5.24	113.02	120.51
3	C	220	ASP	N-CA-C	5.24	117.83	107.98
2	B	953	LEU	CA-C-O	5.24	126.72	120.28
1	A	1378	GLN	CA-C-N	-5.23	114.82	122.46
1	A	1378	GLN	C-N-CA	-5.23	114.82	122.46
1	A	1374	VAL	N-CA-C	-5.23	105.28	110.62
2	B	682	SER	N-CA-C	5.23	117.89	111.82
2	B	825	VAL	CG1-CB-CG2	-5.23	99.29	110.80
4	E	112	TYR	OH-CZ-CE2	5.23	135.60	119.90
1	A	1023	ARG	CA-C-O	-5.23	114.19	120.10
2	B	880	THR	N-CA-C	5.23	121.93	110.80
2	B	612	GLU	O-C-N	-5.22	116.07	122.34
2	B	942	ARG	NE-CZ-NH1	-5.22	116.28	121.50
2	B	722	ASP	OD1-CG-OD2	-5.22	110.37	122.90
6	H	49	VAL	N-CA-C	5.22	114.74	108.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	104	ASN	N-CA-CB	5.22	119.58	110.18
1	A	576	GLN	CB-CA-C	-5.22	99.73	110.38
1	A	384	ASN	N-CA-CB	-5.21	103.44	110.95
1	A	985	ASP	OD1-CG-OD2	5.21	135.41	122.90
2	B	431	TYR	CB-CA-C	-5.21	103.20	111.17
1	A	1239	ARG	CG-CD-NE	-5.21	100.54	112.00
6	H	104	PHE	O-C-N	-5.21	115.66	122.59
1	A	285	PRO	N-CA-CB	5.21	107.88	103.19
1	A	1143	LEU	CA-C-N	-5.21	113.51	120.54
1	A	1143	LEU	C-N-CA	-5.21	113.51	120.54
2	B	380	TYR	O-C-N	-5.21	116.60	122.12
6	H	103	LYS	CA-C-O	-5.21	113.07	120.51
6	H	104	PHE	CA-C-O	5.20	127.95	120.51
1	A	85	ASP	N-CA-C	-5.20	101.98	110.20
4	E	98	ILE	N-CA-CB	5.20	118.63	110.31
8	J	24	LEU	CB-CA-C	-5.20	99.44	110.31
2	B	955	THR	CB-CA-C	-5.20	101.44	112.78
2	B	1210	MET	CA-C-N	-5.20	115.28	123.91
2	B	1210	MET	C-N-CA	-5.20	115.28	123.91
3	C	136	ASP	N-CA-C	5.20	118.42	110.20
1	A	468	PHE	CA-C-N	-5.20	114.51	122.62
1	A	468	PHE	C-N-CA	-5.20	114.51	122.62
1	A	1040	GLN	CG-CD-NE2	-5.20	108.60	116.40
1	A	1165	GLU	N-CA-C	5.20	121.87	110.80
3	C	210	GLU	O-C-N	-5.20	117.56	123.48
1	A	156	ASP	N-CA-C	5.20	121.86	110.80
1	A	563	PRO	CA-C-O	5.20	128.01	121.67
2	B	1085	ILE	O-C-N	-5.20	117.65	123.26
2	B	314	LEU	CA-C-N	-5.19	113.30	120.26
2	B	314	LEU	C-N-CA	-5.19	113.30	120.26
2	B	739	THR	CB-CA-C	-5.19	100.35	109.07
4	E	167	ARG	NE-CZ-NH1	-5.19	116.31	121.50
7	I	42	LEU	N-CA-C	5.19	116.62	109.15
10	L	28	LYS	O-C-N	-5.19	115.69	122.59
2	B	840	ILE	CA-CB-CG2	-5.19	101.68	110.50
4	E	132	ILE	N-CA-CB	-5.19	103.94	111.52
1	A	192	GLY	N-CA-C	-5.18	100.89	113.18
1	A	731	ARG	NE-CZ-NH1	-5.18	116.32	121.50
1	A	586	ILE	CA-C-N	5.18	131.28	122.37
1	A	586	ILE	C-N-CA	5.18	131.28	122.37
1	A	850	VAL	CG1-CB-CG2	-5.18	99.40	110.80
2	B	1097	HIS	CA-C-O	5.18	127.92	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	86	CYS	N-CA-C	5.18	118.56	110.32
2	B	69	LEU	N-CA-C	5.18	117.73	109.65
7	I	68	LEU	CA-C-O	-5.18	115.37	120.19
1	A	237	THR	CA-C-N	5.18	131.03	122.33
1	A	237	THR	C-N-CA	5.18	131.03	122.33
1	A	1192	LEU	N-CA-C	5.18	117.41	109.07
10	L	49	LYS	CA-C-O	5.18	127.91	120.51
1	A	1017	LEU	N-CA-C	-5.17	105.82	111.82
1	A	1135	ARG	CD-NE-CZ	5.17	131.64	124.40
1	A	780	VAL	CB-CA-C	-5.17	105.71	111.35
2	B	912	ILE	CA-C-N	5.17	126.87	120.92
2	B	912	ILE	C-N-CA	5.17	126.87	120.92
2	B	1153	GLU	CG-CD-OE1	-5.17	106.50	118.40
8	J	32	GLU	N-CA-CB	5.17	118.21	109.78
1	A	867	ILE	O-C-N	-5.17	117.31	123.05
2	B	241	ARG	NE-CZ-NH1	5.17	126.67	121.50
2	B	627	PHE	CA-C-O	-5.17	114.58	120.32
4	E	23	VAL	N-CA-CB	-5.17	104.50	110.55
10	L	63	ARG	CB-CA-C	5.17	118.02	109.70
1	A	503	GLN	N-CA-C	-5.17	107.03	113.38
1	A	78	PRO	N-CD-CG	5.16	110.94	103.20
1	A	962	ARG	O-C-N	-5.16	114.69	122.28
1	A	1257	ASP	CA-C-N	-5.16	111.76	120.58
1	A	1257	ASP	C-N-CA	-5.16	111.76	120.58
1	A	1259	MET	CG-SD-CE	5.16	112.25	100.90
2	B	396	ASP	N-CA-C	-5.16	103.22	110.50
2	B	448	ILE	CB-CA-C	-5.16	103.14	110.83
7	I	24	ARG	N-CA-CB	5.16	120.67	111.69
7	I	94	ASP	CA-C-N	5.16	128.54	120.75
7	I	94	ASP	C-N-CA	5.16	128.54	120.75
10	L	33	GLU	N-CA-C	5.16	121.79	110.80
1	A	273	ASN	CA-C-N	5.16	127.53	120.46
1	A	273	ASN	C-N-CA	5.16	127.53	120.46
1	A	434	ARG	CD-NE-CZ	5.16	131.62	124.40
1	A	986	ILE	N-CA-CB	-5.16	105.00	110.62
2	B	860	MET	CB-CA-C	-5.16	100.42	109.71
8	J	61	LEU	CB-CG-CD2	5.16	126.18	110.70
4	E	96	PHE	CB-CA-C	5.16	119.05	110.90
6	H	21	ASN	CA-CB-CG	-5.16	107.44	112.60
7	I	61	ASP	N-CA-C	5.16	118.70	112.93
9	K	78	THR	CB-CA-C	-5.16	100.51	109.64
1	A	451	HIS	CB-CG-CD2	-5.15	124.50	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	790	ASP	CB-CG-OD2	-5.15	106.55	118.40
4	E	127	ILE	O-C-N	5.15	126.97	121.10
1	A	1284	MET	CG-SD-CE	-5.15	89.57	100.90
1	A	1305	VAL	CG1-CB-CG2	-5.15	99.47	110.80
9	K	51	LEU	N-CA-C	5.15	119.55	113.16
3	C	190	ASP	N-CA-C	5.15	116.80	108.41
1	A	1348	LEU	N-CA-C	-5.15	105.67	111.28
2	B	292	ILE	N-CA-C	5.15	120.00	108.88
3	C	219	PHE	O-C-N	5.15	129.25	122.97
4	E	148	GLU	N-CA-CB	5.15	118.27	110.14
1	A	638	GLY	CA-C-N	5.15	124.59	119.24
1	A	638	GLY	C-N-CA	5.15	124.59	119.24
2	B	91	SER	CA-C-N	5.15	128.15	120.95
2	B	91	SER	C-N-CA	5.15	128.15	120.95
1	A	16	GLU	CG-CD-OE2	-5.14	106.57	118.40
2	B	598	GLU	CG-CD-OE2	5.14	130.23	118.40
2	B	790	ASP	CA-C-O	-5.14	115.61	121.68
9	K	72	LYS	N-CA-C	-5.14	99.59	108.69
2	B	1026	LEU	N-CA-C	-5.14	105.75	111.36
4	E	169	ARG	N-CA-CB	-5.14	103.53	111.65
1	A	366	VAL	CA-C-O	5.14	126.84	119.95
2	B	538	ASN	N-CA-CB	-5.14	101.91	110.80
4	E	92	THR	CA-C-N	5.14	127.12	120.44
4	E	92	THR	C-N-CA	5.14	127.12	120.44
2	B	109	THR	CA-C-N	5.14	130.83	121.89
2	B	109	THR	C-N-CA	5.14	130.83	121.89
1	A	53	LEU	CB-CG-CD1	5.14	126.11	110.70
1	A	884	ASP	CB-CG-OD1	-5.14	106.59	118.40
1	A	4	GLN	CB-CA-C	5.13	120.64	110.17
1	A	77	CYS	CB-CA-C	-5.13	101.29	109.51
1	A	846	GLU	CA-C-O	5.13	125.88	119.97
1	A	1344	GLY	CA-C-O	5.13	126.04	120.75
2	B	372	SER	CA-C-O	5.13	125.87	119.97
2	B	395	GLN	CA-C-O	-5.13	116.11	121.55
2	B	562	GLY	CA-C-N	-5.13	113.77	120.95
2	B	562	GLY	C-N-CA	-5.13	113.77	120.95
2	B	579	ARG	NH1-CZ-NH2	5.13	125.97	119.30
1	A	424	ILE	CG1-CB-CG2	-5.13	95.32	110.70
2	B	511	PRO	N-CA-C	-5.13	107.45	113.86
4	E	9	ILE	CB-CA-C	-5.13	105.37	112.24
4	E	164	LEU	CD1-CG-CD2	-5.13	99.52	110.80
2	B	736	THR	N-CA-CB	5.13	119.12	110.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	129	ILE	CA-CB-CG1	5.12	119.11	110.40
1	A	498	ARG	NE-CZ-NH1	-5.12	116.38	121.50
9	K	79	GLU	CB-CA-C	5.12	117.94	110.26
1	A	225	ASN	CA-CB-CG	5.12	117.72	112.60
1	A	454	SER	CA-C-O	-5.12	113.08	119.28
2	B	621	GLU	CG-CD-OE2	5.12	130.18	118.40
2	B	1082	MET	CB-CG-SD	5.12	128.06	112.70
6	H	133	ASN	N-CA-C	5.12	121.71	110.80
8	J	49	MET	N-CA-CB	-5.12	102.59	110.12
1	A	296	LEU	CA-C-N	5.12	128.50	120.82
1	A	296	LEU	C-N-CA	5.12	128.50	120.82
1	A	1027	ALA	N-CA-CB	-5.12	102.80	110.17
1	A	1212	VAL	CB-CA-C	-5.12	105.33	111.88
3	C	35	ARG	CD-NE-CZ	5.12	131.57	124.40
1	A	389	THR	N-CA-CB	5.12	117.43	110.01
2	B	187	SER	CA-CB-OG	-5.12	100.87	111.10
1	A	1214	GLU	N-CA-C	-5.11	106.55	112.89
5	F	150	GLU	CG-CD-OE1	-5.11	106.64	118.40
3	C	29	MET	N-CA-C	-5.11	105.79	111.36
1	A	712	GLU	CA-C-O	-5.11	114.09	119.97
1	A	988	LEU	CD1-CG-CD2	-5.11	99.56	110.80
2	B	213	ILE	CA-C-O	5.11	126.04	120.57
2	B	380	TYR	CA-C-O	5.11	125.97	120.55
4	E	110	PHE	N-CA-CB	-5.11	102.75	110.77
2	B	788	ARG	CA-CB-CG	5.11	124.31	114.10
2	B	914	LYS	CB-CA-C	-5.11	101.12	110.62
1	A	607	ILE	CA-C-O	-5.11	115.44	120.90
2	B	414	ALA	CA-C-N	5.11	127.43	120.54
2	B	414	ALA	C-N-CA	5.11	127.43	120.54
7	I	75	CYS	CA-C-O	-5.11	115.61	120.97
8	J	18	TRP	N-CA-C	5.11	116.92	111.36
3	C	148	ARG	O-C-N	-5.10	117.34	123.06
1	A	437	MET	CB-CA-C	-5.10	99.51	111.09
1	A	55	ASP	O-C-N	5.10	127.19	121.32
4	E	195	VAL	CA-C-O	-5.10	115.07	120.48
6	H	38	LEU	CD1-CG-CD2	-5.10	99.58	110.80
1	A	244	PRO	O-C-N	5.10	127.48	121.46
2	B	824	ILE	N-CA-C	-5.10	102.16	108.89
4	E	3	GLN	CA-CB-CG	5.10	124.29	114.10
4	E	207	ARG	NE-CZ-NH1	5.10	126.60	121.50
1	A	207	ILE	CB-CA-C	-5.09	105.45	111.97
5	F	153	VAL	O-C-N	5.09	129.67	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	567	GLU	CB-CA-C	5.09	120.55	110.42
3	C	72	LEU	N-CA-C	-5.09	100.74	109.24
1	A	1449	SER	CA-C-N	5.09	130.85	121.70
1	A	1449	SER	C-N-CA	5.09	130.85	121.70
2	B	974	PRO	CA-C-N	5.09	130.55	121.75
2	B	974	PRO	C-N-CA	5.09	130.55	121.75
5	F	130	ILE	O-C-N	5.09	124.57	121.37
5	F	131	PRO	CA-C-N	-5.09	114.61	122.59
5	F	131	PRO	C-N-CA	-5.09	114.61	122.59
3	C	268	ASP	CB-CG-OD2	5.08	130.09	118.40
1	A	525	GLN	CG-CD-NE2	-5.08	108.77	116.40
1	A	710	LEU	N-CA-C	5.08	117.21	111.11
2	B	39	ARG	O-C-N	-5.08	116.73	122.12
2	B	908	GLU	N-CA-C	-5.08	104.70	111.87
4	E	98	ILE	CG1-CB-CG2	-5.08	95.45	110.70
2	B	1049	ASP	N-CA-C	5.08	119.57	113.17
1	A	489	LEU	N-CA-C	-5.08	100.76	109.24
2	B	855	PHE	CA-C-O	-5.08	115.21	120.70
2	B	335	GLY	CA-C-N	-5.08	112.97	120.28
2	B	335	GLY	C-N-CA	-5.08	112.97	120.28
4	E	95	THR	CB-CA-C	-5.08	100.02	110.38
1	A	28	ARG	O-C-N	5.08	127.30	122.07
2	B	692	TYR	O-C-N	-5.08	117.25	123.19
4	E	154	ILE	CB-CA-C	-5.08	103.57	110.42
4	E	195	VAL	CA-CB-CG2	-5.07	101.78	110.40
1	A	932	GLU	CA-CB-CG	5.07	124.24	114.10
1	A	991	LYS	CA-C-O	5.07	125.80	120.42
3	C	80	LEU	N-CA-CB	-5.07	102.61	110.57
1	A	460	VAL	CG1-CB-CG2	-5.07	99.65	110.80
1	A	1317	MET	CA-C-O	5.07	125.62	119.49
2	B	1155	SER	CA-CB-OG	5.07	121.23	111.10
1	A	829	VAL	N-CA-C	5.07	115.68	110.36
1	A	673	GLY	CA-C-O	-5.06	114.28	121.52
1	A	989	GLY	CA-C-O	-5.06	115.53	120.75
1	A	1070	GLN	N-CA-C	-5.06	105.46	111.69
1	A	652	VAL	CB-CA-C	-5.06	105.39	112.02
3	C	230	MET	CG-SD-CE	5.06	112.03	100.90
1	A	352	VAL	CA-CB-CG1	5.06	119.00	110.40
1	A	1284	MET	CB-CA-C	-5.06	100.98	109.53
1	A	998	LEU	N-CA-C	5.05	117.48	109.24
1	A	1167	GLU	CA-C-N	5.05	127.30	120.38
1	A	1167	GLU	C-N-CA	5.05	127.30	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	612	GLU	N-CA-C	-5.05	106.70	112.92
3	C	180	TYR	O-C-N	-5.05	117.82	123.48
6	H	79	TRP	N-CA-C	-5.05	101.39	109.23
1	A	121	LEU	N-CA-C	-5.05	105.90	111.71
4	E	139	ALA	CA-C-O	-5.05	113.38	119.49
4	E	181	ALA	N-CA-C	5.05	118.48	112.72
1	A	636	GLU	O-C-N	-5.05	115.49	122.46
2	B	299	GLU	CB-CG-CD	-5.05	104.02	112.60
4	E	3	GLN	N-CA-CB	5.05	119.02	110.49
4	E	24	LYS	N-CA-C	5.05	116.78	111.28
1	A	1165	GLU	O-C-N	-5.05	115.88	122.59
1	A	266	LEU	CB-CA-C	-5.05	99.44	109.99
1	A	398	GLU	N-CA-C	-5.05	100.95	109.07
2	B	702	LEU	N-CA-C	-5.05	99.88	108.26
2	B	1209	ALA	O-C-N	5.04	127.47	122.12
1	A	1012	ARG	CD-NE-CZ	5.04	131.46	124.40
10	L	53	HIS	N-CA-C	5.04	117.83	109.46
2	B	1192	TYR	CA-C-O	5.04	127.16	121.51
8	J	3	VAL	CG1-CB-CG2	5.04	121.89	110.80
1	A	441	PRO	CA-C-N	-5.04	116.18	123.03
1	A	441	PRO	C-N-CA	-5.04	116.18	123.03
2	B	857	ARG	CG-CD-NE	-5.04	100.91	112.00
2	B	577	ALA	O-C-N	5.04	128.65	122.96
1	A	732	LEU	CA-C-O	5.04	126.11	120.82
1	A	266	LEU	CA-CB-CG	5.04	133.93	116.30
2	B	22	SER	CA-C-O	5.04	125.31	119.32
2	B	135	ARG	N-CA-C	-5.04	100.39	108.55
2	B	627	PHE	CB-CA-C	-5.04	100.59	109.70
3	C	182	PRO	N-CD-CG	-5.04	95.65	103.20
2	B	268	THR	CA-CB-CG2	5.03	119.06	110.50
2	B	175	ARG	NE-CZ-NH2	5.03	123.73	119.20
2	B	1041	GLU	N-CA-CB	5.03	117.04	109.34
1	A	1141	THR	OG1-CB-CG2	-5.03	99.24	109.30
2	B	433	GLN	N-CA-CB	5.03	117.81	110.47
2	B	741	CYS	N-CA-C	5.03	117.02	109.23
1	A	968	GLN	N-CA-CB	5.03	118.73	110.39
1	A	1103	GLU	N-CA-C	-5.02	105.88	111.36
1	A	525	GLN	CG-CD-OE1	5.02	130.84	120.80
1	A	1206	ASP	N-CA-C	-5.02	104.31	111.24
2	B	1220	ARG	NH1-CZ-NH2	-5.02	112.77	119.30
4	E	88	VAL	CB-CA-C	5.02	117.86	110.98
2	B	642	ASP	CB-CG-OD1	5.02	129.95	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	710	LEU	CB-CG-CD2	5.02	125.76	110.70
2	B	169	ARG	CA-C-O	5.02	125.67	120.30
2	B	706	GLN	CA-C-N	5.02	124.80	119.28
2	B	706	GLN	C-N-CA	5.02	124.80	119.28
1	A	855	THR	N-CA-CB	5.02	118.49	110.46
1	A	914	GLU	CG-CD-OE1	5.02	129.94	118.40
2	B	408	LEU	N-CA-CB	-5.02	101.51	110.14
2	B	916	THR	N-CA-C	5.02	125.04	111.00
1	A	481	ASP	CA-CB-CG	-5.01	107.58	112.60
1	A	811	GLN	N-CA-C	-5.01	105.70	111.07
1	A	1198	ASP	N-CA-C	5.01	116.93	108.96
2	B	265	SER	CA-CB-OG	5.01	121.13	111.10
1	A	1280	GLU	CG-CD-OE1	-5.01	106.88	118.40
1	A	16	GLU	OE1-CD-OE2	5.01	134.92	122.90
6	H	32	THR	N-CA-C	-5.01	100.13	110.80
6	H	102	TYR	N-CA-CB	-5.01	103.74	110.95
9	K	96	ASN	N-CA-C	-5.01	105.73	111.14
1	A	975	HIS	CB-CA-C	5.01	120.38	110.42
1	A	1411	GLU	CA-C-O	5.01	125.73	120.42
1	A	903	ASN	CB-CA-C	5.00	118.31	109.80
1	A	1215	ARG	N-CA-CB	5.00	117.56	110.16
2	B	873	THR	OG1-CB-CG2	-5.00	99.29	109.30
2	B	959	ASP	OD1-CG-OD2	-5.00	110.89	122.90
2	B	996	ARG	N-CA-C	5.00	116.73	111.28
7	I	62	ILE	CA-C-O	5.00	126.08	120.03

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	204	THR	CB

All (102) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1046	LEU	Mainchain
1	A	1093	LYS	Peptide
1	A	1111	MET	Mainchain
1	A	1119	TYR	Sidechain
1	A	1155	ASP	Peptide,Mainchain
1	A	1220	PHE	Peptide
1	A	1232	ASN	Peptide
1	A	1301	GLU	Mainchain

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Mol	Chain	Res	Type	Group
1	A	1366	ARG	Sidechain
1	A	1384	VAL	Peptide
1	A	1434	ALA	Mainchain
1	A	31	SER	Peptide
1	A	399	HIS	Peptide
1	A	434	ARG	Sidechain
1	A	44	THR	Peptide
1	A	464	PRO	Peptide
1	A	465	TYR	Sidechain
1	A	555	ASP	Peptide
1	A	60	SER	Peptide
1	A	659	HIS	Sidechain
1	A	70	CYS	Peptide
1	A	705	LYS	Peptide
1	A	706	HIS	Peptide
1	A	74	MET	Peptide
1	A	741	ASN	Mainchain
1	A	821	ARG	Sidechain
1	A	936	LEU	Mainchain
2	B	1025	HIS	Sidechain
2	B	104	GLU	Peptide
2	B	107	GLY	Peptide
2	B	1097	HIS	Sidechain
2	B	1101	ASP	Peptide
2	B	1102	LYS	Peptide
2	B	1109	GLY	Peptide
2	B	1141	HIS	Sidechain
2	B	1152	MET	Peptide
2	B	1153	GLU	Peptide
2	B	1155	SER	Peptide
2	B	1221	SER	Peptide
2	B	1222	ARG	Peptide
2	B	238	ALA	Mainchain
2	B	244	LEU	Peptide
2	B	248	SER	Peptide
2	B	369	GLY	Peptide
2	B	431	TYR	Peptide
2	B	518	HIS	Sidechain
2	B	642	ASP	Peptide
2	B	643	ASP	Peptide
2	B	644	GLU	Peptide
2	B	667	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	B	732	SER	Peptide
2	B	868	MET	Peptide
2	B	882	THR	Peptide
2	B	884	ARG	Peptide
2	B	905	VAL	Peptide
2	B	956	THR	Peptide
2	B	963	PHE	Mainchain
2	B	968	VAL	Mainchain
2	B	98	THR	Peptide
3	C	103	ALA	Mainchain
3	C	155	LEU	Peptide,Mainchain
3	C	156	THR	Mainchain
3	C	184	ASN	Peptide
3	C	190	ASP	Peptide
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	119	SER	Peptide
4	E	125	PRO	Peptide
4	E	128	PRO	Peptide
4	E	153	HIS	Sidechain
4	E	207	ARG	Mainchain
4	E	212	ARG	Sidechain
4	E	77	SER	Peptide
6	H	102	TYR	Peptide
6	H	103	LYS	Peptide
6	H	127	GLY	Peptide
6	H	131	ASN	Peptide
6	H	135	LEU	Peptide
6	H	136	LYS	Peptide
6	H	17	PRO	Peptide
6	H	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	3	THR	Peptide,Mainchain

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Mol	Chain	Res	Type	Group
7	I	43	VAL	Mainchain
9	K	6	ARG	Sidechain
9	K	70	ARG	Mainchain
10	L	27	LEU	Peptide
10	L	34	CYS	Peptide
10	L	35	SER	Peptide
10	L	59	ALA	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10625	0	10693	840	0
2	B	8690	0	8713	532	0
3	C	2095	0	2051	145	0
4	E	1760	0	1788	133	0
5	F	670	0	690	51	0
6	H	1068	0	1040	163	0
7	I	990	0	949	71	0
8	J	525	0	535	42	0
9	K	919	0	929	67	0
10	L	364	0	386	53	0
11	A	2	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	I	2	0	0	0	0
11	J	1	0	0	0	0
11	L	1	0	0	0	0
12	A	2	0	0	0	0
13	B	32	0	11	9	0
14	A	11	0	0	3	0
14	B	11	0	0	4	0
14	F	1	0	0	0	0
14	L	1	0	0	1	0
All	All	27772	0	27785	1968	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 36.

All (1968) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:CA	1:A:61:ILE:CB	1.75	1.64
1:A:941:LYS:CD	1:A:941:LYS:CG	1.74	1.64
10:L:61:THR:CB	10:L:61:THR:CG2	1.75	1.64
5:F:72:LYS:CD	5:F:72:LYS:CE	1.76	1.64
1:A:1405:THR:CB	1:A:1405:THR:CA	1.77	1.62
1:A:1132:LYS:CB	1:A:1132:LYS:CG	1.75	1.62
1:A:1055:ARG:CG	1:A:1055:ARG:CD	1.76	1.61
4:E:161:LYS:CD	4:E:161:LYS:CE	1.76	1.61
1:A:46:THR:CA	1:A:46:THR:CB	1.77	1.61
1:A:571:LEU:CD2	1:A:571:LEU:CG	1.78	1.61
2:B:227:LYS:CG	2:B:227:LYS:CD	1.74	1.61
1:A:1081:LEU:CD2	1:A:1081:LEU:CG	1.76	1.60
1:A:1130:GLN:CG	1:A:1130:GLN:CD	1.74	1.60
1:A:1215:ARG:CB	1:A:1215:ARG:CG	1.75	1.60
2:B:531:GLN:CB	2:B:531:GLN:CG	1.77	1.60
3:C:7:GLN:CB	3:C:7:GLN:CG	1.77	1.60
1:A:518:LYS:CE	1:A:518:LYS:CD	1.77	1.60
4:E:54:GLN:CG	4:E:54:GLN:CB	1.78	1.60
7:I:3:THR:CB	7:I:3:THR:CG2	1.75	1.60
1:A:973:ILE:CB	1:A:973:ILE:CG2	1.75	1.60
2:B:115:GLN:CB	2:B:115:GLN:CG	1.76	1.60
1:A:368:LYS:CG	1:A:368:LYS:CD	1.75	1.59
1:A:1102:LYS:CD	1:A:1102:LYS:CE	1.77	1.59
1:A:1261:LYS:CD	1:A:1261:LYS:CE	1.76	1.59
1:A:1385:THR:CB	1:A:1385:THR:CG2	1.75	1.59
7:I:120:GLN:CG	7:I:120:GLN:CB	1.74	1.59
2:B:434:ARG:CG	2:B:434:ARG:CD	1.78	1.59
1:A:274:ILE:CA	1:A:274:ILE:CB	1.78	1.59
1:A:795:GLU:CG	1:A:795:GLU:CD	1.76	1.59
1:A:1262:LYS:CG	1:A:1262:LYS:CD	1.75	1.59
2:B:246:LYS:CA	2:B:246:LYS:C	1.76	1.59
2:B:959:ASP:CB	2:B:959:ASP:CG	1.74	1.59
4:E:131:THR:CA	4:E:131:THR:CB	1.74	1.59
1:A:1080:THR:CA	1:A:1080:THR:CB	1.75	1.59
1:A:1171:GLN:CG	1:A:1171:GLN:CD	1.76	1.59
2:B:436:VAL:CA	2:B:436:VAL:CB	1.78	1.59
10:L:26:THR:CB	10:L:26:THR:CG2	1.75	1.59
2:B:951:GLN:CG	2:B:951:GLN:CD	1.74	1.58
1:A:566:ILE:CB	1:A:566:ILE:CG2	1.75	1.58
4:E:98:ILE:CA	4:E:98:ILE:CB	1.79	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:42:LYS:CD	8:J:42:LYS:CE	1.79	1.58
9:K:20:LYS:CG	9:K:20:LYS:CD	1.77	1.58
1:A:843:LYS:CD	1:A:843:LYS:CE	1.76	1.58
6:H:77:ARG:CB	6:H:77:ARG:CG	1.81	1.58
1:A:1222:ASN:CG	1:A:1222:ASN:CB	1.76	1.58
1:A:1286:LYS:CB	1:A:1286:LYS:CG	1.77	1.58
4:E:37:LEU:CD1	4:E:37:LEU:CG	1.81	1.58
10:L:54:ARG:CG	10:L:54:ARG:CD	1.76	1.58
1:A:1112:LYS:CG	1:A:1112:LYS:CB	1.82	1.58
2:B:305:VAL:CG1	2:B:305:VAL:CB	1.79	1.58
2:B:775:LYS:CB	2:B:775:LYS:CG	1.81	1.57
2:B:1057:LYS:CD	2:B:1057:LYS:CG	1.74	1.57
1:A:1132:LYS:CG	1:A:1132:LYS:CD	1.80	1.57
2:B:958:GLN:CB	2:B:958:GLN:CG	1.76	1.57
3:C:9:LYS:CG	3:C:9:LYS:CD	1.82	1.57
1:A:977:LYS:CB	1:A:977:LYS:CG	1.75	1.57
1:A:1093:LYS:CG	1:A:1093:LYS:CB	1.76	1.57
1:A:1110:ASN:CG	1:A:1110:ASN:CB	1.78	1.57
1:A:1162:VAL:CG1	1:A:1162:VAL:CB	1.80	1.57
2:B:620:ARG:CG	2:B:620:ARG:CD	1.77	1.57
3:C:199:LYS:CD	3:C:199:LYS:CE	1.76	1.57
1:A:423:ASP:CB	1:A:423:ASP:CG	1.76	1.57
1:A:544:ASP:CB	1:A:544:ASP:CG	1.77	1.57
1:A:1109:LYS:CD	1:A:1109:LYS:CG	1.79	1.57
1:A:1272:THR:CG2	1:A:1272:THR:CB	1.76	1.57
1:A:44:THR:CA	1:A:44:THR:CB	1.77	1.56
1:A:74:MET:CB	1:A:74:MET:CG	1.78	1.56
1:A:237:THR:CB	1:A:237:THR:CG2	1.82	1.56
2:B:164:LYS:CE	2:B:164:LYS:CD	1.82	1.56
6:H:9:ILE:CB	6:H:9:ILE:CA	1.76	1.56
6:H:52:GLN:CG	6:H:52:GLN:CD	1.74	1.56
10:L:28:LYS:CA	10:L:28:LYS:C	1.77	1.56
2:B:1097:HIS:CB	2:B:1097:HIS:CA	1.79	1.56
3:C:252:GLN:CG	3:C:252:GLN:CB	1.74	1.56
7:I:45:ARG:CG	7:I:45:ARG:CD	1.82	1.56
2:B:346:GLU:CG	2:B:346:GLU:CD	1.77	1.56
1:A:69:THR:C	1:A:69:THR:CA	1.74	1.56
1:A:295:LEU:CD2	1:A:295:LEU:CG	1.77	1.56
1:A:555:ASP:CB	1:A:555:ASP:CG	1.78	1.56
2:B:191:LYS:CG	2:B:191:LYS:CB	1.81	1.56
2:B:230:ALA:CA	2:B:230:ALA:CB	1.77	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:415:GLN:CG	2:B:415:GLN:CB	1.82	1.56
2:B:598:GLU:CG	2:B:598:GLU:CD	1.76	1.56
4:E:152:LYS:CG	4:E:152:LYS:CD	1.82	1.56
10:L:48:CYS:C	10:L:48:CYS:CA	1.77	1.56
1:A:840:ARG:CG	1:A:840:ARG:CD	1.75	1.55
1:A:1135:ARG:CG	1:A:1135:ARG:CD	1.78	1.55
4:E:129:PRO:CG	4:E:129:PRO:CD	1.75	1.55
1:A:66:LYS:CB	1:A:66:LYS:CG	1.78	1.55
1:A:1003:LYS:CG	1:A:1003:LYS:CB	1.78	1.55
1:A:1187:GLN:CB	1:A:1187:GLN:CG	1.84	1.55
3:C:102:GLN:CB	3:C:102:GLN:CG	1.78	1.55
3:C:116:LYS:CD	3:C:116:LYS:CE	1.79	1.55
2:B:434:ARG:CG	2:B:434:ARG:CB	1.78	1.55
2:B:646:LEU:CD1	2:B:646:LEU:CG	1.81	1.55
1:A:481:ASP:CG	1:A:481:ASP:CB	1.76	1.55
1:A:1445:ILE:CB	1:A:1445:ILE:CG2	1.83	1.55
9:K:26:LYS:CG	9:K:26:LYS:CD	1.77	1.55
2:B:115:GLN:CG	2:B:115:GLN:CD	1.78	1.55
2:B:509:ALA:CA	2:B:509:ALA:CB	1.84	1.55
2:B:986:GLN:CG	2:B:986:GLN:CD	1.75	1.55
2:B:1101:ASP:CB	2:B:1101:ASP:CG	1.77	1.55
4:E:41:ASP:CB	4:E:41:ASP:CG	1.77	1.55
5:F:123:LYS:NZ	5:F:123:LYS:CE	1.67	1.54
2:B:233:PRO:CB	2:B:233:PRO:CG	1.76	1.54
2:B:1102:LYS:CB	2:B:1102:LYS:CG	1.78	1.54
1:A:601:LYS:CD	1:A:601:LYS:CE	1.82	1.54
1:A:1350:LYS:CG	1:A:1350:LYS:CD	1.78	1.54
2:B:227:LYS:NZ	2:B:227:LYS:CE	1.70	1.54
1:A:1109:LYS:CG	1:A:1109:LYS:CB	1.79	1.54
2:B:646:LEU:CG	2:B:646:LEU:CD2	1.81	1.54
2:B:962:LYS:CD	2:B:962:LYS:CE	1.82	1.53
1:A:720:ARG:CG	1:A:720:ARG:CD	1.79	1.53
2:B:477:ALA:CA	2:B:477:ALA:CB	1.85	1.53
2:B:723:VAL:CA	2:B:723:VAL:CB	1.84	1.53
1:A:830:LYS:CE	1:A:830:LYS:CD	1.81	1.53
1:A:1204:ASP:CB	1:A:1204:ASP:CG	1.79	1.53
1:A:1419:ASP:CG	1:A:1419:ASP:CB	1.75	1.53
2:B:723:VAL:CB	2:B:723:VAL:CG1	1.82	1.53
10:L:43:THR:CB	10:L:43:THR:CG2	1.76	1.53
1:A:5:GLN:CG	1:A:5:GLN:CB	1.80	1.53
3:C:154:LYS:CG	3:C:154:LYS:CD	1.82	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:941:LYS:NZ	1:A:941:LYS:CE	1.70	1.53
1:A:1235:LYS:NZ	1:A:1235:LYS:CE	1.69	1.53
4:E:106:GLN:CG	4:E:106:GLN:CD	1.79	1.53
2:B:962:LYS:CD	2:B:962:LYS:CG	1.87	1.52
4:E:162:ARG:CB	4:E:162:ARG:CG	1.86	1.52
9:K:111:LEU:CD1	9:K:111:LEU:CG	1.86	1.52
1:A:934:LYS:CD	1:A:934:LYS:CE	1.87	1.52
2:B:641:GLU:CG	2:B:641:GLU:CD	1.79	1.52
3:C:94:LYS:NZ	3:C:94:LYS:CE	1.67	1.52
2:B:347:LYS:CD	2:B:347:LYS:CE	1.76	1.52
2:B:706:GLN:CB	2:B:706:GLN:CG	1.84	1.51
6:H:104:PHE:C	6:H:104:PHE:CA	1.82	1.51
2:B:1154:ALA:CA	2:B:1154:ALA:CB	1.87	1.51
3:C:50:GLU:CG	3:C:50:GLU:CD	1.77	1.51
2:B:622:LYS:NZ	2:B:622:LYS:CE	1.70	1.51
4:E:191:LYS:NZ	4:E:191:LYS:CE	1.72	1.51
1:A:695:LYS:CE	1:A:695:LYS:CD	1.88	1.51
1:A:728:LYS:CE	1:A:728:LYS:NZ	1.70	1.51
1:A:597:LEU:CD1	1:A:597:LEU:CG	1.87	1.50
1:A:620:LYS:CD	1:A:620:LYS:CE	1.86	1.50
4:E:180:ARG:CG	4:E:180:ARG:CD	1.87	1.50
1:A:830:LYS:CD	1:A:830:LYS:CG	1.87	1.50
1:A:895:LYS:CD	1:A:895:LYS:CE	1.85	1.50
2:B:870:ILE:CA	2:B:870:ILE:CB	1.87	1.50
4:E:152:LYS:CD	4:E:152:LYS:CE	1.86	1.50
1:A:843:LYS:CD	1:A:843:LYS:CG	1.87	1.49
10:L:26:THR:CB	10:L:26:THR:CA	1.89	1.49
2:B:315:LYS:NZ	2:B:315:LYS:CE	1.72	1.49
6:H:139:ASN:CB	6:H:139:ASN:CG	1.86	1.49
1:A:1132:LYS:NZ	1:A:1132:LYS:CE	1.74	1.49
2:B:41:LYS:NZ	2:B:41:LYS:CE	1.72	1.49
3:C:15:LYS:CG	3:C:15:LYS:CD	1.90	1.49
1:A:346:ASP:CB	1:A:346:ASP:CG	1.86	1.48
1:A:978:PRO:CB	1:A:978:PRO:CG	1.78	1.48
10:L:68:GLU:CG	10:L:68:GLU:CD	1.85	1.48
1:A:941:LYS:CD	1:A:941:LYS:CE	1.88	1.48
2:B:199:MET:CE	2:B:199:MET:SD	2.02	1.48
2:B:231:PRO:CB	2:B:231:PRO:CG	1.85	1.47
2:B:531:GLN:CG	2:B:531:GLN:CD	1.88	1.47
4:E:53:PRO:CG	4:E:53:PRO:CB	1.74	1.47
5:F:129:LYS:NZ	5:F:129:LYS:CE	1.72	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:50:MET:SD	4:E:50:MET:CG	2.02	1.47
2:B:432:MET:CE	2:B:432:MET:SD	2.03	1.46
7:I:17:ARG:CG	7:I:17:ARG:CD	1.91	1.46
4:E:93:MET:CG	4:E:93:MET:SD	2.02	1.46
4:E:201:LYS:CG	4:E:201:LYS:CD	1.93	1.45
1:A:705:LYS:CB	1:A:705:LYS:CG	1.90	1.45
1:A:41:MET:CE	1:A:41:MET:SD	2.05	1.45
1:A:676:MET:CE	1:A:676:MET:SD	2.05	1.45
2:B:789:MET:CE	2:B:789:MET:SD	2.05	1.45
1:A:676:MET:SD	1:A:676:MET:CG	2.04	1.44
2:B:999:MET:CG	2:B:999:MET:SD	2.05	1.44
1:A:56:PRO:O	1:A:57:ARG:CD	1.66	1.44
1:A:938:LYS:CD	1:A:938:LYS:CE	1.95	1.44
2:B:1169:MET:CE	2:B:1169:MET:SD	2.05	1.44
3:C:265:MET:CE	3:C:265:MET:SD	2.05	1.44
1:A:248:PRO:CB	1:A:248:PRO:CG	1.78	1.43
1:A:1111:MET:SD	1:A:1111:MET:CG	2.05	1.43
1:A:1350:LYS:NZ	1:A:1350:LYS:CE	1.75	1.43
1:A:728:LYS:CG	1:A:728:LYS:CD	1.92	1.43
2:B:987:LYS:NZ	2:B:987:LYS:CE	1.81	1.43
1:A:1232:ASN:CG	1:A:1232:ASN:CB	1.89	1.43
1:A:1290:LYS:NZ	1:A:1290:LYS:CE	1.80	1.43
2:B:593:PRO:CG	2:B:593:PRO:CB	1.86	1.43
7:I:1:MET:CE	7:I:1:MET:SD	2.07	1.42
2:B:736:THR:CB	2:B:736:THR:CG2	1.96	1.42
13:B:3008:GTP:N9	13:B:3008:GTP:C1'	1.81	1.42
2:B:382:ILE:CG1	2:B:382:ILE:CD1	1.95	1.41
3:C:154:LYS:CD	3:C:154:LYS:CE	1.98	1.41
1:A:1259:MET:SD	1:A:1259:MET:CG	2.09	1.41
2:B:347:LYS:CD	2:B:347:LYS:CG	1.98	1.41
4:E:93:MET:SD	4:E:93:MET:CE	2.08	1.40
8:J:1:MET:CE	8:J:1:MET:SD	2.07	1.40
6:H:19:ARG:CG	6:H:19:ARG:CD	1.98	1.40
4:E:121:MET:CE	4:E:121:MET:SD	2.08	1.40
1:A:620:LYS:CE	1:A:620:LYS:NZ	1.85	1.40
3:C:29:MET:CE	3:C:29:MET:SD	2.10	1.40
1:A:1302:PRO:CG	1:A:1302:PRO:CB	1.95	1.39
4:E:131:THR:CB	4:E:131:THR:CG2	1.99	1.39
4:E:20:LYS:NZ	4:E:20:LYS:CE	1.84	1.38
1:A:74:MET:CE	1:A:74:MET:SD	2.09	1.38
4:E:162:ARG:CG	4:E:162:ARG:CD	2.01	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:1:MET:SD	7:I:1:MET:CG	2.13	1.35
1:A:1444:MET:CE	1:A:1444:MET:SD	2.14	1.35
2:B:1097:HIS:ND1	2:B:1097:HIS:HA	1.37	1.35
7:I:55:THR:CB	7:I:55:THR:CG2	2.05	1.35
4:E:121:MET:SD	4:E:121:MET:CG	2.13	1.34
6:H:104:PHE:O	6:H:106:GLU:N	1.63	1.32
1:A:172:PRO:CG	1:A:185:TRP:CE2	2.11	1.31
1:A:728:LYS:CE	1:A:728:LYS:CD	2.09	1.31
1:A:1259:MET:SD	1:A:1259:MET:CE	2.18	1.30
1:A:437:MET:CE	1:A:437:MET:SD	2.18	1.30
2:B:999:MET:SD	2:B:999:MET:CE	1.20	1.30
4:E:1:MET:CE	4:E:1:MET:SD	2.21	1.29
1:A:156:ASP:O	1:A:158:PRO:CD	1.80	1.28
2:B:705:MET:CE	2:B:705:MET:SD	1.18	1.28
1:A:172:PRO:CD	1:A:185:TRP:CE2	2.18	1.26
7:I:4:PHE:CE1	7:I:13:MET:HE2	1.71	1.25
1:A:304:MET:CE	1:A:304:MET:SD	2.25	1.24
3:C:75:MET:CE	3:C:75:MET:SD	2.25	1.24
1:A:172:PRO:CG	1:A:185:TRP:CZ2	2.18	1.24
1:A:186:LYS:HE2	1:A:197:PRO:CD	1.66	1.24
1:A:172:PRO:CD	1:A:185:TRP:NE1	2.01	1.24
3:C:165:LYS:NZ	3:C:165:LYS:CE	2.01	1.24
1:A:56:PRO:O	1:A:57:ARG:HD2	1.11	1.23
3:C:125:MET:CE	3:C:125:MET:SD	2.27	1.23
1:A:172:PRO:HG2	1:A:185:TRP:CZ2	1.71	1.22
1:A:156:ASP:O	1:A:158:PRO:HD2	1.07	1.21
1:A:369:SER:OG	9:K:2:ASN:ND2	1.73	1.20
1:A:153:PRO:HD3	1:A:161:LEU:CD2	1.71	1.20
1:A:605:MET:CE	1:A:607:ILE:HD11	1.71	1.19
1:A:487:MET:CE	1:A:487:MET:SD	1.09	1.19
2:B:662:MET:CE	2:B:662:MET:SD	2.31	1.18
1:A:535:THR:HG21	1:A:617:VAL:H	1.07	1.16
10:L:68:GLU:OE1	14:L:3006:HOH:O	1.63	1.16
2:B:1019:SER:OG	13:B:3008:GTP:O6	1.61	1.16
9:K:1:MET:SD	9:K:1:MET:CE	2.35	1.15
5:F:103:MET:CE	5:F:103:MET:SD	2.33	1.15
1:A:172:PRO:HD3	1:A:185:TRP:CD1	1.82	1.14
1:A:172:PRO:HD2	1:A:185:TRP:NE1	1.60	1.14
1:A:42:ASP:OD2	1:A:47:ARG:N	1.81	1.14
2:B:101:MET:SD	2:B:101:MET:CE	2.35	1.14
1:A:885:THR:HG21	14:A:3013:HOH:O	1.45	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:PRO:HG3	1:A:185:TRP:CE2	1.80	1.13
2:B:999:MET:SD	2:B:999:MET:HE1	1.77	1.13
1:A:487:MET:CE	1:A:487:MET:CG	2.25	1.12
2:B:846:ILE:HD11	2:B:974:PRO:HB2	1.13	1.12
1:A:708:MET:CE	1:A:708:MET:SD	2.37	1.12
6:H:138:GLU:O	6:H:139:ASN:C	1.92	1.12
1:A:518:LYS:CD	1:A:518:LYS:NZ	2.11	1.11
7:I:45:ARG:HG2	7:I:45:ARG:HH11	1.10	1.11
2:B:705:MET:CE	2:B:705:MET:CG	2.28	1.10
2:B:999:MET:SD	2:B:999:MET:HE3	1.77	1.10
1:A:186:LYS:HE2	1:A:197:PRO:HD3	1.22	1.10
2:B:705:MET:SD	2:B:705:MET:HE2	1.76	1.10
6:H:128:ASN:O	6:H:131:ASN:ND2	1.85	1.09
2:B:130:VAL:HG22	2:B:167:ILE:HD11	1.30	1.09
2:B:999:MET:SD	2:B:999:MET:HE2	1.77	1.09
2:B:705:MET:SD	2:B:705:MET:HE3	1.76	1.09
3:C:54:ASN:OD1	3:C:56:THR:HB	1.53	1.09
1:A:107:CYS:HB2	1:A:148:CYS:SG	1.93	1.08
1:A:567:LYS:HB3	6:H:96:VAL:H	1.16	1.08
2:B:705:MET:SD	2:B:705:MET:HE1	1.76	1.08
2:B:792:MET:SD	2:B:792:MET:CE	2.42	1.08
7:I:4:PHE:HE1	7:I:13:MET:HE2	0.94	1.08
6:H:63:LEU:C	6:H:90:ALA:HB3	1.77	1.07
6:H:106:GLU:O	6:H:107:VAL:C	1.98	1.06
1:A:487:MET:SD	1:A:487:MET:HE3	1.68	1.06
1:A:487:MET:SD	1:A:487:MET:HE2	1.68	1.06
1:A:487:MET:SD	1:A:487:MET:HE1	1.68	1.06
7:I:16:PRO:O	7:I:17:ARG:HD3	1.53	1.06
2:B:1097:HIS:CA	2:B:1097:HIS:ND1	2.12	1.06
1:A:172:PRO:HG3	1:A:185:TRP:CD2	1.88	1.05
7:I:45:ARG:CG	7:I:45:ARG:HH11	1.69	1.05
2:B:999:MET:CG	2:B:999:MET:CE	2.35	1.04
1:A:1233:ASP:O	1:A:1234:GLU:HB3	1.55	1.03
1:A:1285:MET:CE	1:A:1285:MET:SD	2.46	1.03
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.40	1.03
8:J:14:VAL:HG13	8:J:50:ILE:HD11	1.41	1.03
9:K:110:ASN:O	9:K:112:GLN:N	1.92	1.03
2:B:955:THR:HG22	10:L:54:ARG:O	1.57	1.03
4:E:12:LEU:HD21	4:E:58:MET:SD	1.99	1.03
4:E:57:MET:CE	4:E:57:MET:SD	2.47	1.02
2:B:552:MET:CG	2:B:552:MET:SD	2.48	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1134:ILE:O	1:A:1138:ILE:HG13	1.58	1.01
1:A:605:MET:HE2	1:A:607:ILE:CD1	1.89	1.01
1:A:679:ILE:HD11	1:A:732:LEU:HB2	1.42	1.01
1:A:1079:MET:SD	1:A:1359:ASP:OD2	2.19	1.01
1:A:187:LYS:HB2	1:A:194:ALA:HB3	1.44	1.00
1:A:567:LYS:HD3	6:H:95:TYR:CG	1.95	0.99
1:A:605:MET:HE2	1:A:607:ILE:HD11	1.00	0.99
1:A:89:PRO:HB2	1:A:204:THR:HG21	1.39	0.99
1:A:567:LYS:HB3	6:H:96:VAL:N	1.78	0.99
1:A:72:GLU:OE2	2:B:1175:LEU:HD11	1.63	0.98
1:A:325:ILE:C	1:A:327:ALA:H	1.68	0.98
1:A:153:PRO:HD3	1:A:161:LEU:HD22	1.43	0.97
1:A:119:ASN:O	1:A:120:GLU:HB2	1.63	0.97
2:B:643:ASP:O	2:B:644:GLU:HB2	1.63	0.96
1:A:107:CYS:CB	1:A:148:CYS:SG	2.53	0.96
1:A:605:MET:CE	1:A:607:ILE:CD1	2.43	0.96
1:A:172:PRO:HD3	1:A:185:TRP:NE1	1.77	0.96
1:A:186:LYS:CE	1:A:197:PRO:HD3	1.95	0.96
1:A:98:LYS:HB3	1:A:234:MET:HE1	1.48	0.95
1:A:153:PRO:HD3	1:A:161:LEU:HD23	1.48	0.95
2:B:885:MET:CE	2:B:885:MET:SD	2.54	0.95
1:A:186:LYS:HE2	1:A:197:PRO:HD2	1.45	0.95
7:I:78:CYS:SG	7:I:103:CYS:SG	2.64	0.95
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.29	0.95
8:J:2:ILE:HD13	8:J:2:ILE:N	1.80	0.95
1:A:567:LYS:HD2	1:A:568:PRO:HD3	1.48	0.95
1:A:1081:LEU:CD2	1:A:1081:LEU:HG	1.97	0.94
2:B:552:MET:SD	2:B:552:MET:CE	2.55	0.94
1:A:186:LYS:NZ	1:A:195:ASP:HA	1.82	0.94
2:B:1077:THR:HG22	2:B:1079:LYS:H	1.33	0.94
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	1.83	0.94
4:E:63:ASN:O	4:E:64:PRO:O	1.86	0.93
2:B:555:ILE:CD1	2:B:587:HIS:CE1	2.51	0.93
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.03	0.92
1:A:176:LYS:NZ	1:A:178:GLY:O	2.01	0.92
1:A:775:ILE:CG1	1:A:775:ILE:CD1	2.48	0.92
2:B:1190:ASP:O	2:B:1191:ILE:HG13	1.68	0.92
5:F:77:ASP:O	5:F:78:GLN:HB2	1.66	0.92
7:I:116:ASN:HD21	7:I:118:ARG:HB2	1.35	0.92
2:B:846:ILE:CD1	2:B:974:PRO:HB2	2.00	0.92
1:A:531:ILE:HD11	1:A:578:LEU:CD2	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:ARG:CG	1:A:1055:ARG:NE	2.33	0.91
1:A:1079:MET:HG2	1:A:1359:ASP:OD2	1.71	0.91
2:B:130:VAL:H	2:B:167:ILE:HD11	1.32	0.91
6:H:104:PHE:O	6:H:105:GLU:C	2.10	0.91
5:F:81:THR:CG2	5:F:136:ARG:HH11	1.83	0.91
1:A:1236:LEU:O	1:A:1237:ILE:HD12	1.71	0.91
2:B:846:ILE:HD11	2:B:974:PRO:CB	1.98	0.91
1:A:535:THR:CG2	1:A:617:VAL:H	1.84	0.90
6:H:55:LEU:HD22	6:H:144:ILE:HD12	1.53	0.90
7:I:4:PHE:HE1	7:I:13:MET:CE	1.83	0.90
1:A:1242:VAL:HG11	1:A:1259:MET:HE3	1.54	0.90
1:A:1134:ILE:O	1:A:1138:ILE:CG1	2.19	0.89
2:B:58:THR:O	2:B:62:ILE:HG12	1.71	0.89
2:B:1097:HIS:CA	2:B:1097:HIS:CG	2.55	0.89
2:B:620:ARG:CG	2:B:620:ARG:NE	2.36	0.89
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.55	0.89
4:E:117:THR:O	4:E:119:SER:N	2.06	0.89
1:A:369:SER:H	9:K:2:ASN:HD21	1.21	0.89
8:J:1:MET:CE	8:J:1:MET:CG	2.51	0.89
2:B:846:ILE:HD11	2:B:974:PRO:O	1.73	0.88
2:B:775:LYS:CB	2:B:775:LYS:CD	2.51	0.88
6:H:89:LEU:O	6:H:91:ASP:N	2.06	0.88
7:I:45:ARG:HG2	7:I:45:ARG:NH1	1.88	0.88
10:L:48:CYS:C	10:L:48:CYS:HA	1.98	0.88
1:A:795:GLU:HG2	2:B:731:VAL:HG21	1.54	0.88
1:A:1341:ILE:HD12	1:A:1379:GLY:HA2	1.54	0.88
3:C:167:HIS:HD2	3:C:169:LYS:H	1.22	0.88
1:A:1286:LYS:CB	1:A:1286:LYS:CD	2.51	0.88
1:A:89:PRO:HB2	1:A:204:THR:CG2	2.02	0.88
1:A:567:LYS:HD3	6:H:95:TYR:HA	1.54	0.88
1:A:1166:ASP:HB3	1:A:1169:ILE:CG2	2.05	0.88
4:E:147:HIS:HD2	4:E:149:LEU:H	1.17	0.87
1:A:172:PRO:HG3	1:A:185:TRP:CZ2	2.02	0.87
1:A:56:PRO:O	1:A:57:ARG:HD3	1.69	0.87
2:B:555:ILE:HD12	2:B:587:HIS:CE1	2.09	0.87
1:A:567:LYS:CB	6:H:96:VAL:H	1.87	0.87
5:F:93:ILE:CD1	5:F:134:ILE:HD11	2.04	0.87
1:A:1079:MET:CG	1:A:1359:ASP:OD2	2.22	0.87
2:B:1025:HIS:HE1	2:B:1090:THR:HG21	1.41	0.86
3:C:167:HIS:HE1	10:L:70:ARG:O	1.58	0.86
1:A:172:PRO:HD3	1:A:185:TRP:CE2	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:846:ILE:CD1	2:B:974:PRO:O	2.24	0.86
6:H:57:VAL:HG22	6:H:144:ILE:HD11	1.57	0.86
4:E:79:TRP:HB2	4:E:105:PHE:CE1	2.10	0.86
1:A:1134:ILE:CG2	1:A:1138:ILE:HD11	2.06	0.86
10:L:28:LYS:C	10:L:28:LYS:HA	1.98	0.86
1:A:567:LYS:CD	6:H:95:TYR:HA	2.06	0.86
6:H:63:LEU:C	6:H:90:ALA:CB	2.49	0.86
8:J:2:ILE:N	8:J:2:ILE:CD1	2.37	0.85
1:A:567:LYS:CG	1:A:568:PRO:CD	2.54	0.85
1:A:567:LYS:HD3	6:H:95:TYR:CA	2.05	0.85
5:F:123:LYS:NZ	5:F:123:LYS:CD	2.39	0.85
1:A:64:ASN:OD1	1:A:64:ASN:O	1.93	0.85
1:A:1166:ASP:HB3	1:A:1169:ILE:HG21	1.59	0.85
1:A:172:PRO:HG3	1:A:185:TRP:CE3	2.10	0.85
1:A:164:ARG:O	1:A:166:GLY:N	2.08	0.85
1:A:679:ILE:HD12	1:A:729:ALA:HA	1.58	0.85
2:B:104:GLU:OE1	10:L:54:ARG:NE	2.10	0.85
6:H:106:GLU:O	6:H:107:VAL:O	1.94	0.84
1:A:55:ASP:OD1	1:A:55:ASP:O	1.94	0.84
1:A:481:ASP:CG	1:A:481:ASP:CA	2.50	0.84
3:C:46:ILE:HD12	3:C:72:LEU:HD11	1.59	0.84
2:B:542:MET:HE2	2:B:747:MET:HG3	1.58	0.84
7:I:32:CYS:HB2	7:I:34:TYR:H	1.43	0.83
1:A:61:ILE:CB	1:A:61:ILE:HA	2.04	0.83
2:B:1220:ARG:O	2:B:1222:ARG:HD3	1.77	0.83
2:B:542:MET:HG3	2:B:747:MET:CE	2.07	0.83
2:B:477:ALA:CB	2:B:477:ALA:HA	2.08	0.83
4:E:98:ILE:CB	4:E:98:ILE:HA	2.03	0.83
1:A:679:ILE:HD13	1:A:732:LEU:HD12	1.59	0.83
1:A:31:SER:CB	1:A:83:HIS:HD2	1.91	0.83
2:B:286:PHE:HB3	2:B:297:ILE:HD12	1.58	0.83
2:B:431:TYR:CD2	2:B:431:TYR:O	2.31	0.83
1:A:108:MET:H	1:A:171:GLN:HE22	1.23	0.82
13:B:3008:GTP:C1'	13:B:3008:GTP:C8	2.61	0.82
4:E:2:ASP:HB3	4:E:6:GLU:HB2	1.61	0.82
1:A:1233:ASP:O	1:A:1234:GLU:CB	2.26	0.82
2:B:561:TRP:O	2:B:590:HIS:HE1	1.61	0.82
2:B:1051:THR:HG22	2:B:1053:GLU:N	1.93	0.82
1:A:1003:LYS:CG	1:A:1003:LYS:CA	2.56	0.82
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.59	0.82
2:B:1128:LEU:HD12	2:B:1128:LEU:C	2.03	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ILE:O	1:A:327:ALA:N	2.12	0.82
1:A:69:THR:C	1:A:69:THR:HA	2.03	0.81
2:B:25:ILE:HD11	2:B:651:LEU:HD12	1.62	0.81
2:B:644:GLU:OE1	2:B:646:LEU:HB2	1.79	0.81
1:A:55:ASP:N	1:A:56:PRO:CD	2.44	0.81
1:A:531:ILE:HD12	1:A:617:VAL:HB	1.62	0.81
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.63	0.81
2:B:515:HIS:H	2:B:518:HIS:CD2	1.99	0.81
1:A:347:PHE:H	2:B:1107:ALA:HA	1.46	0.81
1:A:156:ASP:C	1:A:158:PRO:CD	2.53	0.81
1:A:901:LEU:H	1:A:926:GLN:NE2	1.77	0.81
1:A:1111:MET:CG	1:A:1111:MET:CE	2.58	0.81
1:A:265:LYS:CD	1:A:302:THR:HG22	2.11	0.81
6:H:138:GLU:O	6:H:140:ALA:N	2.14	0.80
1:A:535:THR:HG21	1:A:617:VAL:N	1.93	0.80
7:I:45:ARG:CG	7:I:45:ARG:NH1	2.45	0.80
2:B:542:MET:HG3	2:B:747:MET:HE3	1.63	0.80
1:A:567:LYS:HG3	1:A:568:PRO:CD	2.10	0.80
1:A:172:PRO:HD3	1:A:185:TRP:CG	2.15	0.80
6:H:130:ARG:HD2	6:H:130:ARG:C	2.06	0.80
1:A:567:LYS:CD	1:A:568:PRO:HD3	2.11	0.80
1:A:982:THR:HG22	1:A:985:ASP:H	1.47	0.80
2:B:515:HIS:H	2:B:518:HIS:HD2	1.25	0.80
6:H:103:LYS:HB3	6:H:105:GLU:OE1	1.82	0.80
6:H:89:LEU:C	6:H:91:ASP:H	1.90	0.79
2:B:417:PHE:CD2	2:B:417:PHE:O	2.36	0.79
2:B:90:ILE:HA	2:B:133:LYS:O	1.83	0.79
5:F:77:ASP:O	5:F:78:GLN:CB	2.28	0.79
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.17	0.79
1:A:265:LYS:NZ	1:A:302:THR:HG21	1.98	0.79
2:B:114:PRO:HD3	2:B:124:TYR:CE1	2.17	0.79
2:B:643:ASP:O	2:B:644:GLU:CB	2.31	0.79
8:J:1:MET:C	8:J:2:ILE:HD13	2.07	0.79
1:A:55:ASP:O	1:A:57:ARG:N	2.15	0.79
2:B:130:VAL:HG22	2:B:167:ILE:CD1	2.10	0.79
4:E:50:MET:SD	4:E:50:MET:CE	2.70	0.79
1:A:596:THR:HG22	1:A:597:LEU:H	1.47	0.78
1:A:1364:ASN:HD22	1:A:1366:ARG:H	1.29	0.78
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.62	0.78
3:C:260:LEU:HD12	3:C:260:LEU:O	1.82	0.78
1:A:567:LYS:HD2	1:A:568:PRO:CD	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:GLY:O	4:E:204:THR:HG21	1.84	0.78
1:A:571:LEU:CD2	1:A:571:LEU:HG	2.08	0.78
1:A:711:ARG:HE	7:I:95:THR:HG22	1.48	0.78
2:B:246:LYS:C	2:B:246:LYS:HA	2.07	0.78
1:A:134:ARG:O	1:A:138:ILE:HG23	1.84	0.78
1:A:941:LYS:CD	1:A:941:LYS:NZ	2.47	0.78
2:B:754:SER:O	2:B:806:THR:HG21	1.84	0.78
1:A:46:THR:CA	1:A:46:THR:HB	2.10	0.77
2:B:281:PRO:HB2	2:B:284:ILE:HD13	1.63	0.77
1:A:1055:ARG:CD	1:A:1055:ARG:CB	2.62	0.77
1:A:1151:GLU:CG	7:I:45:ARG:HD2	2.14	0.77
1:A:636:GLU:OE1	1:A:966:ASN:ND2	2.16	0.77
2:B:431:TYR:CE1	2:B:447:ALA:HB1	2.19	0.77
2:B:1084:GLN:NE2	3:C:192:TRP:H	1.82	0.77
2:B:431:TYR:O	2:B:431:TYR:HD2	1.66	0.77
6:H:104:PHE:O	6:H:106:GLU:CA	2.32	0.77
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.65	0.77
1:A:909:ASP:OD1	1:A:911:SER:N	2.17	0.77
4:E:98:ILE:CA	4:E:98:ILE:HB	2.12	0.77
6:H:77:ARG:O	6:H:78:SER:O	2.03	0.77
1:A:587:HIS:HD2	1:A:966:ASN:OD1	1.69	0.76
6:H:84:ALA:O	6:H:88:SER:OG	2.02	0.76
6:H:91:ASP:OD1	6:H:91:ASP:O	2.01	0.76
1:A:265:LYS:HZ2	1:A:302:THR:HG21	1.48	0.76
2:B:305:VAL:CG1	2:B:305:VAL:CA	2.62	0.76
9:K:111:LEU:CD1	9:K:111:LEU:CB	2.62	0.76
2:B:29:ASP:HB3	2:B:658:ILE:HD12	1.68	0.76
1:A:327:ALA:O	2:B:1206:GLU:OE1	2.03	0.76
1:A:1118:VAL:HB	1:A:1327:ILE:HD12	1.66	0.76
3:C:73:GLN:HE21	3:C:75:MET:H	1.33	0.76
1:A:567:LYS:CD	6:H:95:TYR:CG	2.69	0.75
2:B:680:THR:HG22	2:B:682:SER:H	1.50	0.75
1:A:172:PRO:HD2	1:A:185:TRP:HE1	1.48	0.75
1:A:941:LYS:CD	1:A:941:LYS:CB	2.62	0.75
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.68	0.75
2:B:549:THR:HG22	2:B:628:THR:HB	1.69	0.75
1:A:172:PRO:HG3	1:A:185:TRP:CH2	2.21	0.75
1:A:531:ILE:HD11	1:A:578:LEU:HD22	1.68	0.75
3:C:40:GLU:HA	3:C:163:ILE:HD12	1.69	0.75
1:A:73:GLY:O	1:A:75:ASN:N	2.19	0.75
1:A:172:PRO:CG	1:A:185:TRP:CH2	2.70	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1350:LYS:CD	1:A:1350:LYS:CB	2.65	0.75
1:A:186:LYS:HZ1	1:A:195:ASP:HA	1.50	0.75
1:A:567:LYS:HD3	6:H:95:TYR:CD2	2.21	0.75
8:J:1:MET:C	8:J:2:ILE:CD1	2.60	0.74
6:H:9:ILE:CB	6:H:9:ILE:HA	2.14	0.74
1:A:61:ILE:O	1:A:62:ASP:HB2	1.86	0.74
10:L:47:ARG:HG2	10:L:48:CYS:H	1.53	0.74
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.23	0.74
6:H:123:MET:HE1	6:H:142:LEU:HD13	1.69	0.74
1:A:1259:MET:SD	1:A:1259:MET:CB	2.75	0.74
1:A:1445:ILE:CG2	1:A:1445:ILE:CA	2.65	0.74
2:B:1084:GLN:HE22	3:C:192:TRP:H	1.32	0.74
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.18	0.74
5:F:75:PRO:O	5:F:77:ASP:O	2.06	0.74
7:I:116:ASN:ND2	7:I:118:ARG:HB2	2.03	0.73
4:E:147:HIS:CD2	4:E:149:LEU:H	2.05	0.73
1:A:531:ILE:HD11	1:A:578:LEU:HD21	1.68	0.73
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.86	0.73
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.36	0.73
1:A:1151:GLU:OE2	7:I:45:ARG:HD3	1.88	0.73
1:A:1236:LEU:O	1:A:1237:ILE:CD1	2.36	0.73
2:B:723:VAL:CB	2:B:723:VAL:HA	2.16	0.73
3:C:33:LEU:HD13	3:C:248:ILE:HD13	1.70	0.73
4:E:29:PHE:O	4:E:30:ILE:HD13	1.87	0.73
10:L:34:CYS:O	10:L:34:CYS:SG	2.41	0.73
2:B:1161:HIS:C	2:B:1162:ILE:HD12	2.13	0.73
5:F:111:LEU:O	5:F:113:GLY:N	2.20	0.73
1:A:938:LYS:CE	1:A:938:LYS:CG	2.67	0.73
1:A:328:ARG:HG3	1:A:329:LEU:H	1.53	0.73
1:A:368:LYS:CD	1:A:368:LYS:CB	2.66	0.73
1:A:1134:ILE:HG22	1:A:1138:ILE:HD11	1.69	0.73
1:A:1341:ILE:HD11	1:A:1376:THR:O	1.88	0.73
2:B:1065:GLN:HE22	2:B:1067:ARG:HB2	1.53	0.73
1:A:156:ASP:OD2	1:A:156:ASP:N	2.21	0.73
1:A:172:PRO:HG3	1:A:185:TRP:CZ3	2.24	0.73
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.03	0.73
1:A:156:ASP:O	1:A:158:PRO:HD3	1.84	0.72
2:B:243:ALA:C	2:B:244:LEU:HG	2.14	0.72
2:B:357:GLN:NE2	2:B:368:GLU:HG2	2.03	0.72
6:H:27:GLU:OE1	6:H:39:THR:OG1	2.05	0.72
2:B:531:GLN:CD	2:B:531:GLN:H	1.97	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLU:O	1:A:30:ILE:HD13	1.90	0.72
2:B:242:SER:HG	2:B:363:HIS:HD1	1.36	0.72
2:B:251:ILE:O	2:B:251:ILE:HG22	1.89	0.72
2:B:417:PHE:CD2	2:B:417:PHE:C	2.67	0.72
1:A:46:THR:CB	1:A:46:THR:C	2.63	0.72
1:A:503:GLN:NE2	5:F:90:ARG:NH2	2.38	0.72
1:A:903:ASN:ND2	1:A:905:ASP:H	1.88	0.72
1:A:977:LYS:CG	1:A:977:LYS:CA	2.67	0.72
2:B:515:HIS:N	2:B:518:HIS:HD2	1.88	0.72
2:B:1162:ILE:CD1	2:B:1194:ILE:HG12	2.20	0.72
1:A:566:ILE:CG2	1:A:566:ILE:CA	2.66	0.72
9:K:35:PHE:HE1	9:K:73:LEU:HD12	1.54	0.72
2:B:315:LYS:NZ	2:B:315:LYS:CD	2.50	0.72
5:F:93:ILE:HD11	5:F:134:ILE:CD1	2.19	0.72
1:A:172:PRO:CG	1:A:185:TRP:CD2	2.62	0.72
1:A:1134:ILE:HG23	1:A:1138:ILE:HD11	1.70	0.72
2:B:663:ALA:O	2:B:667:GLN:HG3	1.89	0.72
3:C:102:GLN:CG	3:C:102:GLN:CA	2.66	0.72
2:B:294:ASP:H	7:I:12:ASN:HD22	1.36	0.71
6:H:105:GLU:HG2	6:H:136:LYS:NZ	2.04	0.71
1:A:1336:MET:HE2	1:A:1381:LEU:H	1.55	0.71
2:B:357:GLN:HE21	2:B:368:GLU:HG2	1.56	0.71
2:B:996:ARG:NH1	14:B:3012:HOH:O	2.22	0.71
1:A:154:SER:O	1:A:155:GLU:O	2.08	0.71
3:C:77:ILE:HD12	3:C:80:LEU:HB3	1.73	0.71
1:A:247:ARG:NH1	1:A:263:THR:HG23	2.05	0.71
4:E:112:TYR:CG	4:E:116:ILE:HD11	2.25	0.71
1:A:23:SER:O	1:A:27:VAL:HG23	1.89	0.71
1:A:518:LYS:CD	1:A:518:LYS:HZ2	2.03	0.71
1:A:187:LYS:CB	1:A:194:ALA:HB3	2.19	0.71
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.25	0.71
6:H:6:PHE:CD2	6:H:7:ASP:N	2.59	0.71
1:A:531:ILE:O	1:A:535:THR:HB	1.90	0.71
1:A:1364:ASN:ND2	1:A:1366:ARG:H	1.88	0.71
7:I:4:PHE:CE1	7:I:13:MET:CE	2.62	0.71
1:A:265:LYS:HD3	1:A:302:THR:HG22	1.71	0.71
2:B:294:ASP:H	7:I:12:ASN:ND2	1.87	0.71
1:A:1385:THR:CG2	1:A:1385:THR:CA	2.68	0.71
8:J:1:MET:HB3	8:J:2:ILE:HD13	1.71	0.71
1:A:186:LYS:CE	1:A:197:PRO:CD	2.56	0.71
1:A:605:MET:HE3	1:A:607:ILE:CD1	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:117:THR:O	4:E:118:PRO:C	2.34	0.70
1:A:560:ILE:HD12	1:A:560:ILE:H	1.56	0.70
1:A:1080:THR:CA	1:A:1080:THR:HB	2.13	0.70
1:A:53:LEU:HD23	1:A:54:ASN:N	2.06	0.70
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.55	0.70
4:E:47:CYS:SG	4:E:52:ARG:O	2.50	0.70
1:A:261:ASP:N	1:A:261:ASP:OD1	2.24	0.70
2:B:877:PRO:O	2:B:878:GLN:HG2	1.92	0.70
3:C:8:VAL:HG12	3:C:9:LYS:H	1.56	0.70
4:E:36:GLU:O	4:E:37:LEU:C	2.30	0.70
1:A:107:CYS:SG	1:A:171:GLN:OE1	2.49	0.70
1:A:547:LEU:HB3	9:K:58:PHE:CE1	2.27	0.70
2:B:227:LYS:CG	2:B:227:LYS:CE	2.70	0.70
1:A:42:ASP:OD2	1:A:47:ARG:CA	2.40	0.70
1:A:1162:VAL:CG1	1:A:1162:VAL:CA	2.69	0.70
2:B:484:ASN:OD1	2:B:486:TYR:CE1	2.45	0.70
3:C:18:VAL:HG23	3:C:240:VAL:HG11	1.74	0.70
3:C:172:PRO:O	3:C:235:VAL:HG12	1.90	0.70
9:K:65:HIS:HD2	9:K:67:PHE:H	1.36	0.70
1:A:156:ASP:C	1:A:158:PRO:HD3	2.17	0.70
1:A:369:SER:CB	9:K:2:ASN:ND2	2.54	0.70
1:A:1135:ARG:CG	1:A:1135:ARG:NE	2.53	0.70
1:A:1405:THR:CA	1:A:1405:THR:HB	2.14	0.70
1:A:150:THR:HA	1:A:166:GLY:HA2	1.73	0.70
1:A:1341:ILE:HD12	1:A:1379:GLY:CA	2.21	0.70
3:C:7:GLN:CB	3:C:7:GLN:CD	2.63	0.70
3:C:181:ASP:OD2	3:C:186:LEU:HB2	1.92	0.70
1:A:679:ILE:HD12	1:A:729:ALA:CA	2.21	0.69
1:A:32:VAL:HG23	1:A:33:ALA:H	1.57	0.69
1:A:567:LYS:CD	1:A:568:PRO:CD	2.70	0.69
2:B:119:LEU:O	2:B:965:LYS:NZ	2.24	0.69
2:B:463:THR:HG21	2:B:465:ASN:OD1	1.91	0.69
2:B:645:SER:OG	2:B:646:LEU:N	2.23	0.69
2:B:1025:HIS:CE1	2:B:1090:THR:HG21	2.25	0.69
2:B:1166:CYS:O	2:B:1168:LEU:N	2.25	0.69
6:H:89:LEU:C	6:H:91:ASP:N	2.49	0.69
2:B:1031:LEU:HB2	2:B:1055:ILE:CD1	2.22	0.69
2:B:1077:THR:CG2	2:B:1079:LYS:H	2.05	0.69
1:A:608:ILE:HD12	1:A:613:ILE:HG13	1.74	0.69
2:B:1222:ARG:HH11	2:B:1222:ARG:HB2	1.57	0.69
3:C:209:TYR:HD1	3:C:209:TYR:H	1.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:THR:O	1:A:48:ALA:N	2.26	0.69
1:A:885:THR:CG2	14:A:3013:HOH:O	2.19	0.69
2:B:217:ARG:HD3	2:B:407:ASP:OD2	1.93	0.69
3:C:50:GLU:HB3	10:L:64:LEU:HD13	1.73	0.69
3:C:199:LYS:CD	3:C:199:LYS:NZ	2.56	0.69
7:I:120:GLN:O	7:I:121:PHE:HB2	1.91	0.69
8:J:2:ILE:HG22	8:J:3:VAL:N	2.07	0.69
1:A:282:ASN:C	1:A:283:GLY:O	2.28	0.69
1:A:328:ARG:CG	1:A:329:LEU:H	2.03	0.69
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.75	0.69
1:A:849:MET:HE2	1:A:1061:GLY:HA2	1.74	0.69
1:A:679:ILE:CD1	1:A:729:ALA:HA	2.21	0.69
1:A:840:ARG:CG	1:A:840:ARG:NE	2.54	0.69
2:B:744:HIS:HD2	2:B:746:SER:H	1.41	0.69
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.74	0.69
2:B:839:MET:CE	2:B:1010:LEU:HD11	2.23	0.68
2:B:879:ARG:NH2	2:B:885:MET:HE1	2.08	0.68
2:B:955:THR:CG2	10:L:54:ARG:O	2.39	0.68
4:E:131:THR:CB	4:E:131:THR:C	2.65	0.68
1:A:166:GLY:O	1:A:167:CYS:HB3	1.92	0.68
6:H:105:GLU:H	6:H:105:GLU:CD	2.01	0.68
1:A:351:THR:HG21	2:B:1103:ILE:HG12	1.75	0.68
6:H:103:LYS:O	6:H:115:TYR:HD1	1.76	0.68
5:F:76:LYS:O	5:F:79:ARG:HD2	1.93	0.68
1:A:567:LYS:HE2	6:H:95:TYR:CE2	2.26	0.68
1:A:587:HIS:CE1	1:A:969:GLN:HG2	2.28	0.68
6:H:105:GLU:HG2	6:H:136:LYS:HZ2	1.58	0.68
1:A:122:MET:HE1	1:A:138:ILE:HD13	1.75	0.68
1:A:265:LYS:CE	1:A:302:THR:HG22	2.23	0.68
2:B:841:MET:HE3	2:B:990:ILE:HD11	1.75	0.68
1:A:69:THR:HG22	2:B:1174:LYS:HE2	1.75	0.68
4:E:112:TYR:CD2	4:E:116:ILE:HD11	2.28	0.68
5:F:81:THR:CG2	5:F:136:ARG:NH1	2.56	0.68
6:H:105:GLU:HB3	6:H:107:VAL:HG23	1.76	0.68
1:A:1161:THR:CG2	1:A:1163:ILE:H	2.06	0.68
4:E:98:ILE:O	4:E:101:GLN:HB3	1.93	0.68
9:K:55:LYS:HB2	9:K:81:TYR:CE1	2.28	0.68
1:A:679:ILE:HD13	1:A:732:LEU:CD1	2.24	0.68
1:A:1265:ASN:O	1:A:1266:THR:C	2.35	0.68
1:A:1385:THR:O	1:A:1385:THR:HG22	1.94	0.67
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.01	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:79:TRP:HB2	4:E:105:PHE:CD1	2.28	0.67
6:H:104:PHE:C	6:H:104:PHE:HA	2.10	0.67
1:A:164:ARG:C	1:A:166:GLY:H	2.02	0.67
1:A:834:THR:HG21	1:A:1077:THR:OG1	1.94	0.67
3:C:116:LYS:CD	3:C:116:LYS:NZ	2.56	0.67
1:A:351:THR:CG2	2:B:1103:ILE:HG12	2.24	0.67
1:A:567:LYS:CG	1:A:568:PRO:HD3	2.25	0.67
1:A:184:SER:HB2	1:A:199:LEU:HD23	1.75	0.67
1:A:912:LEU:HD23	1:A:912:LEU:N	2.10	0.67
2:B:435:THR:O	2:B:435:THR:HG22	1.95	0.67
2:B:654:ARG:H	2:B:657:HIS:HD2	1.42	0.67
2:B:1222:ARG:HG2	2:B:1222:ARG:NH1	2.09	0.67
1:A:567:LYS:CB	6:H:95:TYR:HA	2.25	0.67
2:B:51:PHE:CZ	2:B:172:ILE:HD13	2.30	0.67
2:B:227:LYS:CD	2:B:227:LYS:CB	2.70	0.67
2:B:487:THR:HG22	2:B:490:SER:H	1.58	0.67
2:B:1162:ILE:HD13	2:B:1194:ILE:HG12	1.77	0.67
1:A:503:GLN:NE2	5:F:90:ARG:HH21	1.93	0.67
1:A:63:ARG:HA	1:A:74:MET:HG2	1.77	0.67
2:B:90:ILE:HD13	2:B:134:LYS:HA	1.77	0.67
9:K:55:LYS:HB3	9:K:81:TYR:HD1	1.60	0.67
1:A:46:THR:HB	1:A:46:THR:O	1.95	0.67
1:A:172:PRO:HD3	1:A:185:TRP:CD2	2.30	0.67
7:I:3:THR:CG2	7:I:3:THR:CA	2.70	0.67
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.25	0.66
1:A:328:ARG:HA	2:B:1206:GLU:OE1	1.95	0.66
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.75	0.66
9:K:20:LYS:CG	9:K:20:LYS:CE	2.73	0.66
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.25	0.66
9:K:110:ASN:C	9:K:112:GLN:H	2.00	0.66
1:A:567:LYS:CG	6:H:96:VAL:H	2.09	0.66
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.26	0.66
1:A:351:THR:CG2	2:B:1103:ILE:CG1	2.74	0.66
1:A:369:SER:N	9:K:2:ASN:HD21	1.90	0.66
1:A:1350:LYS:CG	1:A:1350:LYS:CE	2.74	0.66
2:B:206:ASN:OD1	2:B:458:LYS:CE	2.44	0.66
2:B:291:ILE:HG22	2:B:297:ILE:HD13	1.76	0.66
6:H:115:TYR:O	6:H:123:MET:O	2.13	0.66
1:A:44:THR:CB	1:A:44:THR:C	2.67	0.66
1:A:265:LYS:NZ	1:A:302:THR:CG2	2.59	0.66
1:A:534:LEU:O	1:A:574:GLY:HA3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.78	0.66
9:K:93:SER:O	9:K:97:LYS:HG3	1.95	0.66
1:A:172:PRO:CD	1:A:185:TRP:CD2	2.79	0.66
1:A:99:ILE:HD13	1:A:235:ILE:HD13	1.77	0.66
4:E:100:ILE:HG22	4:E:101:GLN:N	2.07	0.66
6:H:131:ASN:H	6:H:131:ASN:HD22	1.42	0.66
1:A:57:ARG:HB3	1:A:68:GLN:HG2	1.75	0.65
1:A:135:PHE:CD1	1:A:222:LEU:HD22	2.31	0.65
1:A:172:PRO:HD2	1:A:185:TRP:CE2	2.11	0.65
1:A:537:ARG:NH2	1:A:600:PRO:O	2.29	0.65
2:B:1019:SER:CB	13:B:3008:GTP:O6	2.43	0.65
1:A:224:PHE:CG	1:A:231:PRO:HD3	2.31	0.65
8:J:53:HIS:HE1	8:J:55:ASP:HA	1.62	0.65
8:J:53:HIS:CE1	8:J:54:VAL:C	2.74	0.65
1:A:42:ASP:OD2	1:A:46:THR:C	2.39	0.65
1:A:187:LYS:HB2	1:A:194:ALA:CB	2.21	0.65
1:A:1266:THR:O	1:A:1267:MET:C	2.39	0.65
1:A:919:ILE:HD13	1:A:983:ILE:HD13	1.79	0.65
2:B:228:LYS:O	2:B:261:ARG:NH2	2.29	0.65
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.78	0.65
3:C:167:HIS:CE1	10:L:70:ARG:O	2.47	0.65
9:K:24:ASP:OD1	9:K:74:ARG:NH1	2.29	0.65
2:B:191:LYS:CG	2:B:191:LYS:CA	2.74	0.65
2:B:341:LEU:HD12	2:B:342:GLY:H	1.60	0.65
1:A:960:ILE:O	1:A:964:ILE:HD13	1.97	0.65
1:A:1236:LEU:C	1:A:1237:ILE:CD1	2.70	0.65
1:A:562:THR:CG2	6:H:98:TYR:CD2	2.80	0.65
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.61	0.64
1:A:1151:GLU:HG2	7:I:45:ARG:HD2	1.79	0.64
1:A:1298:TYR:O	1:A:1299:VAL:HG23	1.97	0.64
4:E:152:LYS:CD	4:E:152:LYS:CB	2.75	0.64
7:I:120:GLN:O	7:I:121:PHE:CB	2.45	0.64
1:A:934:LYS:CD	1:A:934:LYS:NZ	2.60	0.64
2:B:115:GLN:CG	2:B:115:GLN:CA	2.74	0.64
2:B:1222:ARG:HH11	2:B:1222:ARG:CG	2.10	0.64
5:F:109:VAL:CG1	5:F:110:ASP:N	2.60	0.64
6:H:89:LEU:HB3	6:H:91:ASP:OD1	1.98	0.64
1:A:1272:THR:CG2	1:A:1272:THR:CA	2.72	0.64
2:B:789:MET:HE3	2:B:965:LYS:HB3	1.78	0.64
2:B:1163:CYS:SG	2:B:1165:ILE:HG13	2.38	0.64
1:A:407:ARG:CD	1:A:413:ILE:HD11	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:ILE:O	2:B:297:ILE:HD11	1.97	0.64
3:C:40:GLU:C	3:C:163:ILE:HD11	2.22	0.64
3:C:41:ILE:N	3:C:163:ILE:HD11	2.13	0.64
4:E:115:ASN:O	4:E:116:ILE:HD13	1.96	0.64
5:F:105:ALA:HB1	5:F:106:PRO:HD2	1.77	0.64
6:H:123:MET:HE3	6:H:142:LEU:HD22	1.79	0.64
3:C:77:ILE:CD1	3:C:80:LEU:HB3	2.28	0.64
6:H:47:PHE:CG	6:H:95:TYR:HD1	2.16	0.64
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.62	0.64
1:A:1172:LEU:O	1:A:1173:HIS:CD2	2.49	0.64
1:A:1155:ASP:O	1:A:1241:ARG:NH2	2.31	0.64
2:B:841:MET:HB2	2:B:990:ILE:HD12	1.78	0.64
3:C:77:ILE:HD12	3:C:77:ILE:O	1.98	0.64
6:H:9:ILE:CB	6:H:9:ILE:C	2.68	0.64
1:A:894:GLU:HB2	1:A:933:TYR:OH	1.98	0.64
8:J:1:MET:CE	8:J:1:MET:CB	2.76	0.64
1:A:84:ILE:HD12	1:A:270:LEU:HD13	1.80	0.63
1:A:446:ARG:HG2	1:A:446:ARG:HH11	1.62	0.63
2:B:94:LYS:HG2	2:B:96:TYR:CE1	2.34	0.63
3:C:40:GLU:HA	3:C:163:ILE:CD1	2.28	0.63
1:A:709:THR:HG22	1:A:712:GLU:H	1.63	0.63
2:B:120:ARG:NH2	2:B:956:THR:O	2.29	0.63
2:B:393:LYS:NZ	2:B:621:GLU:OE2	2.23	0.63
4:E:117:THR:OG1	4:E:120:ALA:CB	2.47	0.63
10:L:26:THR:CA	10:L:26:THR:HB	2.19	0.63
2:B:127:GLY:HA2	2:B:168:GLY:O	1.98	0.63
4:E:152:LYS:CD	4:E:152:LYS:NZ	2.62	0.63
8:J:53:HIS:HE1	8:J:55:ASP:CA	2.10	0.63
9:K:55:LYS:HB2	9:K:81:TYR:CD1	2.34	0.63
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.29	0.63
2:B:879:ARG:HH21	2:B:885:MET:HE1	1.62	0.63
3:C:99:LEU:HD12	3:C:99:LEU:N	2.14	0.63
1:A:11:LEU:HD11	2:B:1195:HIS:CD2	2.34	0.63
1:A:579:SER:HA	1:A:582:ILE:HD12	1.80	0.63
1:A:589:GLN:HB2	1:A:961:ARG:HH22	1.63	0.63
6:H:76:THR:O	6:H:76:THR:HG22	1.99	0.63
1:A:531:ILE:CD1	1:A:578:LEU:HD22	2.29	0.63
2:B:1166:CYS:O	2:B:1167:GLY:C	2.40	0.63
2:B:1222:ARG:NH1	2:B:1222:ARG:CG	2.59	0.63
6:H:32:THR:CG2	6:H:33:GLN:OE1	2.47	0.63
6:H:93:TYR:HB3	6:H:144:ILE:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:SER:HB3	1:A:83:HIS:HD2	1.62	0.63
4:E:161:LYS:CE	4:E:161:LYS:CG	2.69	0.63
1:A:224:PHE:CD2	1:A:231:PRO:HD3	2.34	0.62
1:A:1162:VAL:O	1:A:1162:VAL:HG12	1.98	0.62
2:B:531:GLN:CG	2:B:531:GLN:CA	2.71	0.62
9:K:55:LYS:CB	9:K:81:TYR:CD1	2.82	0.62
2:B:955:THR:HG23	10:L:55:ILE:HA	1.80	0.62
5:F:81:THR:HG23	5:F:136:ARG:HH11	1.62	0.62
6:H:96:VAL:HG22	6:H:143:LEU:HD23	1.80	0.62
1:A:237:THR:CG2	1:A:237:THR:CA	2.73	0.62
2:B:436:VAL:CA	2:B:436:VAL:HB	2.16	0.62
2:B:1084:GLN:C	2:B:1085:ILE:HD12	2.25	0.62
1:A:901:LEU:H	1:A:926:GLN:HE22	1.47	0.62
2:B:100:PRO:HD2	2:B:180:TYR:CZ	2.35	0.62
10:L:58:LYS:O	10:L:59:ALA:HB3	2.00	0.62
2:B:899:ILE:HD12	2:B:911:ILE:HG13	1.80	0.62
6:H:47:PHE:CB	6:H:95:TYR:HD1	2.12	0.62
6:H:63:LEU:HB2	6:H:90:ALA:HB2	1.81	0.62
2:B:884:ARG:NH1	2:B:884:ARG:HG2	2.13	0.62
2:B:1084:GLN:HE22	3:C:192:TRP:N	1.98	0.62
1:A:186:LYS:CD	1:A:197:PRO:HD3	2.29	0.62
1:A:518:LYS:CE	1:A:518:LYS:CG	2.75	0.62
2:B:531:GLN:NE2	2:B:532:ALA:H	1.97	0.62
2:B:787:VAL:O	2:B:787:VAL:CG1	2.47	0.62
6:H:32:THR:HG22	6:H:33:GLN:CD	2.25	0.62
6:H:57:VAL:HG22	6:H:144:ILE:CD1	2.30	0.62
1:A:55:ASP:N	1:A:56:PRO:HD3	2.12	0.62
2:B:1077:THR:HG22	2:B:1079:LYS:N	2.12	0.62
3:C:255:VAL:O	3:C:255:VAL:HG12	1.99	0.62
1:A:84:ILE:HD12	1:A:270:LEU:CD1	2.30	0.62
1:A:328:ARG:HH11	1:A:1405:THR:HG22	1.65	0.61
1:A:837:ILE:HD11	1:A:1102:LYS:HG2	1.81	0.61
3:C:46:ILE:CD1	3:C:72:LEU:HD11	2.29	0.61
2:B:843:GLN:NE2	2:B:846:ILE:CG2	2.62	0.61
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.98	0.61
1:A:1259:MET:SD	1:A:1259:MET:HB2	2.40	0.61
2:B:130:VAL:CG2	2:B:167:ILE:HD11	2.20	0.61
2:B:498:THR:CG2	2:B:537:LYS:HB2	2.30	0.61
1:A:274:ILE:CB	1:A:274:ILE:C	2.70	0.61
1:A:636:GLU:OE2	1:A:962:ARG:HD2	2.01	0.61
1:A:1436:ILE:HD12	1:A:1436:ILE:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:251:ILE:O	2:B:251:ILE:CG2	2.48	0.61
1:A:567:LYS:CE	6:H:95:TYR:CE2	2.83	0.61
1:A:596:THR:HG22	1:A:597:LEU:N	2.11	0.61
1:A:1118:VAL:HB	1:A:1327:ILE:CD1	2.30	0.61
2:B:118:ARG:HH22	2:B:194:GLU:CG	2.12	0.61
1:A:751:SER:O	1:A:752:LYS:HB2	1.99	0.61
1:A:1323:ASP:OD1	1:A:1325:THR:HB	1.99	0.61
2:B:1002:THR:HG21	2:B:1006:ILE:HB	1.83	0.61
6:H:47:PHE:CZ	6:H:146:ARG:HD2	2.36	0.61
6:H:118:PHE:O	6:H:119:GLY:C	2.44	0.61
5:F:81:THR:HG23	5:F:136:ARG:NH1	2.16	0.61
8:J:2:ILE:HG22	8:J:3:VAL:H	1.65	0.61
9:K:12:LEU:N	9:K:12:LEU:HD12	2.15	0.61
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.40	0.61
2:B:128:LEU:O	2:B:167:ILE:HD12	2.00	0.61
4:E:129:PRO:CD	4:E:130:ALA:H	2.13	0.61
5:F:73:ALA:HB2	5:F:143:PHE:CZ	2.35	0.61
6:H:26:ILE:HD12	6:H:42:ILE:HD12	1.81	0.61
1:A:1318:THR:HG23	4:E:11:ARG:HH12	1.66	0.61
1:A:1385:THR:CG2	1:A:1385:THR:C	2.74	0.61
4:E:191:LYS:NZ	4:E:191:LYS:CD	2.64	0.61
6:H:8:ASP:OD2	6:H:9:ILE:N	2.27	0.61
6:H:114:VAL:HG11	6:H:134:ASN:HD22	1.66	0.61
1:A:567:LYS:CB	1:A:568:PRO:CD	2.79	0.60
4:E:65:THR:O	4:E:69:ILE:HG13	2.01	0.60
1:A:72:GLU:OE2	2:B:1175:LEU:CD1	2.45	0.60
6:H:97:MET:HE3	6:H:118:PHE:CG	2.36	0.60
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.01	0.60
2:B:995:ARG:HD2	2:B:997:GLU:OE2	2.01	0.60
3:C:242:GLN:NE2	3:C:246:ARG:HE	1.98	0.60
1:A:858:ASN:HD21	1:A:860:LEU:HB2	1.65	0.60
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.31	0.60
7:I:16:PRO:HG3	7:I:27:PHE:CE2	2.37	0.60
1:A:595:THR:HG22	1:A:596:THR:N	2.16	0.60
2:B:879:ARG:NH2	2:B:885:MET:CE	2.65	0.60
6:H:123:MET:HE1	6:H:142:LEU:CD1	2.31	0.60
1:A:369:SER:CB	9:K:2:ASN:HD21	2.12	0.60
1:A:571:LEU:CD2	1:A:571:LEU:CD1	2.73	0.60
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.01	0.60
8:J:14:VAL:CG1	8:J:50:ILE:HD11	2.23	0.60
1:A:658:LEU:HD12	1:A:658:LEU:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:LYS:CD	1:A:895:LYS:NZ	2.62	0.60
2:B:249:ARG:CZ	2:B:415:GLN:HG3	2.32	0.60
2:B:775:LYS:CB	2:B:775:LYS:HD2	2.31	0.60
1:A:562:THR:HG22	6:H:98:TYR:CD2	2.36	0.60
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.84	0.60
4:E:153:HIS:CE1	4:E:184:VAL:HG11	2.36	0.60
1:A:172:PRO:CD	1:A:185:TRP:CD1	2.59	0.60
1:A:378:GLU:OE1	1:A:434:ARG:HD3	2.02	0.60
1:A:1172:LEU:O	1:A:1173:HIS:CG	2.55	0.60
2:B:885:MET:CE	2:B:885:MET:HB3	2.31	0.60
3:C:252:GLN:HE22	9:K:99:GLY:N	2.00	0.60
2:B:999:MET:CG	2:B:999:MET:HE2	2.31	0.59
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.01	0.59
2:B:787:VAL:O	2:B:787:VAL:HG12	2.02	0.59
2:B:999:MET:CG	2:B:999:MET:HE3	2.31	0.59
3:C:55:THR:O	3:C:55:THR:HG22	2.01	0.59
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.38	0.59
6:H:11:GLN:NE2	6:H:52:GLN:HG2	2.17	0.59
1:A:903:ASN:C	1:A:903:ASN:HD22	2.09	0.59
2:B:680:THR:HG22	2:B:682:SER:N	2.14	0.59
2:B:916:THR:N	2:B:935:ARG:O	2.34	0.59
4:E:37:LEU:HD23	4:E:42:PHE:HB2	1.84	0.59
1:A:353:ILE:HD12	1:A:482:PHE:CE2	2.38	0.59
1:A:265:LYS:CE	1:A:302:THR:CG2	2.80	0.59
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.83	0.59
4:E:78:LEU:HD11	4:E:109:ILE:HD12	1.84	0.59
9:K:55:LYS:CB	9:K:81:TYR:HD1	2.15	0.59
1:A:804:TYR:O	2:B:761:HIS:ND1	2.35	0.59
2:B:862:GLN:HE22	2:B:961:LEU:HD13	1.67	0.59
1:A:189:ARG:HG2	1:A:189:ARG:O	2.03	0.59
1:A:679:ILE:CD1	1:A:732:LEU:HD12	2.32	0.59
1:A:1198:ASP:OD1	1:A:1200:ALA:HB3	2.02	0.59
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.84	0.59
1:A:567:LYS:HB2	6:H:95:TYR:HA	1.83	0.59
1:A:744:LYS:HD3	1:A:748:MET:SD	2.43	0.59
1:A:1263:ILE:O	1:A:1267:MET:HG3	2.03	0.59
1:A:1424:VAL:O	1:A:1428:VAL:HG23	2.02	0.59
2:B:843:GLN:NE2	2:B:846:ILE:HG22	2.16	0.59
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.35	0.59
3:C:252:GLN:CB	3:C:252:GLN:CD	2.72	0.59
1:A:3:GLY:CA	1:A:76:GLU:HG2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:ILE:HD11	1:A:729:ALA:O	2.02	0.59
1:A:903:ASN:ND2	1:A:905:ASP:N	2.50	0.59
2:B:282:ILE:HD11	2:B:317:CYS:HB3	1.85	0.59
2:B:1222:ARG:HH11	2:B:1222:ARG:CB	2.15	0.59
3:C:94:LYS:NZ	3:C:94:LYS:CD	2.59	0.59
4:E:131:THR:CB	4:E:131:THR:HA	2.17	0.59
8:J:53:HIS:ND1	8:J:54:VAL:N	2.50	0.59
1:A:122:MET:HG3	1:A:122:MET:O	2.02	0.59
1:A:1077:THR:HG22	1:A:1078:GLN:NE2	2.17	0.59
6:H:103:LYS:HE3	6:H:135:LEU:O	2.03	0.59
6:H:130:ARG:HD2	6:H:130:ARG:O	2.01	0.59
9:K:65:HIS:CD2	9:K:67:PHE:H	2.19	0.59
1:A:1172:LEU:C	1:A:1173:HIS:CD2	2.81	0.58
2:B:377:PHE:CE2	2:B:381:MET:HE2	2.38	0.58
2:B:1097:HIS:CE1	2:B:1102:LYS:HG3	2.38	0.58
3:C:120:ILE:H	3:C:120:ILE:HD12	1.68	0.58
6:H:32:THR:HB	6:H:33:GLN:OE1	2.03	0.58
1:A:535:THR:O	1:A:575:LYS:HE2	2.03	0.58
2:B:531:GLN:HE21	2:B:532:ALA:H	1.49	0.58
2:B:1221:SER:OG	5:F:72:LYS:HD2	2.02	0.58
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.27	0.58
1:A:683:ILE:HD13	1:A:725:ALA:HB1	1.85	0.58
3:C:239:PRO:O	3:C:242:GLN:HB2	2.03	0.58
1:A:770:VAL:HG23	1:A:775:ILE:HD13	1.85	0.58
1:A:1325:THR:O	4:E:148:GLU:HG2	2.02	0.58
2:B:705:MET:HB3	2:B:706:GLN:HE21	1.67	0.58
2:B:870:ILE:CB	2:B:870:ILE:HA	2.17	0.58
7:I:7:CYS:SG	7:I:32:CYS:SG	3.00	0.58
1:A:40:THR:HG23	1:A:54:ASN:ND2	2.18	0.58
2:B:1097:HIS:HA	2:B:1097:HIS:CG	2.22	0.58
2:B:1154:ALA:CB	2:B:1154:ALA:HA	2.19	0.58
4:E:83:CYS:O	4:E:113:GLN:NE2	2.35	0.58
1:A:280:GLU:HG3	1:A:289:ILE:HD12	1.86	0.58
1:A:464:PRO:O	1:A:465:TYR:O	2.22	0.58
1:A:588:LEU:HD23	1:A:588:LEU:C	2.29	0.58
2:B:134:LYS:O	2:B:135:ARG:HG3	2.03	0.58
6:H:123:MET:CE	6:H:142:LEU:HD22	2.33	0.58
1:A:107:CYS:SG	1:A:148:CYS:CB	2.92	0.58
1:A:247:ARG:HH11	1:A:263:THR:HG23	1.69	0.58
1:A:533:LYS:NZ	1:A:745:GLN:HE22	2.01	0.58
2:B:906:SER:O	2:B:907:GLY:C	2.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:PRO:O	1:A:57:ARG:CG	2.50	0.58
1:A:325:ILE:C	1:A:327:ALA:N	2.37	0.58
1:A:741:ASN:HD22	1:A:741:ASN:C	2.12	0.58
2:B:103:ASN:HB2	2:B:169:ARG:HH22	1.69	0.58
2:B:555:ILE:CD1	2:B:587:HIS:NE2	2.67	0.58
5:F:123:LYS:NZ	5:F:123:LYS:HD2	2.16	0.58
6:H:113:ALA:CB	6:H:124:ARG:HH21	2.17	0.58
7:I:111:THR:HG21	7:I:113:ASP:HB2	1.86	0.58
9:K:88:LYS:O	9:K:89:ASN:C	2.45	0.58
1:A:555:ASP:OD1	9:K:26:LYS:NZ	2.37	0.58
2:B:51:PHE:HZ	2:B:172:ILE:HD13	1.68	0.58
2:B:561:TRP:O	2:B:590:HIS:CE1	2.51	0.58
6:H:91:ASP:OD1	6:H:91:ASP:C	2.45	0.58
6:H:95:TYR:CD2	6:H:95:TYR:C	2.82	0.58
10:L:38:LEU:HG	10:L:39:SER:H	1.67	0.58
2:B:1152:MET:HA	2:B:1152:MET:CE	2.34	0.58
10:L:47:ARG:HG2	10:L:48:CYS:N	2.18	0.58
1:A:154:SER:O	1:A:155:GLU:C	2.47	0.57
1:A:1166:ASP:CB	1:A:1169:ILE:CG2	2.82	0.57
6:H:130:ARG:HB2	6:H:133:ASN:CB	2.33	0.57
7:I:3:THR:CG2	7:I:3:THR:OG1	2.47	0.57
8:J:3:VAL:HA	8:J:53:HIS:CD2	2.39	0.57
8:J:7:CYS:HA	8:J:49:MET:HE3	1.86	0.57
9:K:26:LYS:CD	9:K:26:LYS:CB	2.81	0.57
2:B:914:LYS:H	2:B:938:SER:HB2	1.69	0.57
9:K:35:PHE:CE1	9:K:73:LEU:HD12	2.36	0.57
1:A:362:ASP:OD1	1:A:459:ARG:HD3	2.04	0.57
3:C:80:LEU:HD22	3:C:129:ILE:CD1	2.34	0.57
3:C:252:GLN:HE22	9:K:99:GLY:CA	2.18	0.57
5:F:74:ILE:HD12	5:F:144:GLU:HG2	1.86	0.57
3:C:10:ILE:HD12	9:K:108:GLU:O	2.04	0.57
3:C:55:THR:HB	3:C:152:GLU:H	1.69	0.57
1:A:231:PRO:O	1:A:234:MET:HG3	2.05	0.57
1:A:1080:THR:CB	1:A:1080:THR:N	2.64	0.57
5:F:89:GLU:HG2	5:F:134:ILE:HD13	1.85	0.57
10:L:34:CYS:SG	10:L:36:SER:OG	2.63	0.57
1:A:61:ILE:CA	1:A:61:ILE:CG1	2.78	0.57
1:A:587:HIS:NE2	1:A:969:GLN:HG2	2.19	0.57
2:B:26:THR:O	2:B:27:ALA:C	2.45	0.57
2:B:890:TYR:OH	2:B:936:ASP:OD1	2.19	0.57
6:H:47:PHE:CB	6:H:95:TYR:CD1	2.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:114:VAL:HG11	6:H:134:ASN:ND2	2.18	0.57
7:I:16:PRO:O	7:I:17:ARG:CD	2.42	0.57
1:A:407:ARG:O	1:A:408:ASP:C	2.48	0.57
1:A:351:THR:HG21	2:B:1103:ILE:CG1	2.35	0.57
9:K:18:LYS:HE3	9:K:38:GLU:HG2	1.85	0.57
2:B:167:ILE:HG22	2:B:167:ILE:O	2.05	0.57
2:B:516:ASN:HD22	2:B:516:ASN:H	1.51	0.57
4:E:169:ARG:HD3	5:F:140:ASP:OD2	2.05	0.57
8:J:14:VAL:HG13	8:J:50:ILE:CD1	2.27	0.57
2:B:117:ALA:HA	2:B:122:LEU:HB2	1.86	0.56
3:C:148:ARG:O	3:C:149:LYS:C	2.48	0.56
2:B:95:ILE:HG22	2:B:96:TYR:N	2.20	0.56
2:B:555:ILE:HD13	2:B:587:HIS:CE1	2.37	0.56
1:A:903:ASN:HD21	1:A:905:ASP:HB2	1.70	0.56
1:A:982:THR:HB	1:A:985:ASP:OD2	2.05	0.56
2:B:393:LYS:HZ1	2:B:621:GLU:CD	2.12	0.56
6:H:6:PHE:CG	6:H:7:ASP:N	2.73	0.56
1:A:1236:LEU:C	1:A:1237:ILE:HD13	2.31	0.56
3:C:102:GLN:CG	3:C:102:GLN:N	2.68	0.56
3:C:133:ILE:O	3:C:134:ILE:HD13	2.05	0.56
3:C:178:PHE:C	3:C:178:PHE:CD2	2.84	0.56
1:A:155:GLU:HB2	1:A:156:ASP:OD2	2.06	0.56
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.40	0.56
5:F:114:GLU:HB2	5:F:120:ILE:HD13	1.88	0.56
1:A:34:LYS:O	1:A:35:ILE:C	2.48	0.56
1:A:73:GLY:C	1:A:75:ASN:N	2.61	0.56
1:A:843:LYS:CD	1:A:843:LYS:NZ	2.67	0.56
3:C:209:TYR:N	3:C:209:TYR:CD1	2.73	0.56
1:A:120:GLU:HG2	1:A:123:ARG:HH22	1.70	0.56
1:A:385:ILE:O	1:A:385:ILE:HD13	2.06	0.56
1:A:846:GLU:HA	1:A:1066:VAL:HG23	1.86	0.56
2:B:566:LEU:HD13	2:B:588:GLY:HA2	1.87	0.56
2:B:1152:MET:HA	2:B:1152:MET:HE2	1.87	0.56
3:C:33:LEU:CD1	3:C:248:ILE:HD13	2.36	0.56
4:E:117:THR:OG1	4:E:120:ALA:HB3	2.06	0.56
4:E:129:PRO:HD2	4:E:130:ALA:H	1.70	0.56
6:H:55:LEU:HD22	6:H:144:ILE:CD1	2.33	0.56
1:A:844:ALA:CB	1:A:1384:VAL:HG12	2.35	0.56
2:B:864:LYS:HD2	2:B:871:THR:OG1	2.05	0.56
1:A:44:THR:CA	1:A:44:THR:HB	2.18	0.56
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.71	0.56
3:C:8:VAL:HG12	3:C:9:LYS:N	2.21	0.56
6:H:127:GLY:O	6:H:128:ASN:HB2	2.05	0.56
1:A:84:ILE:CG2	1:A:241:VAL:CG2	2.84	0.55
1:A:567:LYS:HD3	6:H:95:TYR:CB	2.34	0.55
1:A:1127:ASP:HB3	1:A:1130:GLN:H	1.70	0.55
2:B:605:ARG:NE	2:B:639:ILE:HD11	2.21	0.55
6:H:6:PHE:CD2	6:H:6:PHE:C	2.84	0.55
1:A:55:ASP:C	1:A:57:ARG:H	2.09	0.55
1:A:679:ILE:HD12	1:A:729:ALA:CB	2.36	0.55
2:B:900:ALA:O	2:B:901:PRO:C	2.48	0.55
1:A:50:ILE:HG22	1:A:52:GLY:N	2.20	0.55
1:A:1215:ARG:CG	1:A:1215:ARG:CA	2.79	0.55
2:B:436:VAL:CB	2:B:436:VAL:HA	2.20	0.55
2:B:1162:ILE:HD11	2:B:1194:ILE:HG12	1.87	0.55
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.71	0.55
2:B:280:ILE:HD12	2:B:280:ILE:N	2.21	0.55
3:C:265:MET:CE	3:C:265:MET:CG	2.84	0.55
7:I:64:SER:O	7:I:66:PRO:HD3	2.07	0.55
10:L:61:THR:CG2	10:L:61:THR:OG1	2.48	0.55
10:L:51:CYS:SG	10:L:53:HIS:HB2	2.47	0.55
3:C:41:ILE:C	3:C:163:ILE:HD11	2.32	0.55
3:C:180:TYR:OH	3:C:188:HIS:ND1	2.26	0.55
9:K:18:LYS:CE	9:K:38:GLU:OE2	2.55	0.55
1:A:135:PHE:CE1	1:A:222:LEU:HD22	2.42	0.55
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.42	0.55
2:B:68:THR:HG23	2:B:91:SER:HB3	1.89	0.55
2:B:620:ARG:CG	2:B:620:ARG:HE	2.18	0.55
1:A:41:MET:O	1:A:50:ILE:HD11	2.06	0.55
1:A:834:THR:HG21	1:A:1077:THR:CA	2.37	0.55
1:A:1105:LEU:O	1:A:1383:SER:OG	2.23	0.55
2:B:846:ILE:HD11	2:B:974:PRO:C	2.31	0.55
1:A:1146:VAL:O	1:A:1146:VAL:HG13	2.07	0.55
1:A:1445:ILE:CG2	1:A:1445:ILE:HA	2.37	0.55
1:A:840:ARG:CD	1:A:840:ARG:CB	2.79	0.55
2:B:984:HIS:CD2	2:B:1025:HIS:HA	2.42	0.55
3:C:15:LYS:CD	3:C:15:LYS:CB	2.84	0.55
3:C:29:MET:CE	3:C:29:MET:HB2	2.37	0.55
6:H:47:PHE:CG	6:H:95:TYR:CD1	2.95	0.55
1:A:3:GLY:HA3	1:A:76:GLU:HG2	1.90	0.54
1:A:1146:VAL:O	1:A:1146:VAL:CG1	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:THR:HB	2:B:99:LYS:O	2.08	0.54
4:E:147:HIS:CD2	4:E:149:LEU:HB2	2.43	0.54
6:H:32:THR:CB	6:H:33:GLN:OE1	2.55	0.54
1:A:567:LYS:CD	6:H:95:TYR:CD1	2.91	0.54
1:A:597:LEU:CD1	1:A:597:LEU:HG	2.21	0.54
1:A:1261:LYS:CD	1:A:1261:LYS:NZ	2.67	0.54
2:B:1198:TYR:CE1	2:B:1201:LYS:HD2	2.42	0.54
3:C:102:GLN:N	3:C:102:GLN:HG2	2.21	0.54
3:C:116:LYS:CE	3:C:116:LYS:CG	2.81	0.54
6:H:138:GLU:O	6:H:139:ASN:O	2.25	0.54
7:I:98:VAL:HG22	7:I:99:LEU:N	2.20	0.54
9:K:46:ILE:O	9:K:47:ARG:C	2.40	0.54
1:A:540:PHE:O	1:A:541:ILE:HD13	2.07	0.54
1:A:1169:ILE:HD11	1:A:1227:ILE:HD12	1.89	0.54
2:B:526:GLU:HG2	2:B:538:ASN:ND2	2.23	0.54
6:H:4:THR:O	6:H:5:LEU:HD23	2.08	0.54
10:L:28:LYS:O	10:L:59:ALA:HB3	2.07	0.54
1:A:295:LEU:CD2	1:A:295:LEU:CD1	2.79	0.54
1:A:679:ILE:CD1	1:A:732:LEU:HB2	2.25	0.54
2:B:203:PHE:HB3	2:B:205:ILE:CD1	2.36	0.54
6:H:77:ARG:C	6:H:78:SER:O	2.49	0.54
6:H:103:LYS:CB	6:H:105:GLU:OE1	2.54	0.54
1:A:53:LEU:HD23	1:A:54:ASN:H	1.70	0.54
1:A:237:THR:CG2	1:A:237:THR:HB	2.19	0.54
1:A:1151:GLU:CG	7:I:45:ARG:CD	2.85	0.54
2:B:1006:ILE:HD11	8:J:43:ARG:HB2	1.90	0.54
8:J:42:LYS:CE	8:J:42:LYS:CG	2.83	0.54
3:C:19:ASP:C	3:C:19:ASP:OD1	2.50	0.54
4:E:154:ILE:HD13	4:E:199:ILE:HD12	1.90	0.54
7:I:65:ASP:C	7:I:65:ASP:OD1	2.50	0.54
1:A:1226:VAL:HG12	1:A:1227:ILE:N	2.20	0.54
2:B:98:THR:OG1	2:B:127:GLY:O	2.25	0.54
2:B:864:LYS:HG3	2:B:865:LYS:N	2.21	0.54
1:A:487:MET:CG	1:A:487:MET:HE3	2.20	0.54
2:B:360:PHE:O	2:B:361:LEU:C	2.51	0.54
1:A:31:SER:CB	1:A:83:HIS:CD2	2.83	0.54
1:A:369:SER:H	9:K:2:ASN:ND2	2.00	0.54
1:A:903:ASN:HD22	1:A:905:ASP:N	2.05	0.54
1:A:1166:ASP:CA	1:A:1169:ILE:HG22	2.37	0.54
2:B:899:ILE:HG22	2:B:900:ALA:H	1.72	0.54
2:B:983:ARG:HD3	14:B:3009:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:THR:CG2	3:C:44:LEU:N	2.71	0.54
8:J:1:MET:C	8:J:2:ILE:HD12	2.32	0.54
1:A:156:ASP:C	1:A:158:PRO:HD2	2.10	0.53
1:A:446:ARG:HH11	1:A:446:ARG:CG	2.19	0.53
2:B:841:MET:CE	2:B:990:ILE:HD11	2.37	0.53
3:C:102:GLN:CB	3:C:102:GLN:CD	2.78	0.53
6:H:59:ILE:HG22	6:H:60:ALA:N	2.23	0.53
1:A:741:ASN:C	1:A:741:ASN:ND2	2.67	0.53
4:E:117:THR:OG1	4:E:120:ALA:HB2	2.09	0.53
1:A:268:ASP:HB3	1:A:299:HIS:CD2	2.44	0.53
2:B:102:VAL:O	2:B:109:THR:HA	2.09	0.53
3:C:80:LEU:HD12	3:C:94:LYS:O	2.08	0.53
1:A:84:ILE:HG22	1:A:241:VAL:CG2	2.38	0.53
1:A:134:ARG:O	1:A:138:ILE:CG2	2.55	0.53
1:A:189:ARG:O	1:A:190:ALA:CB	2.55	0.53
1:A:518:LYS:NZ	1:A:518:LYS:HD3	2.14	0.53
1:A:601:LYS:CD	1:A:601:LYS:NZ	2.70	0.53
1:A:913:LEU:HD11	1:A:981:LEU:O	2.08	0.53
3:C:40:GLU:OE1	3:C:254:LYS:NZ	2.42	0.53
3:C:80:LEU:HD22	3:C:129:ILE:HD13	1.91	0.53
5:F:109:VAL:HG22	5:F:127:GLU:OE1	2.09	0.53
1:A:172:PRO:HG2	1:A:185:TRP:CH2	2.31	0.53
1:A:636:GLU:OE2	1:A:962:ARG:CD	2.56	0.53
2:B:999:MET:HB3	2:B:1000:PRO:HD2	1.89	0.53
3:C:8:VAL:CG1	3:C:9:LYS:H	2.22	0.53
3:C:70:ILE:HD11	3:C:144:ILE:HD12	1.90	0.53
1:A:1341:ILE:HD12	1:A:1379:GLY:C	2.33	0.53
2:B:620:ARG:HG2	7:I:62:ILE:CD1	2.38	0.53
3:C:242:GLN:HE21	3:C:246:ARG:HH21	1.56	0.53
1:A:93:VAL:HA	1:A:96:ILE:CD1	2.39	0.53
1:A:487:MET:CG	1:A:487:MET:HE2	2.20	0.53
2:B:249:ARG:NH1	2:B:418:LYS:NZ	2.57	0.53
2:B:417:PHE:C	2:B:417:PHE:HD2	2.16	0.53
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.37	0.53
6:H:62:SER:O	6:H:63:LEU:O	2.26	0.53
6:H:105:GLU:C	6:H:107:VAL:N	2.63	0.53
1:A:704:ALA:HB1	1:A:708:MET:O	2.09	0.53
2:B:1002:THR:HG22	2:B:1006:ILE:N	2.24	0.53
5:F:72:LYS:CE	5:F:72:LYS:CG	2.85	0.53
6:H:4:THR:C	6:H:5:LEU:HD23	2.33	0.53
10:L:58:LYS:O	10:L:59:ALA:CB	2.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:HG21	1:A:214:ILE:HG12	1.90	0.53
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.43	0.53
1:A:1151:GLU:HG2	7:I:45:ARG:CD	2.39	0.53
3:C:169:LYS:NZ	10:L:69:ALA:O	2.41	0.53
6:H:37:LYS:O	6:H:125:LEU:HA	2.09	0.53
7:I:49:ILE:HG22	7:I:49:ILE:O	2.09	0.53
1:A:63:ARG:HA	1:A:74:MET:SD	2.49	0.52
1:A:535:THR:HG23	1:A:616:VAL:HA	1.91	0.52
4:E:37:LEU:CD1	4:E:37:LEU:HG	2.20	0.52
4:E:63:ASN:O	4:E:64:PRO:C	2.44	0.52
8:J:1:MET:CB	8:J:1:MET:HE3	2.39	0.52
1:A:693:VAL:HG21	1:A:721:PHE:CE1	2.42	0.52
1:A:752:LYS:HD2	2:B:1015:HIS:O	2.09	0.52
2:B:431:TYR:CE1	2:B:447:ALA:CB	2.91	0.52
2:B:1065:GLN:NE2	2:B:1067:ARG:N	2.56	0.52
1:A:541:ILE:HD11	1:A:656:TRP:HE1	1.73	0.52
6:H:9:ILE:CA	6:H:9:ILE:CG2	2.81	0.52
1:A:964:ILE:CD1	1:A:964:ILE:N	2.72	0.52
1:A:1262:LYS:CG	1:A:1262:LYS:CE	2.82	0.52
4:E:127:ILE:N	4:E:128:PRO:CD	2.72	0.52
1:A:351:THR:HG23	2:B:1103:ILE:CG1	2.40	0.52
1:A:1318:THR:CG2	4:E:11:ARG:HH12	2.22	0.52
2:B:424:LEU:O	2:B:428:ILE:HG13	2.08	0.52
4:E:37:LEU:C	4:E:38:PRO:O	2.50	0.52
4:E:117:THR:C	4:E:119:SER:N	2.67	0.52
6:H:55:LEU:CD2	6:H:144:ILE:HD12	2.33	0.52
1:A:120:GLU:HG2	1:A:123:ARG:NH2	2.25	0.52
1:A:1341:ILE:HD13	4:E:212:ARG:NH2	2.24	0.52
3:C:114:TYR:HB3	3:C:140:ASN:O	2.10	0.52
5:F:83:PRO:HA	5:F:146:TRP:CZ3	2.44	0.52
1:A:42:ASP:OD2	1:A:47:ARG:CG	2.58	0.52
2:B:724:ASP:O	2:B:725:PRO:C	2.51	0.52
2:B:789:MET:CE	2:B:789:MET:CG	2.88	0.52
13:B:3008:GTP:N9	13:B:3008:GTP:C2'	2.68	0.52
6:H:106:GLU:O	6:H:108:SER:N	2.40	0.52
1:A:99:ILE:HG12	1:A:234:MET:HE3	1.91	0.52
1:A:973:ILE:CG2	1:A:973:ILE:CA	2.82	0.52
1:A:186:LYS:HZ3	1:A:195:ASP:HA	1.70	0.52
1:A:973:ILE:CG2	1:A:973:ILE:CG1	2.81	0.52
1:A:1035:TYR:O	1:A:1036:ARG:HB2	2.10	0.52
1:A:1111:MET:HE1	1:A:1331:SER:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1195:LEU:HD11	1:A:1267:MET:HE1	1.92	0.52
1:A:1336:MET:HE2	1:A:1381:LEU:N	2.22	0.52
2:B:59:LEU:HG	2:B:95:ILE:HD13	1.92	0.52
2:B:775:LYS:CG	2:B:775:LYS:CA	2.82	0.52
3:C:94:LYS:NZ	3:C:94:LYS:CG	2.72	0.52
6:H:97:MET:HE3	6:H:118:PHE:CD1	2.45	0.52
7:I:43:VAL:O	7:I:43:VAL:HG12	2.09	0.52
1:A:186:LYS:HG3	1:A:197:PRO:HD3	1.92	0.51
2:B:705:MET:CG	2:B:705:MET:HE3	2.28	0.51
2:B:757:PRO:HG2	2:B:984:HIS:HE1	1.75	0.51
4:E:52:ARG:HG3	4:E:53:PRO:HD3	1.91	0.51
10:L:68:GLU:O	10:L:69:ALA:HB3	2.10	0.51
1:A:186:LYS:NZ	1:A:195:ASP:CA	2.67	0.51
1:A:1143:LEU:O	1:A:1144:LYS:C	2.53	0.51
1:A:1287:TYR:O	1:A:1302:PRO:HA	2.10	0.51
1:A:1341:ILE:CD1	1:A:1379:GLY:HA2	2.36	0.51
2:B:727:LYS:HE2	2:B:1049:ASP:CG	2.35	0.51
2:B:864:LYS:HB2	2:B:871:THR:HA	1.92	0.51
3:C:73:GLN:HA	3:C:133:ILE:HD11	1.91	0.51
7:I:45:ARG:CD	7:I:45:ARG:CB	2.80	0.51
1:A:237:THR:CG2	1:A:237:THR:C	2.82	0.51
1:A:598:LEU:HD21	6:H:124:ARG:HB2	1.92	0.51
1:A:64:ASN:OD1	1:A:64:ASN:C	2.53	0.51
2:B:43:LEU:HD11	2:B:811:TYR:O	2.11	0.51
2:B:705:MET:CE	2:B:705:MET:HG3	2.36	0.51
2:B:843:GLN:HE22	2:B:846:ILE:HG21	1.75	0.51
3:C:209:TYR:HD1	3:C:209:TYR:N	2.08	0.51
7:I:10:CYS:SG	7:I:32:CYS:SG	3.09	0.51
1:A:689:LYS:O	1:A:693:VAL:HG23	2.10	0.51
6:H:113:ALA:HB2	6:H:124:ARG:NH2	2.25	0.51
1:A:551:TYR:CD2	9:K:62:LYS:HD3	2.46	0.51
2:B:744:HIS:CD2	2:B:746:SER:H	2.24	0.51
2:B:792:MET:SD	2:B:857:ARG:NH2	2.84	0.51
2:B:1019:SER:HB2	13:B:3008:GTP:N7	2.26	0.51
4:E:162:ARG:CG	4:E:162:ARG:CA	2.86	0.51
7:I:14:LEU:HB3	7:I:27:PHE:HB3	1.92	0.51
1:A:110:CYS:SG	1:A:167:CYS:SG	3.09	0.51
9:K:18:LYS:HE2	9:K:38:GLU:OE2	2.10	0.51
5:F:81:THR:HG22	5:F:136:ARG:HH11	1.71	0.51
6:H:44:VAL:O	6:H:44:VAL:HG13	2.11	0.51
1:A:135:PHE:HD1	1:A:222:LEU:HD22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ARG:O	1:A:190:ALA:HB3	2.11	0.51
2:B:884:ARG:HG2	2:B:884:ARG:HH11	1.76	0.51
4:E:176:PRO:O	4:E:212:ARG:HA	2.11	0.51
6:H:130:ARG:HB2	6:H:133:ASN:HB3	1.92	0.51
6:H:135:LEU:HD13	6:H:139:ASN:O	2.11	0.51
1:A:351:THR:CG2	2:B:1103:ILE:HG13	2.40	0.51
3:C:196:ASP:HB3	3:C:199:LYS:HG3	1.91	0.51
3:C:214:ASN:O	3:C:217:ASP:HB2	2.11	0.51
1:A:328:ARG:NH1	1:A:1405:THR:HG22	2.24	0.50
2:B:1051:THR:CG2	2:B:1053:GLU:H	2.14	0.50
2:B:486:TYR:CZ	2:B:1096:ARG:NH2	2.79	0.50
1:A:35:ILE:HD13	1:A:241:VAL:HG11	1.93	0.50
1:A:279:LEU:H	1:A:281:HIS:H	1.59	0.50
1:A:1130:GLN:CG	1:A:1130:GLN:NE2	2.65	0.50
2:B:435:THR:O	2:B:435:THR:CG2	2.59	0.50
2:B:436:VAL:CA	2:B:436:VAL:CG2	2.79	0.50
2:B:662:MET:CE	2:B:662:MET:CG	2.90	0.50
3:C:252:GLN:NE2	9:K:99:GLY:H	2.09	0.50
6:H:48:PRO:C	6:H:49:VAL:HG23	2.36	0.50
9:K:111:LEU:N	9:K:111:LEU:HD23	2.27	0.50
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.94	0.50
2:B:435:THR:HG23	2:B:437:GLU:HB2	1.93	0.50
3:C:162:GLY:HA3	3:C:170:TRP:CD2	2.46	0.50
4:E:117:THR:C	4:E:119:SER:H	2.19	0.50
6:H:77:ARG:HB2	6:H:77:ARG:HH11	1.76	0.50
1:A:121:LEU:HB3	1:A:141:LEU:HD21	1.94	0.50
1:A:365:GLY:HA2	1:A:461:LYS:O	2.11	0.50
1:A:679:ILE:HD12	1:A:729:ALA:HB1	1.94	0.50
1:A:1134:ILE:O	1:A:1138:ILE:CD1	2.59	0.50
1:A:1449:SER:HB2	5:F:149:GLU:OE2	2.11	0.50
2:B:167:ILE:HD12	2:B:167:ILE:N	2.26	0.50
5:F:109:VAL:HG12	5:F:110:ASP:N	2.24	0.50
1:A:93:VAL:HA	1:A:96:ILE:HD13	1.94	0.50
1:A:466:SER:CB	2:B:1103:ILE:HD11	2.41	0.50
1:A:587:HIS:CD2	1:A:966:ASN:OD1	2.58	0.50
1:A:664:THR:HG22	1:A:742:ASN:HB3	1.93	0.50
2:B:458:LYS:NZ	2:B:958:GLN:NE2	2.59	0.50
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.47	0.50
2:B:436:VAL:CB	2:B:436:VAL:N	2.69	0.50
2:B:1097:HIS:CB	2:B:1097:HIS:N	2.66	0.50
1:A:1112:LYS:CG	1:A:1112:LYS:CA	2.81	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:4:PRO:HD3	8:J:53:HIS:HD2	1.77	0.50
1:A:63:ARG:HA	1:A:74:MET:CG	2.40	0.50
1:A:89:PRO:CB	1:A:204:THR:HG21	2.28	0.50
2:B:512:ARG:HB2	14:B:3017:HOH:O	2.12	0.50
2:B:843:GLN:NE2	2:B:846:ILE:HG21	2.27	0.50
1:A:55:ASP:N	1:A:56:PRO:HD2	2.25	0.49
1:A:328:ARG:NH1	1:A:1405:THR:CG2	2.75	0.49
1:A:481:ASP:CG	1:A:481:ASP:C	2.80	0.49
1:A:1081:LEU:CD2	1:A:1081:LEU:CD1	2.81	0.49
2:B:516:ASN:H	2:B:516:ASN:ND2	2.10	0.49
2:B:956:THR:HA	2:B:961:LEU:O	2.12	0.49
7:I:16:PRO:HG3	7:I:27:PHE:HE2	1.76	0.49
1:A:69:THR:CG2	2:B:1174:LYS:HE2	2.42	0.49
1:A:913:LEU:HD12	1:A:914:GLU:N	2.27	0.49
1:A:1224:LEU:HG	1:A:1225:PHE:N	2.27	0.49
2:B:345:LYS:O	2:B:346:GLU:C	2.51	0.49
3:C:218:PRO:O	3:C:219:PHE:C	2.55	0.49
3:C:252:GLN:NE2	9:K:99:GLY:N	2.60	0.49
1:A:858:ASN:C	1:A:858:ASN:HD22	2.20	0.49
4:E:63:ASN:C	4:E:64:PRO:O	2.55	0.49
10:L:48:CYS:HB3	10:L:51:CYS:O	2.13	0.49
1:A:853:ASP:O	1:A:854:ASN:HB2	2.12	0.49
1:A:867:ILE:HD12	1:A:1000:LEU:HD21	1.95	0.49
2:B:235:SER:OG	2:B:236:HIS:HD2	1.96	0.49
6:H:103:LYS:HG2	6:H:105:GLU:OE2	2.12	0.49
10:L:26:THR:CG2	10:L:27:LEU:H	2.26	0.49
2:B:1014:PRO:HA	2:B:1017:ILE:HD12	1.94	0.49
2:B:365:THR:HG22	2:B:367:LEU:H	1.76	0.49
3:C:196:ASP:CG	3:C:199:LYS:HG3	2.38	0.49
7:I:55:THR:CG2	7:I:55:THR:HB	2.29	0.49
10:L:30:ILE:HG22	10:L:31:CYS:N	2.27	0.49
10:L:32:ALA:HB2	10:L:55:ILE:HG22	1.93	0.49
1:A:1162:VAL:CG1	1:A:1162:VAL:O	2.61	0.49
2:B:237:VAL:HG12	2:B:238:ALA:N	2.28	0.49
3:C:252:GLN:HE22	9:K:99:GLY:HA2	1.75	0.49
6:H:19:ARG:CD	6:H:19:ARG:HA	2.43	0.49
7:I:4:PHE:CZ	7:I:13:MET:HE2	2.42	0.49
1:A:507:VAL:N	1:A:508:PRO:CD	2.75	0.49
1:A:560:ILE:HD12	1:A:560:ILE:N	2.26	0.49
1:A:983:ILE:N	1:A:983:ILE:HD12	2.28	0.49
2:B:284:ILE:HD11	2:B:321:GLY:HA2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:453:ILE:HG22	2:B:454:THR:N	2.28	0.49
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.95	0.49
4:E:41:ASP:O	4:E:42:PHE:C	2.53	0.49
8:J:53:HIS:ND1	8:J:53:HIS:C	2.70	0.49
1:A:706:HIS:CE1	1:A:1135:ARG:HD3	2.48	0.49
1:A:1151:GLU:OE2	7:I:45:ARG:CD	2.59	0.49
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.95	0.49
2:B:531:GLN:HE21	2:B:532:ALA:N	2.10	0.49
2:B:1190:ASP:C	2:B:1191:ILE:HG13	2.36	0.49
6:H:103:LYS:CE	6:H:135:LEU:O	2.60	0.49
1:A:229:SER:O	1:A:229:SER:OG	2.25	0.49
1:A:481:ASP:CG	1:A:481:ASP:N	2.70	0.49
1:A:1166:ASP:CA	1:A:1169:ILE:CG2	2.91	0.49
1:A:1436:ILE:CD1	2:B:1144:ALA:HB2	2.42	0.49
2:B:121:ASN:HD21	2:B:965:LYS:NZ	2.10	0.49
2:B:821:GLN:OE1	2:B:850:LEU:HD12	2.12	0.49
6:H:81:PRO:C	6:H:82:PRO:O	2.55	0.49
7:I:71:SER:OG	7:I:83:ASN:ND2	2.45	0.49
1:A:599:SER:O	1:A:600:PRO:C	2.56	0.48
1:A:1162:VAL:CG1	1:A:1162:VAL:CG2	2.81	0.48
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.95	0.48
10:L:38:LEU:O	10:L:39:SER:HB2	2.13	0.48
10:L:48:CYS:C	10:L:48:CYS:CB	2.76	0.48
1:A:44:THR:CB	1:A:44:THR:HA	2.21	0.48
1:A:531:ILE:O	1:A:531:ILE:HD13	2.13	0.48
1:A:768:GLN:NE2	1:A:816:HIS:HA	2.28	0.48
1:A:1111:MET:SD	1:A:1111:MET:CB	2.92	0.48
1:A:1161:THR:HG23	1:A:1163:ILE:H	1.77	0.48
6:H:103:LYS:O	6:H:115:TYR:CD1	2.63	0.48
1:A:144:THR:HG22	1:A:145:LYS:N	2.28	0.48
1:A:278:THR:O	1:A:278:THR:HG22	2.13	0.48
1:A:596:THR:HG22	1:A:597:LEU:HD12	1.94	0.48
1:A:1318:THR:HG23	4:E:11:ARG:NH1	2.28	0.48
1:A:1405:THR:CB	1:A:1405:THR:C	2.80	0.48
2:B:498:THR:HG21	2:B:537:LYS:HB2	1.95	0.48
2:B:1006:ILE:HD11	8:J:43:ARG:CB	2.43	0.48
2:B:1153:GLU:OE1	2:B:1153:GLU:HA	2.13	0.48
4:E:65:THR:O	4:E:69:ILE:CG1	2.60	0.48
6:H:89:LEU:O	6:H:90:ALA:C	2.50	0.48
7:I:29:CYS:SG	7:I:31:THR:HB	2.54	0.48
1:A:786:HIS:N	1:A:786:HIS:CD2	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:841:MET:HE3	2:B:990:ILE:CD1	2.42	0.48
8:J:1:MET:CE	8:J:1:MET:HG3	2.43	0.48
1:A:66:LYS:CB	1:A:66:LYS:CD	2.84	0.48
1:A:187:LYS:HD2	1:A:194:ALA:HB2	1.94	0.48
1:A:295:LEU:CD2	1:A:295:LEU:HG	2.19	0.48
1:A:503:GLN:HE21	5:F:90:ARG:HH21	1.61	0.48
3:C:183:TRP:NE1	3:C:207:CYS:HB3	2.28	0.48
6:H:9:ILE:CA	6:H:9:ILE:CG1	2.83	0.48
6:H:33:GLN:C	6:H:35:GLN:H	2.22	0.48
1:A:901:LEU:CD2	1:A:919:ILE:HD12	2.43	0.48
2:B:65:GLU:HG2	2:B:66:ASP:N	2.27	0.48
2:B:213:ILE:HD13	2:B:481:GLN:HG3	1.95	0.48
2:B:350:GLN:HG3	2:B:350:GLN:O	2.13	0.48
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.96	0.48
4:E:5:ASN:O	4:E:9:ILE:HG13	2.13	0.48
6:H:5:LEU:O	6:H:133:ASN:ND2	2.46	0.48
6:H:100:THR:O	6:H:116:TYR:HA	2.13	0.48
1:A:373:THR:O	1:A:373:THR:HG22	2.12	0.48
2:B:230:ALA:CB	2:B:230:ALA:C	2.81	0.48
2:B:313:MET:CE	2:B:386:LEU:HD22	2.39	0.48
2:B:758:PHE:N	2:B:759:PRO:CD	2.76	0.48
2:B:986:GLN:CD	2:B:986:GLN:CB	2.83	0.48
4:E:93:MET:CE	4:E:116:ILE:HG21	2.43	0.48
6:H:98:TYR:C	6:H:118:PHE:HD2	2.21	0.48
7:I:58:VAL:HG11	7:I:109:ILE:HD11	1.96	0.48
9:K:10:PHE:HD1	9:K:11:LEU:HD13	1.78	0.48
1:A:153:PRO:CD	1:A:161:LEU:CD2	2.66	0.48
1:A:466:SER:HB3	2:B:1103:ILE:HD11	1.94	0.48
1:A:476:SER:N	1:A:477:PRO:HD2	2.29	0.48
1:A:518:LYS:CD	1:A:518:LYS:HZ3	2.20	0.48
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.40	0.48
1:A:901:LEU:HD21	1:A:919:ILE:HD12	1.95	0.48
1:A:1102:LYS:CD	1:A:1102:LYS:NZ	2.69	0.48
2:B:1128:LEU:HG	2:B:1128:LEU:O	2.14	0.48
4:E:115:ASN:C	4:E:116:ILE:HD13	2.38	0.48
1:A:92:HIS:HD2	1:A:94:GLY:N	2.12	0.48
1:A:387:ARG:O	1:A:388:LEU:C	2.51	0.48
2:B:1220:ARG:O	2:B:1222:ARG:CD	2.57	0.48
3:C:29:MET:HB2	3:C:29:MET:HE2	1.96	0.48
3:C:131:HIS:O	3:C:132:PRO:C	2.57	0.48
6:H:40:LEU:HD12	6:H:41:ASP:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:H	1:A:56:PRO:HD3	1.77	0.48
1:A:472:LEU:O	1:A:475:THR:HB	2.14	0.48
1:A:664:THR:HG21	1:A:746:MET:CE	2.44	0.48
2:B:121:ASN:N	2:B:121:ASN:HD22	2.11	0.48
2:B:185:THR:HG23	2:B:188:ASP:OD2	2.14	0.48
2:B:203:PHE:HB3	2:B:205:ILE:HD11	1.96	0.48
2:B:498:THR:HG22	2:B:537:LYS:HB2	1.95	0.48
3:C:94:LYS:NZ	3:C:94:LYS:HG2	2.28	0.48
9:K:18:LYS:HE3	9:K:38:GLU:CG	2.44	0.48
9:K:82:ASP:OD1	9:K:83:PRO:HG2	2.14	0.48
5:F:109:VAL:HG13	5:F:110:ASP:N	2.29	0.47
1:A:670:ILE:HD13	2:B:1067:ARG:CZ	2.43	0.47
2:B:117:ALA:O	2:B:207:GLY:HA2	2.14	0.47
3:C:73:GLN:HE21	3:C:75:MET:N	2.08	0.47
1:A:274:ILE:CA	1:A:274:ILE:CG1	2.84	0.47
1:A:1291:VAL:O	1:A:1291:VAL:HG12	2.10	0.47
2:B:705:MET:CG	2:B:705:MET:HE2	2.28	0.47
2:B:864:LYS:O	2:B:961:LEU:CD2	2.62	0.47
2:B:899:ILE:HD12	2:B:911:ILE:HA	1.97	0.47
3:C:180:TYR:CD1	3:C:180:TYR:C	2.93	0.47
3:C:240:VAL:C	3:C:242:GLN:N	2.70	0.47
9:K:65:HIS:CD2	9:K:66:PRO:HD2	2.49	0.47
1:A:64:ASN:O	1:A:66:LYS:N	2.46	0.47
1:A:399:HIS:HE1	1:A:436:ILE:O	1.97	0.47
1:A:720:ARG:O	1:A:724:GLU:HB3	2.14	0.47
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	2.14	0.47
1:A:1436:ILE:HD12	2:B:1144:ALA:HB2	1.97	0.47
4:E:31:THR:O	4:E:32:GLN:C	2.55	0.47
6:H:95:TYR:C	6:H:95:TYR:HD2	2.22	0.47
1:A:84:ILE:HG22	1:A:241:VAL:HG21	1.96	0.47
1:A:138:ILE:HD12	1:A:142:CYS:SG	2.54	0.47
1:A:325:ILE:HG22	2:B:1210:MET:HE2	1.97	0.47
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.28	0.47
2:B:213:ILE:CD1	2:B:481:GLN:CD	2.88	0.47
2:B:1177:HIS:HB2	2:B:1179:GLN:NE2	2.29	0.47
6:H:32:THR:CG2	6:H:33:GLN:CD	2.87	0.47
10:L:47:ARG:CG	10:L:48:CYS:H	2.18	0.47
2:B:101:MET:HA	2:B:110:HIS:O	2.14	0.47
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.96	0.47
7:I:35:VAL:O	7:I:35:VAL:HG23	2.06	0.47
1:A:34:LYS:HG2	1:A:83:HIS:HE1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:LYS:CD	2:B:1015:HIS:O	2.62	0.47
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.96	0.47
1:A:1134:ILE:HG22	1:A:1306:LEU:HD11	1.97	0.47
1:A:1150:SER:OG	7:I:46:HIS:HB3	2.15	0.47
1:A:1287:TYR:CD1	1:A:1305:VAL:HG21	2.49	0.47
2:B:169:ARG:O	2:B:457:LEU:HD12	2.14	0.47
2:B:259:TYR:HB2	2:B:268:THR:HG22	1.97	0.47
2:B:864:LYS:O	2:B:961:LEU:HD23	2.13	0.47
2:B:1212:ILE:O	2:B:1214:PRO:HD3	2.15	0.47
6:H:37:LYS:O	6:H:125:LEU:HD23	2.14	0.47
6:H:76:THR:O	6:H:76:THR:CG2	2.61	0.47
1:A:605:MET:HG3	1:A:607:ILE:HD12	1.97	0.47
1:A:1111:MET:HE1	1:A:1331:SER:CB	2.45	0.47
2:B:97:VAL:HG12	2:B:178:ASN:HD21	1.80	0.47
2:B:393:LYS:NZ	2:B:621:GLU:CD	2.73	0.47
2:B:616:ILE:HD13	2:B:696:GLU:HG3	1.97	0.47
2:B:1002:THR:CG2	2:B:1006:ILE:HB	2.44	0.47
3:C:47:ASP:CG	3:C:47:ASP:O	2.56	0.47
6:H:113:ALA:HA	6:H:125:LEU:O	2.15	0.47
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.97	0.47
1:A:922:ASP:C	1:A:922:ASP:OD1	2.58	0.47
2:B:509:ALA:C	2:B:511:PRO:HD3	2.39	0.47
2:B:955:THR:CG2	10:L:55:ILE:HA	2.45	0.47
3:C:120:ILE:HD12	3:C:120:ILE:N	2.29	0.47
1:A:555:ASP:OD1	9:K:26:LYS:CE	2.63	0.47
6:H:138:GLU:C	6:H:140:ALA:N	2.67	0.47
1:A:413:ILE:N	1:A:413:ILE:HD12	2.30	0.46
1:A:913:LEU:HD12	1:A:913:LEU:C	2.30	0.46
1:A:1111:MET:HE3	1:A:1111:MET:HB2	1.97	0.46
1:A:1445:ILE:HD13	1:A:1445:ILE:N	2.30	0.46
2:B:916:THR:O	2:B:916:THR:HG22	2.14	0.46
3:C:52:GLU:HA	10:L:64:LEU:HD21	1.97	0.46
4:E:61:GLN:HG3	4:E:62:ALA:N	2.29	0.46
6:H:9:ILE:CA	6:H:9:ILE:HB	2.20	0.46
6:H:97:MET:HE2	6:H:142:LEU:HD23	1.97	0.46
2:B:755:ILE:HD12	2:B:814:PHE:CD1	2.51	0.46
2:B:827:ILE:HG12	2:B:1012:ILE:HD11	1.96	0.46
2:B:1027:ILE:HG21	2:B:1027:ILE:HD13	1.56	0.46
1:A:110:CYS:SG	1:A:167:CYS:CB	3.04	0.46
1:A:119:ASN:O	1:A:120:GLU:CB	2.45	0.46
1:A:1154:TYR:CZ	1:A:1156:PRO:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:566:LEU:HD12	2:B:566:LEU:HA	1.78	0.46
2:B:844:SER:O	2:B:847:ASP:HB2	2.15	0.46
1:A:26:GLU:HA	1:A:29:ALA:HB3	1.96	0.46
1:A:46:THR:HB	1:A:46:THR:C	2.37	0.46
1:A:1127:ASP:OD2	1:A:1130:GLN:HB2	2.15	0.46
2:B:134:LYS:HE3	2:B:134:LYS:HB2	1.74	0.46
2:B:458:LYS:HZ1	2:B:958:GLN:NE2	2.12	0.46
2:B:820:GLY:HA3	2:B:1091:TYR:CZ	2.51	0.46
6:H:101:ALA:HA	6:H:116:TYR:H	1.81	0.46
1:A:265:LYS:HZ2	1:A:302:THR:CG2	2.23	0.46
2:B:65:GLU:O	2:B:67:SER:N	2.49	0.46
2:B:1058:LEU:O	2:B:1062:HIS:HD2	1.98	0.46
1:A:145:LYS:HE2	1:A:149:GLU:CD	2.40	0.46
1:A:153:PRO:CD	1:A:161:LEU:HD22	2.30	0.46
1:A:523:ILE:HB	1:A:622:VAL:CG1	2.45	0.46
1:A:567:LYS:HG2	6:H:96:VAL:O	2.14	0.46
1:A:901:LEU:HD11	1:A:919:ILE:HD12	1.98	0.46
1:A:1322:ILE:C	1:A:1322:ILE:HD12	2.41	0.46
2:B:952:VAL:HG22	2:B:966:VAL:HG22	1.97	0.46
10:L:47:ARG:CG	10:L:48:CYS:N	2.75	0.46
1:A:80:HIS:O	1:A:243:PRO:HD3	2.16	0.46
1:A:551:TYR:CE2	9:K:62:LYS:HD3	2.50	0.46
1:A:595:THR:CG2	1:A:596:THR:N	2.77	0.46
1:A:956:LEU:HB3	1:A:957:PRO:HD2	1.97	0.46
1:A:1055:ARG:NE	1:A:1055:ARG:HG3	2.25	0.46
2:B:515:HIS:CB	2:B:518:HIS:CD2	2.98	0.46
2:B:1195:HIS:C	2:B:1196:ILE:HG23	2.40	0.46
6:H:106:GLU:HB2	6:H:113:ALA:HB3	1.96	0.46
9:K:47:ARG:C	9:K:47:ARG:HD2	2.41	0.46
1:A:328:ARG:HH11	1:A:1405:THR:CG2	2.28	0.46
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.43	0.46
2:B:261:ARG:O	2:B:264:SER:N	2.48	0.46
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.80	0.46
4:E:44:ALA:O	4:E:46:TYR:N	2.49	0.46
4:E:61:GLN:HB2	4:E:79:TRP:HE3	1.81	0.46
9:K:78:THR:HG22	9:K:79:GLU:H	1.81	0.46
10:L:26:THR:CG2	10:L:26:THR:OG1	2.57	0.46
1:A:34:LYS:HG2	1:A:83:HIS:CE1	2.51	0.46
2:B:622:LYS:NZ	2:B:622:LYS:CD	2.70	0.46
4:E:55:ARG:O	4:E:58:MET:HB2	2.16	0.46
8:J:53:HIS:HD1	8:J:54:VAL:N	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:919:ILE:HD13	1:A:983:ILE:CD1	2.45	0.46
1:A:920:LEU:HD22	1:A:921:GLY:N	2.31	0.46
2:B:227:LYS:NZ	2:B:236:HIS:HE1	2.13	0.46
2:B:1079:LYS:HG3	3:C:180:TYR:HH	1.80	0.46
4:E:161:LYS:CE	4:E:172:GLU:OE2	2.64	0.46
5:F:89:GLU:CG	5:F:134:ILE:HD13	2.45	0.46
6:H:113:ALA:CB	6:H:124:ARG:NH2	2.79	0.46
6:H:113:ALA:HB2	6:H:124:ARG:HH21	1.81	0.46
1:A:535:THR:CG2	1:A:617:VAL:N	2.66	0.45
1:A:1293:SER:HB2	1:A:1294:PRO:HD2	1.98	0.45
1:A:1362:TYR:CD2	1:A:1362:TYR:C	2.93	0.45
2:B:249:ARG:NH1	2:B:418:LYS:HZ2	2.14	0.45
9:K:98:LEU:O	9:K:99:GLY:C	2.58	0.45
1:A:195:ASP:O	1:A:196:GLU:CB	2.64	0.45
1:A:1258:HIS:O	1:A:1259:MET:C	2.59	0.45
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.98	0.45
1:A:1410:PHE:HD2	2:B:1212:ILE:CD1	2.29	0.45
2:B:723:VAL:CA	2:B:723:VAL:HB	2.23	0.45
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.76	0.45
4:E:12:LEU:CD2	4:E:58:MET:SD	2.88	0.45
5:F:128:LYS:NZ	5:F:151:LEU:O	2.46	0.45
1:A:92:HIS:HD2	1:A:94:GLY:H	1.64	0.45
1:A:436:ILE:HD13	1:A:436:ILE:HG21	1.63	0.45
3:C:15:LYS:O	3:C:240:VAL:CG2	2.64	0.45
6:H:142:LEU:HG	6:H:143:LEU:N	2.26	0.45
8:J:42:LYS:HG3	8:J:43:ARG:N	2.32	0.45
1:A:83:HIS:ND1	1:A:83:HIS:C	2.74	0.45
1:A:98:LYS:O	1:A:102:VAL:HG23	2.15	0.45
1:A:216:VAL:HA	1:A:219:PHE:CE2	2.52	0.45
1:A:264:PHE:O	1:A:267:ALA:HB3	2.17	0.45
1:A:1055:ARG:CG	1:A:1055:ARG:HE	2.27	0.45
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.98	0.45
4:E:55:ARG:O	4:E:56:LYS:C	2.59	0.45
1:A:605:MET:CE	1:A:607:ILE:CG1	2.95	0.45
1:A:1109:LYS:CG	1:A:1109:LYS:CA	2.80	0.45
2:B:121:ASN:HD22	2:B:121:ASN:H	1.63	0.45
2:B:282:ILE:HD11	2:B:317:CYS:SG	2.57	0.45
2:B:642:ASP:HA	2:B:643:ASP:HA	1.29	0.45
7:I:43:VAL:O	7:I:43:VAL:CG1	2.64	0.45
9:K:102:LYS:O	9:K:106:GLU:HB2	2.17	0.45
9:K:110:ASN:C	9:K:112:GLN:N	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:ILE:CB	1:A:622:VAL:HG13	2.45	0.45
1:A:925:LEU:HD23	1:A:925:LEU:HA	1.82	0.45
1:A:1166:ASP:O	1:A:1169:ILE:HG23	2.16	0.45
1:A:1385:THR:CG2	1:A:1385:THR:HB	2.19	0.45
2:B:206:ASN:OD1	2:B:458:LYS:HE3	2.15	0.45
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.65	0.45
2:B:916:THR:HB	2:B:935:ARG:HB2	1.98	0.45
4:E:39:LEU:O	4:E:42:PHE:HB3	2.17	0.45
1:A:127:ALA:O	1:A:128:ILE:C	2.59	0.45
1:A:511:ILE:HD13	1:A:646:PHE:HE1	1.81	0.45
1:A:597:LEU:H	1:A:597:LEU:HD12	1.81	0.45
1:A:771:GLU:CD	2:B:510:LYS:HZ3	2.24	0.45
1:A:908:LEU:HA	1:A:908:LEU:HD23	1.77	0.45
1:A:1192:LEU:HD11	1:A:1239:ARG:HB2	1.99	0.45
2:B:246:LYS:CA	2:B:247:GLY:N	2.66	0.45
3:C:56:THR:CG2	3:C:58:LEU:H	2.29	0.45
5:F:128:LYS:HD3	5:F:128:LYS:HA	1.76	0.45
8:J:53:HIS:CE1	8:J:55:ASP:N	2.85	0.45
8:J:53:HIS:C	8:J:53:HIS:HD1	2.24	0.45
8:J:62:ARG:HE	8:J:62:ARG:HB3	1.29	0.45
1:A:61:ILE:CA	1:A:61:ILE:CG2	2.86	0.45
1:A:1259:MET:O	1:A:1260:LEU:C	2.58	0.45
2:B:361:LEU:HD21	2:B:381:MET:HE1	1.99	0.45
2:B:455:SER:O	2:B:459:TYR:HB3	2.16	0.45
5:F:111:LEU:C	5:F:113:GLY:N	2.75	0.45
9:K:7:PHE:CD1	9:K:7:PHE:C	2.95	0.45
1:A:1172:LEU:C	1:A:1173:HIS:CG	2.94	0.45
2:B:859:TYR:N	2:B:859:TYR:CD1	2.85	0.45
3:C:40:GLU:CD	3:C:254:LYS:NZ	2.75	0.45
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.99	0.45
3:C:80:LEU:HD12	3:C:80:LEU:HA	1.58	0.45
3:C:239:PRO:O	3:C:240:VAL:C	2.59	0.45
4:E:129:PRO:CD	4:E:130:ALA:N	2.78	0.45
7:I:51:ASN:HB2	7:I:118:ARG:CZ	2.46	0.45
1:A:566:ILE:CG2	1:A:566:ILE:HB	2.20	0.44
2:B:210:LYS:HE3	2:B:461:LEU:O	2.17	0.44
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.99	0.44
2:B:1019:SER:OG	13:B:3008:GTP:C6	2.57	0.44
3:C:216:GLY:O	3:C:217:ASP:C	2.60	0.44
4:E:41:ASP:CG	4:E:41:ASP:CA	2.82	0.44
4:E:80:VAL:HG12	4:E:81:GLU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:131:THR:CB	4:E:131:THR:N	2.67	0.44
5:F:107:VAL:HG12	5:F:109:VAL:H	1.81	0.44
7:I:75:CYS:HB3	7:I:110:PHE:CE2	2.52	0.44
1:A:515:GLN:OE1	14:A:3018:HOH:O	2.21	0.44
1:A:560:ILE:O	1:A:561:PRO:C	2.54	0.44
1:A:941:LYS:NZ	1:A:941:LYS:HD3	2.30	0.44
2:B:643:ASP:HB3	2:B:644:GLU:C	2.42	0.44
2:B:806:THR:HG23	2:B:808:ALA:H	1.82	0.44
1:A:543:LEU:O	1:A:543:LEU:HG	2.15	0.44
1:A:1157:ASP:O	1:A:1160:SER:O	2.36	0.44
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.31	0.44
2:B:118:ARG:NH2	2:B:194:GLU:CD	2.73	0.44
2:B:755:ILE:O	2:B:755:ILE:HG22	2.14	0.44
4:E:116:ILE:HG22	4:E:120:ALA:HB3	2.00	0.44
6:H:40:LEU:HD12	6:H:41:ASP:N	2.31	0.44
7:I:120:GLN:O	7:I:121:PHE:CD1	2.71	0.44
1:A:58:LEU:O	1:A:59:GLY:O	2.34	0.44
1:A:328:ARG:NH1	1:A:1405:THR:HB	2.32	0.44
1:A:356:ASP:OD2	1:A:469:ARG:HD3	2.17	0.44
1:A:809:THR:HB	1:A:810:PRO:CD	2.47	0.44
1:A:896:ARG:HD3	1:A:897:TYR:CZ	2.52	0.44
2:B:531:GLN:CD	2:B:531:GLN:N	2.71	0.44
6:H:93:TYR:CD1	6:H:93:TYR:N	2.86	0.44
1:A:503:GLN:HE21	5:F:90:ARG:NH2	2.12	0.44
1:A:531:ILE:CD1	1:A:617:VAL:HB	2.39	0.44
1:A:596:THR:CG2	1:A:597:LEU:N	2.77	0.44
1:A:843:LYS:CE	1:A:843:LYS:CG	2.93	0.44
1:A:901:LEU:CD1	1:A:919:ILE:HD12	2.48	0.44
1:A:982:THR:O	1:A:985:ASP:HB2	2.18	0.44
1:A:1111:MET:CB	1:A:1111:MET:HE3	2.48	0.44
2:B:983:ARG:CD	14:B:3009:HOH:O	2.66	0.44
2:B:1019:SER:CB	13:B:3008:GTP:N7	2.81	0.44
3:C:66:ARG:O	3:C:67:LEU:C	2.53	0.44
4:E:36:GLU:O	4:E:38:PRO:N	2.50	0.44
8:J:1:MET:HE3	8:J:1:MET:CA	2.48	0.44
1:A:557:ASP:OD1	1:A:557:ASP:C	2.61	0.44
1:A:903:ASN:ND2	1:A:903:ASN:C	2.76	0.44
2:B:56:ASP:OD1	2:B:56:ASP:N	2.45	0.44
2:B:755:ILE:O	2:B:755:ILE:CG2	2.66	0.44
3:C:54:ASN:OD1	3:C:56:THR:CB	2.44	0.44
3:C:260:LEU:O	3:C:260:LEU:CD1	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:91:ARG:HD3	7:I:91:ARG:HA	1.77	0.44
10:L:48:CYS:CA	10:L:49:LYS:N	2.66	0.44
1:A:555:ASP:OD1	9:K:26:LYS:HE3	2.17	0.44
1:A:1111:MET:CE	1:A:1111:MET:CB	2.96	0.44
2:B:284:ILE:CD1	2:B:321:GLY:HA2	2.48	0.44
2:B:424:LEU:HD23	2:B:424:LEU:C	2.43	0.44
6:H:10:PHE:HA	6:H:29:ALA:O	2.18	0.44
10:L:38:LEU:HG	10:L:39:SER:N	2.32	0.44
10:L:38:LEU:HD13	10:L:48:CYS:HA	1.99	0.44
1:A:1333:ILE:HD12	1:A:1333:ILE:N	2.33	0.44
2:B:114:PRO:HD3	2:B:124:TYR:HE1	1.78	0.44
2:B:130:VAL:H	2:B:167:ILE:CD1	2.17	0.44
4:E:36:GLU:O	4:E:38:PRO:HD3	2.18	0.44
1:A:41:MET:HE2	1:A:47:ARG:O	2.18	0.44
1:A:793:SER:O	1:A:794:PRO:C	2.58	0.44
1:A:1151:GLU:HG3	7:I:45:ARG:HD2	1.95	0.44
1:A:1166:ASP:HA	1:A:1169:ILE:HG22	1.98	0.44
2:B:969:ARG:HH11	2:B:969:ARG:HD3	1.43	0.44
3:C:252:GLN:CG	3:C:252:GLN:HB3	2.20	0.44
3:C:262:LEU:HA	3:C:262:LEU:HD23	1.78	0.44
4:E:116:ILE:HG22	4:E:120:ALA:CB	2.48	0.44
6:H:95:TYR:CE2	6:H:97:MET:HG3	2.53	0.44
1:A:145:LYS:HE2	1:A:149:GLU:OE1	2.18	0.43
1:A:771:GLU:CD	2:B:510:LYS:NZ	2.76	0.43
1:A:1166:ASP:C	1:A:1169:ILE:HG22	2.43	0.43
2:B:555:ILE:HD12	2:B:587:HIS:HE1	1.75	0.43
1:A:587:HIS:CE1	1:A:609:ASP:H	2.36	0.43
1:A:834:THR:HG21	1:A:1077:THR:N	2.33	0.43
1:A:882:SER:CB	1:A:953:ASN:OD1	2.66	0.43
1:A:979:SER:OG	1:A:981:LEU:HB2	2.18	0.43
1:A:1110:ASN:CG	1:A:1110:ASN:CA	2.80	0.43
2:B:118:ARG:NH2	2:B:194:GLU:CG	2.80	0.43
2:B:276:ILE:HD12	2:B:276:ILE:HG23	1.71	0.43
2:B:323:VAL:O	2:B:323:VAL:CG1	2.65	0.43
2:B:654:ARG:N	2:B:657:HIS:HD2	2.14	0.43
2:B:999:MET:CE	2:B:1011:ILE:HD11	2.48	0.43
2:B:1202:LEU:HD23	2:B:1202:LEU:HA	1.88	0.43
3:C:116:LYS:C	3:C:118:LEU:H	2.26	0.43
4:E:65:THR:O	4:E:66:GLU:C	2.60	0.43
6:H:105:GLU:CD	6:H:105:GLU:N	2.69	0.43
1:A:417:TYR:O	1:A:418:SER:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:MET:HE3	1:A:607:ILE:HG13	2.01	0.43
2:B:199:MET:HE2	2:B:492:LEU:CD2	2.48	0.43
2:B:620:ARG:CD	2:B:620:ARG:CB	2.82	0.43
6:H:27:GLU:OE1	6:H:39:THR:CG2	2.66	0.43
6:H:96:VAL:HA	6:H:142:LEU:O	2.18	0.43
9:K:49:GLU:C	9:K:51:LEU:N	2.76	0.43
1:A:11:LEU:O	1:A:12:ARG:HG2	2.18	0.43
1:A:353:ILE:HD12	1:A:482:PHE:CD2	2.54	0.43
1:A:666:ILE:O	1:A:666:ILE:HD13	2.19	0.43
1:A:676:MET:SD	1:A:676:MET:CB	2.98	0.43
1:A:977:LYS:CG	1:A:977:LYS:HA	2.49	0.43
1:A:1438:THR:HB	2:B:1142:GLY:O	2.18	0.43
2:B:25:ILE:CD1	2:B:651:LEU:HD12	2.41	0.43
2:B:293:PRO:HA	7:I:12:ASN:HD21	1.83	0.43
2:B:387:LEU:HD12	2:B:387:LEU:HA	1.55	0.43
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.76	0.43
3:C:74:SER:HB2	3:C:238:ILE:HD12	2.01	0.43
3:C:179:GLU:CG	3:C:180:TYR:N	2.81	0.43
3:C:196:ASP:CB	3:C:199:LYS:HG3	2.49	0.43
3:C:250:THR:O	3:C:251:LEU:C	2.60	0.43
4:E:213:ILE:O	4:E:213:ILE:HG23	2.17	0.43
7:I:97:MET:HE2	7:I:97:MET:HB3	1.77	0.43
1:A:243:PRO:CB	1:A:245:PRO:HD2	2.46	0.43
1:A:567:LYS:CD	6:H:95:TYR:CD2	2.97	0.43
1:A:901:LEU:HB2	1:A:926:GLN:HE21	1.83	0.43
1:A:1339:LEU:HA	1:A:1339:LEU:HD23	1.77	0.43
1:A:1419:ASP:CG	1:A:1419:ASP:CA	2.78	0.43
2:B:870:ILE:CA	2:B:870:ILE:HB	2.24	0.43
2:B:1150:ARG:HH11	2:B:1150:ARG:HD2	1.45	0.43
5:F:81:THR:HG22	5:F:136:ARG:NH1	2.32	0.43
6:H:82:PRO:O	6:H:83:GLN:HB2	2.18	0.43
1:A:503:GLN:HE22	5:F:90:ARG:NH2	2.14	0.43
2:B:612:GLU:O	2:B:612:GLU:HG3	2.11	0.43
2:B:69:LEU:C	2:B:70:ILE:HD12	2.44	0.43
2:B:896:ASP:OD2	10:L:29:TYR:OH	2.24	0.43
3:C:4:GLU:HG2	3:C:5:GLY:H	1.84	0.43
3:C:40:GLU:C	3:C:163:ILE:CD1	2.91	0.43
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.54	0.43
5:F:114:GLU:CB	5:F:120:ILE:HD13	2.49	0.43
7:I:10:CYS:SG	7:I:31:THR:HG22	2.58	0.43
7:I:55:THR:HG21	7:I:121:PHE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:43:ARG:O	8:J:47:ARG:HG3	2.19	0.43
1:A:34:LYS:CG	1:A:83:HIS:CE1	3.02	0.43
1:A:359:LEU:HA	1:A:359:LEU:HD23	1.75	0.43
1:A:886:ILE:HD12	1:A:943:LEU:HB3	2.01	0.43
1:A:1073:GLY:O	1:A:1074:GLU:C	2.58	0.43
1:A:1383:SER:OG	1:A:1384:VAL:N	2.51	0.43
2:B:169:ARG:HB2	2:B:454:THR:CG2	2.41	0.43
2:B:451:LYS:HA	2:B:454:THR:HB	2.00	0.43
2:B:529:GLU:O	2:B:531:GLN:NE2	2.52	0.43
2:B:863:GLU:OE1	2:B:962:LYS:HD3	2.18	0.43
3:C:163:ILE:HA	3:C:163:ILE:HD13	1.43	0.43
4:E:78:LEU:HD11	4:E:109:ILE:CD1	2.49	0.43
6:H:13:SER:O	6:H:14:GLU:HG3	2.19	0.43
1:A:562:THR:HG21	6:H:98:TYR:CD2	2.53	0.43
1:A:593:GLU:O	1:A:593:GLU:HG2	2.18	0.43
1:A:597:LEU:CD1	1:A:597:LEU:CB	2.86	0.43
1:A:700:ASN:O	7:I:115:LYS:HE3	2.19	0.43
2:B:274:PRO:CG	2:B:359:GLU:HB3	2.48	0.43
1:A:295:LEU:CD2	1:A:295:LEU:CB	2.82	0.43
1:A:853:ASP:OD2	1:A:857:ARG:NH2	2.50	0.43
1:A:908:LEU:O	1:A:909:ASP:C	2.61	0.43
1:A:1169:ILE:HD11	1:A:1227:ILE:CD1	2.48	0.43
2:B:118:ARG:HG3	2:B:204:ILE:CD1	2.47	0.43
3:C:77:ILE:HD11	3:C:80:LEU:HD23	2.00	0.43
4:E:93:MET:HE2	4:E:116:ILE:HG21	2.01	0.43
4:E:112:TYR:CD1	4:E:112:TYR:C	2.97	0.43
6:H:33:GLN:C	6:H:35:GLN:N	2.74	0.43
9:K:18:LYS:HE3	9:K:38:GLU:OE2	2.19	0.43
1:A:14:VAL:N	1:A:1432:GLN:HE22	2.11	0.42
1:A:186:LYS:CG	1:A:197:PRO:HD3	2.48	0.42
1:A:545:GLN:O	1:A:546:VAL:C	2.61	0.42
1:A:563:PRO:HB3	1:A:572:TRP:CD2	2.53	0.42
2:B:132:VAL:HG12	2:B:133:LYS:N	2.34	0.42
2:B:235:SER:C	2:B:236:HIS:CD2	2.97	0.42
2:B:461:LEU:N	2:B:461:LEU:HD12	2.34	0.42
2:B:914:LYS:N	2:B:938:SER:HB2	2.33	0.42
3:C:43:THR:HG23	3:C:44:LEU:N	2.33	0.42
1:A:391:LEU:CD2	1:A:400:PRO:HB2	2.50	0.42
1:A:560:ILE:H	1:A:560:ILE:CD1	2.30	0.42
1:A:973:ILE:CG2	1:A:973:ILE:C	2.92	0.42
1:A:1004:ASN:CG	4:E:167:ARG:HG3	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1165:GLU:H	1:A:1165:GLU:HG2	1.56	0.42
2:B:51:PHE:CE2	2:B:172:ILE:HD13	2.54	0.42
2:B:953:LEU:HD23	2:B:953:LEU:C	2.44	0.42
2:B:1194:ILE:O	2:B:1194:ILE:HG13	2.19	0.42
8:J:6:ARG:HD2	8:J:11:GLY:O	2.18	0.42
1:A:157:ASP:O	1:A:160:GLN:HG3	2.19	0.42
1:A:640:GLN:O	1:A:641:VAL:C	2.59	0.42
1:A:868:TYR:CE1	1:A:1064:VAL:HG13	2.54	0.42
2:B:1169:MET:CE	2:B:1204:PHE:HB2	2.49	0.42
4:E:147:HIS:HD2	4:E:149:LEU:HB2	1.84	0.42
4:E:187:TYR:CD2	4:E:187:TYR:C	2.97	0.42
6:H:32:THR:HG22	6:H:33:GLN:OE1	2.17	0.42
7:I:17:ARG:HG3	7:I:28:GLU:OE1	2.19	0.42
1:A:744:LYS:HD3	1:A:748:MET:CE	2.49	0.42
1:A:1209:MET:O	1:A:1210:GLY:C	2.61	0.42
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.20	0.42
2:B:554:ILE:HD12	2:B:554:ILE:H	1.84	0.42
4:E:37:LEU:CD1	4:E:37:LEU:CB	2.84	0.42
4:E:59:SER:O	4:E:60:PHE:HB3	2.20	0.42
5:F:74:ILE:CD1	5:F:144:GLU:HG2	2.49	0.42
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.85	0.42
9:K:12:LEU:HD12	9:K:12:LEU:H	1.85	0.42
1:A:54:ASN:C	1:A:56:PRO:HD2	2.45	0.42
1:A:599:SER:HB2	1:A:602:ASP:H	1.85	0.42
1:A:722:LEU:HD23	1:A:722:LEU:HA	1.90	0.42
1:A:913:LEU:HD12	1:A:913:LEU:HA	1.61	0.42
2:B:554:ILE:HD12	2:B:554:ILE:N	2.34	0.42
2:B:666:TYR:C	2:B:666:TYR:CD2	2.98	0.42
2:B:996:ARG:HH11	2:B:996:ARG:HD3	1.53	0.42
3:C:7:GLN:CG	3:C:7:GLN:CA	2.87	0.42
6:H:44:VAL:O	6:H:44:VAL:CG1	2.67	0.42
9:K:111:LEU:HD23	9:K:111:LEU:H	1.85	0.42
10:L:34:CYS:HB3	10:L:51:CYS:HB3	2.02	0.42
1:A:195:ASP:O	1:A:196:GLU:HB3	2.20	0.42
2:B:70:ILE:HD12	2:B:70:ILE:N	2.34	0.42
2:B:121:ASN:ND2	2:B:965:LYS:NZ	2.68	0.42
2:B:213:ILE:HD13	2:B:481:GLN:CD	2.45	0.42
2:B:646:LEU:CD1	2:B:646:LEU:CD2	2.95	0.42
2:B:789:MET:CE	2:B:965:LYS:HB3	2.48	0.42
2:B:976:ILE:O	2:B:1099:VAL:HG21	2.19	0.42
8:J:2:ILE:C	8:J:53:HIS:NE2	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:O	1:A:568:PRO:C	2.61	0.42
2:B:286:PHE:CB	2:B:297:ILE:HD12	2.40	0.42
2:B:737:THR:O	2:B:738:PHE:C	2.59	0.42
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.20	0.42
2:B:1002:THR:O	2:B:1005:GLY:N	2.42	0.42
4:E:43:LYS:O	4:E:47:CYS:CB	2.68	0.42
1:A:709:THR:HG22	1:A:711:ARG:N	2.35	0.42
1:A:786:HIS:CD2	1:A:786:HIS:H	2.36	0.42
1:A:982:THR:HB	1:A:985:ASP:CG	2.45	0.42
4:E:79:TRP:HE1	4:E:81:GLU:HB2	1.84	0.42
10:L:49:LYS:O	10:L:50:ASP:HB2	2.20	0.42
1:A:99:ILE:CG1	1:A:234:MET:HE3	2.50	0.42
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.20	0.42
1:A:830:LYS:CD	1:A:830:LYS:CB	2.84	0.42
1:A:1102:LYS:CE	1:A:1102:LYS:CG	2.87	0.42
1:A:1146:VAL:HG12	1:A:1197:LEU:HD22	2.02	0.42
1:A:1385:THR:CG2	1:A:1385:THR:O	2.66	0.42
2:B:95:ILE:HG22	2:B:96:TYR:O	2.20	0.42
2:B:104:GLU:HB2	2:B:108:VAL:HA	2.02	0.42
2:B:757:PRO:HD2	2:B:984:HIS:HE1	1.85	0.42
2:B:773:MET:O	2:B:774:GLY:C	2.55	0.42
2:B:902:GLY:O	10:L:65:VAL:HG11	2.19	0.42
2:B:1006:ILE:CD1	8:J:43:ARG:HD2	2.50	0.42
8:J:16:ASP:OD1	8:J:17:LYS:HG3	2.19	0.42
1:A:93:VAL:HG13	1:A:301:ALA:HB1	2.01	0.41
1:A:230:ARG:NH1	1:A:232:GLU:OE2	2.52	0.41
1:A:837:ILE:O	1:A:838:GLN:C	2.61	0.41
2:B:274:PRO:HG3	2:B:359:GLU:O	2.20	0.41
2:B:282:ILE:HD11	2:B:317:CYS:CB	2.50	0.41
1:A:70:CYS:HB3	2:B:1172:ILE:HG23	2.02	0.41
1:A:492:PRO:HB2	1:A:497:THR:CG2	2.48	0.41
1:A:1134:ILE:O	1:A:1138:ILE:HD11	2.21	0.41
3:C:7:GLN:OE1	9:K:104:ASN:ND2	2.54	0.41
3:C:214:ASN:O	3:C:217:ASP:N	2.54	0.41
4:E:61:GLN:HB2	4:E:79:TRP:CE3	2.56	0.41
6:H:47:PHE:HB2	6:H:95:TYR:HD1	1.83	0.41
7:I:40:SER:CB	7:I:41:PRO:CD	2.97	0.41
1:A:807:GLY:CA	2:B:761:HIS:CE1	3.04	0.41
1:A:1170:ILE:HD13	1:A:1170:ILE:HA	1.96	0.41
2:B:213:ILE:HD11	2:B:481:GLN:CD	2.45	0.41
3:C:27:LEU:O	3:C:28:ALA:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:7:ARG:O	4:E:8:ASN:C	2.62	0.41
9:K:40:HIS:O	9:K:41:THR:C	2.63	0.41
1:A:366:VAL:O	1:A:367:PRO:C	2.59	0.41
1:A:446:ARG:CG	1:A:446:ARG:NH1	2.83	0.41
2:B:408:LEU:O	2:B:409:ALA:C	2.62	0.41
4:E:78:LEU:HG	4:E:79:TRP:N	2.33	0.41
4:E:154:ILE:CD1	4:E:199:ILE:HD12	2.50	0.41
4:E:168:TYR:O	4:E:169:ARG:HB2	2.20	0.41
7:I:71:SER:O	7:I:83:ASN:ND2	2.53	0.41
1:A:95:PHE:O	1:A:99:ILE:HG13	2.21	0.41
1:A:96:ILE:HG21	1:A:176:LYS:HE2	2.03	0.41
1:A:138:ILE:HG13	1:A:139:TRP:N	2.35	0.41
1:A:557:ASP:O	1:A:559:VAL:N	2.53	0.41
1:A:666:ILE:HD12	2:B:1052:VAL:HG11	2.02	0.41
1:A:686:ALA:O	1:A:687:LYS:C	2.61	0.41
1:A:752:LYS:HE2	13:B:3008:GTP:N1	2.35	0.41
1:A:973:ILE:CD1	1:A:1038:THR:HG23	2.51	0.41
1:A:1166:ASP:CB	1:A:1169:ILE:HG21	2.39	0.41
1:A:1237:ILE:HD12	1:A:1237:ILE:HA	1.75	0.41
2:B:28:GLU:OE1	2:B:807:ARG:NH2	2.54	0.41
2:B:900:ALA:HA	10:L:58:LYS:HD2	2.02	0.41
2:B:1189:ILE:N	2:B:1189:ILE:HD12	2.35	0.41
4:E:98:ILE:CA	4:E:98:ILE:CG2	2.88	0.41
5:F:143:PHE:C	5:F:143:PHE:CD1	2.98	0.41
7:I:59:VAL:O	7:I:60:GLN:C	2.60	0.41
7:I:103:CYS:SG	7:I:106:CYS:SG	3.18	0.41
1:A:846:GLU:HA	1:A:1066:VAL:CG2	2.50	0.41
2:B:280:ILE:HD12	2:B:280:ILE:H	1.86	0.41
2:B:625:LYS:C	2:B:626:ILE:HG13	2.46	0.41
4:E:79:TRP:NE1	4:E:81:GLU:HB2	2.36	0.41
4:E:191:LYS:O	4:E:192:ARG:C	2.58	0.41
5:F:128:LYS:NZ	5:F:149:GLU:O	2.48	0.41
6:H:138:GLU:HG2	6:H:139:ASN:N	2.36	0.41
8:J:14:VAL:CG1	8:J:50:ILE:CD1	2.95	0.41
1:A:9:ALA:O	2:B:1193:GLN:OE1	2.39	0.41
1:A:302:THR:O	1:A:303:TYR:C	2.60	0.41
1:A:351:THR:HG23	2:B:1103:ILE:HG12	1.98	0.41
1:A:571:LEU:HA	1:A:571:LEU:HD12	1.70	0.41
1:A:741:ASN:ND2	1:A:743:VAL:H	2.19	0.41
1:A:834:THR:CG2	1:A:1077:THR:OG1	2.66	0.41
2:B:780:VAL:HG21	8:J:56:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:914:LYS:HD2	2:B:937:ALA:HB3	2.02	0.41
2:B:939:THR:HA	2:B:940:PRO:HD3	1.93	0.41
3:C:44:LEU:HD22	3:C:129:ILE:HD12	2.03	0.41
4:E:161:LYS:NZ	4:E:172:GLU:OE2	2.51	0.41
6:H:118:PHE:C	6:H:120:GLY:N	2.76	0.41
6:H:145:ARG:HG2	6:H:145:ARG:NH1	2.36	0.41
1:A:516:SER:OG	1:A:1362:TYR:O	2.39	0.41
1:A:1023:ARG:HH21	1:A:1023:ARG:HD3	1.66	0.41
1:A:59:GLY:C	1:A:60:SER:HG	2.29	0.41
1:A:186:LYS:HD2	1:A:197:PRO:HG3	2.03	0.41
1:A:269:ILE:CD1	1:A:300:VAL:HG22	2.50	0.41
1:A:541:ILE:HG22	1:A:546:VAL:HG23	2.03	0.41
1:A:582:ILE:HA	1:A:583:PRO:HD3	1.92	0.41
1:A:1207:LEU:HD23	1:A:1211:GLN:OE1	2.21	0.41
1:A:1267:MET:HA	1:A:1271:ILE:HD13	2.03	0.41
2:B:90:ILE:HD11	2:B:134:LYS:HE2	2.03	0.41
2:B:199:MET:HE3	2:B:488:TYR:CE1	2.55	0.41
2:B:323:VAL:O	2:B:323:VAL:HG12	2.20	0.41
2:B:1002:THR:O	2:B:1003:ALA:C	2.62	0.41
2:B:1161:HIS:HA	2:B:1192:TYR:O	2.21	0.41
2:B:1179:GLN:HE21	2:B:1179:GLN:HB2	1.70	0.41
2:B:1187:ASN:ND2	2:B:1187:ASN:C	2.79	0.41
3:C:26:ASP:O	3:C:27:LEU:C	2.62	0.41
3:C:29:MET:CE	3:C:29:MET:CB	2.99	0.41
5:F:79:ARG:HH22	5:F:150:GLU:CD	2.29	0.41
5:F:94:LEU:HD23	5:F:94:LEU:HA	1.85	0.41
6:H:142:LEU:HA	6:H:142:LEU:HD12	1.76	0.41
8:J:1:MET:HG3	8:J:60:PHE:HE2	1.86	0.41
10:L:54:ARG:CG	10:L:54:ARG:NE	2.66	0.41
10:L:60:ARG:O	10:L:61:THR:C	2.63	0.41
1:A:93:VAL:HG22	1:A:301:ALA:HA	2.02	0.41
1:A:1220:PHE:HB3	1:A:1224:LEU:HB3	2.03	0.41
4:E:2:ASP:O	4:E:3:GLN:C	2.63	0.41
6:H:48:PRO:C	6:H:49:VAL:CG2	2.94	0.41
1:A:210:ILE:HD13	1:A:210:ILE:HA	1.91	0.40
1:A:274:ILE:CA	1:A:274:ILE:HB	2.21	0.40
1:A:547:LEU:HD22	9:K:58:PHE:CD1	2.56	0.40
1:A:679:ILE:CD1	1:A:729:ALA:O	2.68	0.40
1:A:983:ILE:HD12	1:A:983:ILE:H	1.86	0.40
1:A:1025:ARG:HD3	1:A:1025:ARG:HA	1.88	0.40
1:A:1166:ASP:HB3	1:A:1169:ILE:HG23	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:93:ILE:HD12	5:F:134:ILE:HD11	1.98	0.40
6:H:101:ALA:HA	6:H:116:TYR:HA	2.01	0.40
9:K:27:ALA:HB1	9:K:28:PRO:CD	2.51	0.40
9:K:59:ALA:HA	9:K:74:ARG:O	2.21	0.40
1:A:587:HIS:HE2	1:A:969:GLN:HG2	1.84	0.40
1:A:1004:ASN:OD1	4:E:167:ARG:HG3	2.21	0.40
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.57	0.40
2:B:724:ASP:O	2:B:726:ALA:N	2.54	0.40
3:C:70:ILE:HD11	3:C:144:ILE:CD1	2.51	0.40
4:E:161:LYS:NZ	4:E:193:GLY:O	2.54	0.40
1:A:44:THR:CA	1:A:44:THR:CG2	2.86	0.40
1:A:497:THR:HG21	2:B:1149:GLU:OE1	2.20	0.40
1:A:599:SER:HA	1:A:600:PRO:HD2	1.82	0.40
1:A:1166:ASP:O	1:A:1169:ILE:CG2	2.69	0.40
1:A:1209:MET:SD	1:A:1236:LEU:HD22	2.62	0.40
1:A:1256:GLU:HB3	1:A:1259:MET:HE2	2.03	0.40
2:B:28:GLU:CD	2:B:807:ARG:HH22	2.30	0.40
2:B:361:LEU:N	2:B:362:PRO:CD	2.85	0.40
2:B:840:ILE:HB	2:B:1011:ILE:HB	2.03	0.40
2:B:1065:GLN:NE2	2:B:1067:ARG:HB2	2.28	0.40
3:C:11:ARG:NE	3:C:209:TYR:CE2	2.89	0.40
4:E:43:LYS:O	4:E:47:CYS:HB3	2.21	0.40
1:A:35:ILE:H	1:A:35:ILE:HG13	1.65	0.40
1:A:1003:LYS:CG	1:A:1003:LYS:HA	2.43	0.40
1:A:1132:LYS:O	1:A:1133:LEU:C	2.62	0.40
2:B:121:ASN:HD21	2:B:965:LYS:CE	2.35	0.40
2:B:165:VAL:O	2:B:165:VAL:HG12	2.20	0.40
2:B:377:PHE:CD2	2:B:381:MET:HE2	2.56	0.40
4:E:61:GLN:HE21	4:E:63:ASN:HD21	1.68	0.40
1:A:35:ILE:HA	1:A:52:GLY:O	2.22	0.40
1:A:1098:VAL:N	1:A:1099:PRO:CD	2.84	0.40
1:A:1411:GLU:O	1:A:1412:ALA:C	2.63	0.40
2:B:270:LYS:HB3	2:B:279:ASP:HB3	2.02	0.40
2:B:291:ILE:O	2:B:297:ILE:CD1	2.67	0.40
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.35	0.40
3:C:248:ILE:HD12	9:K:101:LEU:HD12	2.03	0.40
4:E:28:TYR:CE1	4:E:75:MET:CE	3.04	0.40
4:E:76:GLY:HA3	4:E:106:GLN:HB3	2.02	0.40
6:H:103:LYS:HE3	6:H:135:LEU:C	2.47	0.40
7:I:10:CYS:SG	7:I:31:THR:CG2	3.10	0.40
9:K:42:LEU:HA	9:K:42:LEU:HD12	1.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:29:TYR:O	10:L:30:ILE:HG13	2.21	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	1334/1733 (77%)	1196 (90%)	84 (6%)	54 (4%)	2	14
2	B	1071/1224 (88%)	931 (87%)	104 (10%)	36 (3%)	3	17
3	C	264/318 (83%)	225 (85%)	30 (11%)	9 (3%)	3	17
4	E	213/215 (99%)	181 (85%)	20 (9%)	12 (6%)	1	8
5	F	81/155 (52%)	72 (89%)	8 (10%)	1 (1%)	10	40
6	H	129/146 (88%)	89 (69%)	17 (13%)	23 (18%)	0	0
7	I	119/122 (98%)	108 (91%)	10 (8%)	1 (1%)	16	50
8	J	62/70 (89%)	60 (97%)	2 (3%)	0	100	100
9	K	112/120 (93%)	99 (88%)	10 (9%)	3 (3%)	4	22
10	L	44/70 (63%)	25 (57%)	11 (25%)	8 (18%)	0	0
All	All	3429/4173 (82%)	2986 (87%)	296 (9%)	147 (4%)	2	12

All (147) 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	62	ASP
1	A	65	LEU

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Mol	Chain	Res	Type
1	A	69	THR
1	A	72	GLU
1	A	74	MET
1	A	120	GLU
1	A	155	GLU
1	A	156	ASP
1	A	157	ASP
1	A	165	GLY
1	A	190	ALA
1	A	286	HIS
1	A	418	SER
1	A	465	TYR
1	A	567	LYS
1	A	707	GLY
1	A	752	LYS
1	A	885	THR
1	A	1080	THR
1	A	1221	LYS
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
2	B	436	VAL
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
4	E	118	PRO
5	F	73	ALA

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Mol	Chain	Res	Type
6	H	32	THR
6	H	52	GLN
6	H	53	ASP
6	H	78	SER
6	H	90	ALA
6	H	104	PHE
6	H	105	GLU
6	H	116	TYR
6	H	136	LYS
7	I	4	PHE
9	K	111	LEU
10	L	28	LYS
10	L	45	ALA
10	L	50	ASP
1	A	56	PRO
1	A	57	ARG
1	A	158	PRO
1	A	167	CYS
1	A	279	LEU
1	A	326	ARG
1	A	464	PRO
1	A	672	ASP
1	A	975	HIS
1	A	1223	ASP
1	A	1359	ASP
2	B	266	ALA
2	B	432	MET
2	B	451	LYS
2	B	466	TRP
2	B	887	HIS
2	B	1097	HIS
2	B	1105	ALA
3	C	209	TYR
3	C	231	ASN
4	E	44	ALA
4	E	45	LYS
4	E	50	MET
4	E	126	SER
6	H	77	ARG
6	H	81	PRO
6	H	86	ASP
6	H	89	LEU

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Mol	Chain	Res	Type
6	H	107	VAL
6	H	135	LEU
6	H	139	ASN
9	K	99	GLY
10	L	39	SER
10	L	58	LYS
1	A	38	PRO
1	A	60	SER
1	A	278	THR
1	A	1002	GLY
1	A	1255	GLU
2	B	865	LYS
2	B	1155	SER
2	B	1190	ASP
3	C	267	GLN
4	E	74	ASP
6	H	82	PRO
6	H	83	GLN
6	H	128	ASN
9	K	50	LEU
10	L	41	SER
1	A	32	VAL
1	A	75	ASN
1	A	706	HIS
2	B	90	ILE
2	B	447	ALA
2	B	643	ASP
3	C	137	LYS
4	E	2	ASP
4	E	56	LYS
6	H	19	ARG
10	L	46	VAL
1	A	42	ASP
1	A	196	GLU
1	A	599	SER
1	A	958	VAL
1	A	1204	ASP
1	A	1280	GLU
2	B	19	GLU
2	B	137	TYR
2	B	424	LEU
2	B	831	SER

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Mol	Chain	Res	Type
2	B	1189	ILE
4	E	59	SER
6	H	119	GLY
10	L	59	ALA
1	A	400	PRO
2	B	940	PRO
2	B	1017	ILE
3	C	217	ASP
6	H	5	LEU
6	H	103	LYS
1	A	52	GLY
1	A	55	ASP
3	C	126	GLY
4	E	38	PRO
1	A	1123	GLY

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	1183/1520 (78%)	966 (82%)	217 (18%)	2	9
2	B	947/1061 (89%)	768 (81%)	179 (19%)	1	9
3	C	234/274 (85%)	190 (81%)	44 (19%)	1	9
4	E	197/197 (100%)	150 (76%)	47 (24%)	1	4
5	F	73/137 (53%)	62 (85%)	11 (15%)	3	14
6	H	117/128 (91%)	71 (61%)	46 (39%)	0	1
7	I	115/116 (99%)	95 (83%)	20 (17%)	2	10
8	J	59/65 (91%)	46 (78%)	13 (22%)	1	5
9	K	99/102 (97%)	77 (78%)	22 (22%)	1	5
10	L	40/57 (70%)	21 (52%)	19 (48%)	0	0
All	All	3064/3657 (84%)	2446 (80%)	618 (20%)	1	7

All (618) 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	30	ILE
1	A	34	LYS
1	A	36	ARG
1	A	39	GLU
1	A	44	THR
1	A	46	THR
1	A	49	LYS
1	A	58	LEU
1	A	60	SER
1	A	65	LEU
1	A	68	GLN
1	A	74	MET
1	A	84	ILE
1	A	90	VAL
1	A	93	VAL
1	A	98	LYS
1	A	106	VAL
1	A	110	CYS
1	A	112	LYS
1	A	114	LEU
1	A	120	GLU
1	A	121	LEU
1	A	129	LYS
1	A	138	ILE
1	A	141	LEU
1	A	144	THR
1	A	145	LYS
1	A	147	VAL
1	A	148	CYS
1	A	153	PRO
1	A	156	ASP
1	A	158	PRO
1	A	160	GLN
1	A	162	VAL
1	A	167	CYS
1	A	172	PRO
1	A	173	THR
1	A	176	LYS
1	A	191	THR

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Mol	Chain	Res	Type
1	A	195	ASP
1	A	197	PRO
1	A	198	GLU
1	A	201	VAL
1	A	204	THR
1	A	206	GLU
1	A	215	SER
1	A	231	PRO
1	A	235	ILE
1	A	237	THR
1	A	239	LEU
1	A	246	VAL
1	A	247	ARG
1	A	261	ASP
1	A	263	THR
1	A	265	LYS
1	A	269	ILE
1	A	270	LEU
1	A	275	SER
1	A	286	HIS
1	A	294	SER
1	A	302	THR
1	A	329	LEU
1	A	346	ASP
1	A	351	THR
1	A	354	SER
1	A	385	ILE
1	A	409	SER
1	A	413	ILE
1	A	416	ARG
1	A	419	LYS
1	A	449	SER
1	A	451	HIS
1	A	461	LYS
1	A	466	SER
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	493	GLN
1	A	495	GLU
1	A	497	THR
1	A	498	ARG

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Mol	Chain	Res	Type
1	A	504	LEU
1	A	508	PRO
1	A	513	SER
1	A	531	ILE
1	A	535	THR
1	A	537	ARG
1	A	543	LEU
1	A	566	ILE
1	A	571	LEU
1	A	586	ILE
1	A	588	LEU
1	A	590	ARG
1	A	597	LEU
1	A	599	SER
1	A	607	ILE
1	A	616	VAL
1	A	618	GLU
1	A	620	LYS
1	A	622	VAL
1	A	636	GLU
1	A	666	ILE
1	A	679	ILE
1	A	681	GLU
1	A	683	ILE
1	A	688	LYS
1	A	695	LYS
1	A	702	LEU
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	724	GLU
1	A	728	LYS
1	A	735	VAL
1	A	741	ASN
1	A	744	LYS
1	A	794	PRO
1	A	810	PRO
1	A	821	ARG
1	A	830	LYS

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Mol	Chain	Res	Type
1	A	843	LYS
1	A	858	ASN
1	A	880	LYS
1	A	882	SER
1	A	885	THR
1	A	895	LYS
1	A	903	ASN
1	A	907	THR
1	A	909	ASP
1	A	918	GLU
1	A	920	LEU
1	A	964	ILE
1	A	973	ILE
1	A	974	ASP
1	A	979	SER
1	A	982	THR
1	A	984	LYS
1	A	1003	LYS
1	A	1006	ILE
1	A	1015	VAL
1	A	1039	LYS
1	A	1055	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	1118	VAL
1	A	1120	LEU
1	A	1129	GLU
1	A	1133	LEU
1	A	1134	ILE
1	A	1138	ILE
1	A	1141	THR
1	A	1146	VAL
1	A	1161	THR
1	A	1163	ILE
1	A	1165	GLU
1	A	1169	ILE
1	A	1170	ILE

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Mol	Chain	Res	Type
1	A	1171	GLN
1	A	1172	LEU
1	A	1176	LEU
1	A	1187	GLN
1	A	1204	ASP
1	A	1208	THR
1	A	1217	LYS
1	A	1225	PHE
1	A	1230	GLU
1	A	1235	LYS
1	A	1236	LEU
1	A	1237	ILE
1	A	1243	VAL
1	A	1255	GLU
1	A	1258	HIS
1	A	1259	MET
1	A	1260	LEU
1	A	1263	ILE
1	A	1267	MET
1	A	1269	GLU
1	A	1277	GLU
1	A	1281	ARG
1	A	1290	LYS
1	A	1291	VAL
1	A	1293	SER
1	A	1299	VAL
1	A	1309	ASP
1	A	1317	MET
1	A	1318	THR
1	A	1325	THR
1	A	1327	ILE
1	A	1335	ILE
1	A	1336	MET
1	A	1359	ASP
1	A	1361	SER
1	A	1366	ARG
1	A	1372	VAL
1	A	1376	THR
1	A	1377	THR
1	A	1382	THR
1	A	1384	VAL
1	A	1405	THR

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Mol	Chain	Res	Type
1	A	1426	GLU
1	A	1433	MET
1	A	1438	THR
1	A	1445	ILE
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	70	ILE
2	B	89	GLU
2	B	92	PHE
2	B	98	THR
2	B	99	LYS
2	B	102	VAL
2	B	106	ASP
2	B	121	ASN
2	B	128	LEU
2	B	130	VAL
2	B	133	LYS
2	B	134	LYS
2	B	136	THR
2	B	138	GLU
2	B	164	LYS
2	B	167	ILE
2	B	172	ILE
2	B	178	ASN
2	B	179	CYS
2	B	183	GLU
2	B	194	GLU
2	B	204	ILE
2	B	213	ILE
2	B	228	LYS
2	B	242	SER
2	B	244	LEU
2	B	248	SER
2	B	252	SER

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Mol	Chain	Res	Type
2	B	261	ARG
2	B	264	SER
2	B	269	ILE
2	B	277	LYS
2	B	282	ILE
2	B	283	VAL
2	B	297	ILE
2	B	305	VAL
2	B	315	LYS
2	B	324	ILE
2	B	347	LYS
2	B	358	LYS
2	B	367	LEU
2	B	371	GLU
2	B	373	ARG
2	B	384	ARG
2	B	387	LEU
2	B	417	PHE
2	B	422	LYS
2	B	423	LYS
2	B	425	THR
2	B	426	LYS
2	B	434	ARG
2	B	435	THR
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	502	ILE
2	B	513	GLN
2	B	516	ASN
2	B	522	VAL
2	B	524	PRO
2	B	531	GLN
2	B	541	LEU
2	B	547	VAL
2	B	549	THR
2	B	550	ASP
2	B	552	MET
2	B	555	ILE

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Mol	Chain	Res	Type
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	614	SER
2	B	624	LEU
2	B	639	ILE
2	B	641	GLU
2	B	645	SER
2	B	648	HIS
2	B	650	GLU
2	B	651	LEU
2	B	652	LYS
2	B	653	VAL
2	B	666	TYR
2	B	680	THR
2	B	690	VAL
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
2	B	846	ILE
2	B	860	MET
2	B	863	GLU
2	B	864	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

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Mol	Chain	Res	Type
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	893	LEU
2	B	895	ASP
2	B	896	ASP
2	B	908	GLU
2	B	911	ILE
2	B	914	LYS
2	B	933	SER
2	B	938	SER
2	B	948	ILE
2	B	955	THR
2	B	956	THR
2	B	958	GLN
2	B	962	LYS
2	B	964	VAL
2	B	971	THR
2	B	974	PRO
2	B	975	GLN
2	B	983	ARG
2	B	996	ARG
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1010	LEU
2	B	1050	ILE
2	B	1051	THR
2	B	1055	ILE
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	1106	ARG
2	B	1150	ARG
2	B	1152	MET

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Mol	Chain	Res	Type
2	B	1155	SER
2	B	1156	ASP
2	B	1159	ARG
2	B	1162	ILE
2	B	1165	ILE
2	B	1174	LYS
2	B	1175	LEU
2	B	1178	ASN
2	B	1179	GLN
2	B	1182	CYS
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	11	ARG
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	77	ILE
3	C	86	CYS
3	C	93	ASP
3	C	102	GLN
3	C	110	THR
3	C	119	VAL
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	132	PRO
3	C	137	LYS
3	C	154	LYS

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Mol	Chain	Res	Type
3	C	163	ILE
3	C	178	PHE
3	C	184	ASN
3	C	185	LYS
3	C	186	LEU
3	C	197	SER
3	C	199	LYS
3	C	205	LYS
3	C	209	TYR
3	C	214	ASN
3	C	238	ILE
3	C	240	VAL
3	C	245	VAL
3	C	251	LEU
3	C	260	LEU
3	C	264	GLN
3	C	265	MET
3	C	266	ASP
3	C	268	ASP
4	E	3	GLN
4	E	8	ASN
4	E	10	SER
4	E	14	ARG
4	E	33	GLU
4	E	34	GLU
4	E	36	GLU
4	E	37	LEU
4	E	49	SER
4	E	50	MET
4	E	52	ARG
4	E	57	MET
4	E	61	GLN
4	E	69	ILE
4	E	70	SER
4	E	72	PHE
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

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Mol	Chain	Res	Type
4	E	92	THR
4	E	95	THR
4	E	101	GLN
4	E	103	LYS
4	E	107	THR
4	E	116	ILE
4	E	117	THR
4	E	119	SER
4	E	121	MET
4	E	123	LEU
4	E	129	PRO
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	201	LYS
4	E	204	THR
4	E	212	ARG
5	F	72	LYS
5	F	77	ASP
5	F	79	ARG
5	F	81	THR
5	F	82	THR
5	F	97	ARG
5	F	109	VAL
5	F	110	ASP
5	F	111	LEU
5	F	117	PRO
5	F	119	ARG
6	H	4	THR
6	H	5	LEU
6	H	6	PHE
6	H	7	ASP
6	H	9	ILE
6	H	13	SER
6	H	27	GLU

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Mol	Chain	Res	Type
6	H	34	ASP
6	H	35	GLN
6	H	36	CYS
6	H	40	LEU
6	H	42	ILE
6	H	44	VAL
6	H	45	GLU
6	H	46	LEU
6	H	52	GLN
6	H	53	ASP
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	143	LEU
6	H	144	ILE
6	H	145	ARG
7	I	1	MET
7	I	2	THR
7	I	18	GLU

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Mol	Chain	Res	Type
7	I	21	GLU
7	I	24	ARG
7	I	31	THR
7	I	45	ARG
7	I	55	THR
7	I	59	VAL
7	I	76	PRO
7	I	77	LYS
7	I	78	CYS
7	I	81	ARG
7	I	82	GLU
7	I	84	VAL
7	I	95	THR
7	I	116	ASN
7	I	117	LYS
7	I	119	THR
7	I	120	GLN
8	J	1	MET
8	J	2	ILE
8	J	3	VAL
8	J	13	VAL
8	J	14	VAL
8	J	20	SER
8	J	28	ASP
8	J	38	ARG
8	J	42	LYS
8	J	48	ARG
8	J	50	ILE
8	J	62	ARG
8	J	64	ASN
9	K	1	MET
9	K	2	ASN
9	K	11	LEU
9	K	18	LYS
9	K	20	LYS
9	K	31	VAL
9	K	42	LEU
9	K	47	ARG
9	K	51	LEU
9	K	55	LYS
9	K	63	VAL
9	K	73	LEU

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Mol	Chain	Res	Type
9	K	75	ILE
9	K	78	THR
9	K	79	GLU
9	K	93	SER
9	K	106	GLU
9	K	107	THR
9	K	111	LEU
9	K	112	GLN
9	K	113	THR
9	K	114	LEU
10	L	27	LEU
10	L	28	LYS
10	L	33	GLU
10	L	36	SER
10	L	42	ARG
10	L	44	ASP
10	L	46	VAL
10	L	47	ARG
10	L	49	LYS
10	L	50	ASP
10	L	51	CYS
10	L	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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	83	HIS
1	A	92	HIS
1	A	171	GLN
1	A	299	HIS
1	A	399	HIS
1	A	427	GLN
1	A	445	ASN
1	A	451	HIS

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Mol	Chain	Res	Type
1	A	479	ASN
1	A	503	GLN
1	A	510	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	760	GLN
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	994	GLN
1	A	1070	GLN
1	A	1078	GLN
1	A	1124	HIS
1	A	1140	HIS
1	A	1171	GLN
1	A	1173	HIS
1	A	1222	ASN
1	A	1364	ASN
1	A	1378	GLN
1	A	1432	GLN
2	B	60	GLN
2	B	121	ASN
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS
2	B	383	ASN
2	B	395	GLN
2	B	449	ASN
2	B	516	ASN
2	B	518	HIS
2	B	531	GLN
2	B	538	ASN
2	B	587	HIS
2	B	590	HIS
2	B	657	HIS
2	B	706	GLN

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Mol	Chain	Res	Type
2	B	744	HIS
2	B	843	GLN
2	B	862	GLN
2	B	878	GLN
2	B	951	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	1178	ASN
2	B	1179	GLN
2	B	1187	ASN
2	B	1205	GLN
3	C	24	ASN
3	C	73	GLN
3	C	167	HIS
3	C	184	ASN
3	C	242	GLN
3	C	252	GLN
4	E	5	ASN
4	E	61	GLN
4	E	147	HIS
6	H	11	GLN
6	H	131	ASN
6	H	133	ASN
7	I	12	ASN
7	I	46	HIS
7	I	83	ASN
7	I	89	GLN
7	I	116	ASN
8	J	53	HIS
9	K	2	ASN
9	K	65	HIS
9	K	76	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	GTP	B	3008	12	33,34,34	3.13	9 (27%)	50,54,54	3.27	10 (20%)

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	GTP	B	3008	12	1/1/7/7	8/22/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	3008	GTP	C1'-N9	11.99	1.81	1.47
13	B	3008	GTP	C4-N9	9.38	1.62	1.38
13	B	3008	GTP	C8-N9	5.36	1.49	1.37
13	B	3008	GTP	C5-N7	-3.52	1.32	1.39
13	B	3008	GTP	C4-N3	3.35	1.41	1.34
13	B	3008	GTP	C2-N3	3.35	1.41	1.33
13	B	3008	GTP	C5-C4	2.27	1.44	1.38
13	B	3008	GTP	C8-N7	-2.21	1.26	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	3008	GTP	PA-O3A	2.03	1.61	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	3008	GTP	O4'-C1'-N9	13.53	139.03	108.36
13	B	3008	GTP	C1'-N9-C4	10.95	158.82	126.49
13	B	3008	GTP	C8-N9-C4	-8.03	90.97	106.03
13	B	3008	GTP	C1'-N9-C8	-7.93	104.20	126.73
13	B	3008	GTP	N9-C8-N7	5.49	123.58	113.40
13	B	3008	GTP	C5-C4-N3	-3.72	122.47	128.39
13	B	3008	GTP	O4'-C1'-C2'	3.06	113.16	106.62
13	B	3008	GTP	C2'-C3'-C4'	2.40	107.25	102.61
13	B	3008	GTP	C2'-C1'-N9	-2.28	106.91	113.25
13	B	3008	GTP	N9-C4-N3	2.28	130.50	125.95

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	B	3008	GTP	C1'

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	B	3008	GTP	C5'-O5'-PA-O3A
13	B	3008	GTP	O4'-C4'-C5'-O5'
13	B	3008	GTP	C3'-C4'-C5'-O5'
13	B	3008	GTP	PB-O3B-PG-O2G
13	B	3008	GTP	C5'-O5'-PA-O2A
13	B	3008	GTP	C4'-C5'-O5'-PA
13	B	3008	GTP	PB-O3B-PG-O3G
13	B	3008	GTP	C2'-C1'-N9-C4

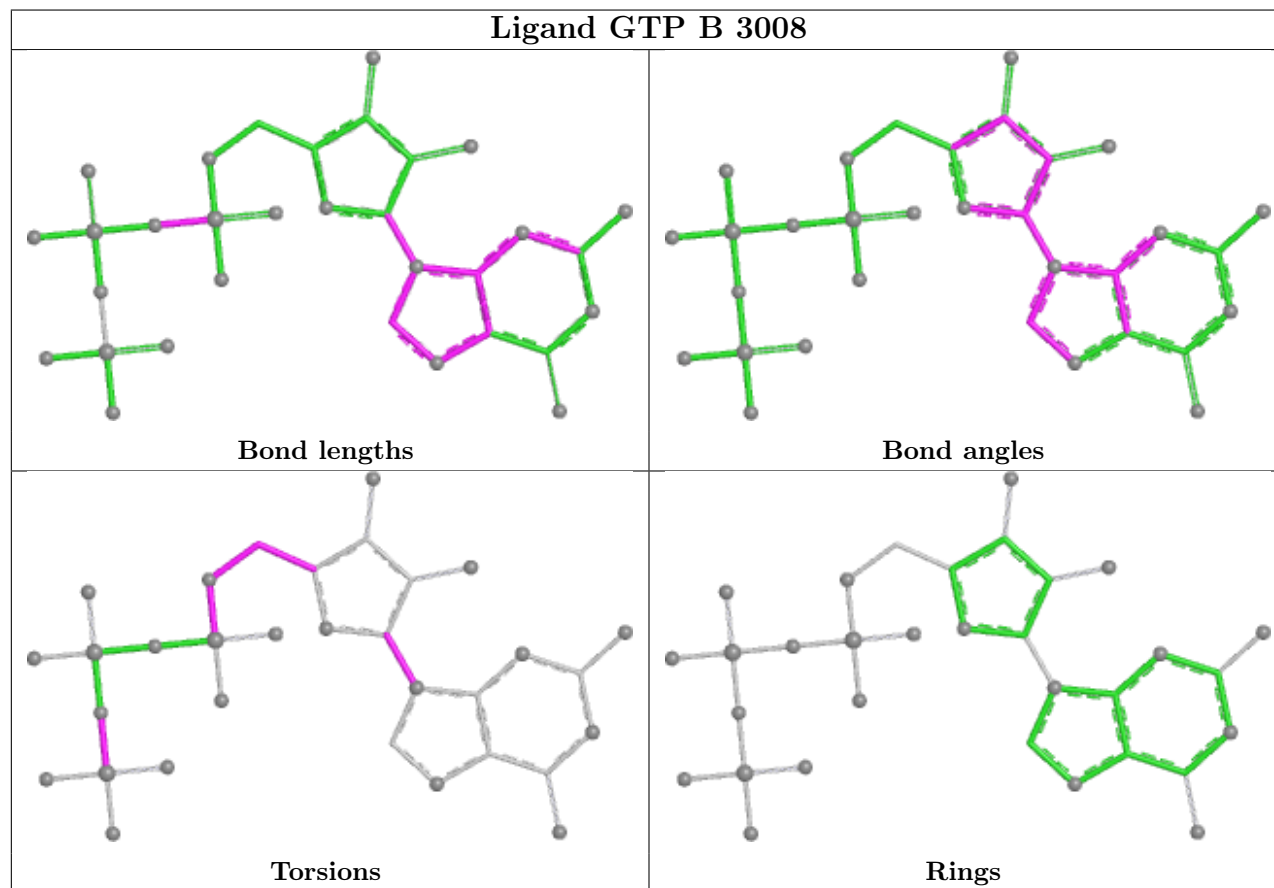
There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	3008	GTP	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	366:VAL	C	367:PRO	N	1.20

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	1351/1733 (77%)	-0.30	21 (1%) 70 47	20, 46, 110, 159	0
2	B	1091/1224 (89%)	-0.26	22 (2%) 65 41	21, 44, 116, 146	0
3	C	266/318 (83%)	-0.31	0 100 100	29, 50, 79, 131	0
4	E	215/215 (100%)	-0.12	3 (1%) 73 51	23, 60, 108, 138	0
5	F	83/155 (53%)	-0.50	0 100 100	24, 45, 71, 80	0
6	H	133/146 (91%)	0.55	7 (5%) 32 16	56, 88, 128, 135	0
7	I	121/122 (99%)	-0.29	4 (3%) 49 28	30, 50, 81, 111	0
8	J	64/70 (91%)	-0.57	0 100 100	31, 42, 71, 81	0
9	K	114/120 (95%)	-0.28	2 (1%) 67 44	31, 58, 79, 86	0
10	L	46/70 (65%)	0.66	2 (4%) 40 21	49, 95, 122, 125	0
All	All	3484/4173 (83%)	-0.24	61 (1%) 67 44	20, 49, 113, 159	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	4.1
2	B	1110	PRO	4.1
1	A	37	PHE	4.1
2	B	883	LEU	3.9
6	H	132	LEU	3.8
6	H	136	LYS	3.6
1	A	1080	THR	3.5
9	K	114	LEU	3.3
2	B	245	GLU	3.3
2	B	643	ASP	3.2
2	B	105	SER	3.1
2	B	733	HIS	3.0
2	B	436	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
6	H	63	LEU	2.8
1	A	327	ALA	2.8
7	I	121	PHE	2.7
1	A	190	ALA	2.7
1	A	53	LEU	2.7
6	H	85	GLY	2.6
2	B	1183	LYS	2.6
1	A	68	GLN	2.6
2	B	1102	LYS	2.5
10	L	25	ALA	2.5
1	A	61	ILE	2.5
2	B	868	MET	2.5
1	A	1081	LEU	2.5
2	B	89	GLU	2.4
6	H	104	PHE	2.4
2	B	882	THR	2.4
4	E	2	ASP	2.4
1	A	188	ASP	2.4
2	B	1107	ALA	2.4
1	A	1173	HIS	2.4
1	A	66	LYS	2.3
1	A	35	ILE	2.3
2	B	502	ILE	2.3
6	H	129	TYR	2.3
1	A	329	LEU	2.3
7	I	1	MET	2.2
1	A	65	LEU	2.2
2	B	1154	ALA	2.2
1	A	148	CYS	2.2
10	L	28	LYS	2.2
2	B	138	GLU	2.2
9	K	2	ASN	2.2
1	A	52	GLY	2.2
7	I	118	ARG	2.2
2	B	137	TYR	2.1
6	H	131	ASN	2.1
1	A	1078	GLN	2.1
2	B	552	MET	2.1
2	B	732	SER	2.1
4	E	90	VAL	2.1
1	A	268	ASP	2.1
2	B	106	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	191	THR	2.1
2	B	880	THR	2.1
7	I	3	THR	2.1
4	E	129	PRO	2.0
2	B	735	ALA	2.0
1	A	1450	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

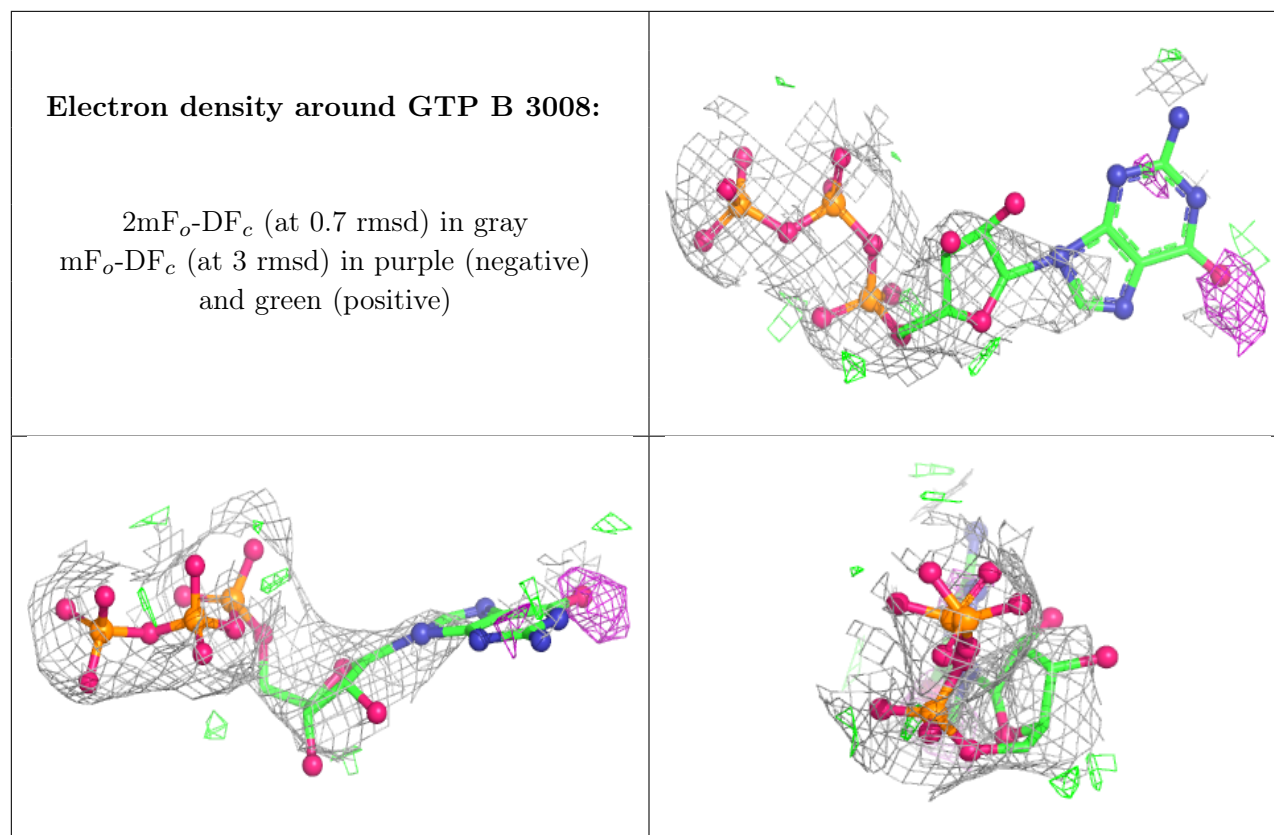
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
13	GTP	B	3008	32/32	0.88	0.14	96,112,119,119	0
12	MN	A	3010	1/1	0.91	0.06	48,48,48,48	0
11	ZN	A	3006	1/1	0.96	0.06	67,67,67,67	0
11	ZN	L	3005	1/1	0.96	0.04	96,96,96,96	0
12	MN	A	3009	1/1	0.98	0.04	36,36,36,36	0
11	ZN	A	3008	1/1	0.99	0.06	91,91,91,91	0
11	ZN	B	3007	1/1	0.99	0.02	64,64,64,64	0
11	ZN	C	3002	1/1	0.99	0.03	53,53,53,53	0
11	ZN	I	3004	1/1	0.99	0.03	80,80,80,80	0
11	ZN	I	3003	1/1	1.00	0.02	59,59,59,59	0
11	ZN	J	3001	1/1	1.00	0.01	47,47,47,47	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.