



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:31 PM GMT

PDB ID : 1TWH
Title : RNA polymerase II complexed with 2'dATP
Authors : Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2004-06-30
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

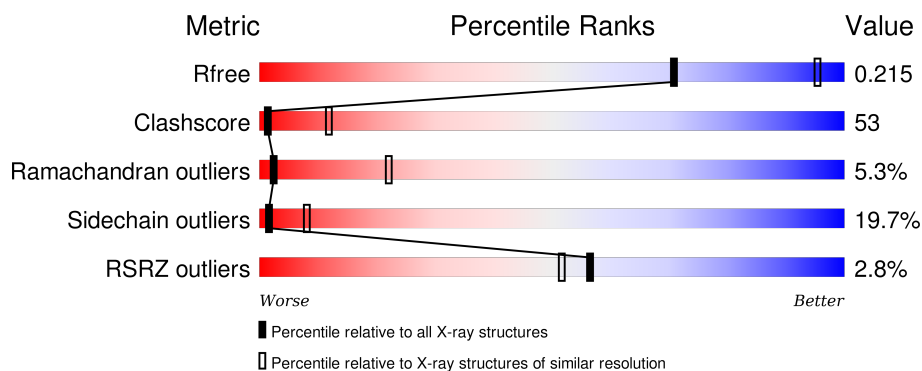
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	1733	<div> <div>2%</div> <div>7% 32% 28% 11% 22%</div> </div>
2	B	1224	<div> <div>4%</div> <div>6% 37% 34% 12% 11%</div> </div>
3	C	318	<div> <div>7% 30% 34% 14% 16%</div> </div>
4	E	215	<div> <div>2%</div> <div>5% 35% 40% 20%</div> </div>
5	F	155	<div> <div>•</div> <div>22% 23% 5% 46%</div> </div>

Continued on next page...

Continued from previous page...

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
12	ZN	C	3002	-	-	X	-
12	ZN	J	3001	-	-	X	-
13	ATP	A	3011	X	-	-	X

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 27728 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II largest subunit.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

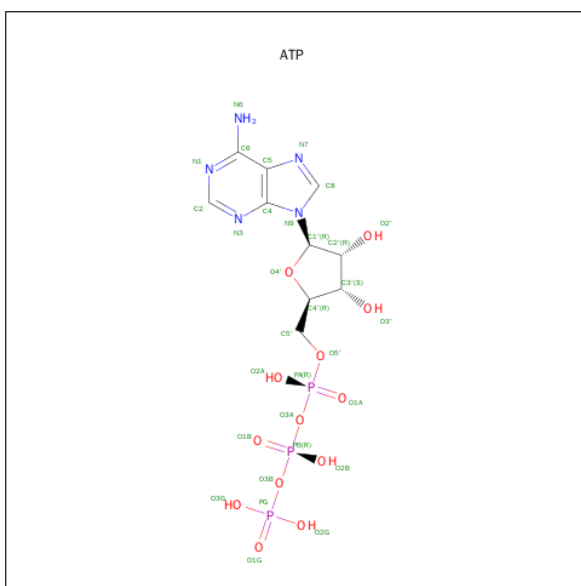
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	J	1	Total	Zn	0	0
			1	1		
12	B	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

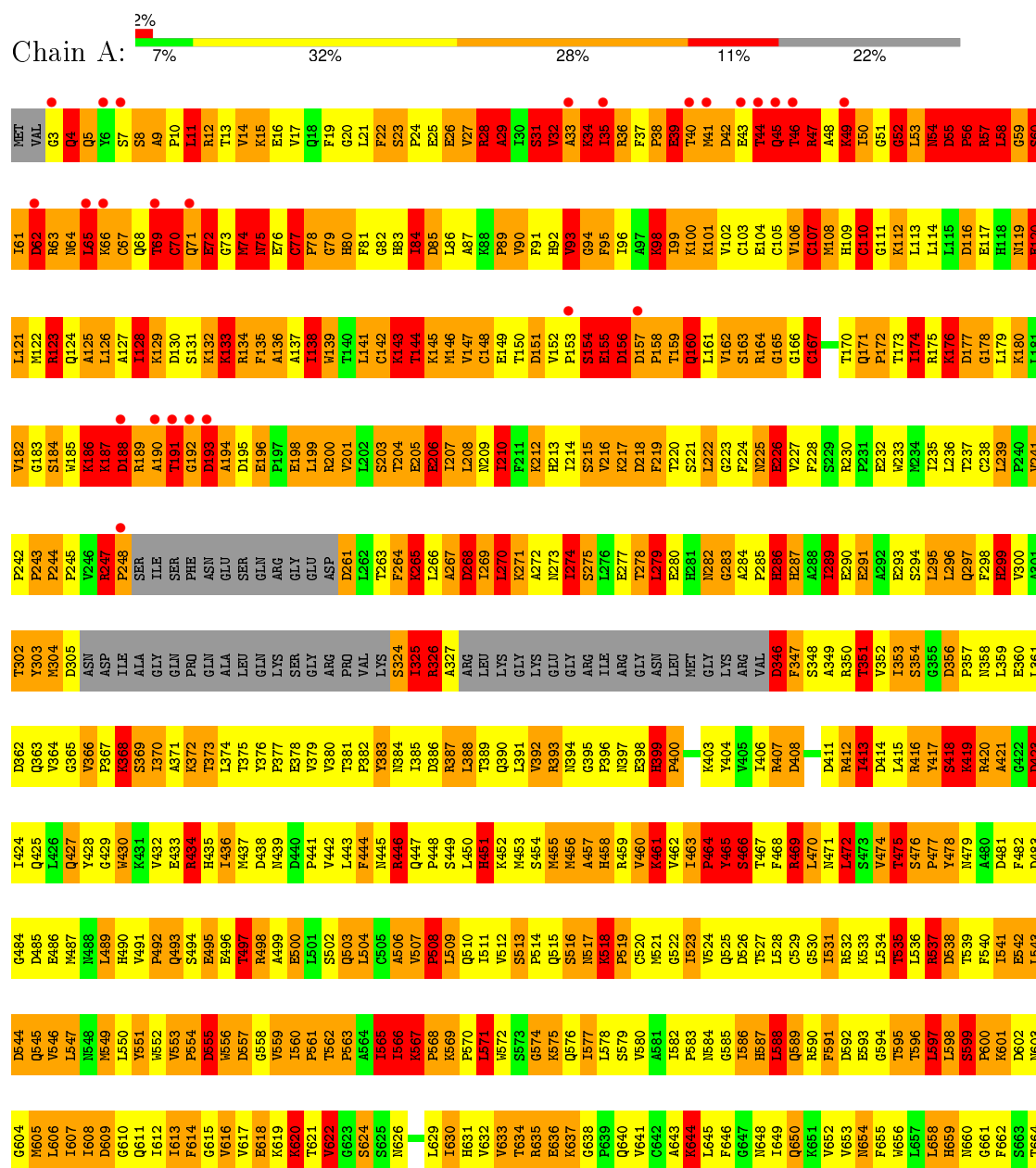
- Molecule 13 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



3 Residue-property plots

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

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

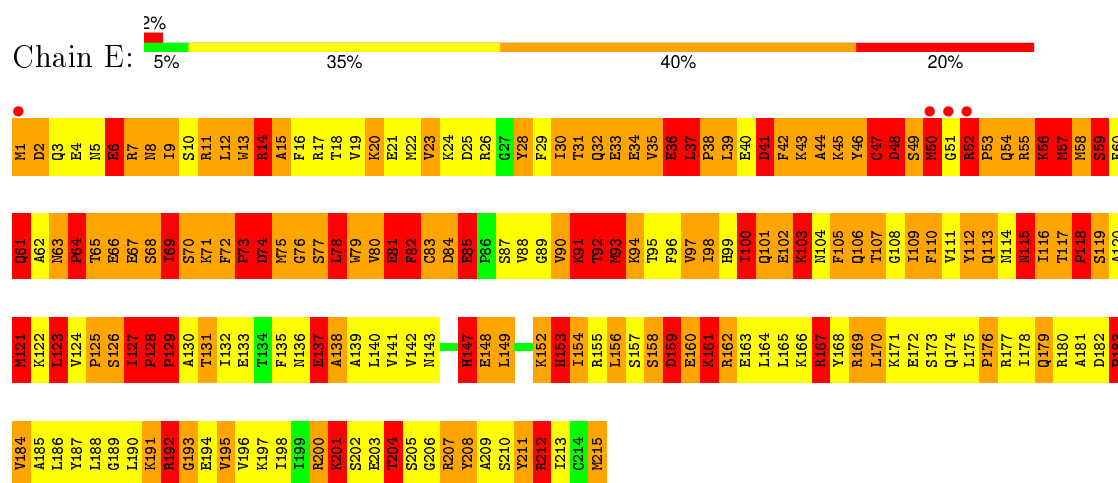




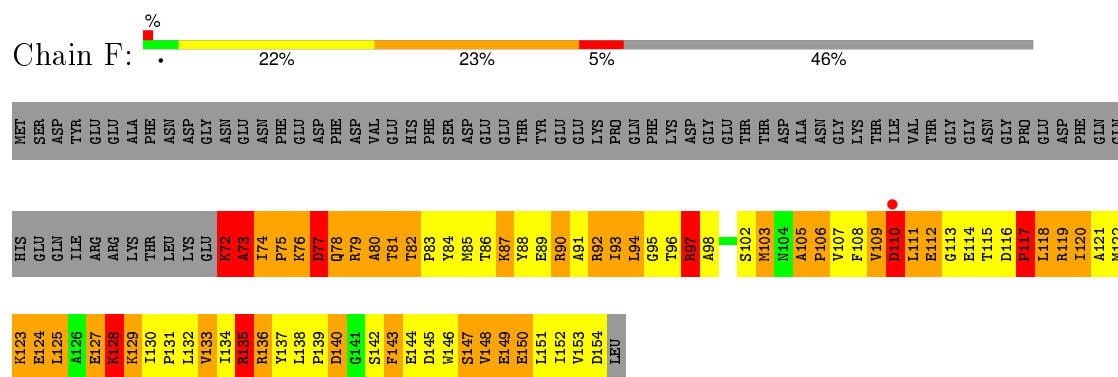
Chain B:



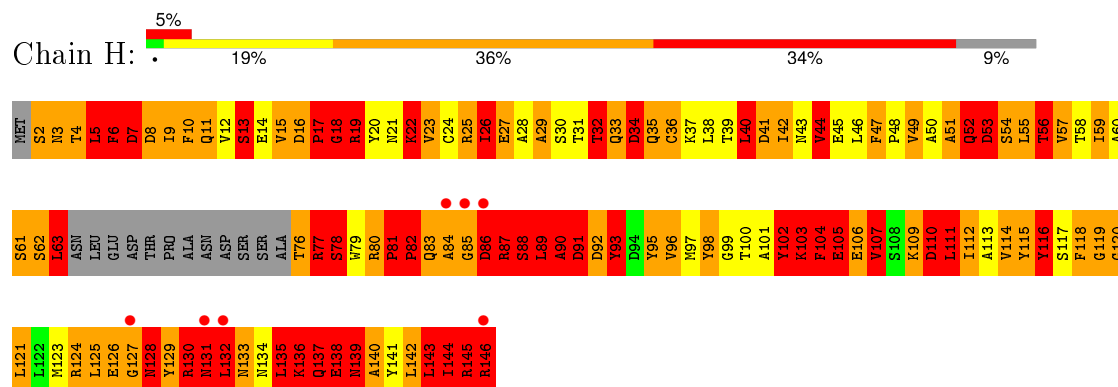




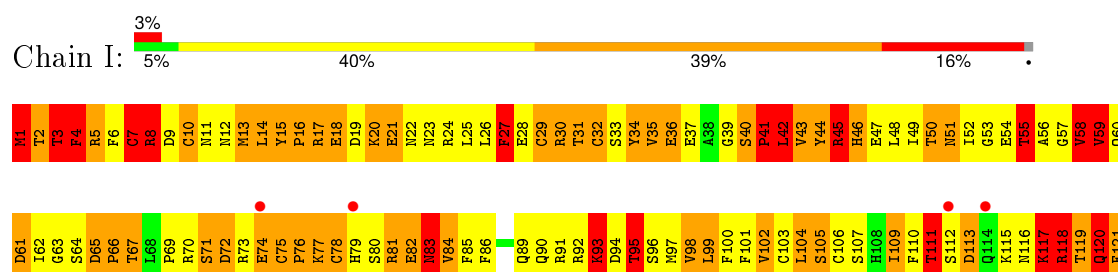
- Molecule 5: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



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




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



SER

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

Chain J: 

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

Chain K: 

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

Chain L: 

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.00 Å 223.00 Å 374.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.40 39.69 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.40) 97.3 (39.69-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 3.32 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.262 0.207 , 0.215	Depositor DCC
R_{free} test set	2055 reflections (2.98%)	DCC
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 50.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 77646 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	27728	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	4.62	2331/10792 (21.6%)	3.06	1145/14601 (7.8%)
2	B	4.57	1918/8860 (21.6%)	3.01	930/11945 (7.8%)
3	C	4.57	476/2133 (22.3%)	2.99	227/2891 (7.9%)
4	E	4.64	405/1796 (22.6%)	2.92	193/2416 (8.0%)
5	F	4.01	117/682 (17.2%)	3.01	56/922 (6.1%)
6	H	4.54	246/1086 (22.7%)	2.94	113/1470 (7.7%)
7	I	5.00	250/1009 (24.8%)	3.19	124/1357 (9.1%)
8	J	4.42	116/533 (21.8%)	3.66	79/715 (11.0%)
9	K	4.36	210/937 (22.4%)	3.12	108/1265 (8.5%)
10	L	5.55	101/366 (27.6%)	3.72	71/485 (14.6%)
All	All	4.60	6170/28194 (21.9%)	3.05	3046/38067 (8.0%)

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	57
2	B	0	55
3	C	0	15
4	E	1	9
5	F	0	1
6	H	0	12
7	I	0	6
9	K	0	2
10	L	0	2
All	All	1	159

All (6170) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1064	VAL	C-O	33.98	1.88	1.23
10	L	68	GLU	CG-CD	32.08	2.00	1.51
1	A	1064	VAL	CA-C	31.22	2.34	1.52
1	A	734	GLU	CD-OE2	30.34	1.59	1.25
2	B	552	MET	CG-SD	28.64	2.55	1.81
2	B	1150	ARG	CZ-NH2	28.27	1.69	1.33
2	B	529	GLU	CD-OE1	27.52	1.55	1.25
2	B	833	TYR	CE1-CZ	-27.51	1.02	1.38
10	L	68	GLU	CD-OE1	27.48	1.55	1.25
2	B	598	GLU	CG-CD	27.37	1.93	1.51
2	B	529	GLU	CD-OE2	26.92	1.55	1.25
2	B	1150	ARG	CZ-NH1	26.72	1.67	1.33
1	A	496	GLU	CD-OE1	26.58	1.54	1.25
1	A	1119	TYR	CE2-CZ	-26.38	1.04	1.38
1	A	206	GLU	CD-OE2	26.08	1.54	1.25
2	B	598	GLU	CD-OE2	25.68	1.53	1.25
7	I	37	GLU	CD-OE1	25.22	1.53	1.25
2	B	194	GLU	CD-OE1	24.60	1.52	1.25
1	A	681	GLU	CD-OE2	24.56	1.52	1.25
4	E	66	GLU	CD-OE2	24.43	1.52	1.25
2	B	239	GLU	CD-OE2	24.43	1.52	1.25
2	B	371	GLU	CD-OE1	24.25	1.52	1.25
1	A	728	LYS	CD-CE	24.02	2.11	1.51
1	A	771	GLU	CD-OE2	23.92	1.51	1.25
1	A	1277	GLU	CD-OE2	23.89	1.51	1.25
1	A	752	LYS	CE-NZ	23.72	2.08	1.49
4	E	208	TYR	CE1-CZ	-23.62	1.07	1.38
1	A	1196	GLU	CD-OE1	23.53	1.51	1.25
2	B	711	GLU	CG-CD	23.34	1.86	1.51
1	A	1064	VAL	CB-CG1	-23.26	1.04	1.52
1	A	938	LYS	CD-CE	23.24	2.09	1.51
4	E	208	TYR	CG-CD2	-23.10	1.09	1.39
1	A	620	LYS	CE-NZ	22.77	2.06	1.49
1	A	931	GLU	CD-OE2	22.76	1.50	1.25
1	A	752	LYS	CD-CE	22.73	2.08	1.51
1	A	1135	ARG	CG-CD	22.64	2.08	1.51
1	A	1280	GLU	CD-OE2	22.41	1.50	1.25
1	A	620	LYS	CD-CE	22.25	2.06	1.51
2	B	346	GLU	CG-CD	21.97	1.84	1.51
4	E	152	LYS	CD-CE	21.81	2.05	1.51
2	B	564	GLU	CD-OE1	21.74	1.49	1.25
1	A	1337	GLU	CD-OE1	21.73	1.49	1.25
1	A	1214	GLU	CD-OE1	21.73	1.49	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	57	MET	SD-CE	21.72	2.99	1.77
7	I	17	ARG	CG-CD	21.68	2.06	1.51
1	A	734	GLU	CD-OE1	21.65	1.49	1.25
1	A	1234	GLU	CD-OE1	21.64	1.49	1.25
1	A	618	GLU	CD-OE2	21.56	1.49	1.25
1	A	795	GLU	CD-OE2	21.20	1.49	1.25
3	C	154	LYS	CD-CE	21.07	2.04	1.51
2	B	211	VAL	CB-CG1	-20.71	1.09	1.52
1	A	44	THR	CA-CB	20.68	2.07	1.53
4	E	162	ARG	CG-CD	20.61	2.03	1.51
2	B	644	GLU	CD-OE1	20.56	1.48	1.25
1	A	941	LYS	CD-CE	20.54	2.02	1.51
2	B	665	GLU	CD-OE2	20.52	1.48	1.25
1	A	226	GLU	CD-OE2	20.44	1.48	1.25
2	B	312	GLU	CD-OE2	20.44	1.48	1.25
5	F	136	ARG	CZ-NH1	-20.43	1.06	1.33
1	A	1015	VAL	CB-CG2	-20.32	1.10	1.52
2	B	346	GLU	CD-OE2	20.13	1.47	1.25
2	B	531	GLN	CG-CD	20.05	1.97	1.51
1	A	1222	ASN	CB-CG	20.04	1.97	1.51
7	I	84	VAL	CB-CG2	-19.96	1.10	1.52
10	L	45	ALA	CA-CB	19.94	1.94	1.52
3	C	78	GLU	CD-OE2	19.90	1.47	1.25
3	C	12	GLU	CD-OE1	19.77	1.47	1.25
4	E	20	LYS	CE-NZ	19.73	1.98	1.49
1	A	196	GLU	CD-OE1	19.70	1.47	1.25
1	A	264	PHE	CB-CG	19.64	1.84	1.51
2	B	164	LYS	CD-CE	19.63	2.00	1.51
2	B	785	TYR	CG-CD2	-19.59	1.13	1.39
2	B	1153	GLU	CD-OE2	19.51	1.47	1.25
2	B	328	GLU	CD-OE2	19.46	1.47	1.25
2	B	785	TYR	CE1-CZ	-19.45	1.13	1.38
2	B	1052	VAL	CB-CG2	-19.38	1.12	1.52
6	H	141	TYR	CE1-CZ	-19.37	1.13	1.38
3	C	166	GLU	CD-OE2	19.25	1.46	1.25
7	I	72	ASP	CB-CG	19.22	1.92	1.51
2	B	650	GLU	CD-OE2	19.14	1.46	1.25
1	A	695	LYS	CD-CE	19.14	1.99	1.51
6	H	139	ASN	CB-CG	19.13	1.95	1.51
2	B	509	ALA	CA-CB	19.00	1.92	1.52
7	I	34	TYR	CE2-CZ	-18.98	1.13	1.38
6	H	45	GLU	CD-OE2	18.93	1.46	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1156	ASP	CB-CG	18.93	1.91	1.51
2	B	1155	SER	CA-CB	18.92	1.81	1.52
2	B	1132	GLU	CG-CD	18.89	1.80	1.51
3	C	78	GLU	CD-OE1	18.85	1.46	1.25
1	A	795	GLU	CG-CD	18.81	1.80	1.51
1	A	430	TRP	CE3-CZ3	-18.79	1.06	1.38
4	E	34	GLU	CD-OE2	18.77	1.46	1.25
1	A	49	LYS	CD-CE	18.77	1.98	1.51
1	A	1119	TYR	CG-CD1	-18.62	1.15	1.39
4	E	67	GLU	CD-OE1	18.47	1.46	1.25
2	B	124	TYR	CE1-CZ	-18.44	1.14	1.38
2	B	666	TYR	CE1-CZ	18.37	1.62	1.38
1	A	464	PRO	C-O	-18.32	0.86	1.23
1	A	1277	GLU	CD-OE1	18.15	1.45	1.25
1	A	496	GLU	CD-OE2	18.14	1.45	1.25
1	A	1349	TYR	CG-CD2	-18.11	1.15	1.39
1	A	1129	GLU	CD-OE1	18.03	1.45	1.25
2	B	908	GLU	CD-OE2	17.99	1.45	1.25
1	A	398	GLU	CD-OE2	17.96	1.45	1.25
1	A	618	GLU	CD-OE1	17.93	1.45	1.25
2	B	1061	GLU	CD-OE1	17.92	1.45	1.25
1	A	346	ASP	CB-CG	17.86	1.89	1.51
7	I	120	GLN	CB-CG	17.86	2.00	1.52
4	E	45	LYS	CD-CE	17.83	1.95	1.51
1	A	1223	ASP	CB-CG	17.81	1.89	1.51
1	A	632	VAL	CB-CG1	-17.75	1.15	1.52
2	B	785	TYR	CD1-CE1	-17.72	1.12	1.39
2	B	96	TYR	CE1-CZ	17.71	1.61	1.38
4	E	50	MET	SD-CE	17.71	2.77	1.77
1	A	1362	TYR	CG-CD2	-17.71	1.16	1.39
1	A	1277	GLU	CG-CD	17.69	1.78	1.51
1	A	1269	GLU	CD-OE1	17.68	1.45	1.25
2	B	347	LYS	CD-CE	17.68	1.95	1.51
2	B	641	GLU	CG-CD	17.68	1.78	1.51
1	A	724	GLU	CD-OE1	17.66	1.45	1.25
6	H	52	GLN	CG-CD	17.66	1.91	1.51
2	B	987	LYS	CE-NZ	17.66	1.93	1.49
7	I	55	THR	CB-CG2	17.65	2.10	1.52
10	L	34	CYS	CB-SG	-17.60	1.52	1.82
3	C	197	SER	CB-OG	17.53	1.65	1.42
1	A	681	GLU	CD-OE1	17.52	1.45	1.25
2	B	344	LYS	CB-CG	17.51	1.99	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	555	ASP	CB-CG	17.51	1.88	1.51
1	A	995	GLU	CD-OE2	17.51	1.45	1.25
2	B	235	SER	CB-OG	-17.49	1.19	1.42
2	B	497	ARG	CZ-NH1	17.47	1.55	1.33
1	A	801	GLU	CD-OE1	17.47	1.44	1.25
1	A	1110	ASN	CB-CG	17.46	1.91	1.51
2	B	434	ARG	CG-CD	17.40	1.95	1.51
2	B	239	GLU	CG-CD	17.37	1.78	1.51
1	A	1074	GLU	CD-OE2	17.36	1.44	1.25
3	C	50	GLU	CD-OE1	17.28	1.44	1.25
1	A	655	PHE	CG-CD2	-17.28	1.12	1.38
4	E	211	TYR	CE1-CZ	-17.27	1.16	1.38
2	B	137	TYR	CB-CG	17.27	1.77	1.51
1	A	1269	GLU	CD-OE2	17.26	1.44	1.25
1	A	1290	LYS	CD-CE	17.23	1.94	1.51
1	A	572	TRP	CZ3-CH2	-17.21	1.12	1.40
6	H	146	ARG	NE-CZ	17.21	1.55	1.33
1	A	945	GLU	CD-OE2	17.20	1.44	1.25
1	A	37	PHE	CE1-CZ	17.19	1.70	1.37
1	A	787	PHE	CE2-CZ	-17.19	1.04	1.37
1	A	1129	GLU	CG-CD	17.17	1.77	1.51
1	A	1425	SER	CB-OG	17.16	1.64	1.42
1	A	897	TYR	CG-CD2	-17.12	1.16	1.39
3	C	3	GLU	CD-OE2	17.11	1.44	1.25
1	A	1337	GLU	CD-OE2	17.11	1.44	1.25
2	B	305	VAL	CB-CG1	17.07	1.88	1.52
2	B	344	LYS	CD-CE	17.04	1.93	1.51
4	E	66	GLU	CG-CD	17.03	1.77	1.51
2	B	502	ILE	CA-CB	17.00	1.94	1.54
1	A	787	PHE	CG-CD1	-17.00	1.13	1.38
1	A	205	GLU	CD-OE1	16.99	1.44	1.25
3	C	165	LYS	CE-NZ	16.99	1.91	1.49
8	J	42	LYS	CD-CE	16.98	1.93	1.51
1	A	870	GLU	CD-OE2	16.95	1.44	1.25
4	E	162	ARG	CB-CG	16.93	1.98	1.52
3	C	170	TRP	CZ3-CH2	-16.92	1.12	1.40
7	I	36	GLU	CG-CD	16.92	1.77	1.51
10	L	50	ASP	CB-CG	16.91	1.87	1.51
10	L	68	GLU	CD-OE2	16.87	1.44	1.25
1	A	16	GLU	CD-OE1	16.87	1.44	1.25
1	A	404	TYR	CG-CD1	-16.87	1.17	1.39
3	C	89	GLU	CD-OE2	16.86	1.44	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	126	GLU	CD-OE1	16.79	1.44	1.25
1	A	1275	GLY	C-O	16.77	1.50	1.23
1	A	751	SER	CB-OG	16.74	1.64	1.42
7	I	1	MET	CG-SD	16.73	2.24	1.81
3	C	195	GLN	CG-CD	16.69	1.89	1.51
2	B	183	GLU	CG-CD	16.68	1.76	1.51
1	A	896	ARG	CZ-NH1	16.66	1.54	1.33
2	B	945	GLU	CD-OE1	16.63	1.44	1.25
2	B	758	PHE	CE1-CZ	16.63	1.69	1.37
2	B	103	ASN	CB-CG	16.61	1.89	1.51
1	A	1350	LYS	CE-NZ	16.60	1.90	1.49
1	A	777	PHE	CG-CD2	-16.59	1.13	1.38
3	C	50	GLU	CG-CD	16.46	1.76	1.51
1	A	206	GLU	CD-OE1	16.45	1.43	1.25
1	A	291	GLU	CG-CD	16.43	1.76	1.51
7	I	34	TYR	CG-CD2	-16.37	1.17	1.39
4	E	211	TYR	CE2-CZ	-16.34	1.17	1.38
1	A	1372	VAL	CB-CG1	-16.32	1.18	1.52
7	I	21	GLU	CD-OE2	16.30	1.43	1.25
6	H	131	ASN	CB-CG	16.30	1.88	1.51
2	B	1132	GLU	CD-OE1	16.30	1.43	1.25
2	B	708	GLU	CD-OE2	16.29	1.43	1.25
1	A	1280	GLU	C-O	-16.27	0.92	1.23
2	B	552	MET	SD-CE	16.21	2.68	1.77
7	I	54	GLU	CD-OE2	16.18	1.43	1.25
1	A	1259	MET	CG-SD	16.16	2.23	1.81
6	H	19	ARG	CG-CD	16.16	1.92	1.51
7	I	117	LYS	CE-NZ	16.15	1.89	1.49
3	C	198	ALA	CA-CB	-16.15	1.18	1.52
2	B	96	TYR	CG-CD1	16.13	1.60	1.39
1	A	1225	PHE	CB-CG	16.08	1.78	1.51
2	B	697	GLU	CD-OE2	16.05	1.43	1.25
2	B	1007	VAL	CB-CG1	-16.03	1.19	1.52
2	B	650	GLU	CD-OE1	16.01	1.43	1.25
4	E	131	THR	CB-CG2	15.97	2.05	1.52
2	B	186	GLU	CD-OE2	15.94	1.43	1.25
2	B	459	TYR	CD2-CE2	15.92	1.63	1.39
1	A	123	ARG	CB-CG	15.90	1.95	1.52
2	B	855	PHE	CG-CD2	-15.90	1.15	1.38
2	B	1154	ALA	CA-CB	15.89	1.85	1.52
1	A	1232	ASN	CB-CG	15.88	1.87	1.51
2	B	646	LEU	CG-CD2	15.88	2.10	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	665	GLU	CD-OE1	15.88	1.43	1.25
1	A	843	LYS	CD-CE	15.87	1.91	1.51
1	A	1034	GLU	CD-OE2	15.86	1.43	1.25
1	A	792	TYR	CE1-CZ	-15.86	1.18	1.38
1	A	1422	ARG	NE-CZ	15.85	1.53	1.33
7	I	93	LYS	CD-CE	15.85	1.90	1.51
2	B	96	TYR	CG-CD2	15.84	1.59	1.39
1	A	931	GLU	CG-CD	15.82	1.75	1.51
3	C	200	GLU	CD-OE2	15.72	1.43	1.25
1	A	427	GLN	CG-CD	15.72	1.87	1.51
1	A	1281	ARG	NE-CZ	15.71	1.53	1.33
8	J	27	GLU	CD-OE1	15.68	1.42	1.25
2	B	951	GLN	CG-CD	15.67	1.87	1.51
2	B	531	GLN	CD-OE1	15.66	1.58	1.24
2	B	692	TYR	CG-CD1	-15.63	1.18	1.39
1	A	1153	TYR	CG-CD1	-15.61	1.18	1.39
1	A	1315	GLU	CD-OE2	15.61	1.42	1.25
3	C	75	MET	SD-CE	15.59	2.65	1.77
2	B	785	TYR	CG-CD1	-15.55	1.19	1.39
2	B	312	GLU	CD-OE1	15.47	1.42	1.25
10	L	29	TYR	CE2-CZ	-15.46	1.18	1.38
1	A	868	TYR	CE2-CZ	-15.46	1.18	1.38
6	H	104	PHE	CA-C	15.41	1.93	1.52
4	E	161	LYS	CD-CE	15.37	1.89	1.51
1	A	1137	ALA	C-O	15.36	1.52	1.23
1	A	155	GLU	CD-OE2	15.35	1.42	1.25
1	A	655	PHE	CE1-CZ	-15.33	1.08	1.37
1	A	551	TYR	CE2-CZ	-15.33	1.18	1.38
1	A	593	GLU	C-O	15.29	1.52	1.23
2	B	811	TYR	CZ-OH	-15.28	1.11	1.37
7	I	82	GLU	CG-CD	15.23	1.74	1.51
7	I	82	GLU	CD-OE1	15.17	1.42	1.25
4	E	191	LYS	CD-CE	15.17	1.89	1.51
5	F	129	LYS	CD-CE	15.17	1.89	1.51
1	A	1304	TRP	CE2-CZ2	-15.15	1.14	1.39
1	A	433	GLU	CD-OE1	15.15	1.42	1.25
2	B	1041	GLU	CD-OE2	15.15	1.42	1.25
1	A	1108	ALA	CA-CB	-15.14	1.20	1.52
1	A	897	TYR	CE1-CZ	-15.12	1.18	1.38
2	B	769	TYR	CD2-CE2	-15.12	1.16	1.39
9	K	32	VAL	CB-CG2	-15.11	1.21	1.52
10	L	29	TYR	CG-CD2	-15.11	1.19	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	961	ARG	CZ-NH2	15.04	1.52	1.33
2	B	1188	LYS	CD-CE	15.04	1.88	1.51
9	K	79	GLU	CD-OE1	15.03	1.42	1.25
2	B	459	TYR	CD1-CE1	15.03	1.61	1.39
7	I	28	GLU	CD-OE1	15.03	1.42	1.25
1	A	1230	GLU	CD-OE1	15.02	1.42	1.25
9	K	111	LEU	C-O	15.01	1.51	1.23
1	A	293	GLU	CD-OE2	15.01	1.42	1.25
1	A	1135	ARG	CZ-NH2	15.01	1.52	1.33
1	A	16	GLU	CD-OE2	15.00	1.42	1.25
3	C	3	GLU	CD-OE1	14.99	1.42	1.25
1	A	551	TYR	CG-CD2	-14.93	1.19	1.39
2	B	811	TYR	CE2-CZ	-14.93	1.19	1.38
2	B	833	TYR	CG-CD2	-14.90	1.19	1.39
4	E	40	GLU	CD-OE1	14.90	1.42	1.25
2	B	962	LYS	CD-CE	14.88	1.88	1.51
6	H	129	TYR	CE1-CZ	14.88	1.57	1.38
1	A	1132	LYS	CD-CE	14.82	1.88	1.51
1	A	1171	GLN	CG-CD	14.79	1.85	1.51
4	E	211	TYR	CG-CD2	-14.76	1.20	1.39
1	A	1280	GLU	CG-CD	14.75	1.74	1.51
2	B	1137	CYS	CB-SG	-14.72	1.57	1.82
4	E	208	TYR	CG-CD1	-14.70	1.20	1.39
7	I	27	PHE	CE1-CZ	-14.70	1.09	1.37
5	F	149	GLU	CG-CD	14.68	1.74	1.51
2	B	31	TRP	CG-CD1	-14.66	1.16	1.36
10	L	26	THR	CA-CB	14.66	1.91	1.53
2	B	569	TYR	CE1-CZ	-14.66	1.19	1.38
8	J	38	ARG	CB-CG	14.66	1.92	1.52
1	A	895	LYS	CD-CE	14.65	1.87	1.51
1	A	942	PHE	CD2-CE2	-14.63	1.09	1.39
1	A	995	GLU	CD-OE1	14.63	1.41	1.25
2	B	296	GLU	CD-OE2	14.63	1.41	1.25
1	A	934	LYS	CD-CE	14.62	1.87	1.51
1	A	1102	LYS	CG-CD	14.60	2.02	1.52
1	A	1109	LYS	CD-CE	14.59	1.87	1.51
2	B	1146	PHE	CE2-CZ	-14.57	1.09	1.37
3	C	210	GLU	CD-OE2	14.57	1.41	1.25
9	K	91	CYS	CB-SG	-14.56	1.57	1.82
2	B	875	GLU	CG-CD	14.55	1.73	1.51
3	C	18	VAL	CB-CG2	-14.53	1.22	1.52
9	K	61	TYR	CG-CD2	-14.50	1.20	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	GLY	C-O	14.48	1.46	1.23
10	L	63	ARG	NE-CZ	14.48	1.51	1.33
6	H	20	TYR	CE2-CZ	-14.48	1.19	1.38
2	B	303	TYR	CD2-CE2	-14.47	1.17	1.39
1	A	801	GLU	CD-OE2	14.46	1.41	1.25
4	E	168	TYR	CE2-CZ	-14.46	1.19	1.38
5	F	149	GLU	CD-OE2	14.46	1.41	1.25
7	I	8	ARG	CZ-NH1	14.43	1.51	1.33
3	C	219	PHE	CE1-CZ	-14.42	1.09	1.37
1	A	1230	GLU	CD-OE2	14.40	1.41	1.25
9	K	16	GLU	CD-OE2	14.38	1.41	1.25
1	A	1239	ARG	CG-CD	14.38	1.87	1.51
2	B	1050	ILE	C-O	-14.37	0.96	1.23
9	K	108	GLU	CD-OE2	14.37	1.41	1.25
3	C	66	ARG	NE-CZ	-14.35	1.14	1.33
2	B	769	TYR	CD1-CE1	-14.32	1.17	1.39
1	A	813	PHE	CE2-CZ	-14.31	1.10	1.37
1	A	933	TYR	CE2-CZ	-14.31	1.20	1.38
1	A	703	THR	CB-CG2	14.31	1.99	1.52
2	B	968	VAL	CB-CG2	-14.30	1.22	1.52
7	I	45	ARG	CG-CD	14.28	1.87	1.51
1	A	186	LYS	CD-CE	14.27	1.86	1.51
2	B	380	TYR	CE2-CZ	-14.25	1.20	1.38
2	B	723	VAL	CB-CG2	14.23	1.82	1.52
8	J	21	TYR	CG-CD2	-14.23	1.20	1.39
2	B	183	GLU	CD-OE1	14.22	1.41	1.25
2	B	328	GLU	CB-CG	14.21	1.79	1.52
1	A	1214	GLU	CD-OE2	14.21	1.41	1.25
1	A	1447	GLU	CD-OE1	14.20	1.41	1.25
2	B	31	TRP	CZ3-CH2	-14.20	1.17	1.40
2	B	681	TRP	CG-CD1	-14.19	1.16	1.36
4	E	1	MET	CG-SD	14.18	2.18	1.81
1	A	795	GLU	CD-OE1	14.18	1.41	1.25
2	B	434	ARG	CB-CG	14.17	1.90	1.52
2	B	216	GLU	CD-OE2	14.16	1.41	1.25
2	B	436	VAL	CA-CB	14.14	1.84	1.54
3	C	209	TYR	CE2-CZ	14.13	1.56	1.38
10	L	62	LYS	CD-CE	14.13	1.86	1.51
1	A	1235	LYS	CD-CE	14.09	1.86	1.51
1	A	518	LYS	CD-CE	14.09	1.86	1.51
1	A	681	GLU	CG-CD	14.08	1.73	1.51
2	B	588	GLY	C-O	14.08	1.46	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	190	TYR	CE2-CZ	-14.07	1.20	1.38
1	A	1131	ALA	CA-CB	-14.06	1.23	1.52
1	A	792	TYR	CG-CD2	-14.06	1.20	1.39
1	A	677	ARG	CZ-NH1	14.05	1.51	1.33
1	A	1234	GLU	CG-CD	14.05	1.73	1.51
2	B	692	TYR	CG-CD2	-14.04	1.20	1.39
2	B	65	GLU	CG-CD	14.03	1.73	1.51
1	A	1287	TYR	CG-CD1	14.03	1.57	1.39
6	H	126	GLU	CG-CD	14.03	1.73	1.51
8	J	29	GLU	CD-OE1	14.03	1.41	1.25
1	A	1228	TRP	CD2-CE2	-14.01	1.24	1.41
2	B	742	GLU	CD-OE2	-14.00	1.10	1.25
2	B	346	GLU	CD-OE1	13.98	1.41	1.25
1	A	466	SER	CB-OG	-13.98	1.24	1.42
1	A	1447	GLU	CD-OE2	13.97	1.41	1.25
3	C	125	MET	SD-CE	13.96	2.56	1.77
9	K	61	TYR	CE1-CZ	-13.96	1.20	1.38
6	H	19	ARG	CB-CG	13.94	1.90	1.52
1	A	728	LYS	CG-CD	13.91	1.99	1.52
1	A	744	LYS	CD-CE	13.91	1.86	1.51
3	C	154	LYS	CG-CD	13.90	1.99	1.52
1	A	196	GLU	CD-OE2	13.88	1.41	1.25
6	H	20	TYR	CE1-CZ	-13.88	1.20	1.38
4	E	90	VAL	CB-CG1	13.87	1.81	1.52
1	A	1109	LYS	CG-CD	13.87	1.99	1.52
1	A	205	GLU	CG-CD	13.86	1.72	1.51
7	I	18	GLU	CD-OE1	13.81	1.40	1.25
2	B	27	ALA	CA-CB	-13.80	1.23	1.52
2	B	1032	SER	CB-OG	13.80	1.60	1.42
1	A	601	LYS	CD-CE	13.77	1.85	1.51
2	B	653	VAL	CB-CG2	-13.77	1.24	1.52
2	B	895	ASP	CB-CG	13.77	1.80	1.51
4	E	67	GLU	CD-OE2	13.77	1.40	1.25
4	E	208	TYR	CB-CG	13.77	1.72	1.51
2	B	101	MET	SD-CE	13.76	2.54	1.77
2	B	766	ARG	CZ-NH1	13.76	1.50	1.33
2	B	1146	PHE	CG-CD1	-13.75	1.18	1.38
3	C	15	LYS	CB-CG	13.75	1.89	1.52
1	A	1417	GLU	CD-OE1	13.74	1.40	1.25
1	A	1264	GLU	CD-OE2	-13.74	1.10	1.25
1	A	496	GLU	CG-CD	13.73	1.72	1.51
2	B	853	SER	CB-OG	13.73	1.60	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	350	ARG	NE-CZ	-13.72	1.15	1.33
1	A	1214	GLU	CG-CD	13.72	1.72	1.51
3	C	114	TYR	CE2-CZ	-13.71	1.20	1.38
1	A	1118	VAL	CB-CG2	-13.70	1.24	1.52
2	B	785	TYR	CE2-CZ	-13.70	1.20	1.38
3	C	49	VAL	CB-CG2	-13.69	1.24	1.52
6	H	19	ARG	CZ-NH2	13.68	1.50	1.33
1	A	1132	LYS	CE-NZ	13.67	1.83	1.49
1	A	552	TRP	CD2-CE2	-13.64	1.25	1.41
1	A	1034	GLU	CG-CD	13.63	1.72	1.51
1	A	1274	ARG	CZ-NH1	13.62	1.50	1.33
1	A	880	LYS	C-O	-13.62	0.97	1.23
3	C	195	GLN	CD-OE1	13.61	1.53	1.24
7	I	74	GLU	CD-OE2	13.61	1.40	1.25
2	B	833	TYR	CE2-CZ	-13.60	1.20	1.38
1	A	643	ALA	CA-CB	-13.60	1.23	1.52
2	B	415	GLN	CB-CG	13.57	1.89	1.52
6	H	23	VAL	CA-CB	-13.57	1.26	1.54
1	A	879	GLU	CD-OE1	13.56	1.40	1.25
7	I	54	GLU	CD-OE1	13.55	1.40	1.25
1	A	833	GLU	CD-OE1	13.54	1.40	1.25
2	B	723	VAL	CB-CG1	13.54	1.81	1.52
1	A	984	LYS	CE-NZ	13.54	1.82	1.49
1	A	990	VAL	CB-CG1	-13.54	1.24	1.52
2	B	1061	GLU	CD-OE2	13.54	1.40	1.25
1	A	839	ARG	NE-CZ	13.53	1.50	1.33
2	B	1192	TYR	CG-CD1	-13.53	1.21	1.39
8	J	63	TYR	CG-CD2	-13.52	1.21	1.39
4	E	162	ARG	NE-CZ	13.51	1.50	1.33
1	A	551	TYR	CE1-CZ	-13.51	1.21	1.38
3	C	157	CYS	CB-SG	-13.51	1.59	1.82
3	C	9	LYS	CD-CE	13.50	1.85	1.51
6	H	116	TYR	CG-CD1	13.48	1.56	1.39
2	B	459	TYR	CG-CD1	13.48	1.56	1.39
1	A	734	GLU	CG-CD	13.47	1.72	1.51
8	J	44	TYR	CG-CD2	-13.47	1.21	1.39
2	B	892	LYS	CD-CE	13.45	1.84	1.51
2	B	333	PHE	CG-CD2	-13.44	1.18	1.38
2	B	21	GLU	CD-OE2	13.43	1.40	1.25
3	C	210	GLU	CD-OE1	13.43	1.40	1.25
9	K	20	LYS	CD-CE	13.41	1.84	1.51
1	A	731	ARG	C-O	-13.40	0.97	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	ASN	CG-OD1	13.40	1.53	1.24
1	A	1005	GLU	CD-OE1	13.39	1.40	1.25
2	B	519	TRP	CZ3-CH2	-13.39	1.18	1.40
10	L	28	LYS	CE-NZ	13.38	1.82	1.49
1	A	120	GLU	CD-OE1	13.38	1.40	1.25
2	B	418	LYS	CD-CE	13.38	1.84	1.51
2	B	1087	PHE	CD2-CE2	-13.37	1.12	1.39
2	B	996	ARG	CZ-NH1	13.37	1.50	1.33
2	B	1186	ASP	CB-CG	13.37	1.79	1.51
7	I	100	PHE	CG-CD2	-13.37	1.18	1.38
8	J	21	TYR	CE1-CZ	-13.36	1.21	1.38
2	B	1221	SER	CA-CB	13.35	1.73	1.52
1	A	677	ARG	CZ-NH2	13.35	1.50	1.33
1	A	747	VAL	CB-CG1	-13.34	1.24	1.52
1	A	552	TRP	CZ3-CH2	-13.31	1.18	1.40
1	A	469	ARG	CD-NE	-13.31	1.23	1.46
4	E	168	TYR	CD2-CE2	13.30	1.59	1.39
1	A	858	ASN	CB-CG	-13.30	1.20	1.51
3	C	205	LYS	CD-CE	13.30	1.84	1.51
2	B	699	GLU	N-CA	-13.28	1.19	1.46
1	A	507	VAL	CB-CG2	-13.28	1.25	1.52
2	B	169	ARG	CZ-NH2	13.28	1.50	1.33
2	B	31	TRP	CD2-CE2	-13.26	1.25	1.41
3	C	12	GLU	CD-OE2	13.25	1.40	1.25
3	C	94	LYS	CE-NZ	13.25	1.82	1.49
1	A	1351	GLU	CD-OE2	13.23	1.40	1.25
2	B	65	GLU	CD-OE2	13.23	1.40	1.25
1	A	551	TYR	CG-CD1	-13.23	1.22	1.39
3	C	220	ASP	CB-CG	13.22	1.79	1.51
1	A	893	PHE	CG-CD1	-13.22	1.19	1.38
1	A	1287	TYR	CD2-CE2	13.20	1.59	1.39
10	L	47	ARG	CG-CD	13.20	1.84	1.51
1	A	677	ARG	NE-CZ	13.19	1.50	1.33
1	A	268	ASP	CB-CG	13.19	1.79	1.51
9	K	2	ASN	C-O	13.19	1.48	1.23
1	A	1129	GLU	CD-OE2	13.18	1.40	1.25
1	A	830	LYS	CG-CD	13.15	1.97	1.52
1	A	1426	GLU	CD-OE1	13.14	1.40	1.25
5	F	87	LYS	CD-CE	13.13	1.84	1.51
1	A	1103	GLU	CD-OE2	13.12	1.40	1.25
6	H	20	TYR	CG-CD2	-13.12	1.22	1.39
1	A	1232	ASN	CG-OD1	13.12	1.52	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	20	LYS	CD-CE	13.12	1.84	1.51
4	E	187	TYR	CG-CD1	-13.11	1.22	1.39
1	A	1023	ARG	CZ-NH1	-13.11	1.16	1.33
2	B	409	ALA	CA-CB	-13.10	1.25	1.52
1	A	1112	LYS	CD-CE	13.09	1.83	1.51
1	A	1353	TYR	CG-CD1	-13.09	1.22	1.39
1	A	1291	VAL	CA-CB	-13.09	1.27	1.54
1	A	1304	TRP	CE3-CZ3	-13.09	1.16	1.38
1	A	106	VAL	CB-CG2	-13.08	1.25	1.52
1	A	1301	GLU	CD-OE1	13.08	1.40	1.25
2	B	641	GLU	CD-OE2	13.07	1.40	1.25
1	A	1232	ASN	C-O	13.07	1.48	1.23
2	B	994	TYR	CE2-CZ	-13.07	1.21	1.38
4	E	137	GLU	CD-OE1	13.07	1.40	1.25
2	B	1219	ASP	CB-CG	13.07	1.79	1.51
1	A	217	LYS	CD-CE	13.07	1.83	1.51
1	A	227	VAL	C-O	13.06	1.48	1.23
2	B	371	GLU	CG-CD	13.05	1.71	1.51
2	B	706	GLN	CG-CD	13.04	1.81	1.51
1	A	1153	TYR	CE2-CZ	-13.04	1.21	1.38
2	B	963	PHE	CB-CG	-13.03	1.29	1.51
3	C	196	ASP	CB-CG	13.02	1.79	1.51
1	A	117	GLU	CD-OE1	13.00	1.40	1.25
1	A	1003	LYS	CD-CE	13.00	1.83	1.51
1	A	1337	GLU	CG-CD	13.00	1.71	1.51
4	E	82	PHE	CE2-CZ	13.00	1.62	1.37
1	A	738	LYS	CE-NZ	12.99	1.81	1.49
6	H	2	SER	CA-CB	12.99	1.72	1.52
6	H	107	VAL	CB-CG1	12.98	1.80	1.52
2	B	531	GLN	CB-CG	12.97	1.87	1.52
1	A	941	LYS	CE-NZ	12.96	1.81	1.49
1	A	376	TYR	CG-CD1	-12.96	1.22	1.39
4	E	179	GLN	CD-OE1	12.96	1.52	1.24
1	A	157	ASP	CB-CG	12.95	1.78	1.51
2	B	903	VAL	CA-CB	-12.95	1.27	1.54
1	A	1290	LYS	CE-NZ	12.94	1.81	1.49
4	E	46	TYR	CD2-CE2	12.94	1.58	1.39
3	C	82	TYR	CZ-OH	12.93	1.59	1.37
2	B	1083	ALA	CA-CB	-12.93	1.25	1.52
2	B	581	PHE	CG-CD1	-12.92	1.19	1.38
3	C	194	GLU	CD-OE2	12.92	1.39	1.25
1	A	5	GLN	CB-CG	12.90	1.87	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	666	TYR	CD2-CE2	12.88	1.58	1.39
3	C	4	GLU	CD-OE1	12.88	1.39	1.25
1	A	914	GLU	CD-OE1	12.86	1.39	1.25
1	A	597	LEU	CG-CD1	12.85	1.99	1.51
1	A	460	VAL	CB-CG2	-12.85	1.25	1.52
1	A	188	ASP	CB-CG	12.85	1.78	1.51
1	A	524	VAL	CB-CG2	-12.84	1.25	1.52
2	B	1206	GLU	CD-OE1	12.84	1.39	1.25
1	A	1154	TYR	CE2-CZ	12.83	1.55	1.38
1	A	193	ASP	CB-CG	12.82	1.78	1.51
1	A	478	TYR	CD1-CE1	-12.82	1.20	1.39
2	B	908	GLU	CB-CG	12.82	1.76	1.52
7	I	57	GLY	C-O	-12.81	1.03	1.23
2	B	870	ILE	CA-CB	12.81	1.84	1.54
1	A	37	PHE	CG-CD2	12.80	1.57	1.38
2	B	319	GLU	CD-OE1	12.79	1.39	1.25
1	A	12	ARG	CZ-NH1	12.79	1.49	1.33
2	B	627	PHE	CD1-CE1	-12.79	1.13	1.39
1	A	149	GLU	CD-OE2	12.78	1.39	1.25
2	B	477	ALA	CA-CB	12.77	1.79	1.52
1	A	1417	GLU	CG-CD	12.76	1.71	1.51
2	B	1069	PHE	CE1-CZ	-12.76	1.13	1.37
1	A	1255	GLU	CD-OE2	12.75	1.39	1.25
1	A	1196	GLU	CD-OE2	12.74	1.39	1.25
1	A	1012	ARG	CG-CD	12.74	1.83	1.51
1	A	705	LYS	CB-CG	12.74	1.86	1.52
2	B	1198	TYR	CD2-CE2	12.73	1.58	1.39
9	K	35	PHE	CG-CD1	-12.73	1.19	1.38
1	A	1280	GLU	CD-OE1	12.73	1.39	1.25
1	A	977	LYS	CB-CG	12.72	1.86	1.52
2	B	315	LYS	CE-NZ	12.72	1.80	1.49
2	B	1106	ARG	CG-CD	12.72	1.83	1.51
9	K	12	LEU	CG-CD1	12.71	1.98	1.51
9	K	71	PHE	CD2-CE2	-12.70	1.13	1.39
2	B	768	THR	CA-C	12.70	1.85	1.52
2	B	262	GLU	CD-OE1	12.69	1.39	1.25
4	E	54	GLN	CB-CG	12.66	1.86	1.52
4	E	85	GLU	CD-OE1	12.66	1.39	1.25
4	E	34	GLU	CG-CD	12.66	1.71	1.51
1	A	25	GLU	CD-OE1	12.66	1.39	1.25
9	K	61	TYR	CE2-CZ	-12.65	1.22	1.38
3	C	81	GLU	C-O	12.65	1.47	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	769	TYR	CB-CG	12.64	1.70	1.51
9	K	36	GLU	CD-OE2	12.62	1.39	1.25
1	A	1160	SER	CB-OG	12.62	1.58	1.42
1	A	264	PHE	CD2-CE2	12.60	1.64	1.39
2	B	986	GLN	CG-CD	12.60	1.80	1.51
1	A	689	LYS	CD-CE	12.59	1.82	1.51
1	A	1080	THR	CB-CG2	12.59	1.93	1.52
1	A	836	TYR	CZ-OH	12.59	1.59	1.37
2	B	246	LYS	CA-C	12.57	1.85	1.52
3	C	255	VAL	CB-CG2	-12.57	1.26	1.52
1	A	1130	GLN	CG-CD	12.54	1.79	1.51
1	A	620	LYS	CB-CG	12.53	1.86	1.52
1	A	516	SER	CB-OG	12.52	1.58	1.42
1	A	28	ARG	CG-CD	12.51	1.83	1.51
7	I	15	TYR	CD1-CE1	12.50	1.58	1.39
7	I	28	GLU	CD-OE2	12.50	1.39	1.25
3	C	116	LYS	CD-CE	12.49	1.82	1.51
2	B	1064	TYR	CG-CD2	-12.48	1.23	1.39
2	B	1164	GLY	C-O	12.46	1.43	1.23
4	E	187	TYR	CE1-CZ	-12.46	1.22	1.38
7	I	100	PHE	CE1-CZ	-12.45	1.13	1.37
1	A	1206	ASP	CB-CG	12.45	1.77	1.51
2	B	935	ARG	NE-CZ	12.44	1.49	1.33
1	A	678	GLU	CG-CD	12.44	1.70	1.51
1	A	491	VAL	CB-CG1	-12.43	1.26	1.52
9	K	35	PHE	CG-CD2	-12.43	1.20	1.38
5	F	105	ALA	CA-CB	-12.42	1.26	1.52
1	A	148	CYS	CB-SG	-12.40	1.61	1.82
2	B	242	SER	CB-OG	12.40	1.58	1.42
1	A	610	GLY	C-O	12.40	1.43	1.23
1	A	843	LYS	CG-CD	12.38	1.94	1.52
4	E	81	GLU	CD-OE1	12.38	1.39	1.25
4	E	102	GLU	CG-CD	12.38	1.70	1.51
1	A	423	ASP	CB-CG	12.38	1.77	1.51
2	B	536	VAL	CB-CG1	-12.38	1.26	1.52
1	A	264	PHE	CG-CD1	12.38	1.57	1.38
3	C	138	GLU	CD-OE1	12.35	1.39	1.25
1	A	282	ASN	CB-CG	12.35	1.79	1.51
2	B	226	PHE	CD1-CE1	12.34	1.64	1.39
6	H	77	ARG	NE-CZ	12.34	1.49	1.33
5	F	146	TRP	CB-CG	-12.34	1.28	1.50
3	C	89	GLU	CG-CD	12.32	1.70	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	PHE	CE1-CZ	12.32	1.60	1.37
2	B	328	GLU	CG-CD	12.32	1.70	1.51
4	E	41	ASP	CB-CG	12.31	1.77	1.51
1	A	1419	ASP	CB-CG	12.31	1.77	1.51
3	C	180	TYR	CG-CD1	-12.29	1.23	1.39
2	B	994	TYR	CD1-CE1	-12.28	1.21	1.39
1	A	633	VAL	CB-CG2	12.27	1.78	1.52
1	A	1405	THR	CA-CB	12.27	1.85	1.53
6	H	20	TYR	CG-CD1	-12.26	1.23	1.39
1	A	468	PHE	CE2-CZ	-12.26	1.14	1.37
2	B	959	ASP	CB-CG	12.25	1.77	1.51
2	B	838	SER	CB-OG	-12.24	1.26	1.42
6	H	77	ARG	CB-CG	12.24	1.85	1.52
1	A	155	GLU	CG-CD	12.24	1.70	1.51
9	K	108	GLU	CD-OE1	12.24	1.39	1.25
1	A	1293	SER	CB-OG	-12.23	1.26	1.42
1	A	593	GLU	CD-OE2	12.23	1.39	1.25
9	K	1	MET	SD-CE	12.22	2.46	1.77
1	A	1262	LYS	CG-CD	12.22	1.94	1.52
3	C	163	ILE	CA-CB	-12.20	1.26	1.54
2	B	106	ASP	CB-CG	12.19	1.77	1.51
1	A	188	ASP	CA-C	12.19	1.84	1.52
2	B	620	ARG	CZ-NH2	12.18	1.48	1.33
1	A	1235	LYS	CE-NZ	12.16	1.79	1.49
2	B	1134	GLU	CD-OE1	12.16	1.39	1.25
2	B	191	LYS	CD-CE	12.15	1.81	1.51
1	A	1053	PHE	CE1-CZ	-12.15	1.14	1.37
2	B	908	GLU	CG-CD	12.15	1.70	1.51
9	K	16	GLU	CD-OE1	12.15	1.39	1.25
3	C	215	GLU	CG-CD	12.14	1.70	1.51
2	B	785	TYR	CD2-CE2	-12.14	1.21	1.39
2	B	1019	SER	CB-OG	-12.13	1.26	1.42
2	B	1086	PHE	CG-CD2	-12.12	1.20	1.38
1	A	1298	TYR	CG-CD2	-12.12	1.23	1.39
1	A	931	GLU	CD-OE1	12.12	1.39	1.25
1	A	304	MET	SD-CE	12.12	2.45	1.77
4	E	162	ARG	CZ-NH1	12.11	1.48	1.33
1	A	149	GLU	CD-OE1	12.09	1.39	1.25
2	B	328	GLU	CD-OE1	12.09	1.39	1.25
2	B	414	ALA	CA-CB	-12.09	1.27	1.52
2	B	986	GLN	CB-CG	12.09	1.85	1.52
1	A	585	GLY	C-O	12.08	1.43	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	670	ILE	CA-CB	-12.08	1.27	1.54
1	A	469	ARG	CG-CD	12.07	1.82	1.51
1	A	1285	MET	SD-CE	12.06	2.45	1.77
3	C	219	PHE	CG-CD2	-12.06	1.20	1.38
2	B	479	VAL	CB-CG1	-12.06	1.27	1.52
1	A	177	ASP	CB-CG	12.05	1.77	1.51
4	E	66	GLU	CD-OE1	12.04	1.38	1.25
6	H	146	ARG	CZ-NH2	12.03	1.48	1.33
2	B	875	GLU	CB-CG	12.03	1.75	1.52
2	B	1101	ASP	CB-CG	12.03	1.77	1.51
1	A	549	MET	SD-CE	-12.02	1.10	1.77
6	H	14	GLU	CD-OE1	12.01	1.38	1.25
2	B	995	ARG	CD-NE	-11.99	1.26	1.46
2	B	567	GLU	CD-OE2	11.99	1.38	1.25
1	A	1287	TYR	C-O	11.98	1.46	1.23
2	B	775	LYS	CB-CG	11.98	1.84	1.52
2	B	1224	PHE	CD2-CE2	11.98	1.63	1.39
4	E	44	ALA	CA-CB	11.98	1.77	1.52
4	E	208	TYR	CD2-CE2	-11.98	1.21	1.39
2	B	975	GLN	CD-NE2	11.97	1.62	1.32
1	A	1359	ASP	CB-CG	11.96	1.76	1.51
2	B	67	SER	CA-CB	11.96	1.70	1.52
2	B	567	GLU	CD-OE1	11.96	1.38	1.25
1	A	676	MET	CG-SD	11.95	2.12	1.81
3	C	152	GLU	CD-OE1	11.95	1.38	1.25
2	B	200	GLY	C-O	-11.94	1.04	1.23
5	F	103	MET	SD-CE	11.93	2.44	1.77
6	H	41	ASP	CB-CG	11.92	1.76	1.51
1	A	144	THR	CB-CG2	11.91	1.91	1.52
7	I	44	TYR	CD2-CE2	11.91	1.57	1.39
6	H	98	TYR	CD1-CE1	11.90	1.57	1.39
3	C	164	ALA	CA-CB	-11.89	1.27	1.52
1	A	1349	TYR	C-O	-11.88	1.00	1.23
2	B	197	PHE	CG-CD1	-11.88	1.21	1.38
2	B	620	ARG	CZ-NH1	11.87	1.48	1.33
2	B	348	ARG	NE-CZ	-11.86	1.17	1.33
2	B	459	TYR	CE1-CZ	11.85	1.53	1.38
2	B	620	ARG	CG-CD	11.84	1.81	1.51
5	F	80	ALA	CA-CB	11.84	1.77	1.52
7	I	34	TYR	CD1-CE1	-11.83	1.21	1.39
8	J	27	GLU	CD-OE2	11.83	1.38	1.25
1	A	1268	LEU	N-CA	-11.83	1.22	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	933	SER	CA-C	11.82	1.83	1.52
10	L	42	ARG	NE-CZ	11.82	1.48	1.33
4	E	57	MET	CG-SD	11.82	2.11	1.81
7	I	34	TYR	CE1-CZ	-11.81	1.23	1.38
9	K	58	PHE	CB-CG	11.81	1.71	1.51
3	C	114	TYR	CE1-CZ	-11.80	1.23	1.38
3	C	253	LYS	CD-CE	11.79	1.80	1.51
2	B	595	ARG	CG-CD	11.78	1.81	1.51
2	B	935	ARG	CG-CD	11.78	1.81	1.51
2	B	251	ILE	CB-CG2	11.78	1.89	1.52
3	C	64	ALA	CA-CB	-11.78	1.27	1.52
1	A	1110	ASN	CG-ND2	11.77	1.62	1.32
1	A	932	GLU	CD-OE2	11.77	1.38	1.25
7	I	21	GLU	CD-OE1	11.76	1.38	1.25
4	E	52	ARG	CB-CG	11.76	1.84	1.52
3	C	78	GLU	CG-CD	11.73	1.69	1.51
6	H	63	LEU	C-O	11.73	1.45	1.23
1	A	1162	VAL	CB-CG1	11.73	1.77	1.52
2	B	830	TYR	CE1-CZ	-11.71	1.23	1.38
2	B	619	ILE	CA-CB	-11.71	1.27	1.54
1	A	829	VAL	CB-CG2	11.70	1.77	1.52
2	B	1171	VAL	C-O	11.70	1.45	1.23
4	E	103	LYS	CD-CE	11.70	1.80	1.51
2	B	184	ALA	CA-CB	-11.70	1.27	1.52
2	B	915	THR	CA-CB	11.69	1.83	1.53
3	C	102	GLN	CB-CG	11.69	1.84	1.52
8	J	26	GLN	CB-CG	11.69	1.84	1.52
1	A	1050	GLU	CD-OE1	11.67	1.38	1.25
9	K	93	SER	CB-OG	11.66	1.57	1.42
2	B	279	ASP	CB-CG	11.66	1.76	1.51
1	A	893	PHE	CE1-CZ	-11.65	1.15	1.37
2	B	19	GLU	CD-OE2	11.64	1.38	1.25
2	B	690	VAL	CB-CG1	-11.63	1.28	1.52
2	B	1086	PHE	CG-CD1	-11.63	1.21	1.38
1	A	738	LYS	C-O	-11.62	1.01	1.23
9	K	79	GLU	CG-CD	11.61	1.69	1.51
8	J	26	GLN	CG-CD	11.61	1.77	1.51
1	A	205	GLU	CB-CG	11.60	1.74	1.52
2	B	885	MET	SD-CE	11.60	2.42	1.77
3	C	15	LYS	CG-CD	11.60	1.91	1.52
2	B	124	TYR	CE2-CZ	-11.59	1.23	1.38
1	A	351	THR	C-O	-11.58	1.01	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1064	TYR	CE2-CZ	-11.57	1.23	1.38
7	I	56	ALA	C-O	-11.57	1.01	1.23
1	A	123	ARG	NE-CZ	11.56	1.48	1.33
2	B	706	GLN	CB-CG	11.56	1.83	1.52
2	B	275	TYR	CE2-CZ	-11.56	1.23	1.38
2	B	1153	GLU	CD-OE1	11.56	1.38	1.25
2	B	595	ARG	NE-CZ	11.55	1.48	1.33
4	E	201	LYS	CG-CD	11.55	1.91	1.52
10	L	29	TYR	CE1-CZ	-11.54	1.23	1.38
1	A	840	ARG	CG-CD	11.54	1.80	1.51
2	B	852	ARG	CZ-NH1	-11.54	1.18	1.33
2	B	662	MET	CG-SD	-11.54	1.51	1.81
1	A	1194	ARG	CB-CG	11.53	1.83	1.52
1	A	1287	TYR	CD1-CE1	11.53	1.56	1.39
1	A	1055	ARG	CG-CD	11.51	1.80	1.51
2	B	589	VAL	CB-CG2	-11.51	1.28	1.52
1	A	1018	PHE	CG-CD1	-11.51	1.21	1.38
2	B	872	GLU	CG-CD	11.51	1.69	1.51
4	E	191	LYS	CE-NZ	11.51	1.77	1.49
9	K	88	LYS	CE-NZ	11.51	1.77	1.49
1	A	945	GLU	CD-OE1	11.49	1.38	1.25
5	F	123	LYS	CE-NZ	11.49	1.77	1.49
1	A	1291	VAL	CB-CG1	-11.48	1.28	1.52
7	I	101	PHE	CB-CG	-11.48	1.31	1.51
4	E	43	LYS	CB-CG	11.48	1.83	1.52
2	B	186	GLU	CD-OE1	11.48	1.38	1.25
2	B	137	TYR	CG-CD1	11.47	1.54	1.39
2	B	764	SER	CB-OG	-11.47	1.27	1.42
10	L	54	ARG	CG-CD	11.47	1.80	1.51
2	B	958	GLN	CB-CG	11.47	1.83	1.52
7	I	93	LYS	CE-NZ	11.46	1.77	1.49
1	A	1025	ARG	CG-CD	-11.46	1.23	1.51
1	A	1144	LYS	CD-CE	11.45	1.79	1.51
1	A	326	ARG	CG-CD	11.45	1.80	1.51
7	I	15	TYR	CD2-CE2	11.45	1.56	1.39
1	A	1302	PRO	C-O	11.44	1.46	1.23
3	C	234	SER	CB-OG	11.44	1.57	1.42
6	H	129	TYR	CE2-CZ	11.43	1.53	1.38
2	B	191	LYS	CB-CG	11.43	1.83	1.52
1	A	556	TRP	CE3-CZ3	-11.42	1.19	1.38
1	A	958	VAL	CB-CG1	-11.42	1.28	1.52
3	C	42	PRO	CA-CB	-11.42	1.30	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1204	ASP	CB-CG	11.42	1.75	1.51
7	I	74	GLU	CB-CG	11.42	1.73	1.52
1	A	482	PHE	CE1-CZ	-11.41	1.15	1.37
1	A	28	ARG	CZ-NH2	11.40	1.47	1.33
2	B	239	GLU	CD-OE1	11.40	1.38	1.25
2	B	963	PHE	CE2-CZ	11.40	1.59	1.37
1	A	770	VAL	CB-CG1	-11.39	1.28	1.52
1	A	556	TRP	CE2-CZ2	-11.38	1.20	1.39
9	K	67	PHE	CG-CD2	-11.38	1.21	1.38
1	A	474	VAL	CB-CG1	-11.38	1.28	1.52
2	B	51	PHE	CD2-CE2	-11.36	1.16	1.39
2	B	804	GLY	C-O	-11.36	1.05	1.23
9	K	111	LEU	CG-CD1	11.36	1.93	1.51
6	H	104	PHE	CE2-CZ	11.36	1.58	1.37
1	A	209	ASN	CG-ND2	11.35	1.61	1.32
1	A	688	LYS	CD-CE	11.34	1.79	1.51
1	A	1015	VAL	CB-CG1	-11.34	1.29	1.52
3	C	81	GLU	CD-OE2	11.34	1.38	1.25
1	A	1018	PHE	CG-CD2	-11.32	1.21	1.38
2	B	1046	PRO	N-CD	-11.31	1.32	1.47
8	J	24	LEU	C-O	-11.31	1.01	1.23
1	A	516	SER	CA-CB	-11.31	1.35	1.52
2	B	459	TYR	CE2-CZ	11.30	1.53	1.38
2	B	1192	TYR	CG-CD2	-11.30	1.24	1.39
9	K	109	TRP	CZ3-CH2	-11.29	1.22	1.40
8	J	63	TYR	CG-CD1	-11.29	1.24	1.39
1	A	1328	TYR	CD2-CE2	-11.28	1.22	1.39
2	B	40	GLU	CD-OE1	11.27	1.38	1.25
10	L	62	LYS	CE-NZ	11.26	1.77	1.49
7	I	74	GLU	CG-CD	11.25	1.68	1.51
2	B	983	ARG	CZ-NH2	-11.25	1.18	1.33
2	B	18	PHE	CB-CG	11.24	1.70	1.51
2	B	266	ALA	C-O	11.24	1.44	1.23
8	J	45	CYS	CB-SG	11.24	2.01	1.82
2	B	736	THR	CB-CG2	11.23	1.89	1.52
9	K	88	LYS	CD-CE	11.23	1.79	1.51
2	B	369	GLY	CA-C	11.23	1.69	1.51
4	E	147	HIS	CG-CD2	11.22	1.54	1.35
1	A	687	LYS	CE-NZ	11.22	1.77	1.49
3	C	255	VAL	CA-CB	-11.21	1.31	1.54
1	A	978	PRO	CB-CG	11.20	2.06	1.50
2	B	668	ASP	CB-CG	11.20	1.75	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1255	GLU	CG-CD	11.20	1.68	1.51
7	I	1	MET	CA-CB	11.20	1.78	1.53
2	B	547	VAL	CB-CG1	-11.20	1.29	1.52
6	H	19	ARG	CZ-NH1	11.20	1.47	1.33
2	B	959	ASP	C-O	11.20	1.44	1.23
3	C	84	ARG	CB-CG	11.20	1.82	1.52
1	A	1450	LEU	CG-CD2	11.20	1.93	1.51
2	B	266	ALA	CA-CB	11.20	1.75	1.52
1	A	1005	GLU	CD-OE2	11.18	1.38	1.25
6	H	51	ALA	CA-CB	11.18	1.75	1.52
4	E	28	TYR	CG-CD1	-11.17	1.24	1.39
1	A	459	ARG	CD-NE	-11.16	1.27	1.46
1	A	198	GLU	CD-OE2	11.16	1.38	1.25
1	A	368	LYS	CG-CD	11.15	1.90	1.52
2	B	183	GLU	CB-CG	11.14	1.73	1.52
3	C	199	LYS	CB-CG	11.14	1.82	1.52
2	B	345	LYS	CD-CE	11.13	1.79	1.51
1	A	1121	GLU	CD-OE2	11.12	1.37	1.25
2	B	810	GLU	CD-OE1	11.12	1.37	1.25
1	A	593	GLU	CD-OE1	11.12	1.37	1.25
1	A	1365	TYR	CE2-CZ	-11.12	1.24	1.38
1	A	274	ILE	CA-CB	11.11	1.80	1.54
1	A	1225	PHE	CG-CD1	11.11	1.55	1.38
1	A	1285	MET	CG-SD	11.11	2.10	1.81
2	B	249	ARG	CG-CD	11.11	1.79	1.51
2	B	120	ARG	CB-CG	11.11	1.82	1.52
2	B	105	SER	CA-CB	11.10	1.69	1.52
1	A	264	PHE	CE2-CZ	11.10	1.58	1.37
1	A	1256	GLU	CD-OE2	11.10	1.37	1.25
2	B	779	GLY	C-O	-11.10	1.05	1.23
2	B	1140	ALA	N-CA	-11.09	1.24	1.46
2	B	592	ASN	CG-OD1	11.09	1.48	1.24
3	C	127	ARG	N-CA	11.09	1.68	1.46
1	A	37	PHE	CD2-CE2	11.09	1.61	1.39
1	A	434	ARG	CD-NE	-11.09	1.27	1.46
1	A	1426	GLU	CG-CD	11.09	1.68	1.51
2	B	45	SER	CA-CB	11.09	1.69	1.52
2	B	1155	SER	CB-OG	11.08	1.56	1.42
2	B	1224	PHE	CD1-CE1	11.08	1.61	1.39
2	B	643	ASP	C-O	-11.07	1.02	1.23
1	A	977	LYS	CE-NZ	11.07	1.76	1.49
9	K	26	LYS	CE-NZ	11.07	1.76	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1091	TYR	CG-CD2	-11.06	1.24	1.39
1	A	290	GLU	CD-OE1	11.06	1.37	1.25
2	B	38	PHE	CG-CD1	-11.06	1.22	1.38
3	C	23	SER	CA-CB	11.05	1.69	1.52
1	A	304	MET	CG-SD	11.05	2.09	1.81
1	A	673	GLY	C-O	-11.05	1.05	1.23
2	B	627	PHE	CD2-CE2	-11.05	1.17	1.39
1	A	1018	PHE	CD1-CE1	11.04	1.61	1.39
1	A	117	GLU	CD-OE2	11.04	1.37	1.25
2	B	622	LYS	CE-NZ	11.03	1.76	1.49
8	J	42	LYS	CG-CD	11.03	1.90	1.52
1	A	950	GLY	CA-C	11.01	1.69	1.51
1	A	476	SER	C-O	-11.01	1.02	1.23
8	J	43	ARG	CG-CD	11.01	1.79	1.51
4	E	28	TYR	CE1-CZ	-11.01	1.24	1.38
6	H	102	TYR	CG-CD2	-11.00	1.24	1.39
1	A	177	ASP	CG-OD2	11.00	1.50	1.25
2	B	351	TYR	CG-CD1	-11.00	1.24	1.39
4	E	91	LYS	CB-CG	11.00	1.82	1.52
1	A	271	LYS	CD-CE	10.99	1.78	1.51
1	A	725	ALA	CA-CB	-10.99	1.29	1.52
3	C	267	GLN	CA-C	10.99	1.81	1.52
3	C	134	ILE	CA-CB	-10.98	1.29	1.54
9	K	54	ARG	NE-CZ	10.97	1.47	1.33
1	A	708	MET	SD-CE	10.95	2.39	1.77
2	B	1188	LYS	CG-CD	10.95	1.89	1.52
5	F	142	SER	CB-OG	-10.95	1.28	1.42
2	B	426	LYS	CD-CE	10.95	1.78	1.51
2	B	640	VAL	CB-CG1	-10.94	1.29	1.52
2	B	569	TYR	CG-CD2	-10.94	1.25	1.39
1	A	82	GLY	C-O	-10.93	1.06	1.23
3	C	155	LEU	C-O	10.93	1.44	1.23
1	A	406	ILE	CA-CB	-10.93	1.29	1.54
1	A	1065	GLY	N-CA	-10.93	1.29	1.46
6	H	87	ARG	CG-CD	10.92	1.79	1.51
2	B	1155	SER	N-CA	10.91	1.68	1.46
4	E	135	PHE	CG-CD1	-10.91	1.22	1.38
2	B	704	ALA	C-O	-10.91	1.02	1.23
1	A	264	PHE	CG-CD2	10.90	1.55	1.38
2	B	641	GLU	CD-OE1	10.90	1.37	1.25
2	B	178	ASN	C-O	-10.89	1.02	1.23
1	A	1155	ASP	CB-CG	-10.88	1.28	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	106	GLU	CD-OE2	10.88	1.37	1.25
3	C	95	CYS	CB-SG	10.88	2.00	1.82
10	L	25	ALA	CA-CB	10.88	1.75	1.52
1	A	155	GLU	CD-OE1	10.87	1.37	1.25
1	A	1261	LYS	CD-CE	10.87	1.78	1.51
2	B	552	MET	CB-CG	10.86	1.86	1.51
1	A	954	TRP	CG-CD1	-10.85	1.21	1.36
3	C	191	TYR	CG-CD1	10.85	1.53	1.39
2	B	848	ARG	CZ-NH2	10.84	1.47	1.33
1	A	544	ASP	CB-CG	10.84	1.74	1.51
2	B	754	SER	CB-OG	10.84	1.56	1.42
1	A	1326	ARG	C-O	-10.84	1.02	1.23
1	A	1264	GLU	CD-OE1	-10.83	1.13	1.25
2	B	166	PHE	CB-CG	-10.82	1.32	1.51
1	A	644	LYS	CE-NZ	10.81	1.76	1.49
1	A	1196	GLU	CG-CD	10.81	1.68	1.51
2	B	666	TYR	CD1-CE1	10.81	1.55	1.39
2	B	60	GLN	CB-CG	-10.79	1.23	1.52
2	B	265	SER	CB-OG	10.79	1.56	1.42
2	B	401	PHE	CD2-CE2	-10.80	1.17	1.39
4	E	115	ASN	CB-CG	10.79	1.75	1.51
9	K	93	SER	CA-CB	10.79	1.69	1.52
3	C	192	TRP	CE3-CZ3	-10.78	1.20	1.38
1	A	1109	LYS	CB-CG	10.77	1.81	1.52
2	B	665	GLU	CG-CD	10.77	1.68	1.51
2	B	667	GLN	CD-OE1	10.77	1.47	1.24
3	C	137	LYS	CD-CE	10.77	1.78	1.51
1	A	1149	ALA	C-O	10.76	1.43	1.23
2	B	568	ASP	CB-CG	10.76	1.74	1.51
1	A	25	GLU	CD-OE2	10.75	1.37	1.25
2	B	815	ARG	CZ-NH2	10.75	1.47	1.33
1	A	368	LYS	CD-CE	10.75	1.78	1.51
5	F	129	LYS	CE-NZ	10.75	1.75	1.49
1	A	864	ILE	C-O	10.74	1.43	1.23
1	A	1301	GLU	CD-OE2	10.74	1.37	1.25
6	H	115	TYR	CZ-OH	10.74	1.56	1.37
2	B	798	TYR	CG-CD1	-10.74	1.25	1.39
2	B	137	TYR	CG-CD2	10.74	1.53	1.39
3	C	120	ILE	CA-CB	-10.73	1.30	1.54
1	A	1353	TYR	CG-CD2	-10.73	1.25	1.39
1	A	1414	ALA	CA-CB	-10.73	1.29	1.52
1	A	32	VAL	C-O	10.73	1.43	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	7	ARG	CB-CG	10.73	1.81	1.52
1	A	61	ILE	CA-CB	10.73	1.79	1.54
2	B	970	THR	CA-CB	-10.72	1.25	1.53
1	A	874	ASP	CG-OD2	10.71	1.50	1.25
1	A	1262	LYS	CD-CE	10.71	1.78	1.51
1	A	71	GLN	CG-CD	10.71	1.75	1.51
2	B	874	PHE	CD2-CE2	-10.70	1.17	1.39
3	C	191	TYR	CG-CD2	-10.71	1.25	1.39
2	B	1176	ASN	CB-CG	10.70	1.75	1.51
2	B	1073	TYR	CE1-CZ	-10.70	1.24	1.38
2	B	451	LYS	CG-CD	10.69	1.88	1.52
4	E	66	GLU	CB-CG	10.69	1.72	1.52
1	A	3	GLY	N-CA	10.69	1.62	1.46
1	A	1314	SER	CB-OG	10.68	1.56	1.42
1	A	616	VAL	CA-CB	-10.68	1.32	1.54
4	E	192	ARG	NE-CZ	10.68	1.47	1.33
1	A	186	LYS	CB-CG	10.68	1.81	1.52
2	B	360	PHE	CG-CD2	-10.68	1.22	1.38
1	A	755	PHE	CB-CG	10.67	1.69	1.51
8	J	57	ILE	CA-CB	-10.67	1.30	1.54
2	B	1097	HIS	CA-CB	10.67	1.77	1.53
1	A	1112	LYS	CE-NZ	10.66	1.75	1.49
2	B	245	GLU	CG-CD	10.66	1.68	1.51
1	A	1256	GLU	CG-CD	10.66	1.68	1.51
4	E	16	PHE	CD1-CE1	-10.66	1.18	1.39
4	E	163	GLU	CD-OE1	10.65	1.37	1.25
2	B	57	TYR	CE2-CZ	-10.64	1.24	1.38
2	B	1106	ARG	NE-CZ	10.64	1.46	1.33
2	B	371	GLU	CD-OE2	10.63	1.37	1.25
2	B	1064	TYR	CZ-OH	10.62	1.55	1.37
1	A	1012	ARG	C-O	10.62	1.43	1.23
2	B	30	SER	C-O	-10.62	1.03	1.23
10	L	48	CYS	CA-C	10.61	1.80	1.52
1	A	779	PHE	CE1-CZ	-10.61	1.17	1.37
3	C	19	ASP	CB-CG	-10.61	1.29	1.51
2	B	227	LYS	CD-CE	10.59	1.77	1.51
2	B	1090	THR	CB-CG2	-10.59	1.17	1.52
9	K	110	ASN	CB-CG	10.59	1.75	1.51
2	B	327	ARG	CZ-NH1	10.59	1.46	1.33
8	J	54	VAL	CA-CB	-10.59	1.32	1.54
4	E	190	LEU	C-O	10.58	1.43	1.23
2	B	39	ARG	CB-CG	10.58	1.81	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	722	ASP	CB-CG	10.58	1.74	1.51
1	A	1422	ARG	CZ-NH2	10.57	1.46	1.33
5	F	84	TYR	CG-CD1	-10.56	1.25	1.39
2	B	994	TYR	CD2-CE2	-10.56	1.23	1.39
1	A	622	VAL	CB-CG1	-10.56	1.30	1.52
1	A	992	ASP	CB-CG	10.56	1.74	1.51
1	A	70	CYS	CB-SG	10.55	2.00	1.82
1	A	1428	VAL	CB-CG1	-10.55	1.30	1.52
1	A	217	LYS	CG-CD	10.54	1.88	1.52
3	C	181	ASP	C-O	-10.54	1.03	1.23
2	B	735	ALA	N-CA	10.54	1.67	1.46
1	A	656	TRP	CD2-CE3	-10.54	1.24	1.40
1	A	1326	ARG	CZ-NH1	-10.53	1.19	1.33
1	A	40	THR	CA-CB	10.53	1.80	1.53
5	F	154	ASP	CB-CG	10.53	1.73	1.51
6	H	11	GLN	CA-C	-10.53	1.25	1.52
1	A	191	THR	CA-CB	10.52	1.80	1.53
1	A	19	PHE	CD1-CE1	-10.51	1.18	1.39
2	B	193	LYS	CD-CE	10.51	1.77	1.51
1	A	469	ARG	NE-CZ	-10.51	1.19	1.33
1	A	1024	SER	CB-OG	10.51	1.55	1.42
2	B	811	TYR	CG-CD1	-10.51	1.25	1.39
2	B	875	GLU	CD-OE2	10.51	1.37	1.25
1	A	491	VAL	CB-CG2	-10.50	1.30	1.52
2	B	595	ARG	CD-NE	10.50	1.64	1.46
3	C	208	GLU	CD-OE2	10.50	1.37	1.25
1	A	1350	LYS	CG-CD	10.49	1.88	1.52
4	E	46	TYR	CD1-CE1	10.49	1.55	1.39
1	A	1187	GLN	CB-CG	10.49	1.80	1.52
1	A	616	VAL	CB-CG1	-10.48	1.30	1.52
6	H	137	GLN	CG-CD	10.46	1.75	1.51
9	K	7	PHE	CB-CG	-10.46	1.33	1.51
3	C	57	VAL	CB-CG2	-10.46	1.30	1.52
1	A	566	ILE	CB-CG2	10.45	1.85	1.52
10	L	65	VAL	CB-CG2	10.45	1.74	1.52
2	B	381	MET	SD-CE	-10.45	1.19	1.77
2	B	769	TYR	CE2-CZ	-10.45	1.25	1.38
3	C	179	GLU	C-O	-10.45	1.03	1.23
2	B	627	PHE	CE2-CZ	-10.44	1.17	1.37
1	A	25	GLU	CG-CD	10.44	1.67	1.51
2	B	855	PHE	CG-CD1	-10.44	1.23	1.38
1	A	49	LYS	CG-CD	10.43	1.88	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	130	VAL	CB-CG2	-10.43	1.30	1.52
9	K	16	GLU	CG-CD	10.43	1.67	1.51
1	A	390	GLN	C-O	10.43	1.43	1.23
1	A	556	TRP	CD2-CE3	-10.42	1.24	1.40
3	C	23	SER	CB-OG	10.42	1.55	1.42
4	E	7	ARG	NE-CZ	10.42	1.46	1.33
1	A	205	GLU	CD-OE2	10.41	1.37	1.25
1	A	947	PHE	CG-CD1	-10.40	1.23	1.38
1	A	430	TRP	CD2-CE2	-10.40	1.28	1.41
8	J	63	TYR	CE2-CZ	-10.40	1.25	1.38
2	B	994	TYR	CE1-CZ	-10.38	1.25	1.38
3	C	199	LYS	CD-CE	10.38	1.77	1.51
9	K	5	ASP	C-O	10.38	1.43	1.23
1	A	705	LYS	CA-CB	10.38	1.76	1.53
2	B	958	GLN	CG-CD	10.37	1.75	1.51
6	H	104	PHE	CG-CD1	10.37	1.54	1.38
1	A	1228	TRP	CG-CD1	-10.36	1.22	1.36
2	B	738	PHE	CD2-CE2	-10.36	1.18	1.39
2	B	1156	ASP	CA-CB	10.36	1.76	1.53
1	A	1023	ARG	NE-CZ	-10.35	1.19	1.33
1	A	1419	ASP	CG-OD1	10.35	1.49	1.25
2	B	369	GLY	C-O	10.35	1.40	1.23
2	B	1148	LYS	CD-CE	10.35	1.77	1.51
2	B	691	GLU	CD-OE2	10.34	1.37	1.25
1	A	656	TRP	CG-CD2	-10.34	1.26	1.43
1	A	1315	GLU	CD-OE1	10.34	1.37	1.25
1	A	1379	GLY	N-CA	-10.34	1.30	1.46
7	I	94	ASP	CB-CG	10.33	1.73	1.51
2	B	228	LYS	CD-CE	10.33	1.77	1.51
1	A	1315	GLU	CG-CD	10.32	1.67	1.51
2	B	89	GLU	CG-CD	10.32	1.67	1.51
7	I	32	CYS	CB-SG	-10.32	1.64	1.82
5	F	114	GLU	CD-OE1	10.31	1.36	1.25
8	J	44	TYR	CE1-CZ	-10.31	1.25	1.38
2	B	120	ARG	CZ-NH1	10.31	1.46	1.33
2	B	646	LEU	CG-CD1	10.31	1.90	1.51
1	A	515	GLN	CD-OE1	10.30	1.46	1.24
1	A	69	THR	CA-C	10.30	1.79	1.52
1	A	1307	GLU	CD-OE1	10.29	1.36	1.25
7	I	21	GLU	CG-CD	10.29	1.67	1.51
1	A	230	ARG	CZ-NH1	10.29	1.46	1.33
1	A	392	VAL	CA-CB	-10.28	1.33	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1115	SER	CB-OG	10.28	1.55	1.42
2	B	855	PHE	CE1-CZ	-10.28	1.17	1.37
1	A	685	GLU	CD-OE2	10.27	1.36	1.25
4	E	202	SER	C-O	-10.27	1.03	1.23
1	A	4	GLN	CB-CG	10.27	1.80	1.52
1	A	771	GLU	CD-OE1	10.26	1.36	1.25
1	A	833	GLU	CG-CD	10.26	1.67	1.51
2	B	999	MET	SD-CE	-10.26	1.20	1.77
2	B	1183	LYS	CD-CE	10.26	1.76	1.51
3	C	127	ARG	CZ-NH1	10.25	1.46	1.33
1	A	1256	GLU	CD-OE1	10.25	1.36	1.25
7	I	93	LYS	CG-CD	10.25	1.87	1.52
7	I	78	CYS	CB-SG	10.25	1.99	1.82
4	E	168	TYR	CG-CD1	-10.24	1.25	1.39
4	E	34	GLU	CD-OE1	10.24	1.36	1.25
1	A	177	ASP	CG-OD1	10.24	1.48	1.25
2	B	525	ALA	C-O	10.22	1.42	1.23
1	A	776	ALA	C-O	-10.22	1.03	1.23
2	B	1129	ARG	CZ-NH1	10.22	1.46	1.33
7	I	75	CYS	C-O	-10.22	1.03	1.23
1	A	130	ASP	CB-CG	10.21	1.73	1.51
2	B	994	TYR	CG-CD2	-10.21	1.25	1.39
6	H	139	ASN	CA-CB	10.21	1.79	1.53
2	B	351	TYR	CE2-CZ	-10.20	1.25	1.38
4	E	21	GLU	CG-CD	10.20	1.67	1.51
2	B	123	THR	CA-CB	-10.19	1.26	1.53
7	I	1	MET	CB-CG	10.19	1.83	1.51
1	A	1434	ALA	CA-CB	-10.19	1.31	1.52
2	B	1094	ARG	NE-CZ	-10.19	1.19	1.33
2	B	347	LYS	CG-CD	10.18	1.87	1.52
2	B	797	TYR	CE1-CZ	-10.18	1.25	1.38
7	I	74	GLU	CD-OE1	10.18	1.36	1.25
2	B	852	ARG	CZ-NH2	-10.18	1.19	1.33
2	B	1217	TYR	CD1-CE1	-10.17	1.24	1.39
1	A	178	GLY	C-O	-10.17	1.07	1.23
1	A	404	TYR	CE2-CZ	-10.17	1.25	1.38
6	H	131	ASN	CA-CB	10.17	1.79	1.53
7	I	51	ASN	C-O	-10.16	1.04	1.23
1	A	1236	LEU	C-O	-10.15	1.04	1.23
2	B	458	LYS	CD-CE	10.15	1.76	1.51
2	B	116	GLU	CD-OE1	10.15	1.36	1.25
1	A	1045	VAL	CA-CB	-10.14	1.33	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	14	GLU	CD-OE2	10.14	1.36	1.25
2	B	246	LYS	N-CA	10.13	1.66	1.46
1	A	720	ARG	CG-CD	10.13	1.77	1.51
6	H	63	LEU	CA-C	10.13	1.79	1.52
2	B	962	LYS	CE-NZ	10.12	1.74	1.49
2	B	322	PHE	CD2-CE2	-10.12	1.19	1.39
2	B	396	ASP	CG-OD1	10.12	1.48	1.25
4	E	42	PHE	CB-CG	-10.12	1.34	1.51
1	A	190	ALA	CA-CB	10.11	1.73	1.52
3	C	125	MET	CG-SD	10.11	2.07	1.81
2	B	965	LYS	CD-CE	10.10	1.76	1.51
1	A	933	TYR	CG-CD1	-10.10	1.26	1.39
2	B	598	GLU	CD-OE1	10.10	1.36	1.25
10	L	67	PHE	CG-CD1	-10.10	1.23	1.38
1	A	957	PRO	CA-CB	-10.09	1.33	1.53
3	C	187	LYS	CE-NZ	10.09	1.74	1.49
1	A	465	TYR	CG-CD2	-10.08	1.26	1.39
2	B	57	TYR	CG-CD1	-10.08	1.26	1.39
2	B	699	GLU	CA-CB	-10.08	1.31	1.53
7	I	65	ASP	CB-CG	-10.08	1.30	1.51
3	C	201	TRP	CD2-CE3	-10.07	1.25	1.40
1	A	291	GLU	CD-OE2	10.07	1.36	1.25
2	B	531	GLN	CD-NE2	10.07	1.58	1.32
2	B	657	HIS	CA-CB	-10.07	1.31	1.53
1	A	123	ARG	CD-NE	10.07	1.63	1.46
7	I	71	SER	C-O	10.07	1.42	1.23
1	A	808	LEU	C-O	-10.06	1.04	1.23
3	C	170	TRP	CD2-CE3	-10.06	1.25	1.40
1	A	655	PHE	CG-CD1	-10.06	1.23	1.38
5	F	124	GLU	CD-OE1	-10.06	1.14	1.25
1	A	813	PHE	CG-CD1	-10.05	1.23	1.38
1	A	1036	ARG	CZ-NH1	10.05	1.46	1.33
2	B	632	ARG	NE-CZ	-10.05	1.20	1.33
2	B	256	VAL	CB-CG1	-10.05	1.31	1.52
4	E	67	GLU	CG-CD	10.05	1.67	1.51
1	A	143	LYS	CE-NZ	10.04	1.74	1.49
1	A	804	TYR	CD1-CE1	10.04	1.54	1.39
1	A	393	ARG	CD-NE	10.04	1.63	1.46
1	A	885	THR	N-CA	-10.03	1.26	1.46
1	A	45	GLN	CA-C	10.03	1.79	1.52
1	A	264	PHE	CD1-CE1	10.03	1.59	1.39
1	A	295	LEU	CG-CD2	10.03	1.89	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	346	ASP	CG-OD2	10.03	1.48	1.25
2	B	963	PHE	C-O	10.03	1.42	1.23
1	A	1447	GLU	CG-CD	10.02	1.67	1.51
6	H	45	GLU	CD-OE1	10.02	1.36	1.25
1	A	346	ASP	C-O	-10.02	1.04	1.23
1	A	933	TYR	CE1-CZ	-10.02	1.25	1.38
1	A	792	TYR	C-O	-10.02	1.04	1.23
1	A	1228	TRP	CB-CG	10.02	1.68	1.50
4	E	189	GLY	C-O	10.02	1.39	1.23
1	A	933	TYR	CG-CD2	-10.01	1.26	1.39
1	A	1001	ARG	CZ-NH2	10.01	1.46	1.33
1	A	1328	TYR	CE1-CZ	-10.01	1.25	1.38
1	A	375	THR	C-O	-10.00	1.04	1.23
4	E	7	ARG	CD-NE	10.00	1.63	1.46
7	I	105	SER	CB-OG	10.00	1.55	1.42
1	A	1151	GLU	CD-OE1	10.00	1.36	1.25
1	A	1159	ARG	NE-CZ	9.99	1.46	1.33
1	A	162	VAL	CB-CG2	9.99	1.73	1.52
1	A	821	ARG	CD-NE	-9.98	1.29	1.46
2	B	423	LYS	CD-CE	9.98	1.76	1.51
1	A	971	PHE	CG-CD1	-9.98	1.23	1.38
4	E	46	TYR	C-O	9.98	1.42	1.23
9	K	66	PRO	CA-C	-9.98	1.32	1.52
3	C	106	GLU	CG-CD	9.98	1.67	1.51
5	F	109	VAL	CB-CG2	-9.98	1.31	1.52
1	A	787	PHE	CG-CD2	-9.98	1.23	1.38
4	E	20	LYS	CD-CE	9.98	1.76	1.51
9	K	35	PHE	CE1-CZ	-9.97	1.18	1.37
1	A	571	LEU	CG-CD2	9.97	1.88	1.51
4	E	66	GLU	CA-CB	9.97	1.75	1.53
5	F	84	TYR	CD1-CE1	9.97	1.54	1.39
1	A	582	ILE	C-O	9.96	1.42	1.23
2	B	625	LYS	CE-NZ	9.96	1.74	1.49
2	B	1224	PHE	CE1-CZ	9.96	1.56	1.37
9	K	54	ARG	CZ-NH1	9.96	1.46	1.33
2	B	368	GLU	CA-CB	9.96	1.75	1.53
1	A	892	ALA	CA-CB	-9.94	1.31	1.52
1	A	577	ILE	CA-CB	-9.94	1.31	1.54
1	A	1347	ALA	C-O	-9.94	1.04	1.23
2	B	204	ILE	CA-CB	-9.93	1.32	1.54
9	K	1	MET	N-CA	9.93	1.66	1.46
2	B	459	TYR	CG-CD2	9.93	1.52	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	112	GLU	CD-OE2	9.93	1.36	1.25
7	I	35	VAL	CB-CG2	-9.92	1.32	1.52
7	I	92	ARG	C-O	9.92	1.42	1.23
8	J	3	VAL	CA-CB	-9.92	1.33	1.54
2	B	245	GLU	C-O	9.91	1.42	1.23
2	B	607	GLY	C-O	-9.91	1.07	1.23
5	F	83	PRO	C-O	9.91	1.43	1.23
2	B	137	TYR	CE1-CZ	9.90	1.51	1.38
2	B	37	PHE	CD2-CE2	9.90	1.59	1.39
1	A	359	LEU	CA-CB	-9.90	1.30	1.53
3	C	172	PRO	CA-C	-9.89	1.33	1.52
1	A	393	ARG	CG-CD	9.89	1.76	1.51
9	K	20	LYS	CG-CD	9.88	1.86	1.52
10	L	64	LEU	CG-CD1	9.88	1.88	1.51
2	B	792	MET	SD-CE	9.88	2.33	1.77
6	H	129	TYR	CG-CD2	9.87	1.51	1.39
2	B	703	ILE	C-O	9.87	1.42	1.23
1	A	843	LYS	C-O	-9.87	1.04	1.23
1	A	147	VAL	CB-CG2	9.86	1.73	1.52
1	A	291	GLU	CD-OE1	9.86	1.36	1.25
8	J	18	TRP	CZ3-CH2	-9.85	1.24	1.40
1	A	1221	LYS	CB-CG	9.85	1.79	1.52
2	B	1139	ILE	C-O	-9.85	1.04	1.23
1	A	139	TRP	CD2-CE2	-9.85	1.29	1.41
2	B	181	LEU	C-O	9.85	1.42	1.23
3	C	177	GLU	CD-OE2	9.85	1.36	1.25
2	B	1047	PHE	CG-CD1	-9.84	1.24	1.38
2	B	353	LYS	CG-CD	9.84	1.85	1.52
2	B	520	GLY	C-O	-9.84	1.07	1.23
7	I	22	ASN	C-O	9.84	1.42	1.23
7	I	117	LYS	CD-CE	9.84	1.75	1.51
1	A	305	ASP	N-CA	9.83	1.66	1.46
2	B	184	ALA	C-O	-9.83	1.04	1.23
2	B	96	TYR	CE2-CZ	9.82	1.51	1.38
2	B	263	GLY	C-O	9.82	1.39	1.23
2	B	303	TYR	CG-CD2	-9.82	1.26	1.39
1	A	591	PHE	CE2-CZ	9.82	1.56	1.37
1	A	198	GLU	CB-CG	9.81	1.70	1.52
1	A	1365	TYR	CE1-CZ	9.81	1.51	1.38
4	E	208	TYR	CZ-OH	9.81	1.54	1.37
4	E	110	PHE	CE2-CZ	-9.80	1.18	1.37
1	A	1159	ARG	CZ-NH1	9.80	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1311	VAL	N-CA	-9.79	1.26	1.46
1	A	1035	TYR	CG-CD1	-9.79	1.26	1.39
2	B	359	GLU	CD-OE1	9.79	1.36	1.25
3	C	257	SER	CB-OG	9.79	1.54	1.42
1	A	873	MET	C-O	-9.79	1.04	1.23
1	A	1297	GLU	CG-CD	9.79	1.66	1.51
3	C	79	GLN	CD-OE1	9.79	1.45	1.24
8	J	8	PHE	CG-CD2	-9.79	1.24	1.38
3	C	256	ALA	CA-CB	-9.78	1.31	1.52
4	E	195	VAL	CB-CG1	-9.78	1.32	1.52
1	A	696	GLU	CD-OE2	9.78	1.36	1.25
4	E	59	SER	C-O	9.78	1.42	1.23
2	B	219	ALA	CA-CB	9.77	1.73	1.52
1	A	662	PHE	CE1-CZ	-9.77	1.18	1.37
3	C	89	GLU	CD-OE1	9.77	1.36	1.25
7	I	30	ARG	CG-CD	9.77	1.76	1.51
5	F	118	LEU	CG-CD1	-9.77	1.15	1.51
2	B	278	GLN	CB-CG	-9.76	1.26	1.52
1	A	52	GLY	C-O	-9.76	1.08	1.23
2	B	1018	PRO	CA-C	-9.76	1.33	1.52
1	A	1304	TRP	C-O	9.75	1.41	1.23
2	B	426	LYS	CE-NZ	9.74	1.73	1.49
2	B	707	PRO	N-CD	-9.74	1.34	1.47
4	E	130	ALA	CA-CB	9.74	1.72	1.52
1	A	567	LYS	CD-CE	9.73	1.75	1.51
1	A	1256	GLU	N-CA	9.73	1.65	1.46
4	E	186	LEU	CA-C	-9.73	1.27	1.52
3	C	86	CYS	CB-SG	9.72	1.98	1.82
1	A	412	ARG	CG-CD	9.72	1.76	1.51
1	A	591	PHE	CE1-CZ	-9.72	1.18	1.37
1	A	1126	ALA	CA-CB	-9.72	1.32	1.52
8	J	3	VAL	CB-CG2	-9.72	1.32	1.52
1	A	396	PRO	CB-CG	-9.71	1.01	1.50
1	A	1274	ARG	CZ-NH2	9.71	1.45	1.33
1	A	1281	ARG	CZ-NH2	9.71	1.45	1.33
1	A	593	GLU	CG-CD	9.71	1.66	1.51
2	B	866	TYR	CG-CD1	9.71	1.51	1.39
3	C	210	GLU	CG-CD	9.69	1.66	1.51
1	A	962	ARG	CG-CD	9.69	1.76	1.51
1	A	601	LYS	CE-NZ	9.68	1.73	1.49
2	B	814	PHE	CG-CD2	-9.68	1.24	1.38
1	A	699	ALA	C-O	-9.68	1.04	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	253	THR	CA-CB	-9.68	1.28	1.53
1	A	979	SER	CB-OG	9.68	1.54	1.42
4	E	211	TYR	CG-CD1	-9.68	1.26	1.39
2	B	576	ASP	C-O	9.67	1.41	1.23
1	A	14	VAL	C-O	-9.67	1.04	1.23
1	A	813	PHE	CD2-CE2	9.67	1.58	1.39
1	A	661	GLY	CA-C	9.66	1.67	1.51
2	B	1023	VAL	CB-CG2	-9.66	1.32	1.52
4	E	75	MET	C-O	9.65	1.41	1.23
2	B	866	TYR	CE2-CZ	9.65	1.51	1.38
1	A	465	TYR	CD1-CE1	-9.64	1.24	1.39
5	F	87	LYS	CE-NZ	9.63	1.73	1.49
2	B	1069	PHE	CE2-CZ	-9.63	1.19	1.37
4	E	135	PHE	CE1-CZ	-9.62	1.19	1.37
2	B	949	VAL	CB-CG1	-9.62	1.32	1.52
4	E	79	TRP	CG-CD1	9.62	1.50	1.36
2	B	993	THR	C-O	-9.61	1.05	1.23
2	B	1070	GLU	C-O	-9.61	1.05	1.23
4	E	23	VAL	C-O	9.61	1.41	1.23
6	H	85	GLY	CA-C	9.61	1.67	1.51
7	I	45	ARG	CD-NE	9.60	1.62	1.46
1	A	866	PHE	CG-CD1	-9.60	1.24	1.38
3	C	82	TYR	CG-CD2	-9.60	1.26	1.39
1	A	425	GLN	CG-CD	9.60	1.73	1.51
3	C	127	ARG	C-O	9.60	1.41	1.23
1	A	1291	VAL	CB-CG2	9.59	1.73	1.52
1	A	74	MET	SD-CE	9.59	2.31	1.77
7	I	84	VAL	CB-CG1	-9.59	1.32	1.52
1	A	1111	MET	CG-SD	9.59	2.06	1.81
2	B	561	TRP	CB-CG	-9.59	1.32	1.50
1	A	81	PHE	CG-CD1	-9.58	1.24	1.38
1	A	652	VAL	CB-CG1	-9.56	1.32	1.52
1	A	498	ARG	NE-CZ	-9.56	1.20	1.33
1	A	668	ASP	N-CA	-9.56	1.27	1.46
4	E	69	ILE	CA-CB	-9.56	1.32	1.54
6	H	11	GLN	CB-CG	9.56	1.78	1.52
6	H	130	ARG	NE-CZ	-9.56	1.20	1.33
4	E	193	GLY	C-O	9.56	1.39	1.23
1	A	880	LYS	CG-CD	9.55	1.84	1.52
6	H	79	TRP	CB-CG	-9.55	1.33	1.50
1	A	9	ALA	CA-CB	9.55	1.72	1.52
2	B	115	GLN	CD-NE2	9.54	1.56	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1102	LYS	CB-CG	9.55	1.78	1.52
8	J	5	VAL	CB-CG1	-9.54	1.32	1.52
1	A	430	TRP	CE2-CZ2	-9.54	1.23	1.39
2	B	99	LYS	CD-CE	9.54	1.75	1.51
2	B	814	PHE	CE1-CZ	-9.54	1.19	1.37
6	H	88	SER	N-CA	9.54	1.65	1.46
2	B	601	ARG	CZ-NH2	9.53	1.45	1.33
1	A	104	GLU	CD-OE2	9.53	1.36	1.25
2	B	18	PHE	CA-CB	9.53	1.75	1.53
3	C	181	ASP	CA-C	-9.53	1.28	1.52
7	I	4	PHE	CE2-CZ	9.53	1.55	1.37
1	A	4	GLN	CG-CD	9.53	1.73	1.51
1	A	813	PHE	N-CA	-9.53	1.27	1.46
3	C	194	GLU	CD-OE1	9.53	1.36	1.25
1	A	941	LYS	CG-CD	9.52	1.84	1.52
3	C	159	ALA	C-O	-9.52	1.05	1.23
2	B	358	LYS	CB-CG	9.52	1.78	1.52
1	A	72	GLU	CD-OE1	9.52	1.36	1.25
3	C	199	LYS	CG-CD	9.52	1.84	1.52
1	A	216	VAL	CA-CB	-9.51	1.34	1.54
2	B	134	LYS	CB-CG	9.51	1.78	1.52
1	A	446	ARG	CZ-NH1	9.51	1.45	1.33
1	A	1092	LYS	CB-CG	9.51	1.78	1.52
1	A	1349	TYR	CE1-CZ	-9.51	1.26	1.38
1	A	750	GLY	C-O	-9.50	1.08	1.23
2	B	364	ILE	CA-CB	-9.50	1.32	1.54
1	A	659	HIS	CA-CB	-9.50	1.33	1.53
2	B	401	PHE	CG-CD2	-9.50	1.24	1.38
9	K	54	ARG	CZ-NH2	9.50	1.45	1.33
2	B	218	SER	CB-OG	9.50	1.54	1.42
1	A	185	TRP	CG-CD2	-9.49	1.27	1.43
1	A	1057	VAL	CB-CG2	-9.49	1.32	1.52
1	A	135	PHE	CG-CD1	-9.49	1.24	1.38
1	A	1045	VAL	CB-CG1	-9.49	1.32	1.52
2	B	270	LYS	CE-NZ	9.49	1.72	1.49
1	A	671	ALA	CA-CB	-9.48	1.32	1.52
3	C	15	LYS	CE-NZ	9.48	1.72	1.49
7	I	102	VAL	CB-CG1	-9.48	1.32	1.52
1	A	1299	VAL	CB-CG1	-9.47	1.32	1.52
2	B	949	VAL	CA-CB	-9.47	1.34	1.54
3	C	252	GLN	CG-CD	9.47	1.72	1.51
1	A	872	GLY	CA-C	-9.47	1.36	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1097	GLY	C-O	-9.47	1.08	1.23
2	B	296	GLU	CD-OE1	9.46	1.36	1.25
2	B	733	HIS	CA-C	9.46	1.77	1.52
1	A	724	GLU	CG-CD	9.46	1.66	1.51
9	K	56	VAL	CA-CB	9.46	1.74	1.54
3	C	231	ASN	CB-CG	9.45	1.72	1.51
7	I	17	ARG	NE-CZ	9.45	1.45	1.33
1	A	839	ARG	CZ-NH2	9.45	1.45	1.33
1	A	274	ILE	CB-CG2	9.45	1.82	1.52
2	B	516	ASN	C-O	-9.45	1.05	1.23
1	A	895	LYS	CE-NZ	9.45	1.72	1.49
1	A	987	VAL	CA-CB	-9.45	1.34	1.54
1	A	569	LYS	CE-NZ	9.45	1.72	1.49
2	B	773	MET	CG-SD	-9.45	1.56	1.81
4	E	1	MET	SD-CE	9.44	2.30	1.77
2	B	884	ARG	NE-CZ	9.44	1.45	1.33
1	A	572	TRP	CB-CG	-9.44	1.33	1.50
1	A	1278	ASN	CG-OD1	9.44	1.44	1.24
2	B	1106	ARG	CZ-NH2	9.43	1.45	1.33
4	E	104	ASN	CG-OD1	9.43	1.44	1.24
1	A	24	PRO	C-O	9.43	1.42	1.23
1	A	1341	ILE	CA-CB	-9.43	1.33	1.54
2	B	25	ILE	CB-CG2	9.43	1.82	1.52
2	B	121	ASN	CB-CG	9.43	1.72	1.51
2	B	871	THR	CA-CB	9.42	1.77	1.53
2	B	681	TRP	CD2-CE2	-9.42	1.30	1.41
1	A	428	TYR	CB-CG	-9.42	1.37	1.51
1	A	961	ARG	NE-CZ	9.42	1.45	1.33
2	B	336	ARG	CZ-NH1	9.42	1.45	1.33
2	B	582	VAL	CB-CG1	-9.42	1.33	1.52
2	B	1132	GLU	CB-CG	9.42	1.70	1.52
2	B	1146	PHE	C-O	-9.41	1.05	1.23
4	E	56	LYS	CG-CD	9.41	1.84	1.52
3	C	228	PHE	CG-CD1	-9.41	1.24	1.38
4	E	31	THR	CB-CG2	9.41	1.83	1.52
1	A	840	ARG	NE-CZ	9.41	1.45	1.33
1	A	932	GLU	CD-OE1	9.41	1.36	1.25
2	B	1163	CYS	CA-CB	9.41	1.74	1.53
5	F	136	ARG	NE-CZ	-9.41	1.20	1.33
6	H	85	GLY	C-O	9.41	1.38	1.23
8	J	3	VAL	CB-CG1	-9.40	1.33	1.52
4	E	118	PRO	CB-CG	9.40	1.97	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	444	PHE	CD1-CE1	-9.40	1.20	1.39
10	L	44	ASP	C-O	9.40	1.41	1.23
1	A	804	TYR	CG-CD2	-9.39	1.26	1.39
9	K	61	TYR	CD2-CE2	9.39	1.53	1.39
3	C	267	GLN	N-CA	9.39	1.65	1.46
3	C	230	MET	CG-SD	9.38	2.05	1.81
1	A	37	PHE	CD1-CE1	9.38	1.58	1.39
2	B	169	ARG	CZ-NH1	9.38	1.45	1.33
3	C	75	MET	CB-CG	-9.38	1.21	1.51
3	C	154	LYS	CB-CG	9.38	1.77	1.52
1	A	379	VAL	CB-CG1	-9.38	1.33	1.52
2	B	259	TYR	CE1-CZ	-9.38	1.26	1.38
3	C	137	LYS	CG-CD	9.38	1.84	1.52
3	C	79	GLN	CG-CD	9.38	1.72	1.51
6	H	115	TYR	CG-CD2	-9.37	1.26	1.39
1	A	284	ALA	CA-CB	9.37	1.72	1.52
1	A	1049	ILE	CA-CB	-9.37	1.33	1.54
1	A	46	THR	CA-CB	9.37	1.77	1.53
4	E	37	LEU	CG-CD1	9.37	1.86	1.51
10	L	70	ARG	NE-CZ	9.36	1.45	1.33
4	E	91	LYS	CA-CB	9.35	1.74	1.53
1	A	1305	VAL	CB-CG1	-9.35	1.33	1.52
2	B	60	GLN	C-O	-9.35	1.05	1.23
9	K	26	LYS	CD-CE	9.35	1.74	1.51
3	C	214	ASN	CB-CG	9.35	1.72	1.51
2	B	884	ARG	CG-CD	9.34	1.75	1.51
1	A	70	CYS	N-CA	9.34	1.65	1.46
1	A	777	PHE	CE2-CZ	-9.34	1.19	1.37
4	E	54	GLN	CG-CD	9.34	1.72	1.51
1	A	180	LYS	CB-CG	9.34	1.77	1.52
1	A	934	LYS	CE-NZ	9.33	1.72	1.49
1	A	1188	GLN	CG-CD	9.32	1.72	1.51
2	B	115	GLN	CG-CD	9.32	1.72	1.51
2	B	368	GLU	CG-CD	9.32	1.66	1.51
2	B	522	VAL	CA-CB	-9.32	1.35	1.54
2	B	1198	TYR	CD1-CE1	9.32	1.53	1.39
2	B	899	ILE	CA-CB	-9.32	1.33	1.54
6	H	111	LEU	CG-CD1	9.32	1.86	1.51
7	I	47	GLU	CG-CD	9.31	1.66	1.51
2	B	935	ARG	CD-NE	9.31	1.62	1.46
3	C	114	TYR	CG-CD2	-9.31	1.27	1.39
2	B	362	PRO	N-CD	-9.31	1.34	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1040	GLN	CG-CD	9.31	1.72	1.51
2	B	265	SER	CA-CB	9.30	1.67	1.52
1	A	865	GLN	CG-CD	9.30	1.72	1.51
6	H	20	TYR	CD1-CE1	-9.30	1.25	1.39
2	B	965	LYS	CE-NZ	9.30	1.72	1.49
3	C	199	LYS	C-O	-9.29	1.05	1.23
2	B	96	TYR	CD2-CE2	9.29	1.53	1.39
1	A	815	PHE	CG-CD2	-9.29	1.24	1.38
2	B	561	TRP	CG-CD1	-9.28	1.23	1.36
3	C	51	VAL	C-O	-9.29	1.05	1.23
1	A	99	ILE	C-O	9.28	1.41	1.23
1	A	767	GLN	CB-CG	-9.28	1.27	1.52
1	A	1349	TYR	CZ-OH	9.28	1.53	1.37
6	H	32	THR	CA-CB	9.28	1.77	1.53
2	B	648	HIS	C-O	-9.27	1.05	1.23
3	C	229	TYR	CE1-CZ	-9.27	1.26	1.38
1	A	674	PRO	N-CA	-9.27	1.31	1.47
1	A	198	GLU	C-O	-9.27	1.05	1.23
2	B	694	ASP	CB-CG	9.27	1.71	1.51
2	B	1183	LYS	CA-CB	9.27	1.74	1.53
3	C	26	ASP	CG-OD1	9.26	1.46	1.25
1	A	1077	THR	C-O	-9.26	1.05	1.23
2	B	1092	TYR	CG-CD2	-9.25	1.27	1.39
3	C	39	ALA	CA-CB	-9.25	1.33	1.52
1	A	604	GLY	C-O	-9.24	1.08	1.23
1	A	1064	VAL	N-CA	-9.24	1.27	1.46
2	B	807	ARG	CB-CG	9.24	1.77	1.52
7	I	98	VAL	CB-CG1	9.24	1.72	1.52
1	A	1383	SER	CA-CB	-9.24	1.39	1.52
2	B	635	ARG	CZ-NH2	-9.23	1.21	1.33
4	E	52	ARG	NE-CZ	9.23	1.45	1.33
2	B	389	ALA	CA-CB	-9.23	1.33	1.52
2	B	830	TYR	CG-CD1	-9.23	1.27	1.39
1	A	1001	ARG	C-O	9.23	1.40	1.23
2	B	370	PHE	CG-CD1	9.23	1.52	1.38
1	A	806	ARG	CZ-NH2	9.23	1.45	1.33
1	A	193	ASP	CA-CB	9.22	1.74	1.53
1	A	685	GLU	CG-CD	9.22	1.65	1.51
2	B	851	PHE	CB-CG	9.21	1.67	1.51
1	A	302	THR	CB-CG2	9.21	1.82	1.52
1	A	648	ASN	CB-CG	-9.21	1.29	1.51
2	B	668	ASP	CG-OD1	9.20	1.46	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1100	ARG	CZ-NH2	-9.20	1.21	1.33
4	E	102	GLU	CD-OE1	9.20	1.35	1.25
8	J	8	PHE	CD2-CE2	9.20	1.57	1.39
3	C	143	LEU	C-O	-9.19	1.05	1.23
1	A	1212	VAL	CB-CG1	-9.19	1.33	1.52
1	A	1222	ASN	CA-CB	9.19	1.77	1.53
6	H	15	VAL	C-O	9.19	1.40	1.23
3	C	87	PHE	CD2-CE2	9.18	1.57	1.39
1	A	752	LYS	CA-CB	-9.18	1.33	1.53
2	B	620	ARG	CB-CG	9.18	1.77	1.52
2	B	621	GLU	CD-OE2	9.18	1.35	1.25
2	B	698	GLU	CD-OE1	9.18	1.35	1.25
1	A	1372	VAL	CA-CB	-9.18	1.35	1.54
2	B	393	LYS	CD-CE	9.18	1.74	1.51
6	H	93	TYR	CE2-CZ	9.18	1.50	1.38
5	F	135	ARG	CG-CD	9.17	1.74	1.51
6	H	96	VAL	CB-CG2	-9.17	1.33	1.52
9	K	79	GLU	CD-OE2	9.17	1.35	1.25
1	A	187	LYS	C-O	9.17	1.40	1.23
2	B	697	GLU	C-O	-9.17	1.05	1.23
1	A	593	GLU	CB-CG	9.16	1.69	1.52
1	A	1420	ASP	CG-OD2	9.16	1.46	1.25
6	H	38	LEU	CG-CD1	-9.16	1.18	1.51
2	B	754	SER	CA-CB	-9.16	1.39	1.52
1	A	1350	LYS	CD-CE	9.16	1.74	1.51
8	J	60	PHE	CE1-CZ	-9.16	1.20	1.37
1	A	98	LYS	CD-CE	9.15	1.74	1.51
2	B	622	LYS	CB-CG	9.15	1.77	1.52
2	B	962	LYS	CG-CD	9.15	1.83	1.52
1	A	1198	ASP	C-O	9.15	1.40	1.23
7	I	29	CYS	C-O	9.15	1.40	1.23
3	C	180	TYR	CE2-CZ	-9.15	1.26	1.38
9	K	85	ASP	CB-CG	9.15	1.71	1.51
1	A	1239	ARG	CZ-NH2	-9.14	1.21	1.33
1	A	704	ALA	C-O	9.14	1.40	1.23
5	F	78	GLN	CG-CD	9.14	1.72	1.51
2	B	220	GLY	CA-C	-9.14	1.37	1.51
2	B	1224	PHE	CG-CD2	9.13	1.52	1.38
1	A	23	SER	C-O	9.13	1.40	1.23
2	B	19	GLU	CG-CD	9.13	1.65	1.51
1	A	468	PHE	CG-CD1	-9.13	1.25	1.38
2	B	1102	LYS	CD-CE	9.13	1.74	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	7	CYS	C-O	9.12	1.40	1.23
4	E	98	ILE	CB-CG2	9.12	1.81	1.52
4	E	187	TYR	CG-CD2	-9.12	1.27	1.39
6	H	57	VAL	CB-CG2	9.12	1.72	1.52
1	A	91	PHE	CG-CD1	-9.12	1.25	1.38
7	I	36	GLU	CA-CB	-9.12	1.33	1.53
2	B	131	ASP	CB-CG	9.12	1.70	1.51
2	B	1130	PHE	CE1-CZ	-9.12	1.20	1.37
5	F	92	ARG	CB-CG	-9.11	1.27	1.52
1	A	1042	PHE	CE2-CZ	9.11	1.54	1.37
2	B	817	LEU	N-CA	-9.11	1.28	1.46
1	A	403	LYS	CD-CE	9.11	1.74	1.51
3	C	95	CYS	C-O	-9.11	1.06	1.23
1	A	464	PRO	CA-C	-9.10	1.34	1.52
7	I	111	THR	C-O	-9.10	1.06	1.23
2	B	453	ILE	CB-CG2	-9.09	1.24	1.52
1	A	1359	ASP	CG-OD1	9.09	1.46	1.25
6	H	27	GLU	CA-C	9.09	1.76	1.52
1	A	1318	THR	CB-CG2	9.09	1.82	1.52
1	A	49	LYS	CE-NZ	9.09	1.71	1.49
3	C	49	VAL	C-O	-9.08	1.06	1.23
3	C	12	GLU	N-CA	-9.08	1.28	1.46
7	I	84	VAL	CA-CB	-9.07	1.35	1.54
1	A	283	GLY	C-O	9.07	1.38	1.23
2	B	846	ILE	CA-CB	9.07	1.75	1.54
6	H	44	VAL	CB-CG1	9.07	1.71	1.52
10	L	43	THR	CB-CG2	9.06	1.82	1.52
1	A	187	LYS	CA-C	9.06	1.76	1.52
1	A	1074	GLU	C-O	-9.06	1.06	1.23
2	B	388	CYS	CB-SG	-9.06	1.66	1.82
2	B	705	MET	SD-CE	-9.06	1.27	1.77
2	B	994	TYR	CG-CD1	-9.06	1.27	1.39
2	B	705	MET	CG-SD	9.06	2.04	1.81
8	J	26	GLN	CD-OE1	9.06	1.43	1.24
6	H	112	ILE	CB-CG2	-9.05	1.24	1.52
8	J	24	LEU	CG-CD2	-9.05	1.18	1.51
1	A	472	LEU	CG-CD2	-9.05	1.18	1.51
9	K	79	GLU	CB-CG	9.04	1.69	1.52
1	A	951	GLU	CD-OE1	9.04	1.35	1.25
1	A	1273	LEU	C-O	9.04	1.40	1.23
2	B	365	THR	C-O	9.04	1.40	1.23
9	K	63	VAL	CB-CG1	-9.04	1.33	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	ASN	C-O	9.04	1.40	1.23
2	B	1192	TYR	CB-CG	-9.04	1.38	1.51
9	K	68	PHE	CG-CD2	-9.04	1.25	1.38
1	A	971	PHE	CE2-CZ	-9.03	1.20	1.37
2	B	944	THR	CB-CG2	9.04	1.82	1.52
4	E	7	ARG	CG-CD	9.03	1.74	1.51
2	B	370	PHE	CE2-CZ	9.03	1.54	1.37
4	E	207	ARG	CG-CD	9.03	1.74	1.51
7	I	51	ASN	CB-CG	9.02	1.71	1.51
5	F	116	ASP	C-O	-9.02	1.06	1.23
2	B	96	TYR	CB-CG	9.01	1.65	1.51
2	B	129	PHE	CD1-CE1	-9.01	1.21	1.39
4	E	106	GLN	CG-CD	9.01	1.71	1.51
2	B	1061	GLU	CB-CG	9.01	1.69	1.52
7	I	99	LEU	C-O	-9.01	1.06	1.23
1	A	81	PHE	CE2-CZ	-9.01	1.20	1.37
2	B	870	ILE	N-CA	9.01	1.64	1.46
7	I	118	ARG	CG-CD	9.01	1.74	1.51
1	A	578	LEU	CG-CD1	-9.01	1.18	1.51
1	A	596	THR	C-O	-9.01	1.06	1.23
2	B	237	VAL	CA-CB	-9.01	1.35	1.54
2	B	322	PHE	CG-CD2	-9.00	1.25	1.38
3	C	126	GLY	C-O	9.00	1.38	1.23
1	A	226	GLU	CB-CG	9.00	1.69	1.52
4	E	196	VAL	CB-CG1	-9.00	1.33	1.52
1	A	478	TYR	CG-CD2	-9.00	1.27	1.39
1	A	652	VAL	CB-CG2	-8.99	1.33	1.52
2	B	831	SER	CB-OG	-8.99	1.30	1.42
1	A	135	PHE	CE2-CZ	-8.99	1.20	1.37
1	A	838	GLN	CB-CG	8.99	1.76	1.52
1	A	1298	TYR	CG-CD1	-8.99	1.27	1.39
1	A	1298	TYR	CE1-CZ	-8.99	1.26	1.38
2	B	262	GLU	CG-CD	8.99	1.65	1.51
1	A	1105	LEU	CA-C	-8.99	1.29	1.52
2	B	833	TYR	CG-CD1	-8.99	1.27	1.39
6	H	132	LEU	CA-CB	8.99	1.74	1.53
9	K	99	GLY	C-O	8.99	1.38	1.23
1	A	370	ILE	C-O	-8.98	1.06	1.23
2	B	529	GLU	CG-CD	8.98	1.65	1.51
3	C	68	GLY	N-CA	8.98	1.59	1.46
7	I	82	GLU	CB-CG	8.98	1.69	1.52
6	H	138	GLU	CD-OE2	8.98	1.35	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	LYS	CG-CD	8.98	1.82	1.52
1	A	1047	SER	CB-OG	8.98	1.53	1.42
2	B	1183	LYS	CB-CG	8.97	1.76	1.52
2	B	479	VAL	CA-CB	-8.97	1.35	1.54
3	C	241	ASP	CB-CG	8.96	1.70	1.51
1	A	551	TYR	CD1-CE1	-8.96	1.25	1.39
1	A	1036	ARG	CZ-NH2	8.96	1.44	1.33
7	I	98	VAL	CB-CG2	-8.96	1.34	1.52
2	B	758	PHE	CA-CB	-8.96	1.34	1.53
2	B	770	GLN	CD-NE2	8.96	1.55	1.32
7	I	18	GLU	CD-OE2	8.96	1.35	1.25
10	L	65	VAL	CA-CB	-8.95	1.35	1.54
2	B	479	VAL	C-O	-8.95	1.06	1.23
2	B	592	ASN	CB-CG	8.94	1.71	1.51
2	B	572	HIS	CA-CB	8.94	1.73	1.53
1	A	101	LYS	CE-NZ	8.94	1.71	1.49
2	B	233	PRO	CB-CG	8.94	1.94	1.50
1	A	393	ARG	NE-CZ	8.94	1.44	1.33
3	C	196	ASP	CG-OD1	8.94	1.46	1.25
1	A	1225	PHE	CE1-CZ	8.93	1.54	1.37
1	A	1284	MET	CB-CG	-8.93	1.22	1.51
1	A	1383	SER	CB-OG	8.93	1.53	1.42
2	B	319	GLU	CG-CD	8.93	1.65	1.51
2	B	652	LYS	CD-CE	8.93	1.73	1.51
2	B	97	VAL	CB-CG1	-8.93	1.34	1.52
2	B	573	GLN	CG-CD	8.93	1.71	1.51
3	C	121	VAL	CB-CG2	-8.93	1.34	1.52
1	A	404	TYR	CB-CG	-8.92	1.38	1.51
1	A	1040	GLN	C-O	-8.92	1.06	1.23
1	A	1187	GLN	CA-CB	8.92	1.73	1.53
1	A	1080	THR	CA-CB	8.92	1.76	1.53
2	B	1061	GLU	CG-CD	8.92	1.65	1.51
3	C	193	TYR	CE2-CZ	-8.92	1.26	1.38
1	A	1420	ASP	CG-OD1	8.92	1.45	1.25
7	I	70	ARG	NE-CZ	-8.92	1.21	1.33
2	B	202	TYR	CG-CD1	-8.91	1.27	1.39
1	A	1331	SER	C-O	8.91	1.40	1.23
1	A	509	LEU	CA-CB	-8.90	1.33	1.53
1	A	905	ASP	CG-OD2	8.90	1.45	1.25
7	I	8	ARG	CB-CG	8.90	1.76	1.52
1	A	504	LEU	CG-CD1	-8.90	1.19	1.51
1	A	1139	GLU	CD-OE2	-8.90	1.15	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1012	ILE	CB-CG2	-8.89	1.25	1.52
1	A	1352	VAL	C-O	-8.88	1.06	1.23
1	A	427	GLN	CB-CG	8.88	1.76	1.52
2	B	904	ARG	C-O	-8.88	1.06	1.23
10	L	36	SER	CB-OG	8.88	1.53	1.42
3	C	50	GLU	CB-CG	8.88	1.69	1.52
3	C	267	GLN	CG-CD	8.88	1.71	1.51
2	B	887	HIS	C-O	8.88	1.40	1.23
1	A	1137	ALA	CA-CB	-8.88	1.33	1.52
2	B	118	ARG	CD-NE	-8.88	1.31	1.46
2	B	831	SER	CA-CB	-8.88	1.39	1.52
8	J	54	VAL	CB-CG2	-8.88	1.34	1.52
1	A	806	ARG	CZ-NH1	8.87	1.44	1.33
1	A	1411	GLU	CG-CD	8.87	1.65	1.51
2	B	1057	LYS	CD-CE	8.87	1.73	1.51
4	E	79	TRP	C-O	-8.87	1.06	1.23
2	B	979	LYS	CB-CG	-8.87	1.28	1.52
7	I	86	PHE	C-O	-8.87	1.06	1.23
2	B	370	PHE	CD2-CE2	8.87	1.56	1.39
2	B	1215	ARG	CG-CD	8.86	1.74	1.51
1	A	546	VAL	CB-CG2	-8.86	1.34	1.52
4	E	169	ARG	CG-CD	8.86	1.74	1.51
9	K	88	LYS	CG-CD	8.86	1.82	1.52
2	B	1185	CYS	CB-SG	-8.85	1.67	1.82
7	I	89	GLN	CG-CD	-8.85	1.30	1.51
1	A	36	ARG	NE-CZ	8.85	1.44	1.33
1	A	133	LYS	CE-NZ	8.84	1.71	1.49
1	A	1218	GLN	CG-CD	8.84	1.71	1.51
2	B	110	HIS	CA-C	8.84	1.75	1.52
2	B	874	PHE	CD1-CE1	-8.84	1.21	1.39
1	A	1362	TYR	CZ-OH	8.84	1.52	1.37
3	C	261	ALA	C-O	-8.84	1.06	1.23
7	I	24	ARG	N-CA	8.84	1.64	1.46
1	A	721	PHE	CE2-CZ	-8.82	1.20	1.37
5	F	77	ASP	CG-OD1	8.82	1.45	1.25
1	A	1093	LYS	CG-CD	8.82	1.82	1.52
1	A	1316	VAL	CB-CG2	-8.82	1.34	1.52
1	A	350	ARG	CZ-NH2	-8.81	1.21	1.33
10	L	43	THR	CA-CB	8.81	1.76	1.53
2	B	1091	TYR	CA-C	-8.81	1.30	1.52
2	B	202	TYR	CD2-CE2	8.81	1.52	1.39
1	A	720	ARG	NE-CZ	8.80	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	108	GLY	C-O	-8.80	1.09	1.23
1	A	775	ILE	CA-CB	-8.80	1.34	1.54
1	A	1058	VAL	CB-CG2	-8.80	1.34	1.52
2	B	488	TYR	CG-CD2	-8.80	1.27	1.39
1	A	1433	MET	CA-C	-8.79	1.30	1.52
2	B	124	TYR	CA-CB	-8.79	1.34	1.53
2	B	745	PRO	CG-CD	8.79	1.79	1.50
3	C	202	PRO	N-CD	-8.79	1.35	1.47
7	I	44	TYR	CG-CD1	-8.79	1.27	1.39
2	B	772	ALA	CA-CB	8.79	1.71	1.52
1	A	1062	GLU	CG-CD	-8.79	1.38	1.51
1	A	1338	VAL	CB-CG2	-8.79	1.34	1.52
1	A	1412	ALA	CA-CB	8.79	1.71	1.52
2	B	933	SER	C-O	8.77	1.40	1.23
2	B	1108	ARG	NE-CZ	8.77	1.44	1.33
6	H	3	ASN	CB-CG	8.77	1.71	1.51
1	A	963	ILE	CB-CG2	-8.77	1.25	1.52
1	A	364	VAL	CB-CG2	-8.76	1.34	1.52
1	A	1374	VAL	C-O	8.76	1.40	1.23
7	I	94	ASP	CA-CB	8.76	1.73	1.53
1	A	121	LEU	CG-CD1	8.75	1.84	1.51
6	H	2	SER	N-CA	8.75	1.63	1.46
1	A	1221	LYS	CG-CD	8.74	1.82	1.52
3	C	209	TYR	CD1-CE1	8.74	1.52	1.39
7	I	23	ASN	CB-CG	8.74	1.71	1.51
2	B	227	LYS	CG-CD	8.74	1.82	1.52
2	B	262	GLU	CD-OE2	8.73	1.35	1.25
1	A	464	PRO	C-N	-8.73	1.14	1.34
2	B	584	GLY	C-O	8.73	1.37	1.23
2	B	826	ALA	C-O	-8.73	1.06	1.23
3	C	13	ALA	C-O	-8.73	1.06	1.23
1	A	1119	TYR	CG-CD2	-8.73	1.27	1.39
2	B	711	GLU	CD-OE2	8.73	1.35	1.25
7	I	6	PHE	CB-CG	-8.73	1.36	1.51
5	F	148	VAL	C-O	8.73	1.40	1.23
1	A	1318	THR	C-O	-8.73	1.06	1.23
3	C	209	TYR	CD2-CE2	8.73	1.52	1.39
1	A	27	VAL	CB-CG1	8.72	1.71	1.52
2	B	1149	GLU	CA-C	-8.72	1.30	1.52
1	A	163	SER	CA-CB	8.72	1.66	1.52
2	B	1191	ILE	CA-CB	-8.72	1.34	1.54
7	I	51	ASN	CG-OD1	8.72	1.43	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195	ASP	C-O	8.72	1.40	1.23
1	A	572	TRP	CE2-CZ2	-8.71	1.25	1.39
2	B	336	ARG	CZ-NH2	8.72	1.44	1.33
7	I	72	ASP	CG-OD1	8.71	1.45	1.25
7	I	43	VAL	CB-CG1	-8.71	1.34	1.52
1	A	1262	LYS	CB-CG	8.70	1.76	1.52
2	B	275	TYR	CG-CD1	-8.70	1.27	1.39
1	A	1214	GLU	CB-CG	8.70	1.68	1.52
2	B	813	LYS	CD-CE	8.70	1.73	1.51
2	B	1181	GLU	CA-CB	8.70	1.73	1.53
4	E	43	LYS	CE-NZ	8.70	1.70	1.49
9	K	102	LYS	CD-CE	8.70	1.73	1.51
2	B	202	TYR	CB-CG	-8.69	1.38	1.51
1	A	537	ARG	CZ-NH1	8.69	1.44	1.33
7	I	80	SER	CB-OG	8.69	1.53	1.42
1	A	76	GLU	CD-OE2	8.68	1.35	1.25
2	B	1008	PRO	CG-CD	-8.68	1.22	1.50
1	A	1153	TYR	C-O	8.68	1.39	1.23
3	C	15	LYS	CD-CE	8.68	1.73	1.51
2	B	466	TRP	CE3-CZ3	-8.68	1.23	1.38
3	C	29	MET	CG-SD	-8.68	1.58	1.81
1	A	17	VAL	CA-CB	-8.67	1.36	1.54
2	B	1101	ASP	CA-C	8.67	1.75	1.52
2	B	1106	ARG	CD-NE	8.67	1.61	1.46
1	A	599	SER	CB-OG	-8.67	1.30	1.42
1	A	805	LEU	CA-C	-8.67	1.30	1.52
6	H	43	ASN	CB-CG	8.67	1.71	1.51
4	E	98	ILE	CA-CB	8.67	1.74	1.54
1	A	360	GLU	C-O	-8.66	1.06	1.23
2	B	169	ARG	NE-CZ	8.66	1.44	1.33
7	I	30	ARG	CA-CB	-8.66	1.34	1.53
1	A	1328	TYR	CB-CG	8.66	1.64	1.51
6	H	34	ASP	CB-CG	8.66	1.70	1.51
2	B	1157	ALA	CA-CB	8.66	1.70	1.52
2	B	1217	TYR	CG-CD1	-8.66	1.27	1.39
1	A	1225	PHE	CD1-CE1	8.66	1.56	1.39
1	A	31	SER	C-O	8.66	1.39	1.23
1	A	280	GLU	CD-OE1	8.65	1.35	1.25
2	B	451	LYS	CD-CE	8.65	1.72	1.51
2	B	1086	PHE	CE2-CZ	-8.65	1.21	1.37
1	A	787	PHE	CD2-CE2	-8.65	1.22	1.39
1	A	944	ARG	CZ-NH2	-8.65	1.21	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	245	GLU	CA-C	8.65	1.75	1.52
9	K	4	PRO	C-O	8.65	1.40	1.23
10	L	26	THR	CB-CG2	8.65	1.80	1.52
1	A	28	ARG	NE-CZ	8.64	1.44	1.33
1	A	1446	ASP	CB-CG	8.63	1.69	1.51
2	B	1189	ILE	CB-CG2	8.64	1.79	1.52
3	C	79	GLN	CD-NE2	8.64	1.54	1.32
1	A	421	ALA	N-CA	-8.63	1.29	1.46
5	F	77	ASP	CG-OD2	8.63	1.45	1.25
1	A	1159	ARG	CG-CD	8.63	1.73	1.51
2	B	1004	GLU	CD-OE1	8.63	1.35	1.25
9	K	41	THR	CB-CG2	-8.63	1.23	1.52
2	B	245	GLU	CD-OE2	8.63	1.35	1.25
1	A	897	TYR	CE2-CZ	-8.62	1.27	1.38
2	B	579	ARG	CG-CD	8.62	1.73	1.51
2	B	250	PHE	CG-CD2	8.62	1.51	1.38
2	B	624	LEU	CG-CD1	-8.62	1.20	1.51
9	K	67	PHE	CE2-CZ	-8.62	1.21	1.37
2	B	525	ALA	N-CA	-8.61	1.29	1.46
1	A	716	ASP	CG-OD1	8.61	1.45	1.25
1	A	1056	SER	CA-CB	-8.61	1.40	1.52
1	A	506	ALA	C-O	-8.60	1.07	1.23
1	A	1264	GLU	CA-C	-8.60	1.30	1.52
2	B	51	PHE	CD1-CE1	-8.59	1.22	1.39
2	B	429	PHE	CE1-CZ	8.59	1.53	1.37
7	I	37	GLU	CG-CD	8.59	1.64	1.51
1	A	893	PHE	CG-CD2	-8.59	1.25	1.38
4	E	52	ARG	CG-CD	8.58	1.73	1.51
1	A	1234	GLU	CB-CG	8.58	1.68	1.52
2	B	581	PHE	C-O	8.58	1.39	1.23
4	E	194	GLU	C-O	-8.58	1.07	1.23
1	A	568	PRO	CB-CG	-8.58	1.07	1.50
1	A	298	PHE	CE1-CZ	8.58	1.53	1.37
1	A	1194	ARG	CD-NE	-8.58	1.31	1.46
2	B	723	VAL	CA-CB	8.57	1.72	1.54
1	A	905	ASP	N-CA	-8.57	1.29	1.46
1	A	1112	LYS	CB-CG	8.57	1.75	1.52
2	B	747	MET	SD-CE	-8.57	1.29	1.77
1	A	85	ASP	C-O	8.57	1.39	1.23
1	A	1420	ASP	CB-CG	8.57	1.69	1.51
4	E	47	CYS	CA-C	8.57	1.75	1.52
1	A	720	ARG	CD-NE	8.56	1.61	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	106	ASP	CG-OD2	8.56	1.45	1.25
2	B	114	PRO	CG-CD	-8.56	1.22	1.50
9	K	21	ILE	CB-CG2	-8.56	1.26	1.52
2	B	264	SER	CB-OG	8.56	1.53	1.42
4	E	167	ARG	CZ-NH2	8.56	1.44	1.33
6	H	92	ASP	CB-CG	8.56	1.69	1.51
1	A	922	ASP	N-CA	-8.55	1.29	1.46
2	B	1069	PHE	C-O	8.55	1.39	1.23
1	A	193	ASP	N-CA	8.55	1.63	1.46
2	B	790	ASP	CB-CG	8.55	1.69	1.51
1	A	1303	GLU	C-O	-8.54	1.07	1.23
1	A	1217	LYS	CE-NZ	8.54	1.70	1.49
2	B	894	ASP	CB-CG	8.54	1.69	1.51
2	B	1100	ASP	CB-CG	8.54	1.69	1.51
8	J	18	TRP	CE2-CZ2	-8.54	1.25	1.39
10	L	29	TYR	CG-CD1	-8.54	1.28	1.39
2	B	135	ARG	CG-CD	8.53	1.73	1.51
2	B	793	ALA	C-O	-8.53	1.07	1.23
1	A	1284	MET	CA-C	-8.53	1.30	1.52
1	A	1144	LYS	CG-CD	8.52	1.81	1.52
1	A	1159	ARG	CZ-NH2	8.51	1.44	1.33
6	H	146	ARG	CZ-NH1	8.51	1.44	1.33
2	B	31	TRP	CD2-CE3	-8.51	1.27	1.40
2	B	271	ALA	CA-CB	-8.51	1.34	1.52
2	B	766	ARG	N-CA	-8.51	1.29	1.46
7	I	44	TYR	N-CA	8.51	1.63	1.46
2	B	581	PHE	CE2-CZ	-8.51	1.21	1.37
2	B	660	LYS	C-O	8.51	1.39	1.23
3	C	148	ARG	CD-NE	8.50	1.60	1.46
4	E	94	LYS	CG-CD	8.50	1.81	1.52
1	A	326	ARG	NE-CZ	8.50	1.44	1.33
1	A	1092	LYS	CD-CE	8.50	1.72	1.51
1	A	1162	VAL	CB-CG2	8.50	1.70	1.52
3	C	253	LYS	C-O	8.49	1.39	1.23
1	A	430	TRP	CZ3-CH2	-8.49	1.26	1.40
3	C	179	GLU	CD-OE2	-8.49	1.16	1.25
1	A	66	LYS	CB-CG	8.49	1.75	1.52
1	A	1353	TYR	CE2-CZ	-8.49	1.27	1.38
2	B	380	TYR	CD2-CE2	-8.49	1.26	1.39
1	A	1153	TYR	CD2-CE2	-8.48	1.26	1.39
4	E	81	GLU	CG-CD	-8.48	1.39	1.51
1	A	1385	THR	CA-C	8.48	1.75	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	76	THR	CB-CG2	8.48	1.80	1.52
2	B	711	GLU	CD-OE1	8.47	1.34	1.25
2	B	816	GLU	CD-OE2	8.47	1.34	1.25
6	H	2	SER	CA-C	8.47	1.75	1.52
1	A	420	ARG	CB-CG	-8.47	1.29	1.52
1	A	603	ASN	N-CA	-8.47	1.29	1.46
2	B	1071	VAL	CB-CG2	-8.47	1.35	1.52
1	A	347	PHE	N-CA	8.47	1.63	1.46
1	A	219	PHE	CA-CB	-8.47	1.35	1.53
1	A	474	VAL	CA-CB	-8.46	1.36	1.54
1	A	1297	GLU	CD-OE2	8.47	1.34	1.25
2	B	978	ASP	CG-OD2	8.46	1.44	1.25
4	E	130	ALA	C-O	8.47	1.39	1.23
2	B	1149	GLU	CG-CD	8.46	1.64	1.51
6	H	136	LYS	CD-CE	8.46	1.72	1.51
9	K	83	PRO	CB-CG	-8.46	1.07	1.50
1	A	372	LYS	CD-CE	-8.46	1.30	1.51
10	L	61	THR	CB-CG2	8.46	1.80	1.52
6	H	115	TYR	CE2-CZ	8.46	1.49	1.38
2	B	228	LYS	CB-CG	8.46	1.75	1.52
2	B	993	THR	CA-CB	-8.46	1.31	1.53
2	B	1040	ASN	CB-CG	-8.46	1.31	1.51
1	A	940	ARG	CG-CD	8.46	1.73	1.51
1	A	679	ILE	C-O	8.45	1.39	1.23
1	A	1320	PRO	CA-C	-8.45	1.35	1.52
2	B	534	GLY	N-CA	-8.45	1.33	1.46
9	K	94	ILE	CB-CG2	-8.45	1.26	1.52
1	A	1298	TYR	CE2-CZ	-8.45	1.27	1.38
1	A	465	TYR	CE1-CZ	-8.45	1.27	1.38
1	A	944	ARG	CA-CB	-8.45	1.35	1.53
1	A	277	GLU	CD-OE2	8.44	1.34	1.25
2	B	692	TYR	CE1-CZ	-8.44	1.27	1.38
5	F	108	PHE	CE2-CZ	8.44	1.53	1.37
6	H	131	ASN	CA-C	8.44	1.74	1.52
1	A	861	GLY	C-O	-8.43	1.10	1.23
1	A	1423	GLY	C-O	-8.43	1.10	1.23
2	B	811	TYR	CD1-CE1	8.43	1.51	1.39
3	C	208	GLU	CG-CD	8.43	1.64	1.51
6	H	95	TYR	CD1-CE1	8.43	1.51	1.39
2	B	1224	PHE	N-CA	8.43	1.63	1.46
4	E	192	ARG	CD-NE	8.43	1.60	1.46
10	L	40	LEU	CB-CG	8.43	1.76	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	220	GLY	C-O	-8.42	1.10	1.23
2	B	327	ARG	CZ-NH2	8.42	1.44	1.33
3	C	245	VAL	CA-CB	-8.42	1.37	1.54
3	C	170	TRP	CB-CG	-8.42	1.35	1.50
4	E	28	TYR	CE2-CZ	-8.41	1.27	1.38
6	H	136	LYS	CA-C	8.41	1.74	1.52
1	A	346	ASP	CA-CB	8.41	1.72	1.53
1	A	693	VAL	CA-CB	-8.41	1.37	1.54
10	L	50	ASP	CA-C	8.41	1.74	1.52
1	A	912	LEU	CA-C	-8.40	1.31	1.52
2	B	768	THR	CB-OG1	8.40	1.60	1.43
2	B	116	GLU	CD-OE2	8.40	1.34	1.25
4	E	200	ARG	NE-CZ	-8.40	1.22	1.33
5	F	114	GLU	CD-OE2	8.40	1.34	1.25
2	B	1153	GLU	CG-CD	8.40	1.64	1.51
4	E	118	PRO	CG-CD	8.40	1.78	1.50
3	C	138	GLU	CD-OE2	8.39	1.34	1.25
2	B	694	ASP	CG-OD2	8.39	1.44	1.25
4	E	148	GLU	CD-OE1	-8.39	1.16	1.25
1	A	373	THR	CB-CG2	-8.38	1.24	1.52
3	C	166	GLU	CG-CD	8.38	1.64	1.51
3	C	216	GLY	C-O	8.38	1.37	1.23
1	A	1120	LEU	CG-CD1	8.38	1.82	1.51
1	A	1211	GLN	CG-CD	8.38	1.70	1.51
2	B	38	PHE	CD1-CE1	-8.38	1.22	1.39
1	A	165	GLY	C-O	8.37	1.37	1.23
1	A	1076	ALA	CA-CB	8.37	1.70	1.52
2	B	1049	ASP	CB-CG	8.37	1.69	1.51
1	A	1190	PRO	CB-CG	8.37	1.91	1.50
2	B	780	VAL	CB-CG1	-8.37	1.35	1.52
1	A	419	LYS	C-O	-8.37	1.07	1.23
4	E	210	SER	CA-CB	-8.37	1.40	1.52
2	B	435	THR	CA-C	8.36	1.74	1.52
6	H	20	TYR	CD2-CE2	-8.36	1.26	1.39
1	A	1410	PHE	CD1-CE1	-8.36	1.22	1.39
2	B	910	VAL	CB-CG1	8.36	1.70	1.52
3	C	248	ILE	CA-CB	-8.36	1.35	1.54
3	C	211	ASP	CG-OD2	8.36	1.44	1.25
4	E	131	THR	C-O	-8.36	1.07	1.23
8	J	14	VAL	CA-CB	-8.36	1.37	1.54
10	L	33	GLU	CD-OE2	8.36	1.34	1.25
7	I	47	GLU	CD-OE2	8.35	1.34	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1212	VAL	CB-CG2	-8.35	1.35	1.52
1	A	1328	TYR	CE2-CZ	-8.35	1.27	1.38
5	F	110	ASP	CG-OD1	8.35	1.44	1.25
1	A	503	GLN	CD-OE1	8.34	1.42	1.24
1	A	1226	VAL	CB-CG1	-8.34	1.35	1.52
2	B	287	ARG	CA-CB	-8.34	1.35	1.53
1	A	130	ASP	CG-OD1	8.33	1.44	1.25
1	A	1287	TYR	CE2-CZ	8.33	1.49	1.38
3	C	263	THR	CB-CG2	8.33	1.79	1.52
2	B	733	HIS	N-CA	8.33	1.63	1.46
1	A	641	VAL	CA-CB	-8.33	1.37	1.54
2	B	1015	HIS	CE1-NE2	8.32	1.51	1.32
6	H	85	GLY	N-CA	8.32	1.58	1.46
1	A	718	VAL	CB-CG2	-8.32	1.35	1.52
1	A	1412	ALA	C-O	-8.32	1.07	1.23
3	C	58	LEU	N-CA	-8.32	1.29	1.46
1	A	1209	MET	N-CA	-8.32	1.29	1.46
1	A	1228	TRP	CZ3-CH2	-8.32	1.26	1.40
9	K	61	TYR	CZ-OH	-8.32	1.23	1.37
4	E	113	GLN	CB-CG	8.32	1.75	1.52
1	A	44	THR	CB-CG2	8.31	1.79	1.52
1	A	1365	TYR	CG-CD1	-8.31	1.28	1.39
2	B	1069	PHE	CG-CD2	-8.31	1.26	1.38
1	A	781	ASP	C-O	8.31	1.39	1.23
2	B	883	LEU	CA-CB	8.31	1.72	1.53
9	K	102	LYS	CG-CD	8.31	1.80	1.52
1	A	898	ARG	C-O	-8.30	1.07	1.23
2	B	394	ASP	CB-CG	8.30	1.69	1.51
2	B	455	SER	CB-OG	8.30	1.53	1.42
8	J	29	GLU	CD-OE2	8.30	1.34	1.25
1	A	696	GLU	N-CA	-8.30	1.29	1.46
1	A	1365	TYR	CD1-CE1	8.30	1.51	1.39
1	A	1417	GLU	CB-CG	8.30	1.68	1.52
9	K	26	LYS	CB-CG	8.30	1.75	1.52
1	A	822	GLU	C-O	-8.30	1.07	1.23
2	B	746	SER	CB-OG	-8.30	1.31	1.42
2	B	815	ARG	CD-NE	-8.30	1.32	1.46
1	A	1048	ASN	CG-ND2	8.29	1.53	1.32
1	A	1080	THR	CA-C	8.29	1.74	1.52
1	A	590	ARG	CZ-NH2	-8.29	1.22	1.33
2	B	94	LYS	CB-CG	8.29	1.75	1.52
7	I	37	GLU	CD-OE2	8.29	1.34	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	765	VAL	CB-CG1	-8.29	1.35	1.52
6	H	77	ARG	CG-CD	8.29	1.72	1.51
1	A	272	ALA	CA-CB	8.28	1.69	1.52
1	A	1238	ILE	CB-CG2	8.29	1.78	1.52
1	A	1270	ASN	C-O	8.29	1.39	1.23
1	A	1305	VAL	C-O	-8.29	1.07	1.23
1	A	395	GLY	C-O	-8.28	1.10	1.23
2	B	678	GLU	CG-CD	8.28	1.64	1.51
1	A	1289	ARG	NE-CZ	-8.28	1.22	1.33
2	B	916	THR	CB-CG2	8.28	1.79	1.52
1	A	793	SER	C-O	-8.27	1.07	1.23
9	K	74	ARG	CZ-NH1	-8.27	1.22	1.33
1	A	1324	PRO	N-CD	-8.27	1.36	1.47
2	B	1060	ARG	CB-CG	-8.27	1.30	1.52
2	B	21	GLU	CG-CD	8.27	1.64	1.51
2	B	617	ARG	CZ-NH2	-8.27	1.22	1.33
7	I	75	CYS	CA-C	-8.27	1.31	1.52
2	B	1154	ALA	C-O	8.26	1.39	1.23
2	B	38	PHE	CG-CD2	-8.26	1.26	1.38
2	B	1086	PHE	CE1-CZ	-8.26	1.21	1.37
2	B	1065	GLN	CB-CG	-8.25	1.30	1.52
1	A	728	LYS	CE-NZ	8.25	1.69	1.49
2	B	368	GLU	CD-OE2	8.25	1.34	1.25
2	B	245	GLU	CB-CG	8.25	1.67	1.52
2	B	1012	ILE	CB-CG1	-8.25	1.30	1.54
4	E	29	PHE	CD2-CE2	-8.25	1.22	1.39
1	A	1159	ARG	CB-CG	8.25	1.74	1.52
2	B	235	SER	CA-CB	-8.25	1.40	1.52
2	B	106	ASP	CA-C	8.25	1.74	1.52
4	E	135	PHE	CE2-CZ	-8.25	1.21	1.37
2	B	1087	PHE	CE1-CZ	-8.24	1.21	1.37
2	B	706	GLN	CD-NE2	8.24	1.53	1.32
1	A	654	ASN	N-CA	-8.23	1.29	1.46
1	A	705	LYS	CE-NZ	8.23	1.69	1.49
7	I	17	ARG	CA-C	-8.23	1.31	1.52
9	K	110	ASN	CG-OD1	8.23	1.42	1.24
2	B	54	PHE	CD1-CE1	-8.23	1.22	1.39
2	B	333	PHE	CE1-CZ	-8.23	1.21	1.37
6	H	91	ASP	CA-C	8.23	1.74	1.52
9	K	85	ASP	CA-CB	8.23	1.72	1.53
1	A	165	GLY	CA-C	8.23	1.65	1.51
2	B	49	ASP	CB-CG	8.23	1.69	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	104	PHE	CE1-CZ	8.23	1.52	1.37
1	A	792	TYR	CA-CB	-8.22	1.35	1.53
4	E	71	LYS	CB-CG	8.22	1.74	1.52
7	I	66	PRO	CA-C	-8.22	1.36	1.52
2	B	751	VAL	CA-CB	-8.22	1.37	1.54
1	A	894	GLU	CG-CD	8.22	1.64	1.51
1	A	1165	GLU	CD-OE2	8.22	1.34	1.25
2	B	125	SER	CA-CB	8.22	1.65	1.52
2	B	204	ILE	C-O	-8.22	1.07	1.23
1	A	696	GLU	CD-OE1	-8.22	1.16	1.25
2	B	287	ARG	CG-CD	8.22	1.72	1.51
1	A	656	TRP	CG-CD1	-8.21	1.25	1.36
1	A	681	GLU	C-O	8.22	1.39	1.23
9	K	74	ARG	NE-CZ	-8.22	1.22	1.33
1	A	176	LYS	CG-CD	8.21	1.80	1.52
1	A	1385	THR	CB-CG2	8.21	1.79	1.52
2	B	891	ASP	CB-CG	8.21	1.69	1.51
6	H	98	TYR	CE2-CZ	8.21	1.49	1.38
10	L	27	LEU	CA-C	8.21	1.74	1.52
1	A	53	LEU	C-O	8.21	1.39	1.23
1	A	348	SER	CA-CB	-8.21	1.40	1.52
2	B	265	SER	C-O	8.21	1.39	1.23
2	B	651	LEU	CG-CD2	-8.21	1.21	1.51
1	A	915	SER	CA-CB	8.21	1.65	1.52
2	B	496	ARG	CD-NE	-8.21	1.32	1.46
2	B	1069	PHE	CB-CG	-8.21	1.37	1.51
2	B	1137	CYS	C-O	-8.21	1.07	1.23
9	K	30	ALA	CA-CB	-8.20	1.35	1.52
1	A	189	ARG	N-CA	8.20	1.62	1.46
1	A	360	GLU	CD-OE2	8.20	1.34	1.25
4	E	179	GLN	CA-CB	-8.20	1.35	1.53
2	B	105	SER	C-O	8.20	1.39	1.23
2	B	380	TYR	CG-CD1	-8.20	1.28	1.39
4	E	52	ARG	C-O	8.20	1.39	1.23
7	I	44	TYR	CD1-CE1	8.20	1.51	1.39
1	A	1173	HIS	CA-C	8.20	1.74	1.52
1	A	199	LEU	CG-CD1	8.20	1.82	1.51
1	A	379	VAL	CB-CG2	8.19	1.70	1.52
1	A	1067	LEU	CG-CD1	-8.20	1.21	1.51
6	H	19	ARG	NE-CZ	8.19	1.43	1.33
1	A	1226	VAL	CA-CB	-8.19	1.37	1.54
2	B	981	ALA	CA-CB	-8.19	1.35	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	878	GLN	CG-CD	8.19	1.69	1.51
1	A	1102	LYS	CD-CE	8.18	1.71	1.51
1	A	1384	VAL	CB-CG2	8.18	1.70	1.52
2	B	522	VAL	CB-CG2	-8.18	1.35	1.52
2	B	174	LEU	C-O	-8.18	1.07	1.23
2	B	563	MET	CG-SD	8.17	2.02	1.81
1	A	186	LYS	CG-CD	8.17	1.80	1.52
1	A	225	ASN	C-O	8.17	1.38	1.23
1	A	1129	GLU	CB-CG	8.17	1.67	1.52
2	B	1158	PHE	C-O	-8.17	1.07	1.23
1	A	552	TRP	CG-CD1	-8.17	1.25	1.36
1	A	1417	GLU	CD-OE2	8.17	1.34	1.25
2	B	373	ARG	CZ-NH1	8.17	1.43	1.33
3	C	94	LYS	CB-CG	8.17	1.74	1.52
4	E	8	ASN	CG-ND2	8.17	1.53	1.32
1	A	232	GLU	CD-OE1	8.16	1.34	1.25
1	A	692	ASP	CB-CG	8.16	1.68	1.51
4	E	212	ARG	CG-CD	8.16	1.72	1.51
2	B	327	ARG	C-O	-8.15	1.07	1.23
1	A	134	ARG	CB-CG	-8.15	1.30	1.52
1	A	34	LYS	CG-CD	8.15	1.80	1.52
1	A	497	THR	C-O	-8.15	1.07	1.23
2	B	194	GLU	CD-OE2	8.15	1.34	1.25
1	A	226	GLU	CG-CD	8.14	1.64	1.51
2	B	1193	GLN	C-O	-8.14	1.07	1.23
3	C	62	PHE	CD1-CE1	-8.14	1.23	1.39
2	B	751	VAL	CB-CG1	-8.14	1.35	1.52
5	F	73	ALA	N-CA	8.14	1.62	1.46
1	A	125	ALA	C-O	-8.13	1.07	1.23
1	A	529	CYS	C-N	-8.14	1.18	1.33
2	B	589	VAL	CB-CG1	-8.13	1.35	1.52
1	A	991	LYS	CE-NZ	8.13	1.69	1.49
2	B	1007	VAL	CB-CG2	-8.13	1.35	1.52
2	B	320	ASP	CB-CG	8.13	1.68	1.51
3	C	35	ARG	CG-CD	8.13	1.72	1.51
3	C	62	PHE	CG-CD2	8.13	1.50	1.38
1	A	771	GLU	CA-C	-8.12	1.31	1.52
1	A	1149	ALA	CA-CB	-8.12	1.35	1.52
1	A	996	ASN	N-CA	-8.12	1.30	1.46
4	E	30	ILE	C-O	-8.12	1.07	1.23
9	K	23	PRO	CB-CG	8.12	1.90	1.50
10	L	66	GLN	CD-OE1	8.12	1.41	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	91	ALA	CA-CB	-8.12	1.35	1.52
3	C	84	ARG	C-O	-8.12	1.07	1.23
7	I	120	GLN	CA-CB	8.11	1.71	1.53
5	F	79	ARG	NE-CZ	-8.10	1.22	1.33
1	A	800	VAL	CA-CB	-8.10	1.37	1.54
2	B	215	GLN	CB-CG	-8.10	1.30	1.52
4	E	21	GLU	CD-OE1	8.10	1.34	1.25
6	H	120	GLY	C-O	8.10	1.36	1.23
1	A	419	LYS	CE-NZ	-8.10	1.28	1.49
2	B	138	GLU	N-CA	8.10	1.62	1.46
2	B	604	ARG	NE-CZ	-8.10	1.22	1.33
3	C	109	SER	CA-CB	8.10	1.65	1.52
1	A	792	TYR	CE2-CZ	-8.09	1.28	1.38
2	B	57	TYR	CE1-CZ	-8.09	1.28	1.38
1	A	553	VAL	CB-CG1	-8.09	1.35	1.52
1	A	1107	VAL	C-O	8.09	1.38	1.23
3	C	84	ARG	CG-CD	8.09	1.72	1.51
2	B	250	PHE	CE1-CZ	8.09	1.52	1.37
2	B	304	ASP	CB-CG	8.09	1.68	1.51
2	B	579	ARG	NE-CZ	-8.08	1.22	1.33
8	J	47	ARG	NE-CZ	-8.08	1.22	1.33
8	J	64	ASN	CG-OD1	8.08	1.41	1.24
4	E	53	PRO	CB-CG	8.07	1.90	1.50
4	E	142	VAL	CB-CG1	-8.07	1.35	1.52
1	A	717	ASN	CG-OD1	8.07	1.41	1.24
1	A	814	PHE	CD1-CE1	-8.07	1.23	1.39
2	B	980	PHE	CE1-CZ	8.07	1.52	1.37
1	A	949	ASP	C-O	-8.07	1.08	1.23
1	A	1155	ASP	CA-CB	-8.07	1.36	1.53
1	A	1223	ASP	CG-OD1	8.07	1.44	1.25
2	B	436	VAL	CA-C	8.07	1.74	1.52
2	B	567	GLU	CB-CG	8.07	1.67	1.52
4	E	85	GLU	CG-CD	8.07	1.64	1.51
1	A	172	PRO	CA-C	-8.06	1.36	1.52
1	A	1239	ARG	CZ-NH1	8.06	1.43	1.33
2	B	249	ARG	C-O	8.06	1.38	1.23
1	A	462	VAL	C-O	8.06	1.38	1.23
2	B	652	LYS	CE-NZ	8.06	1.69	1.49
4	E	102	GLU	CB-CG	8.06	1.67	1.52
10	L	47	ARG	NE-CZ	8.05	1.43	1.33
1	A	412	ARG	NE-CZ	-8.05	1.22	1.33
9	K	22	ASP	C-O	8.05	1.38	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	ILE	CB-CG2	8.05	1.77	1.52
1	A	1034	GLU	C-O	8.04	1.38	1.23
1	A	1221	LYS	CE-NZ	8.04	1.69	1.49
2	B	759	PRO	C-O	8.04	1.39	1.23
7	I	54	GLU	C-O	-8.04	1.08	1.23
1	A	16	GLU	CG-CD	8.04	1.64	1.51
1	A	69	THR	CA-CB	8.04	1.74	1.53
1	A	1345	ARG	CZ-NH2	-8.04	1.22	1.33
3	C	260	LEU	CG-CD2	8.04	1.81	1.51
6	H	131	ASN	N-CA	8.04	1.62	1.46
7	I	33	SER	CB-OG	8.04	1.52	1.42
2	B	1071	VAL	CB-CG1	-8.03	1.35	1.52
2	B	376	PHE	CE2-CZ	-8.03	1.22	1.37
1	A	1421	CYS	C-O	-8.03	1.08	1.23
4	E	109	ILE	CB-CG2	-8.03	1.27	1.52
5	F	102	SER	CB-OG	-8.03	1.31	1.42
4	E	93	MET	CG-SD	8.03	2.02	1.81
1	A	851	HIS	CA-CB	-8.02	1.36	1.53
2	B	967	ARG	CB-CG	-8.02	1.30	1.52
3	C	47	ASP	CB-CG	8.02	1.68	1.51
6	H	6	PHE	CG-CD2	-8.02	1.26	1.38
1	A	1189	SER	C-O	-8.02	1.08	1.23
2	B	108	VAL	CB-CG2	8.02	1.69	1.52
8	J	61	LEU	CA-CB	-8.02	1.35	1.53
1	A	1222	ASN	CG-OD1	8.01	1.41	1.24
2	B	299	GLU	CD-OE1	8.01	1.34	1.25
2	B	702	LEU	N-CA	-8.01	1.30	1.46
2	B	329	THR	N-CA	-8.01	1.30	1.46
1	A	268	ASP	CA-CB	8.01	1.71	1.53
5	F	122	MET	SD-CE	-8.01	1.33	1.77
1	A	1268	LEU	CG-CD2	-8.01	1.22	1.51
2	B	809	MET	C-O	-8.01	1.08	1.23
4	E	52	ARG	CZ-NH1	8.01	1.43	1.33
5	F	142	SER	C-O	-8.01	1.08	1.23
7	I	35	VAL	C-O	-8.00	1.08	1.23
1	A	1110	ASN	CG-OD1	8.00	1.41	1.24
3	C	13	ALA	CA-CB	-8.00	1.35	1.52
3	C	123	ASN	CB-CG	8.00	1.69	1.51
1	A	971	PHE	CB-CG	-8.00	1.37	1.51
2	B	322	PHE	CE1-CZ	-8.00	1.22	1.37
2	B	912	ILE	CA-CB	-8.00	1.36	1.54
2	B	417	PHE	CD1-CE1	-7.99	1.23	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1092	TYR	CE2-CZ	-7.99	1.28	1.38
9	K	61	TYR	CD1-CE1	7.99	1.51	1.39
8	J	42	LYS	C-O	7.99	1.38	1.23
1	A	614	PHE	CE2-CZ	-7.99	1.22	1.37
4	E	185	ALA	CA-CB	-7.99	1.35	1.52
2	B	914	LYS	C-O	7.99	1.38	1.23
7	I	86	PHE	CE1-CZ	7.99	1.52	1.37
6	H	98	TYR	CB-CG	-7.98	1.39	1.51
1	A	1096	SER	CA-CB	7.98	1.65	1.52
2	B	963	PHE	CE1-CZ	7.98	1.52	1.37
6	H	22	LYS	CB-CG	7.98	1.74	1.52
2	B	702	LEU	CG-CD2	-7.98	1.22	1.51
3	C	8	VAL	CA-CB	-7.98	1.38	1.54
1	A	529	CYS	CB-SG	-7.97	1.68	1.82
1	A	662	PHE	CG-CD2	-7.97	1.26	1.38
1	A	712	GLU	CD-OE2	7.97	1.34	1.25
2	B	54	PHE	C-O	-7.97	1.08	1.23
2	B	627	PHE	CB-CG	7.97	1.65	1.51
1	A	1378	GLN	CG-CD	7.97	1.69	1.51
1	A	154	SER	CB-OG	-7.97	1.31	1.42
1	A	1441	PHE	CB-CG	-7.97	1.37	1.51
10	L	29	TYR	N-CA	7.97	1.62	1.46
4	E	206	GLY	CA-C	-7.96	1.39	1.51
3	C	17	ASN	CB-CG	7.96	1.69	1.51
4	E	57	MET	CB-CG	7.96	1.76	1.51
1	A	1099	PRO	CA-C	-7.96	1.36	1.52
2	B	769	TYR	N-CA	-7.96	1.30	1.46
6	H	14	GLU	CG-CD	7.96	1.63	1.51
1	A	369	SER	CA-CB	-7.96	1.41	1.52
2	B	285	ILE	CA-CB	-7.96	1.36	1.54
2	B	393	LYS	CG-CD	7.96	1.79	1.52
2	B	1023	VAL	CA-CB	-7.96	1.38	1.54
2	B	542	MET	SD-CE	-7.96	1.33	1.77
6	H	136	LYS	CA-CB	7.96	1.71	1.53
1	A	1114	PRO	N-CD	-7.96	1.36	1.47
1	A	264	PHE	CA-CB	7.95	1.71	1.53
3	C	34	ARG	NE-CZ	-7.95	1.22	1.33
1	A	668	ASP	CA-CB	-7.95	1.36	1.53
1	A	1096	SER	CB-OG	7.95	1.52	1.42
2	B	39	ARG	NE-CZ	7.95	1.43	1.33
2	B	1127	GLY	N-CA	7.95	1.57	1.46
4	E	102	GLU	CD-OE2	7.95	1.34	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	602	ASP	CA-CB	-7.94	1.36	1.53
2	B	1045	SER	CA-CB	-7.94	1.41	1.52
2	B	70	ILE	CA-CB	7.94	1.73	1.54
7	I	109	ILE	CB-CG2	-7.94	1.28	1.52
3	C	50	GLU	CD-OE2	7.94	1.34	1.25
1	A	518	LYS	CB-CG	-7.94	1.31	1.52
1	A	1112	LYS	CG-CD	7.94	1.79	1.52
2	B	259	TYR	C-O	-7.94	1.08	1.23
7	I	102	VAL	CB-CG2	-7.94	1.36	1.52
2	B	835	GLN	C-O	-7.94	1.08	1.23
1	A	979	SER	CA-CB	7.93	1.64	1.52
2	B	483	LEU	CG-CD1	-7.93	1.22	1.51
7	I	82	GLU	CA-CB	7.93	1.71	1.53
5	F	95	GLY	C-O	-7.93	1.10	1.23
6	H	3	ASN	CG-OD1	7.93	1.41	1.24
1	A	849	MET	SD-CE	-7.93	1.33	1.77
2	B	905	VAL	CB-CG1	-7.92	1.36	1.52
8	J	7	CYS	CA-CB	7.92	1.71	1.53
9	K	26	LYS	CG-CD	7.92	1.79	1.52
4	E	17	ARG	CZ-NH2	7.92	1.43	1.33
10	L	38	LEU	CG-CD1	7.92	1.81	1.51
1	A	1349	TYR	CD1-CE1	-7.92	1.27	1.39
2	B	488	TYR	CE1-CZ	-7.92	1.28	1.38
2	B	827	ILE	N-CA	-7.92	1.30	1.46
4	E	153	HIS	C-O	-7.92	1.08	1.23
10	L	67	PHE	CE2-CZ	-7.92	1.22	1.37
1	A	498	ARG	CB-CG	-7.92	1.31	1.52
1	A	407	ARG	C-O	7.91	1.38	1.23
1	A	1187	GLN	CG-CD	7.91	1.69	1.51
1	A	1203	ASN	CG-ND2	7.91	1.52	1.32
2	B	870	ILE	CB-CG2	7.91	1.77	1.52
2	B	1092	TYR	CE1-CZ	-7.91	1.28	1.38
1	A	917	SER	CA-CB	-7.91	1.41	1.52
2	B	37	PHE	CE2-CZ	-7.91	1.22	1.37
2	B	322	PHE	CD1-CE1	-7.91	1.23	1.39
4	E	28	TYR	CD2-CE2	7.91	1.51	1.39
8	J	24	LEU	C-N	-7.91	1.15	1.34
4	E	49	SER	CA-C	7.91	1.73	1.52
1	A	886	ILE	CB-CG2	-7.90	1.28	1.52
3	C	190	ASP	C-O	-7.90	1.08	1.23
4	E	105	PHE	CB-CG	-7.90	1.38	1.51
1	A	373	THR	C-O	-7.90	1.08	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	19	GLU	N-CA	7.90	1.62	1.46
2	B	40	GLU	CB-CG	7.90	1.67	1.52
2	B	337	ARG	CD-NE	-7.89	1.33	1.46
2	B	605	ARG	NE-CZ	-7.89	1.22	1.33
1	A	45	GLN	CB-CG	7.89	1.73	1.52
1	A	248	PRO	CB-CG	7.89	1.89	1.50
7	I	118	ARG	CD-NE	7.89	1.59	1.46
9	K	71	PHE	CE1-CZ	-7.89	1.22	1.37
1	A	271	LYS	CG-CD	7.89	1.79	1.52
1	A	1299	VAL	C-O	7.89	1.38	1.23
2	B	65	GLU	CD-OE1	7.89	1.34	1.25
4	E	112	TYR	CZ-OH	7.89	1.51	1.37
9	K	70	ARG	CG-CD	7.89	1.71	1.51
2	B	178	ASN	CG-OD1	7.88	1.41	1.24
1	A	1362	TYR	CE2-CZ	7.88	1.48	1.38
1	A	836	TYR	CE2-CZ	7.88	1.48	1.38
1	A	1243	VAL	CB-CG2	7.88	1.69	1.52
4	E	16	PHE	CG-CD2	-7.88	1.26	1.38
3	C	38	ILE	CB-CG2	-7.88	1.28	1.52
3	C	219	PHE	CD2-CE2	-7.88	1.23	1.39
9	K	11	LEU	CG-CD1	7.87	1.80	1.51
2	B	624	LEU	CA-CB	-7.87	1.35	1.53
2	B	462	ALA	CA-CB	-7.87	1.35	1.52
8	J	7	CYS	CB-SG	-7.87	1.68	1.82
1	A	684	ALA	CA-CB	7.86	1.69	1.52
1	A	1407	GLU	CD-OE2	7.86	1.34	1.25
6	H	6	PHE	CB-CG	-7.86	1.38	1.51
2	B	812	LEU	C-O	-7.86	1.08	1.23
2	B	380	TYR	CG-CD2	-7.86	1.28	1.39
2	B	583	ASN	CG-OD1	-7.86	1.06	1.24
1	A	779	PHE	CA-CB	-7.85	1.36	1.53
1	A	572	TRP	CZ2-CH2	-7.85	1.22	1.37
2	B	358	LYS	CE-NZ	7.85	1.68	1.49
3	C	61	GLU	CD-OE1	-7.85	1.17	1.25
1	A	1256	GLU	CB-CG	7.85	1.67	1.52
2	B	1132	GLU	CD-OE2	7.85	1.34	1.25
1	A	123	ARG	CG-CD	7.85	1.71	1.51
4	E	200	ARG	CB-CG	-7.85	1.31	1.52
10	L	47	ARG	CD-NE	7.85	1.59	1.46
2	B	411	PRO	C-O	7.84	1.39	1.23
6	H	47	PHE	CD1-CE1	-7.84	1.23	1.39
1	A	305	ASP	CB-CG	7.84	1.68	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	819	ALA	CA-CB	-7.84	1.35	1.52
1	A	1406	VAL	CB-CG1	7.84	1.69	1.52
1	A	1438	THR	CA-CB	-7.84	1.32	1.53
1	A	800	VAL	CB-CG1	-7.84	1.36	1.52
2	B	1064	TYR	CD1-CE1	-7.84	1.27	1.39
3	C	28	ALA	CA-CB	-7.84	1.35	1.52
1	A	954	TRP	CD2-CE2	-7.84	1.31	1.41
2	B	401	PHE	CD1-CE1	-7.84	1.23	1.39
4	E	138	ALA	CA-CB	-7.84	1.35	1.52
7	I	2	THR	CA-CB	-7.84	1.32	1.53
2	B	810	GLU	CG-CD	7.83	1.63	1.51
1	A	1259	MET	SD-CE	7.83	2.21	1.77
9	K	68	PHE	CE1-CZ	-7.83	1.22	1.37
2	B	20	ASP	C-O	-7.82	1.08	1.23
2	B	961	LEU	CG-CD1	7.82	1.80	1.51
9	K	54	ARG	CD-NE	7.82	1.59	1.46
2	B	449	ASN	CB-CG	7.82	1.69	1.51
3	C	227	THR	CA-CB	7.82	1.73	1.53
1	A	513	SER	CB-OG	7.82	1.52	1.42
6	H	9	ILE	CA-CB	7.82	1.72	1.54
2	B	870	ILE	CG1-CD1	7.81	2.04	1.50
2	B	589	VAL	CA-CB	-7.81	1.38	1.54
9	K	105	PHE	CE1-CZ	7.81	1.52	1.37
2	B	203	PHE	CD2-CE2	-7.81	1.23	1.39
2	B	758	PHE	CE2-CZ	-7.81	1.22	1.37
2	B	1183	LYS	CG-CD	7.81	1.78	1.52
1	A	882	SER	C-O	-7.81	1.08	1.23
3	C	51	VAL	CB-CG1	-7.80	1.36	1.52
1	A	1211	GLN	CB-CG	7.80	1.73	1.52
1	A	1419	ASP	CG-OD2	7.80	1.43	1.25
3	C	137	LYS	CB-CG	7.80	1.73	1.52
1	A	474	VAL	CB-CG2	-7.80	1.36	1.52
3	C	162	GLY	C-O	7.80	1.36	1.23
2	B	466	TRP	C-O	7.80	1.38	1.23
1	A	1029	ARG	NE-CZ	-7.80	1.23	1.33
2	B	561	TRP	CZ3-CH2	7.80	1.52	1.40
2	B	1043	ASP	CG-OD2	7.80	1.43	1.25
2	B	65	GLU	CB-CG	7.80	1.67	1.52
2	B	563	MET	C-O	-7.79	1.08	1.23
2	B	824	ILE	C-O	-7.79	1.08	1.23
2	B	1224	PHE	CG-CD1	7.79	1.50	1.38
1	A	966	ASN	N-CA	-7.79	1.30	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	589	GLN	CD-NE2	7.78	1.52	1.32
1	A	589	GLN	CD-OE1	7.78	1.41	1.24
4	E	186	LEU	N-CA	-7.78	1.30	1.46
2	B	1106	ARG	CA-C	7.78	1.73	1.52
2	B	1128	LEU	N-CA	7.78	1.61	1.46
2	B	1145	SER	N-CA	-7.78	1.30	1.46
1	A	898	ARG	NE-CZ	7.78	1.43	1.33
2	B	641	GLU	C-O	-7.78	1.08	1.23
2	B	381	MET	CG-SD	7.78	2.01	1.81
2	B	662	MET	SD-CE	7.78	2.21	1.77
2	B	933	SER	CA-CB	7.78	1.64	1.52
1	A	416	ARG	CA-C	-7.77	1.32	1.52
6	H	116	TYR	CE1-CZ	7.77	1.48	1.38
1	A	1385	THR	C-O	7.77	1.38	1.23
2	B	223	VAL	C-O	-7.77	1.08	1.23
2	B	403	LYS	CB-CG	7.77	1.73	1.52
9	K	53	ASP	CB-CG	7.76	1.68	1.51
1	A	1326	ARG	CG-CD	7.76	1.71	1.51
2	B	551	PRO	N-CD	-7.76	1.36	1.47
2	B	770	GLN	CG-CD	-7.76	1.33	1.51
2	B	1006	ILE	CA-CB	-7.76	1.37	1.54
3	C	35	ARG	C-O	7.75	1.38	1.23
7	I	15	TYR	CG-CD1	-7.75	1.29	1.39
2	B	249	ARG	CB-CG	7.75	1.73	1.52
4	E	112	TYR	CE1-CZ	-7.75	1.28	1.38
1	A	210	ILE	CB-CG2	-7.75	1.28	1.52
1	A	579	SER	C-O	7.75	1.38	1.23
1	A	637	LYS	CE-NZ	7.75	1.68	1.49
3	C	185	LYS	CB-CG	7.75	1.73	1.52
1	A	1003	LYS	CG-CD	7.75	1.78	1.52
1	A	1441	PHE	CG-CD1	-7.75	1.27	1.38
4	E	147	HIS	CB-CG	7.74	1.64	1.50
2	B	679	TYR	CE1-CZ	-7.74	1.28	1.38
4	E	179	GLN	CB-CG	-7.74	1.31	1.52
3	C	18	VAL	C-O	-7.74	1.08	1.23
2	B	323	VAL	CB-CG2	7.74	1.69	1.52
2	B	613	VAL	CB-CG1	-7.73	1.36	1.52
2	B	1067	ARG	CZ-NH2	-7.73	1.23	1.33
1	A	1311	VAL	C-O	7.73	1.38	1.23
2	B	1064	TYR	CG-CD1	-7.73	1.29	1.39
4	E	29	PHE	CD1-CE1	-7.73	1.23	1.39
8	J	21	TYR	CE2-CZ	-7.73	1.28	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1300	LYS	CD-CE	7.73	1.70	1.51
7	I	106	CYS	CB-SG	7.73	1.95	1.82
2	B	649	LYS	C-O	7.72	1.38	1.23
1	A	462	VAL	CA-CB	-7.72	1.38	1.54
5	F	77	ASP	C-O	7.72	1.38	1.23
8	J	62	ARG	C-O	-7.72	1.08	1.23
1	A	885	THR	C-O	7.72	1.38	1.23
2	B	1100	ASP	CA-CB	7.72	1.71	1.53
3	C	154	LYS	CE-NZ	7.72	1.68	1.49
2	B	394	ASP	CG-OD2	7.72	1.43	1.25
1	A	969	GLN	CD-OE1	7.71	1.41	1.24
2	B	1097	HIS	CA-C	7.71	1.73	1.52
1	A	28	ARG	C-O	7.71	1.38	1.23
3	C	54	ASN	CB-CG	-7.71	1.33	1.51
1	A	830	LYS	CE-NZ	7.71	1.68	1.49
2	B	248	SER	CA-CB	7.71	1.64	1.52
3	C	56	THR	CB-CG2	-7.71	1.26	1.52
9	K	81	TYR	CG-CD2	-7.71	1.29	1.39
1	A	1187	GLN	C-O	7.71	1.38	1.23
1	A	596	THR	CB-CG2	7.70	1.77	1.52
1	A	303	TYR	CG-CD2	-7.70	1.29	1.39
1	A	507	VAL	CB-CG1	-7.70	1.36	1.52
2	B	249	ARG	NE-CZ	7.70	1.43	1.33
2	B	586	TRP	CE3-CZ3	-7.70	1.25	1.38
3	C	215	GLU	CD-OE1	7.70	1.34	1.25
1	A	1362	TYR	CE1-CZ	-7.70	1.28	1.38
2	B	332	ASP	C-O	-7.70	1.08	1.23
1	A	664	THR	CA-C	-7.70	1.32	1.52
1	A	946	VAL	CA-CB	-7.69	1.38	1.54
2	B	192	LEU	CG-CD2	7.69	1.80	1.51
1	A	1167	GLU	CA-CB	7.69	1.70	1.53
7	I	58	VAL	CB-CG2	7.69	1.69	1.52
1	A	787	PHE	CE1-CZ	-7.69	1.22	1.37
2	B	1098	MET	CG-SD	7.69	2.01	1.81
6	H	32	THR	C-O	7.68	1.38	1.23
4	E	162	ARG	CD-NE	7.68	1.59	1.46
7	I	30	ARG	CZ-NH1	7.68	1.43	1.33
1	A	1448	GLU	N-CA	7.68	1.61	1.46
1	A	556	TRP	CZ3-CH2	-7.68	1.27	1.40
7	I	3	THR	CB-CG2	7.68	1.77	1.52
10	L	50	ASP	CA-CB	7.68	1.70	1.53
2	B	103	ASN	C-O	7.67	1.38	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	690	VAL	C-O	-7.67	1.08	1.23
3	C	205	LYS	CG-CD	7.67	1.78	1.52
1	A	1188	GLN	C-O	7.67	1.38	1.23
2	B	41	LYS	C-O	7.67	1.38	1.23
2	B	202	TYR	CE2-CZ	-7.67	1.28	1.38
2	B	570	VAL	CB-CG1	-7.67	1.36	1.52
2	B	745	PRO	N-CD	-7.67	1.37	1.47
2	B	880	THR	CB-CG2	7.67	1.77	1.52
2	B	737	THR	CB-CG2	-7.67	1.27	1.52
5	F	84	TYR	CG-CD2	-7.67	1.29	1.39
2	B	1135	ARG	CG-CD	-7.66	1.32	1.51
2	B	1176	ASN	CG-OD1	7.66	1.40	1.24
9	K	39	ASP	CA-C	-7.66	1.33	1.52
1	A	247	ARG	CA-C	7.66	1.72	1.52
1	A	650	GLN	CD-OE1	-7.66	1.07	1.24
3	C	37	MET	CG-SD	-7.66	1.61	1.81
2	B	375	ALA	CA-CB	-7.66	1.36	1.52
2	B	587	HIS	N-CA	-7.66	1.31	1.46
1	A	561	PRO	CA-CB	7.66	1.68	1.53
2	B	859	TYR	CG-CD1	-7.66	1.29	1.39
4	E	60	PHE	CG-CD1	7.66	1.50	1.38
1	A	469	ARG	C-O	-7.65	1.08	1.23
1	A	614	PHE	CG-CD1	-7.65	1.27	1.38
3	C	175	ALA	N-CA	-7.65	1.31	1.46
3	C	268	ASP	CA-C	7.65	1.72	1.52
9	K	8	GLU	CD-OE2	7.65	1.34	1.25
9	K	59	ALA	CA-CB	-7.65	1.36	1.52
2	B	870	ILE	C-O	7.65	1.37	1.23
2	B	1005	GLY	C-O	7.65	1.35	1.23
2	B	679	TYR	CE2-CZ	-7.65	1.28	1.38
10	L	69	ALA	CA-CB	-7.64	1.36	1.52
1	A	457	ALA	N-CA	-7.64	1.31	1.46
7	I	56	ALA	CA-CB	-7.64	1.36	1.52
1	A	805	LEU	CA-CB	-7.64	1.36	1.53
6	H	88	SER	CA-CB	7.64	1.64	1.52
2	B	646	LEU	CB-CG	7.63	1.74	1.52
3	C	9	LYS	CG-CD	7.63	1.78	1.52
1	A	514	PRO	CG-CD	-7.63	1.25	1.50
2	B	315	LYS	CB-CG	-7.63	1.31	1.52
4	E	168	TYR	CD1-CE1	7.63	1.50	1.39
1	A	942	PHE	C-N	-7.63	1.16	1.34
1	A	1288	ASP	CG-OD1	7.63	1.42	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	643	ASP	CB-CG	7.63	1.67	1.51
5	F	76	LYS	CG-CD	7.63	1.78	1.52
7	I	19	ASP	CG-OD2	7.63	1.42	1.25
8	J	2	ILE	N-CA	-7.62	1.31	1.46
2	B	348	ARG	CB-CG	-7.62	1.31	1.52
1	A	698	GLN	CG-CD	7.62	1.68	1.51
2	B	362	PRO	CB-CG	-7.62	1.11	1.50
2	B	1214	PRO	C-O	7.62	1.38	1.23
4	E	180	ARG	CG-CD	7.62	1.71	1.51
1	A	188	ASP	CA-CB	7.62	1.70	1.53
7	I	119	THR	N-CA	7.61	1.61	1.46
3	C	200	GLU	C-O	7.61	1.37	1.23
6	H	87	ARG	CD-NE	7.61	1.59	1.46
6	H	30	SER	C-O	7.61	1.37	1.23
7	I	28	GLU	CG-CD	7.61	1.63	1.51
2	B	1138	MET	CG-SD	-7.61	1.61	1.81
1	A	1092	LYS	C-O	7.61	1.37	1.23
7	I	120	GLN	CG-CD	7.60	1.68	1.51
1	A	708	MET	CA-CB	-7.60	1.37	1.53
1	A	819	GLY	CA-C	-7.60	1.39	1.51
1	A	902	LEU	N-CA	-7.60	1.31	1.46
6	H	47	PHE	CG-CD2	-7.60	1.27	1.38
2	B	656	GLY	C-O	7.60	1.35	1.23
4	E	11	ARG	NE-CZ	-7.60	1.23	1.33
7	I	113	ASP	C-O	-7.60	1.08	1.23
10	L	33	GLU	C-O	7.60	1.37	1.23
1	A	724	GLU	N-CA	-7.60	1.31	1.46
2	B	697	GLU	CD-OE1	7.60	1.34	1.25
2	B	1189	ILE	CG1-CD1	7.60	2.02	1.50
1	A	949	ASP	CB-CG	-7.59	1.35	1.51
1	A	44	THR	N-CA	7.59	1.61	1.46
7	I	112	SER	CA-CB	-7.59	1.41	1.52
1	A	532	ARG	CZ-NH1	7.59	1.43	1.33
1	A	681	GLU	CB-CG	7.59	1.66	1.52
2	B	1017	ILE	CG1-CD1	-7.58	0.98	1.50
1	A	948	VAL	CA-CB	-7.58	1.38	1.54
1	A	192	GLY	CA-C	7.58	1.64	1.51
2	B	286	PHE	CE1-CZ	-7.58	1.23	1.37
1	A	815	PHE	CE2-CZ	-7.58	1.23	1.37
2	B	456	GLY	N-CA	7.58	1.57	1.46
2	B	997	GLU	CD-OE1	7.58	1.33	1.25
7	I	28	GLU	C-O	-7.58	1.08	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1354	ASN	CB-CG	7.57	1.68	1.51
2	B	135	ARG	NE-CZ	7.57	1.42	1.33
3	C	116	LYS	CE-NZ	7.57	1.68	1.49
1	A	1163	ILE	CB-CG2	-7.57	1.29	1.52
2	B	1072	MET	C-O	7.57	1.37	1.23
3	C	36	VAL	CB-CG2	-7.57	1.36	1.52
3	C	75	MET	CG-SD	-7.57	1.61	1.81
3	C	71	PRO	N-CD	-7.57	1.37	1.47
4	E	142	VAL	C-O	7.57	1.37	1.23
1	A	466	SER	N-CA	7.57	1.61	1.46
2	B	1064	TYR	CD2-CE2	-7.57	1.28	1.39
1	A	773	LYS	C-O	-7.56	1.08	1.23
2	B	803	LEU	CA-CB	-7.56	1.36	1.53
1	A	695	LYS	CE-NZ	7.56	1.68	1.49
1	A	1147	THR	CB-CG2	-7.56	1.27	1.52
2	B	325	GLN	CB-CG	-7.56	1.32	1.52
1	A	1093	LYS	CD-CE	7.56	1.70	1.51
2	B	814	PHE	CE2-CZ	-7.56	1.23	1.37
2	B	291	ILE	CB-CG2	-7.56	1.29	1.52
2	B	1130	PHE	CG-CD2	-7.55	1.27	1.38
2	B	954	VAL	CB-CG1	-7.55	1.36	1.52
1	A	1167	GLU	CG-CD	7.55	1.63	1.51
7	I	28	GLU	N-CA	-7.55	1.31	1.46
8	J	64	ASN	CB-CG	7.55	1.68	1.51
1	A	1344	GLY	C-O	-7.54	1.11	1.23
2	B	246	LYS	CA-CB	7.54	1.70	1.53
2	B	1172	ILE	CB-CG2	7.54	1.76	1.52
7	I	66	PRO	CA-CB	-7.54	1.38	1.53
1	A	1320	PRO	CA-CB	-7.54	1.38	1.53
1	A	667	GLY	CA-C	7.54	1.64	1.51
1	A	719	VAL	CB-CG1	-7.54	1.37	1.52
1	A	817	ALA	CA-CB	-7.54	1.36	1.52
1	A	36	ARG	CG-CD	7.53	1.70	1.51
1	A	724	GLU	CD-OE2	7.53	1.33	1.25
2	B	905	VAL	C-O	-7.53	1.09	1.23
10	L	28	LYS	CD-CE	7.53	1.70	1.51
2	B	316	PRO	C-O	7.53	1.38	1.23
1	A	350	ARG	C-O	-7.53	1.09	1.23
2	B	635	ARG	C-O	-7.53	1.09	1.23
2	B	884	ARG	CZ-NH1	7.53	1.42	1.33
4	E	93	MET	SD-CE	7.53	2.20	1.77
6	H	59	ILE	CA-CB	-7.53	1.37	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	130	VAL	CA-C	7.53	1.72	1.52
2	B	1186	ASP	CA-CB	7.53	1.70	1.53
8	J	1	MET	CA-CB	-7.53	1.37	1.53
2	B	344	LYS	CG-CD	7.52	1.78	1.52
1	A	1355	VAL	CB-CG2	-7.52	1.37	1.52
1	A	1130	GLN	CD-NE2	7.52	1.51	1.32
1	A	781	ASP	CA-CB	-7.52	1.37	1.53
1	A	1229	SER	C-O	7.51	1.37	1.23
2	B	261	ARG	CZ-NH1	7.51	1.42	1.33
7	I	101	PHE	CD2-CE2	7.51	1.54	1.39
1	A	170	THR	C-O	7.51	1.37	1.23
1	A	1199	ARG	CZ-NH1	7.51	1.42	1.33
1	A	94	GLY	C-O	7.51	1.35	1.23
2	B	728	ARG	NE-CZ	-7.51	1.23	1.33
4	E	1	MET	CB-CG	7.51	1.75	1.51
5	F	137	TYR	CE1-CZ	-7.50	1.28	1.38
1	A	974	ASP	CA-C	-7.50	1.33	1.52
2	B	283	VAL	CB-CG2	-7.50	1.37	1.52
4	E	139	ALA	CA-CB	7.50	1.68	1.52
2	B	166	PHE	CD1-CE1	-7.50	1.24	1.39
2	B	695	ALA	C-O	-7.50	1.09	1.23
3	C	124	LEU	C-O	7.50	1.37	1.23
8	J	13	VAL	N-CA	-7.50	1.31	1.46
3	C	104	PHE	CE2-CZ	7.50	1.51	1.37
3	C	16	ASP	C-O	-7.49	1.09	1.23
7	I	8	ARG	N-CA	7.49	1.61	1.46
1	A	22	PHE	CE1-CZ	7.49	1.51	1.37
1	A	718	VAL	CB-CG1	-7.49	1.37	1.52
1	A	1422	ARG	CZ-NH1	7.49	1.42	1.33
3	C	12	GLU	CA-CB	-7.49	1.37	1.53
4	E	128	PRO	CA-CB	7.49	1.68	1.53
2	B	798	TYR	CD1-CE1	7.49	1.50	1.39
8	J	8	PHE	N-CA	7.49	1.61	1.46
1	A	587	HIS	CA-CB	7.49	1.70	1.53
1	A	1008	GLN	CD-OE1	7.49	1.40	1.24
2	B	502	ILE	N-CA	7.49	1.61	1.46
2	B	1188	LYS	CE-NZ	7.49	1.67	1.49
2	B	1223	ASP	C-O	7.49	1.37	1.23
2	B	784	ASN	C-O	-7.48	1.09	1.23
1	A	792	TYR	CD1-CE1	-7.48	1.28	1.39
1	A	1234	GLU	CD-OE2	7.48	1.33	1.25
2	B	1159	ARG	CB-CG	7.48	1.72	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	441	PRO	CG-CD	-7.48	1.25	1.50
1	A	640	GLN	CD-NE2	7.48	1.51	1.32
1	A	1074	GLU	CG-CD	7.47	1.63	1.51
1	A	1269	GLU	N-CA	7.47	1.61	1.46
1	A	80	HIS	C-O	7.47	1.37	1.23
1	A	875	ALA	CA-CB	-7.47	1.36	1.52
2	B	446	LEU	C-O	7.47	1.37	1.23
1	A	794	PRO	N-CD	-7.47	1.37	1.47
6	H	56	THR	CA-CB	7.47	1.72	1.53
4	E	21	GLU	CD-OE2	7.46	1.33	1.25
1	A	1138	ILE	C-O	7.46	1.37	1.23
5	F	90	ARG	CZ-NH2	-7.46	1.23	1.33
2	B	302	CYS	CB-SG	-7.46	1.69	1.82
1	A	774	ARG	NE-CZ	7.46	1.42	1.33
1	A	946	VAL	CB-CG1	-7.46	1.37	1.52
4	E	136	ASN	CG-ND2	7.46	1.51	1.32
1	A	223	GLY	C-O	7.45	1.35	1.23
1	A	289	ILE	CB-CG2	-7.45	1.29	1.52
1	A	1289	ARG	C-O	-7.45	1.09	1.23
3	C	156	THR	CB-CG2	7.45	1.76	1.52
1	A	920	LEU	CA-CB	-7.45	1.36	1.53
3	C	249	ASP	CG-OD2	7.45	1.42	1.25
2	B	759	PRO	CA-C	-7.45	1.38	1.52
3	C	144	ILE	CB-CG2	-7.45	1.29	1.52
1	A	537	ARG	CZ-NH2	7.45	1.42	1.33
2	B	1046	PRO	CB-CG	-7.45	1.12	1.50
1	A	1218	GLN	CB-CG	7.45	1.72	1.52
2	B	1014	PRO	CA-C	-7.45	1.38	1.52
1	A	28	ARG	CZ-NH1	7.44	1.42	1.33
1	A	132	LYS	CG-CD	7.44	1.77	1.52
1	A	731	ARG	CZ-NH1	7.44	1.42	1.33
7	I	93	LYS	CA-CB	7.44	1.70	1.53
1	A	895	LYS	CG-CD	7.44	1.77	1.52
1	A	1448	GLU	CA-C	7.44	1.72	1.52
2	B	580	VAL	CA-CB	-7.44	1.39	1.54
4	E	155	ARG	CZ-NH1	7.44	1.42	1.33
9	K	114	LEU	CA-CB	7.44	1.70	1.53
2	B	859	TYR	CA-CB	-7.43	1.37	1.53
1	A	101	LYS	CB-CG	7.43	1.72	1.52
1	A	1080	THR	N-CA	7.43	1.61	1.46
2	B	38	PHE	CD2-CE2	-7.43	1.24	1.39
2	B	172	ILE	CA-CB	-7.43	1.37	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	LYS	CD-CE	7.43	1.69	1.51
2	B	248	SER	N-CA	7.43	1.61	1.46
6	H	90	ALA	CA-CB	-7.43	1.36	1.52
4	E	44	ALA	C-O	7.43	1.37	1.23
10	L	70	ARG	CZ-NH1	7.43	1.42	1.33
3	C	116	LYS	C-O	7.43	1.37	1.23
3	C	228	PHE	CG-CD2	-7.43	1.27	1.38
4	E	189	GLY	N-CA	-7.42	1.34	1.46
9	K	45	LEU	C-O	7.42	1.37	1.23
1	A	43	GLU	CD-OE2	7.42	1.33	1.25
2	B	814	PHE	CD1-CE1	-7.42	1.24	1.39
7	I	4	PHE	CB-CG	-7.42	1.38	1.51
1	A	446	ARG	NE-CZ	-7.42	1.23	1.33
1	A	1118	VAL	C-O	-7.42	1.09	1.23
2	B	286	PHE	CG-CD2	-7.42	1.27	1.38
2	B	465	ASN	C-O	7.42	1.37	1.23
6	H	78	SER	CA-C	-7.42	1.33	1.52
1	A	1410	PHE	CG-CD2	-7.41	1.27	1.38
3	C	209	TYR	CG-CD2	7.41	1.48	1.39
2	B	564	GLU	CD-OE2	7.41	1.33	1.25
1	A	508	PRO	N-CD	-7.41	1.37	1.47
2	B	1057	LYS	CG-CD	7.41	1.77	1.52
1	A	1222	ASN	CG-ND2	7.41	1.51	1.32
1	A	640	GLN	CD-OE1	7.41	1.40	1.24
1	A	1053	PHE	CG-CD2	-7.40	1.27	1.38
1	A	714	PHE	CD1-CE1	-7.40	1.24	1.39
1	A	954	TRP	CB-CG	-7.40	1.36	1.50
2	B	323	VAL	CA-CB	-7.40	1.39	1.54
2	B	546	SER	CA-C	-7.40	1.33	1.52
2	B	1096	ARG	C-O	-7.40	1.09	1.23
4	E	23	VAL	CA-CB	-7.40	1.39	1.54
1	A	860	LEU	CG-CD1	7.40	1.79	1.51
6	H	136	LYS	CB-CG	7.39	1.72	1.52
2	B	191	LYS	CG-CD	7.39	1.77	1.52
1	A	15	LYS	C-O	-7.39	1.09	1.23
2	B	797	TYR	CD2-CE2	7.39	1.50	1.39
2	B	908	GLU	CD-OE1	7.39	1.33	1.25
2	B	448	ILE	CA-CB	7.39	1.71	1.54
3	C	11	ARG	C-O	7.39	1.37	1.23
2	B	855	PHE	CE2-CZ	-7.38	1.23	1.37
3	C	149	LYS	CD-CE	7.38	1.69	1.51
1	A	954	TRP	CZ3-CH2	-7.38	1.28	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1013	ASP	CG-OD2	7.38	1.42	1.25
10	L	46	VAL	CB-CG2	7.38	1.68	1.52
1	A	655	PHE	CD1-CE1	-7.38	1.24	1.39
6	H	104	PHE	C-O	7.38	1.37	1.23
1	A	414	ASP	CB-CG	-7.38	1.36	1.51
2	B	46	GLN	CG-CD	-7.38	1.34	1.51
3	C	70	ILE	C-N	-7.38	1.20	1.34
3	C	148	ARG	CB-CG	-7.38	1.32	1.52
1	A	491	VAL	CA-CB	-7.37	1.39	1.54
1	A	1068	ALA	CA-CB	-7.37	1.36	1.52
8	J	63	TYR	CD1-CE1	-7.37	1.28	1.39
1	A	191	THR	CB-CG2	7.37	1.76	1.52
1	A	1171	GLN	CB-CG	7.37	1.72	1.52
1	A	606	LEU	N-CA	-7.37	1.31	1.46
2	B	724	ASP	C-N	-7.37	1.20	1.34
1	A	95	PHE	CD1-CE1	7.36	1.53	1.39
1	A	508	PRO	C-O	7.36	1.38	1.23
1	A	1002	GLY	C-O	7.36	1.35	1.23
2	B	654	ARG	CG-CD	-7.36	1.33	1.51
2	B	634	TYR	CE2-CZ	-7.36	1.28	1.38
1	A	482	PHE	C-N	-7.36	1.17	1.34
1	A	1157	ASP	CB-CG	7.36	1.67	1.51
1	A	900	ASP	CB-CG	-7.35	1.36	1.51
1	A	383	TYR	CE2-CZ	-7.35	1.28	1.38
1	A	479	ASN	CA-C	-7.35	1.33	1.52
1	A	1214	GLU	C-O	7.35	1.37	1.23
2	B	987	LYS	CA-CB	-7.35	1.37	1.53
1	A	904	THR	CB-OG1	7.35	1.57	1.43
2	B	634	TYR	CE1-CZ	-7.35	1.28	1.38
1	A	780	VAL	CB-CG1	-7.35	1.37	1.52
10	L	66	GLN	CG-CD	7.35	1.68	1.51
1	A	429	GLY	C-O	7.35	1.35	1.23
9	K	68	PHE	CB-CG	-7.35	1.38	1.51
1	A	1298	TYR	CD1-CE1	7.34	1.50	1.39
2	B	1019	SER	C-O	7.34	1.37	1.23
1	A	20	GLY	C-O	7.34	1.35	1.23
7	I	27	PHE	CG-CD2	-7.34	1.27	1.38
8	J	24	LEU	CA-C	-7.34	1.33	1.52
1	A	416	ARG	CG-CD	7.34	1.70	1.51
1	A	965	GLN	CD-NE2	7.34	1.51	1.32
3	C	178	PHE	CD2-CE2	-7.34	1.24	1.39
7	I	115	LYS	CE-NZ	7.34	1.67	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1198	TYR	CE1-CZ	7.34	1.48	1.38
3	C	193	TYR	CD2-CE2	7.33	1.50	1.39
1	A	767	GLN	CA-CB	-7.33	1.37	1.53
1	A	1162	VAL	CA-C	-7.33	1.33	1.52
2	B	63	ILE	CB-CG2	-7.33	1.30	1.52
4	E	17	ARG	NE-CZ	7.33	1.42	1.33
10	L	27	LEU	CB-CG	7.33	1.73	1.52
2	B	164	LYS	CG-CD	7.33	1.77	1.52
1	A	196	GLU	CG-CD	7.32	1.62	1.51
2	B	1024	ALA	CA-CB	-7.32	1.37	1.52
6	H	107	VAL	CA-CB	7.32	1.70	1.54
3	C	191	TYR	CD1-CE1	7.32	1.50	1.39
9	K	36	GLU	CG-CD	7.32	1.62	1.51
1	A	1256	GLU	CA-CB	7.32	1.70	1.53
2	B	57	TYR	CD2-CE2	7.31	1.50	1.39
1	A	1345	ARG	CZ-NH1	-7.31	1.23	1.33
2	B	863	GLU	CD-OE1	-7.31	1.17	1.25
1	A	769	SER	CB-OG	7.31	1.51	1.42
2	B	733	HIS	C-O	7.31	1.37	1.23
3	C	16	ASP	CG-OD2	7.31	1.42	1.25
3	C	28	ALA	C-O	7.31	1.37	1.23
1	A	1277	GLU	CB-CG	7.31	1.66	1.52
10	L	62	LYS	CB-CG	7.31	1.72	1.52
1	A	878	ILE	CA-CB	-7.30	1.38	1.54
2	B	345	LYS	C-O	-7.30	1.09	1.23
2	B	910	VAL	CB-CG2	-7.30	1.37	1.52
2	B	1020	ARG	CG-CD	-7.30	1.33	1.51
4	E	133	GLU	CG-CD	7.30	1.62	1.51
7	I	14	LEU	CG-CD1	-7.30	1.24	1.51
6	H	20	TYR	C-O	7.30	1.37	1.23
2	B	1086	PHE	CA-C	-7.30	1.33	1.52
1	A	462	VAL	CB-CG1	-7.30	1.37	1.52
1	A	129	LYS	CB-CG	7.30	1.72	1.52
5	F	84	TYR	CZ-OH	7.30	1.50	1.37
6	H	115	TYR	CD2-CE2	-7.30	1.28	1.39
2	B	734	HIS	C-O	7.29	1.37	1.23
9	K	81	TYR	CD2-CE2	-7.29	1.28	1.39
1	A	53	LEU	CG-CD1	7.29	1.78	1.51
2	B	1055	ILE	C-O	-7.29	1.09	1.23
3	C	55	THR	CB-CG2	-7.29	1.28	1.52
4	E	55	ARG	CZ-NH1	-7.29	1.23	1.33
8	J	49	MET	SD-CE	-7.29	1.37	1.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	916	THR	CA-C	7.29	1.71	1.52
1	A	960	ILE	CB-CG2	-7.29	1.30	1.52
2	B	1146	PHE	CE1-CZ	-7.29	1.23	1.37
3	C	242	GLN	CD-OE1	7.29	1.40	1.24
6	H	43	ASN	CG-ND2	7.29	1.51	1.32
6	H	109	LYS	CA-C	7.29	1.71	1.52
2	B	384	ARG	CD-NE	7.28	1.58	1.46
2	B	792	MET	CG-SD	7.28	2.00	1.81
1	A	387	ARG	CZ-NH2	-7.28	1.23	1.33
2	B	44	VAL	CB-CG1	-7.28	1.37	1.52
2	B	54	PHE	CD2-CE2	-7.28	1.24	1.39
1	A	721	PHE	CG-CD2	-7.28	1.27	1.38
2	B	104	GLU	CD-OE2	7.28	1.33	1.25
1	A	1162	VAL	CA-CB	-7.28	1.39	1.54
8	J	23	ASN	CG-ND2	7.27	1.51	1.32
1	A	1119	TYR	CD2-CE2	7.27	1.50	1.39
1	A	1196	GLU	CA-CB	-7.27	1.38	1.53
2	B	357	GLN	CA-C	-7.27	1.34	1.52
6	H	61	SER	C-O	7.27	1.37	1.23
2	B	89	GLU	CA-C	7.27	1.71	1.52
2	B	1150	ARG	C-N	-7.27	1.17	1.34
2	B	711	GLU	CA-C	7.27	1.71	1.52
3	C	87	PHE	CG-CD2	-7.27	1.27	1.38
6	H	26	ILE	CA-CB	-7.27	1.38	1.54
2	B	780	VAL	CB-CG2	-7.27	1.37	1.52
3	C	97	VAL	C-O	-7.27	1.09	1.23
2	B	406	LEU	CG-CD2	-7.27	1.25	1.51
1	A	469	ARG	CB-CG	7.26	1.72	1.52
1	A	1417	GLU	CA-CB	7.26	1.70	1.53
2	B	679	TYR	C-O	7.26	1.37	1.23
2	B	851	PHE	CE1-CZ	7.26	1.51	1.37
1	A	1268	LEU	CA-CB	-7.26	1.37	1.53
4	E	159	ASP	CG-OD1	7.26	1.42	1.25
7	I	100	PHE	CE2-CZ	-7.26	1.23	1.37
1	A	529	CYS	CA-C	-7.26	1.34	1.52
8	J	1	MET	CG-SD	-7.26	1.62	1.81
1	A	427	GLN	CD-NE2	7.26	1.50	1.32
1	A	868	TYR	CG-CD2	7.26	1.48	1.39
4	E	110	PHE	CA-C	-7.26	1.34	1.52
1	A	812	GLU	CG-CD	7.25	1.62	1.51
2	B	1154	ALA	CA-C	7.25	1.71	1.52
4	E	26	ARG	CZ-NH2	-7.25	1.23	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	844	ALA	N-CA	-7.25	1.31	1.46
2	B	246	LYS	CB-CG	7.25	1.72	1.52
2	B	423	LYS	CG-CD	7.25	1.77	1.52
3	C	237	SER	CA-CB	-7.25	1.42	1.52
10	L	33	GLU	CA-C	7.25	1.71	1.52
1	A	900	ASP	CA-C	-7.25	1.34	1.52
4	E	7	ARG	CZ-NH1	7.25	1.42	1.33
9	K	67	PHE	N-CA	-7.25	1.31	1.46
1	A	1365	TYR	CB-CG	-7.25	1.40	1.51
6	H	22	LYS	CE-NZ	7.25	1.67	1.49
7	I	110	PHE	CD1-CE1	7.25	1.53	1.39
1	A	1114	PRO	CA-C	-7.25	1.38	1.52
2	B	904	ARG	NE-CZ	-7.25	1.23	1.33
1	A	90	VAL	CB-CG1	-7.25	1.37	1.52
4	E	121	MET	CG-SD	7.25	2.00	1.81
1	A	1286	LYS	CE-NZ	7.24	1.67	1.49
8	J	18	TRP	CA-CB	-7.24	1.38	1.53
1	A	398	GLU	CD-OE1	7.24	1.33	1.25
1	A	864	ILE	CA-CB	-7.24	1.38	1.54
1	A	1146	VAL	CB-CG1	-7.24	1.37	1.52
1	A	1308	THR	CB-CG2	-7.24	1.28	1.52
2	B	992	ILE	CB-CG2	-7.24	1.30	1.52
4	E	25	ASP	C-O	7.24	1.37	1.23
9	K	35	PHE	CD2-CE2	-7.24	1.24	1.39
8	J	63	TYR	C-O	-7.24	1.09	1.23
8	J	4	PRO	CA-CB	-7.24	1.39	1.53
3	C	232	VAL	CA-CB	-7.23	1.39	1.54
2	B	242	SER	C-O	-7.23	1.09	1.23
2	B	308	TRP	CE2-CZ2	-7.23	1.27	1.39
9	K	113	THR	C-O	7.23	1.37	1.23
1	A	1355	VAL	CB-CG1	-7.23	1.37	1.52
1	A	36	ARG	CB-CG	7.23	1.72	1.52
2	B	660	LYS	N-CA	-7.23	1.31	1.46
2	B	805	THR	C-O	-7.23	1.09	1.23
2	B	638	PHE	CE1-CZ	-7.23	1.23	1.37
2	B	411	PRO	N-CD	-7.22	1.37	1.47
1	A	714	PHE	CD2-CE2	-7.22	1.24	1.39
2	B	57	TYR	CB-CG	7.22	1.62	1.51
9	K	46	ILE	CG1-CD1	-7.22	1.00	1.50
10	L	65	VAL	CA-C	-7.22	1.34	1.52
2	B	279	ASP	CG-OD2	7.21	1.42	1.25
1	A	540	PHE	CG-CD2	-7.21	1.27	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	496	ARG	CA-CB	-7.21	1.38	1.53
1	A	686	ALA	CA-C	-7.21	1.34	1.52
1	A	927	VAL	CA-CB	-7.21	1.39	1.54
1	A	1221	LYS	CD-CE	7.21	1.69	1.51
4	E	113	GLN	CA-CB	7.21	1.69	1.53
2	B	1190	ASP	C-O	-7.21	1.09	1.23
3	C	180	TYR	CD1-CE1	7.21	1.50	1.39
2	B	35	SER	CA-CB	-7.20	1.42	1.52
2	B	1091	TYR	CB-CG	-7.20	1.40	1.51
1	A	175	ARG	CB-CG	7.20	1.72	1.52
2	B	976	ILE	C-N	-7.20	1.20	1.33
1	A	1035	TYR	CE2-CZ	-7.20	1.29	1.38
1	A	601	LYS	CG-CD	7.20	1.76	1.52
1	A	685	GLU	CD-OE1	7.20	1.33	1.25
1	A	673	GLY	CA-C	-7.20	1.40	1.51
2	B	325	GLN	CG-CD	7.20	1.67	1.51
2	B	880	THR	CA-C	7.20	1.71	1.52
3	C	108	GLU	CD-OE2	7.19	1.33	1.25
2	B	448	ILE	N-CA	7.19	1.60	1.46
9	K	84	LYS	CE-NZ	7.19	1.67	1.49
10	L	40	LEU	CG-CD2	7.19	1.78	1.51
1	A	552	TRP	CD2-CE3	-7.19	1.29	1.40
8	J	62	ARG	CZ-NH1	7.19	1.42	1.33
9	K	91	CYS	CA-CB	-7.19	1.38	1.53
1	A	544	ASP	CG-OD1	7.19	1.41	1.25
1	A	835	GLY	C-O	7.19	1.35	1.23
1	A	1151	GLU	CG-CD	7.19	1.62	1.51
10	L	37	LYS	CD-CE	7.19	1.69	1.51
1	A	969	GLN	CD-NE2	7.19	1.50	1.32
2	B	523	CYS	CA-C	-7.19	1.34	1.52
5	F	76	LYS	CE-NZ	7.18	1.67	1.49
2	B	604	ARG	CD-NE	-7.18	1.34	1.46
7	I	73	ARG	CZ-NH2	7.18	1.42	1.33
1	A	795	GLU	C-O	-7.18	1.09	1.23
2	B	227	LYS	CE-NZ	7.18	1.67	1.49
2	B	308	TRP	N-CA	-7.18	1.31	1.46
1	A	633	VAL	CB-CG1	-7.18	1.37	1.52
1	A	62	ASP	N-CA	7.18	1.60	1.46
1	A	396	PRO	N-CD	-7.17	1.37	1.47
2	B	886	LYS	CE-NZ	7.17	1.67	1.49
2	B	755	ILE	C-O	7.17	1.36	1.23
2	B	320	ASP	CG-OD1	7.17	1.41	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	147	HIS	CD2-NE2	-7.17	1.22	1.38
1	A	899	VAL	CB-CG2	-7.17	1.37	1.52
1	A	827	THR	CB-CG2	7.16	1.75	1.52
1	A	990	VAL	CA-CB	-7.16	1.39	1.54
2	B	486	TYR	CG-CD2	7.16	1.48	1.39
5	F	83	PRO	N-CA	-7.16	1.35	1.47
1	A	175	ARG	C-O	7.15	1.36	1.23
1	A	1165	GLU	CD-OE1	7.15	1.33	1.25
2	B	466	TRP	CA-C	7.15	1.71	1.52
10	L	69	ALA	CA-C	-7.15	1.34	1.52
1	A	427	GLN	CD-OE1	7.15	1.39	1.24
2	B	350	GLN	N-CA	-7.15	1.32	1.46
2	B	485	ARG	CG-CD	-7.15	1.34	1.51
2	B	1106	ARG	CB-CG	7.15	1.71	1.52
1	A	1378	GLN	C-N	-7.15	1.20	1.33
7	I	113	ASP	CA-C	-7.15	1.34	1.52
1	A	404	TYR	CA-CB	-7.14	1.38	1.53
1	A	174	ILE	N-CA	-7.14	1.32	1.46
1	A	1038	THR	CA-C	-7.14	1.34	1.52
1	A	1255	GLU	CD-OE1	7.14	1.33	1.25
3	C	132	PRO	N-CD	-7.14	1.37	1.47
3	C	240	VAL	CA-C	-7.14	1.34	1.52
1	A	921	GLY	CA-C	7.14	1.63	1.51
2	B	797	TYR	CE2-CZ	-7.14	1.29	1.38
3	C	234	SER	CA-CB	-7.14	1.42	1.52
1	A	519	PRO	CA-C	-7.13	1.38	1.52
1	A	1414	ALA	N-CA	-7.13	1.32	1.46
7	I	95	THR	C-O	-7.13	1.09	1.23
6	H	87	ARG	CB-CG	7.13	1.71	1.52
8	J	3	VAL	C-N	-7.13	1.20	1.34
10	L	63	ARG	CD-NE	7.13	1.58	1.46
1	A	455	MET	C-O	-7.13	1.09	1.23
2	B	368	GLU	CB-CG	7.13	1.65	1.52
1	A	521	MET	CG-SD	-7.13	1.62	1.81
4	E	103	LYS	CE-NZ	7.13	1.66	1.49
1	A	478	TYR	CG-CD1	-7.13	1.29	1.39
1	A	572	TRP	CD2-CE2	-7.13	1.32	1.41
1	A	688	LYS	CE-NZ	7.13	1.66	1.49
1	A	1362	TYR	CD2-CE2	-7.13	1.28	1.39
2	B	557	PHE	CB-CG	-7.13	1.39	1.51
2	B	989	THR	CB-CG2	-7.12	1.28	1.52
2	B	198	ASP	CB-CG	-7.12	1.36	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	811	TYR	CB-CG	-7.12	1.41	1.51
2	B	1030	LEU	CA-C	-7.12	1.34	1.52
6	H	35	GLN	C-O	7.12	1.36	1.23
1	A	290	GLU	CB-CG	-7.12	1.38	1.52
1	A	489	LEU	C-O	-7.12	1.09	1.23
3	C	244	VAL	CB-CG2	-7.12	1.37	1.52
9	K	5	ASP	CG-OD2	7.12	1.41	1.25
1	A	475	THR	C-O	-7.11	1.09	1.23
2	B	257	LYS	CE-NZ	7.11	1.66	1.49
8	J	48	ARG	CZ-NH1	-7.11	1.23	1.33
10	L	27	LEU	CA-CB	7.11	1.70	1.53
5	F	97	ARG	CB-CG	-7.11	1.33	1.52
1	A	57	ARG	C-O	-7.11	1.09	1.23
10	L	50	ASP	C-O	7.11	1.36	1.23
1	A	37	PHE	CE2-CZ	7.11	1.50	1.37
2	B	41	LYS	CE-NZ	7.11	1.66	1.49
1	A	449	SER	CB-OG	7.11	1.51	1.42
2	B	136	THR	C-O	7.11	1.36	1.23
2	B	567	GLU	CG-CD	7.11	1.62	1.51
2	B	1130	PHE	N-CA	-7.11	1.32	1.46
9	K	64	GLU	C-O	-7.11	1.09	1.23
1	A	589	GLN	CG-CD	7.11	1.67	1.51
1	A	901	LEU	CG-CD2	-7.11	1.25	1.51
1	A	1107	VAL	N-CA	-7.11	1.32	1.46
1	A	1261	LYS	CE-NZ	7.11	1.66	1.49
1	A	380	VAL	CB-CG2	-7.10	1.38	1.52
3	C	203	GLN	CD-NE2	7.10	1.50	1.32
4	E	8	ASN	CG-OD1	7.10	1.39	1.24
6	H	35	GLN	CG-CD	7.10	1.67	1.51
2	B	116	GLU	CA-C	-7.10	1.34	1.52
2	B	728	ARG	CG-CD	7.10	1.69	1.51
6	H	117	SER	CB-OG	7.10	1.51	1.42
1	A	290	GLU	CD-OE2	7.09	1.33	1.25
1	A	923	LEU	C-O	7.09	1.36	1.23
1	A	934	LYS	CG-CD	7.09	1.76	1.52
2	B	839	MET	CG-SD	7.09	1.99	1.81
2	B	959	ASP	CG-OD2	7.09	1.41	1.25
9	K	42	LEU	CA-C	-7.09	1.34	1.52
1	A	511	ILE	CB-CG2	-7.09	1.30	1.52
2	B	124	TYR	CG-CD2	-7.09	1.29	1.39
2	B	1057	LYS	C-O	7.09	1.36	1.23
7	I	11	ASN	CG-OD1	-7.09	1.08	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	79	TRP	CZ3-CH2	-7.09	1.28	1.40
1	A	956	LEU	C-O	-7.09	1.09	1.23
1	A	1218	GLN	CA-C	-7.09	1.34	1.52
2	B	515	HIS	CG-CD2	-7.09	1.23	1.35
3	C	174	ALA	C-O	-7.09	1.09	1.23
6	H	141	TYR	CA-CB	-7.09	1.38	1.53
2	B	650	GLU	CG-CD	7.08	1.62	1.51
4	E	76	GLY	C-O	-7.08	1.12	1.23
1	A	133	LYS	CD-CE	7.08	1.69	1.51
2	B	581	PHE	CB-CG	-7.08	1.39	1.51
1	A	521	MET	SD-CE	-7.08	1.38	1.77
2	B	60	GLN	CG-CD	-7.08	1.34	1.51
2	B	205	ILE	N-CA	-7.08	1.32	1.46
1	A	1023	ARG	C-O	-7.08	1.09	1.23
1	A	1242	VAL	CB-CG2	-7.08	1.38	1.52
3	C	100	THR	CA-CB	-7.08	1.34	1.53
4	E	85	GLU	CA-CB	7.08	1.69	1.53
1	A	1237	ILE	CA-CB	-7.07	1.38	1.54
2	B	879	ARG	CG-CD	7.07	1.69	1.51
4	E	19	VAL	CB-CG1	-7.07	1.38	1.52
6	H	138	GLU	CG-CD	7.07	1.62	1.51
2	B	241	ARG	C-O	-7.07	1.09	1.23
2	B	358	LYS	CD-CE	7.07	1.69	1.51
4	E	179	GLN	CD-NE2	7.07	1.50	1.32
2	B	1095	LEU	CA-CB	-7.07	1.37	1.53
4	E	74	ASP	CA-C	7.07	1.71	1.52
1	A	81	PHE	CE1-CZ	-7.07	1.24	1.37
1	A	836	TYR	CG-CD2	7.07	1.48	1.39
1	A	1225	PHE	CE2-CZ	7.07	1.50	1.37
4	E	32	GLN	CG-CD	7.07	1.67	1.51
1	A	465	TYR	CD2-CE2	-7.06	1.28	1.39
1	A	655	PHE	CE2-CZ	-7.06	1.24	1.37
2	B	418	LYS	CG-CD	7.06	1.76	1.52
2	B	855	PHE	CD2-CE2	7.06	1.53	1.39
2	B	995	ARG	NE-CZ	-7.06	1.23	1.33
1	A	1311	VAL	CB-CG2	-7.06	1.38	1.52
1	A	1291	VAL	C-O	-7.06	1.09	1.23
2	B	969	ARG	NE-CZ	-7.06	1.23	1.33
2	B	1023	VAL	N-CA	-7.06	1.32	1.46
3	C	192	TRP	CB-CG	7.06	1.62	1.50
7	I	16	PRO	CG-CD	7.06	1.74	1.50
1	A	693	VAL	CB-CG2	-7.06	1.38	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1365	TYR	CD2-CE2	7.06	1.50	1.39
2	B	1102	LYS	N-CA	7.06	1.60	1.46
3	C	122	SER	CB-OG	7.06	1.51	1.42
9	K	67	PHE	CG-CD1	-7.06	1.28	1.38
2	B	1186	ASP	N-CA	7.06	1.60	1.46
1	A	22	PHE	CD1-CE1	-7.05	1.25	1.39
2	B	347	LYS	CB-CG	7.05	1.71	1.52
2	B	801	LYS	CG-CD	7.05	1.76	1.52
1	A	673	GLY	C-N	-7.05	1.20	1.34
2	B	288	ALA	C-O	7.05	1.36	1.23
6	H	44	VAL	C-O	7.05	1.36	1.23
1	A	1168	GLU	CG-CD	7.05	1.62	1.51
2	B	315	LYS	CA-CB	-7.05	1.38	1.53
3	C	212	PRO	C-O	-7.05	1.09	1.23
3	C	98	VAL	CB-CG1	-7.05	1.38	1.52
3	C	82	TYR	CG-CD1	-7.04	1.29	1.39
1	A	1433	MET	SD-CE	-7.04	1.38	1.77
2	B	1193	GLN	C-N	-7.04	1.17	1.34
1	A	26	GLU	CG-CD	7.04	1.62	1.51
1	A	714	PHE	CG-CD1	-7.04	1.28	1.38
1	A	808	LEU	N-CA	-7.04	1.32	1.46
2	B	681	TRP	CA-C	-7.04	1.34	1.52
1	A	822	GLU	CD-OE2	7.04	1.33	1.25
1	A	961	ARG	CG-CD	7.03	1.69	1.51
1	A	1191	TRP	CB-CG	-7.03	1.37	1.50
2	B	1127	GLY	CA-C	7.03	1.63	1.51
2	B	1198	TYR	CB-CG	-7.03	1.41	1.51
3	C	196	ASP	CG-OD2	7.03	1.41	1.25
1	A	641	VAL	CB-CG2	7.03	1.67	1.52
2	B	988	GLY	C-O	-7.03	1.12	1.23
2	B	991	GLY	C-O	-7.03	1.12	1.23
9	K	35	PHE	CB-CG	-7.03	1.39	1.51
1	A	139	TRP	CZ3-CH2	-7.03	1.28	1.40
2	B	63	ILE	CA-C	7.03	1.71	1.52
9	K	61	TYR	C-O	-7.03	1.09	1.23
2	B	886	LYS	CD-CE	7.03	1.68	1.51
1	A	1360	GLY	CA-C	7.03	1.63	1.51
2	B	797	TYR	CG-CD2	-7.03	1.30	1.39
1	A	1039	LYS	CE-NZ	7.02	1.66	1.49
1	A	1103	GLU	C-O	7.02	1.36	1.23
4	E	11	ARG	CZ-NH2	7.02	1.42	1.33
1	A	1208	THR	N-CA	-7.02	1.32	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1410	PHE	CE2-CZ	-7.02	1.24	1.37
4	E	24	LYS	CE-NZ	7.02	1.66	1.49
1	A	1294	PRO	CG-CD	-7.02	1.27	1.50
7	I	62	ILE	C-N	-7.02	1.20	1.33
9	K	67	PHE	CE1-CZ	-7.02	1.24	1.37
1	A	510	GLN	CA-CB	-7.01	1.38	1.53
1	A	747	VAL	C-O	-7.01	1.10	1.23
2	B	18	PHE	C-O	7.01	1.36	1.23
8	J	44	TYR	CZ-OH	7.01	1.49	1.37
1	A	779	PHE	CG-CD1	-7.01	1.28	1.38
4	E	122	LYS	CE-NZ	7.01	1.66	1.49
6	H	10	PHE	CD2-CE2	7.01	1.53	1.39
1	A	36	ARG	C-O	-7.01	1.10	1.23
2	B	325	GLN	CD-OE1	7.01	1.39	1.24
2	B	1023	VAL	CB-CG1	-7.01	1.38	1.52
4	E	191	LYS	CB-CG	7.01	1.71	1.52
1	A	604	GLY	CA-C	-7.01	1.40	1.51
1	A	1127	ASP	CG-OD2	7.01	1.41	1.25
8	J	50	ILE	C-O	7.01	1.36	1.23
1	A	151	ASP	CB-CG	7.00	1.66	1.51
2	B	351	TYR	CG-CD2	-7.00	1.30	1.39
1	A	1075	PRO	C-O	-7.00	1.09	1.23
2	B	203	PHE	CG-CD1	-7.00	1.28	1.38
9	K	10	PHE	CD2-CE2	-7.00	1.25	1.39
5	F	77	ASP	CB-CG	7.00	1.66	1.51
1	A	656	TRP	CD2-CE2	-7.00	1.32	1.41
3	C	62	PHE	CE1-CZ	7.00	1.50	1.37
6	H	142	LEU	CA-CB	-7.00	1.37	1.53
3	C	252	GLN	CD-OE1	7.00	1.39	1.24
10	L	70	ARG	C-OXT	-6.99	1.10	1.23
2	B	1204	PHE	CD1-CE1	6.99	1.53	1.39
5	F	137	TYR	CA-CB	-6.99	1.38	1.53
1	A	1092	LYS	CG-CD	6.99	1.76	1.52
2	B	797	TYR	CD1-CE1	6.99	1.49	1.39
4	E	72	PHE	CD1-CE1	-6.99	1.25	1.39
2	B	742	GLU	CG-CD	-6.99	1.41	1.51
2	B	813	LYS	C-N	-6.99	1.18	1.34
1	A	376	TYR	CG-CD2	-6.98	1.30	1.39
1	A	461	LYS	C-O	6.98	1.36	1.23
2	B	37	PHE	C-O	6.98	1.36	1.23
2	B	499	ASN	CG-ND2	6.98	1.50	1.32
3	C	235	VAL	CB-CG1	-6.98	1.38	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1167	GLU	CB-CG	6.98	1.65	1.52
1	A	1223	ASP	CG-OD2	6.98	1.41	1.25
2	B	1008	PRO	CA-CB	-6.98	1.39	1.53
1	A	655	PHE	CD2-CE2	-6.98	1.25	1.39
3	C	136	ASP	CG-OD1	-6.98	1.09	1.25
1	A	912	LEU	C-N	-6.98	1.18	1.34
2	B	173	MET	CB-CG	6.98	1.73	1.51
7	I	63	GLY	N-CA	-6.98	1.35	1.46
1	A	171	GLN	CD-NE2	6.97	1.50	1.32
2	B	1191	ILE	CB-CG2	-6.97	1.31	1.52
3	C	26	ASP	CB-CG	6.97	1.66	1.51
2	B	49	ASP	C-O	-6.97	1.10	1.23
2	B	586	TRP	CD2-CE2	-6.97	1.32	1.41
4	E	8	ASN	CB-CG	6.97	1.67	1.51
6	H	6	PHE	CA-C	-6.97	1.34	1.52
1	A	1315	GLU	CB-CG	6.96	1.65	1.52
2	B	838	SER	CA-CB	-6.96	1.42	1.52
1	A	653	VAL	CB-CG2	-6.96	1.38	1.52
1	A	705	LYS	CG-CD	6.96	1.76	1.52
1	A	35	ILE	CA-C	6.96	1.71	1.52
1	A	412	ARG	CZ-NH1	6.96	1.42	1.33
2	B	389	ALA	N-CA	-6.96	1.32	1.46
4	E	167	ARG	NE-CZ	-6.96	1.24	1.33
1	A	1237	ILE	N-CA	-6.96	1.32	1.46
1	A	819	GLY	C-N	-6.95	1.20	1.33
2	B	1085	ILE	CG1-CD1	-6.95	1.02	1.50
4	E	39	LEU	C-O	6.95	1.36	1.23
4	E	35	VAL	CB-CG1	-6.95	1.38	1.52
2	B	486	TYR	CA-CB	-6.95	1.38	1.53
2	B	804	GLY	CA-C	-6.95	1.40	1.51
1	A	836	TYR	CA-C	6.95	1.71	1.52
2	B	957	ASN	CA-C	6.95	1.71	1.52
2	B	682	SER	CB-OG	-6.94	1.33	1.42
1	A	478	TYR	CE1-CZ	-6.93	1.29	1.38
1	A	818	MET	C-N	-6.93	1.20	1.33
1	A	22	PHE	CE2-CZ	-6.93	1.24	1.37
3	C	102	GLN	C-O	6.93	1.36	1.23
1	A	12	ARG	NE-CZ	6.93	1.42	1.33
3	C	87	PHE	CB-CG	-6.93	1.39	1.51
3	C	98	VAL	CB-CG2	-6.93	1.38	1.52
1	A	1358	SER	CB-OG	6.93	1.51	1.42
1	A	846	GLU	CG-CD	6.93	1.62	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	608	ASP	CG-OD1	6.93	1.41	1.25
10	L	70	ARG	CZ-NH2	-6.93	1.24	1.33
2	B	210	LYS	C-O	-6.92	1.10	1.23
2	B	536	VAL	CB-CG2	-6.92	1.38	1.52
6	H	35	GLN	CA-C	6.92	1.71	1.52
1	A	96	ILE	CG1-CD1	-6.92	1.02	1.50
1	A	1225	PHE	CG-CD2	6.92	1.49	1.38
2	B	782	LEU	CG-CD2	-6.92	1.26	1.51
10	L	38	LEU	N-CA	-6.92	1.32	1.46
1	A	881	GLN	N-CA	-6.92	1.32	1.46
2	B	519	TRP	CD2-CE2	-6.92	1.33	1.41
9	K	96	ASN	C-O	6.92	1.36	1.23
1	A	439	ASN	CB-CG	-6.91	1.35	1.51
5	F	97	ARG	NE-CZ	-6.91	1.24	1.33
1	A	553	VAL	C-N	-6.91	1.21	1.34
1	A	678	GLU	CD-OE2	6.91	1.33	1.25
1	A	1345	ARG	NE-CZ	-6.91	1.24	1.33
2	B	128	LEU	CA-C	-6.91	1.34	1.52
2	B	1027	ILE	N-CA	-6.91	1.32	1.46
1	A	537	ARG	CA-CB	6.91	1.69	1.53
3	C	83	SER	CB-OG	-6.91	1.33	1.42
2	B	666	TYR	CZ-OH	6.91	1.49	1.37
3	C	86	CYS	N-CA	6.91	1.60	1.46
1	A	366	VAL	C-N	-6.91	1.21	1.34
2	B	172	ILE	CG1-CD1	6.90	1.98	1.50
6	H	91	ASP	C-O	6.90	1.36	1.23
3	C	114	TYR	CD2-CE2	-6.90	1.28	1.39
3	C	97	VAL	CA-CB	-6.90	1.40	1.54
1	A	477	PRO	CA-C	-6.90	1.39	1.52
4	E	204	THR	CA-CB	-6.90	1.35	1.53
8	J	17	LYS	CD-CE	6.90	1.68	1.51
9	K	6	ARG	CA-CB	-6.90	1.38	1.53
9	K	62	LYS	C-O	6.90	1.36	1.23
1	A	874	ASP	C-O	-6.90	1.10	1.23
2	B	1132	GLU	C-O	6.90	1.36	1.23
3	C	103	ALA	C-O	-6.90	1.10	1.23
9	K	47	ARG	CZ-NH1	6.90	1.42	1.33
2	B	190	TYR	CD2-CE2	6.90	1.49	1.39
2	B	872	GLU	CD-OE1	6.90	1.33	1.25
2	B	1158	PHE	CB-CG	-6.90	1.39	1.51
6	H	20	TYR	CZ-OH	-6.90	1.26	1.37
1	A	938	LYS	CE-NZ	6.89	1.66	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	88	TYR	CG-CD1	-6.89	1.30	1.39
1	A	201	VAL	CB-CG1	6.89	1.67	1.52
1	A	920	LEU	CA-C	-6.89	1.35	1.52
1	A	1371	LEU	C-O	6.89	1.36	1.23
2	B	895	ASP	CG-OD2	6.89	1.41	1.25
4	E	177	ARG	C-O	-6.89	1.10	1.23
1	A	1336	MET	CG-SD	-6.89	1.63	1.81
2	B	417	PHE	CD2-CE2	-6.89	1.25	1.39
2	B	1139	ILE	C-N	6.89	1.49	1.34
3	C	267	GLN	CB-CG	6.89	1.71	1.52
2	B	136	THR	CA-CB	6.89	1.71	1.53
1	A	753	GLY	C-O	-6.89	1.12	1.23
1	A	1076	ALA	C-O	-6.89	1.10	1.23
2	B	250	PHE	CB-CG	6.89	1.63	1.51
1	A	390	GLN	CD-OE1	6.88	1.39	1.24
9	K	73	LEU	C-O	6.88	1.36	1.23
1	A	708	MET	CB-CG	-6.88	1.29	1.51
3	C	150	GLY	N-CA	6.88	1.56	1.46
4	E	183	PRO	CB-CG	-6.88	1.15	1.50
5	F	72	LYS	CD-CE	6.88	1.68	1.51
9	K	5	ASP	CB-CG	6.88	1.66	1.51
9	K	21	ILE	C-O	-6.88	1.10	1.23
4	E	45	LYS	CG-CD	6.88	1.75	1.52
1	A	1188	GLN	CD-OE1	6.88	1.39	1.24
2	B	203	PHE	N-CA	6.88	1.60	1.46
2	B	852	ARG	CB-CG	-6.88	1.33	1.52
2	B	1196	ILE	CA-CB	-6.88	1.39	1.54
7	I	95	THR	CB-CG2	-6.88	1.29	1.52
1	A	391	LEU	N-CA	6.88	1.60	1.46
2	B	796	LEU	C-O	-6.87	1.10	1.23
1	A	832	ALA	C-O	6.87	1.36	1.23
5	F	121	ALA	C-O	-6.87	1.10	1.23
10	L	42	ARG	CD-NE	6.87	1.58	1.46
3	C	60	ASP	CG-OD2	6.87	1.41	1.25
1	A	183	GLY	CA-C	-6.87	1.40	1.51
3	C	7	GLN	CB-CG	6.87	1.71	1.52
1	A	220	THR	N-CA	6.87	1.60	1.46
1	A	1035	TYR	CE1-CZ	-6.87	1.29	1.38
2	B	604	ARG	CZ-NH2	-6.87	1.24	1.33
2	B	1217	TYR	CG-CD2	-6.87	1.30	1.39
3	C	9	LYS	CE-NZ	6.87	1.66	1.49
7	I	6	PHE	CG-CD2	-6.87	1.28	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217	LYS	CB-CG	6.87	1.71	1.52
3	C	165	LYS	CD-CE	6.87	1.68	1.51
1	A	958	VAL	N-CA	6.86	1.60	1.46
1	A	1081	LEU	CG-CD2	6.86	1.77	1.51
2	B	271	ALA	C-O	-6.86	1.10	1.23
2	B	995	ARG	CZ-NH2	6.86	1.42	1.33
1	A	34	LYS	CB-CG	6.86	1.71	1.52
2	B	553	PRO	CA-CB	-6.86	1.39	1.53
4	E	133	GLU	CD-OE2	6.86	1.33	1.25
4	E	174	GLN	CD-OE1	6.86	1.39	1.24
7	I	96	SER	CA-CB	6.86	1.63	1.52
1	A	16	GLU	N-CA	6.86	1.60	1.46
1	A	1191	TRP	C-O	6.86	1.36	1.23
1	A	1272	THR	CB-CG2	6.85	1.75	1.52
2	B	1087	PHE	CD1-CE1	-6.85	1.25	1.39
5	F	150	GLU	CD-OE2	6.85	1.33	1.25
1	A	417	TYR	CE2-CZ	6.85	1.47	1.38
1	A	933	TYR	CB-CG	-6.85	1.41	1.51
3	C	56	THR	CA-CB	-6.85	1.35	1.53
3	C	124	LEU	CA-C	6.85	1.70	1.52
2	B	482	VAL	CA-CB	-6.85	1.40	1.54
3	C	142	VAL	CB-CG1	6.85	1.67	1.52
10	L	29	TYR	C-O	-6.85	1.10	1.23
1	A	134	ARG	CG-CD	6.85	1.69	1.51
1	A	174	ILE	CB-CG2	-6.84	1.31	1.52
2	B	947	GLY	CA-C	-6.84	1.40	1.51
5	F	146	TRP	CZ3-CH2	-6.84	1.29	1.40
4	E	35	VAL	CA-CB	-6.84	1.40	1.54
1	A	49	LYS	N-CA	6.84	1.60	1.46
1	A	591	PHE	CG-CD2	-6.84	1.28	1.38
1	A	1102	LYS	CB-CG	6.84	1.71	1.52
1	A	1078	GLN	CG-CD	6.84	1.66	1.51
2	B	337	ARG	NE-CZ	-6.84	1.24	1.33
1	A	731	ARG	CA-CB	-6.83	1.39	1.53
9	K	69	ALA	C-O	-6.83	1.10	1.23
1	A	34	LYS	C-O	-6.83	1.10	1.23
1	A	247	ARG	C-O	6.83	1.36	1.23
1	A	413	ILE	C-O	-6.83	1.10	1.23
2	B	986	GLN	C-O	6.83	1.36	1.23
1	A	143	LYS	CG-CD	6.83	1.75	1.52
1	A	542	GLU	CD-OE2	6.83	1.33	1.25
1	A	980	ASP	C-O	6.83	1.36	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	15	TYR	N-CA	-6.83	1.32	1.46
7	I	90	GLN	CG-CD	-6.83	1.35	1.51
1	A	882	SER	CB-OG	-6.83	1.33	1.42
2	B	95	ILE	CB-CG2	-6.83	1.31	1.52
2	B	1046	PRO	CA-C	6.83	1.66	1.52
1	A	1039	LYS	CD-CE	6.83	1.68	1.51
8	J	37	SER	CA-CB	-6.83	1.42	1.52
1	A	285	PRO	CA-C	-6.83	1.39	1.52
1	A	1003	LYS	C-O	6.83	1.36	1.23
1	A	1412	ALA	CA-C	-6.83	1.35	1.52
2	B	711	GLU	CA-CB	-6.83	1.39	1.53
4	E	31	THR	CA-C	-6.83	1.35	1.52
1	A	814	PHE	CE1-CZ	-6.82	1.24	1.37
2	B	343	ILE	CA-CB	-6.82	1.39	1.54
2	B	283	VAL	C-O	-6.82	1.10	1.23
2	B	739	THR	CA-C	-6.82	1.35	1.52
4	E	129	PRO	CG-CD	6.82	1.73	1.50
2	B	782	LEU	CG-CD1	-6.82	1.26	1.51
5	F	80	ALA	N-CA	-6.82	1.32	1.46
1	A	603	ASN	CA-C	-6.82	1.35	1.52
2	B	237	VAL	CB-CG1	-6.82	1.38	1.52
7	I	13	MET	N-CA	-6.82	1.32	1.46
2	B	255	GLN	CA-CB	-6.82	1.39	1.53
3	C	82	TYR	N-CA	6.82	1.59	1.46
5	F	147	SER	CA-CB	6.82	1.63	1.52
9	K	71	PHE	CG-CD2	-6.82	1.28	1.38
3	C	140	ASN	CB-CG	6.81	1.66	1.51
6	H	52	GLN	CB-CG	6.81	1.71	1.52
6	H	145	ARG	NE-CZ	6.81	1.42	1.33
2	B	859	TYR	CD2-CE2	6.81	1.49	1.39
4	E	112	TYR	CG-CD1	-6.81	1.30	1.39
1	A	568	PRO	CA-C	-6.81	1.39	1.52
3	C	94	LYS	CD-CE	6.81	1.68	1.51
3	C	138	GLU	CG-CD	6.81	1.62	1.51
4	E	71	LYS	N-CA	6.81	1.59	1.46
2	B	360	PHE	CE1-CZ	-6.80	1.24	1.37
3	C	104	PHE	CD2-CE2	6.80	1.52	1.39
2	B	1224	PHE	CB-CG	6.80	1.62	1.51
10	L	59	ALA	N-CA	6.80	1.59	1.46
2	B	116	GLU	CG-CD	6.80	1.62	1.51
2	B	1063	GLY	CA-C	-6.80	1.41	1.51
1	A	782	ARG	NE-CZ	6.80	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1108	ARG	CA-C	6.80	1.70	1.52
3	C	194	GLU	C-O	6.80	1.36	1.23
2	B	825	VAL	CB-CG2	-6.79	1.38	1.52
3	C	178	PHE	CE2-CZ	-6.79	1.24	1.37
9	K	36	GLU	CA-CB	-6.79	1.39	1.53
1	A	851	HIS	CB-CG	-6.79	1.37	1.50
2	B	734	HIS	C-N	6.79	1.49	1.34
2	B	736	THR	CB-OG1	-6.79	1.29	1.43
1	A	765	VAL	CB-CG2	6.79	1.67	1.52
3	C	183	TRP	CE2-CZ2	-6.79	1.28	1.39
1	A	423	ASP	C-O	6.79	1.36	1.23
3	C	10	ILE	CG1-CD1	-6.79	1.03	1.50
5	F	108	PHE	CG-CD1	6.78	1.49	1.38
2	B	681	TRP	CZ3-CH2	-6.78	1.29	1.40
1	A	486	GLU	CD-OE2	-6.78	1.18	1.25
1	A	1283	VAL	CB-CG2	-6.78	1.38	1.52
2	B	333	PHE	CE2-CZ	-6.78	1.24	1.37
1	A	920	LEU	CG-CD2	-6.78	1.26	1.51
1	A	1447	GLU	CB-CG	6.78	1.65	1.52
2	B	20	ASP	CG-OD1	6.78	1.41	1.25
2	B	710	LEU	CG-CD1	-6.78	1.26	1.51
3	C	35	ARG	CD-NE	-6.78	1.34	1.46
4	E	85	GLU	CD-OE2	6.78	1.33	1.25
9	K	34	THR	C-N	-6.78	1.18	1.34
1	A	1338	VAL	CA-CB	-6.77	1.40	1.54
1	A	1164	PRO	CG-CD	6.77	1.73	1.50
1	A	1309	ASP	CA-C	-6.77	1.35	1.52
1	A	658	LEU	CG-CD1	-6.77	1.26	1.51
2	B	515	HIS	CB-CG	-6.77	1.37	1.50
1	A	302	THR	CA-CB	6.77	1.71	1.53
2	B	909	ASP	C-O	-6.77	1.10	1.23
5	F	88	TYR	CD2-CE2	-6.77	1.29	1.39
1	A	1227	ILE	C-O	-6.76	1.10	1.23
2	B	328	GLU	CA-CB	6.76	1.68	1.53
2	B	611	PRO	N-CD	-6.76	1.38	1.47
2	B	986	GLN	CA-C	6.76	1.70	1.52
6	H	127	GLY	N-CA	6.76	1.56	1.46
1	A	1422	ARG	CB-CG	-6.76	1.34	1.52
3	C	20	PHE	CE2-CZ	6.76	1.50	1.37
1	A	67	CYS	CB-SG	6.76	1.93	1.82
1	A	833	GLU	CB-CG	6.76	1.65	1.52
2	B	592	ASN	CG-ND2	6.76	1.49	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	857	ARG	CB-CG	-6.76	1.34	1.52
9	K	112	GLN	CG-CD	6.76	1.66	1.51
2	B	634	TYR	CB-CG	6.76	1.61	1.51
2	B	25	ILE	CA-C	-6.76	1.35	1.52
2	B	876	LYS	CD-CE	6.75	1.68	1.51
2	B	911	ILE	N-CA	-6.75	1.32	1.46
4	E	135	PHE	CG-CD2	-6.75	1.28	1.38
2	B	1018	PRO	N-CA	-6.75	1.35	1.47
4	E	104	ASN	C-O	6.75	1.36	1.23
1	A	556	TRP	CG-CD2	-6.75	1.32	1.43
1	A	609	ASP	CG-OD1	6.75	1.40	1.25
2	B	401	PHE	C-O	-6.75	1.10	1.23
1	A	560	ILE	CA-CB	-6.75	1.39	1.54
4	E	215	MET	SD-CE	6.75	2.15	1.77
1	A	580	VAL	CB-CG2	-6.75	1.38	1.52
1	A	702	LEU	C-O	6.75	1.36	1.23
1	A	1263	ILE	CG1-CD1	6.75	1.97	1.50
1	A	1328	TYR	CD1-CE1	-6.75	1.29	1.39
6	H	135	LEU	CG-CD2	6.75	1.76	1.51
1	A	25	GLU	CB-CG	6.75	1.65	1.52
1	A	636	GLU	C-O	6.75	1.36	1.23
3	C	208	GLU	CB-CG	6.75	1.65	1.52
1	A	522	GLY	N-CA	6.74	1.56	1.46
2	B	1069	PHE	CG-CD1	-6.74	1.28	1.38
3	C	127	ARG	CG-CD	-6.74	1.35	1.51
1	A	353	ILE	CB-CG1	-6.74	1.35	1.54
2	B	951	GLN	CB-CG	6.74	1.70	1.52
5	F	129	LYS	CG-CD	6.74	1.75	1.52
8	J	48	ARG	CZ-NH2	-6.74	1.24	1.33
9	K	66	PRO	N-CD	-6.74	1.38	1.47
1	A	899	VAL	CB-CG1	-6.74	1.38	1.52
2	B	1062	HIS	CB-CG	-6.73	1.38	1.50
2	B	1072	MET	SD-CE	-6.73	1.40	1.77
2	B	487	THR	CA-CB	-6.73	1.35	1.53
2	B	434	ARG	NE-CZ	6.73	1.41	1.33
2	B	502	ILE	CB-CG2	6.73	1.73	1.52
1	A	886	ILE	C-N	-6.73	1.21	1.33
2	B	398	ARG	CZ-NH1	6.73	1.41	1.33
1	A	1322	ILE	CB-CG2	-6.73	1.31	1.52
9	K	55	LYS	CE-NZ	6.72	1.65	1.49
6	H	86	ASP	CA-C	6.72	1.70	1.52
2	B	119	LEU	CA-CB	-6.72	1.38	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1281	ARG	CZ-NH1	6.72	1.41	1.33
2	B	788	ARG	CD-NE	-6.72	1.35	1.46
2	B	1033	LYS	CB-CG	-6.72	1.34	1.52
7	I	45	ARG	C-O	6.72	1.36	1.23
1	A	91	PHE	CE1-CZ	-6.72	1.24	1.37
9	K	62	LYS	CE-NZ	-6.72	1.32	1.49
2	B	668	ASP	CG-OD2	6.71	1.40	1.25
1	A	768	GLN	CB-CG	-6.71	1.34	1.52
2	B	1149	GLU	CD-OE2	6.71	1.33	1.25
3	C	209	TYR	CG-CD1	6.71	1.47	1.39
1	A	1359	ASP	CG-OD2	6.71	1.40	1.25
1	A	879	GLU	CG-CD	6.71	1.62	1.51
2	B	368	GLU	CD-OE1	6.71	1.33	1.25
3	C	195	GLN	C-O	-6.71	1.10	1.23
2	B	996	ARG	N-CA	-6.71	1.32	1.46
1	A	891	ALA	C-O	-6.70	1.10	1.23
3	C	12	GLU	CG-CD	6.70	1.62	1.51
1	A	913	LEU	CA-CB	6.70	1.69	1.53
2	B	798	TYR	CZ-OH	6.70	1.49	1.37
4	E	171	LYS	CD-CE	6.70	1.68	1.51
1	A	43	GLU	CD-OE1	6.70	1.33	1.25
1	A	264	PHE	CA-C	6.70	1.70	1.52
2	B	271	ALA	CA-C	-6.70	1.35	1.52
4	E	16	PHE	C-O	6.70	1.36	1.23
2	B	745	PRO	CA-C	-6.70	1.39	1.52
2	B	245	GLU	CD-OE1	6.70	1.33	1.25
4	E	56	LYS	CB-CG	6.70	1.70	1.52
1	A	1444	MET	SD-CE	6.69	2.15	1.77
1	A	1438	THR	CB-CG2	-6.69	1.30	1.52
2	B	658	ILE	CA-CB	-6.69	1.39	1.54
2	B	1171	VAL	CA-CB	-6.69	1.40	1.54
1	A	852	TYR	CA-CB	-6.69	1.39	1.53
2	B	220	GLY	N-CA	-6.69	1.36	1.46
3	C	78	GLU	C-O	-6.69	1.10	1.23
1	A	900	ASP	N-CA	6.69	1.59	1.46
1	A	128	ILE	CB-CG2	-6.68	1.32	1.52
2	B	1109	GLY	CA-C	6.68	1.62	1.51
1	A	1114	PRO	CA-CB	-6.68	1.40	1.53
2	B	118	ARG	CG-CD	6.68	1.68	1.51
2	B	196	PRO	N-CD	-6.68	1.38	1.47
1	A	1136	SER	CB-OG	6.68	1.50	1.42
3	C	65	HIS	N-CA	-6.68	1.32	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	76	ASP	CG-OD1	6.68	1.40	1.25
5	F	137	TYR	CA-C	-6.68	1.35	1.52
4	E	95	THR	CB-CG2	6.68	1.74	1.52
1	A	559	VAL	CB-CG2	-6.68	1.38	1.52
1	A	1144	LYS	C-O	-6.68	1.10	1.23
2	B	377	PHE	CB-CG	-6.67	1.40	1.51
2	B	48	LEU	CG-CD2	-6.67	1.27	1.51
1	A	920	LEU	CB-CG	-6.67	1.33	1.52
2	B	1101	ASP	CA-CB	6.67	1.68	1.53
3	C	102	GLN	CG-CD	6.67	1.66	1.51
7	I	5	ARG	CG-CD	6.67	1.68	1.51
7	I	65	ASP	N-CA	6.67	1.59	1.46
9	K	50	LEU	C-O	-6.67	1.10	1.23
10	L	49	LYS	CD-CE	6.67	1.68	1.51
1	A	1260	LEU	C-O	-6.67	1.10	1.23
2	B	568	ASP	C-O	-6.67	1.10	1.23
2	B	1183	LYS	C-O	6.67	1.36	1.23
1	A	189	ARG	CA-C	6.66	1.70	1.52
1	A	1116	LEU	CB-CG	-6.66	1.33	1.52
1	A	1304	TRP	CD2-CE2	-6.66	1.33	1.41
2	B	667	GLN	CG-CD	6.66	1.66	1.51
3	C	67	LEU	C-O	6.66	1.36	1.23
6	H	140	ALA	CA-CB	-6.66	1.38	1.52
8	J	41	LEU	CG-CD2	-6.66	1.27	1.51
2	B	800	GLN	CD-NE2	6.66	1.49	1.32
1	A	1381	LEU	N-CA	6.66	1.59	1.46
2	B	391	ASP	CB-CG	6.66	1.65	1.51
2	B	1181	GLU	N-CA	6.66	1.59	1.46
8	J	39	LEU	CA-C	-6.66	1.35	1.52
2	B	362	PRO	N-CA	-6.66	1.35	1.47
1	A	578	LEU	N-CA	6.65	1.59	1.46
3	C	113	VAL	C-O	-6.65	1.10	1.23
6	H	114	VAL	CB-CG1	-6.65	1.38	1.52
7	I	62	ILE	C-O	-6.65	1.10	1.23
2	B	764	SER	C-N	-6.65	1.21	1.34
2	B	679	TYR	CG-CD2	-6.65	1.30	1.39
2	B	1087	PHE	CG-CD1	-6.65	1.28	1.38
2	B	1108	ARG	CZ-NH1	6.65	1.41	1.33
8	J	38	ARG	N-CA	-6.65	1.33	1.46
2	B	788	ARG	CB-CG	6.65	1.70	1.52
1	A	408	ASP	CG-OD2	6.65	1.40	1.25
3	C	145	CYS	CA-CB	-6.65	1.39	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	303	TYR	CZ-OH	6.64	1.49	1.37
2	B	848	ARG	CA-CB	-6.64	1.39	1.53
1	A	124	GLN	CG-CD	6.64	1.66	1.51
7	I	20	LYS	CE-NZ	6.64	1.65	1.49
1	A	1100	ARG	CA-C	-6.64	1.35	1.52
2	B	259	TYR	CG-CD1	-6.64	1.30	1.39
2	B	862	GLN	CG-CD	6.64	1.66	1.51
2	B	1217	TYR	CE1-CZ	-6.64	1.29	1.38
3	C	106	GLU	CD-OE1	6.64	1.32	1.25
3	C	135	GLN	CG-CD	6.64	1.66	1.51
9	K	111	LEU	CA-C	6.64	1.70	1.52
1	A	497	THR	CB-CG2	-6.64	1.30	1.52
4	E	50	MET	CA-C	6.64	1.70	1.52
1	A	669	THR	N-CA	-6.63	1.33	1.46
2	B	936	ASP	CB-CG	6.63	1.65	1.51
2	B	1143	ALA	CA-CB	-6.63	1.38	1.52
2	B	1182	CYS	N-CA	6.63	1.59	1.46
3	C	167	HIS	CA-CB	-6.63	1.39	1.53
2	B	528	PRO	CA-CB	-6.63	1.40	1.53
2	B	705	MET	C-O	-6.63	1.10	1.23
6	H	98	TYR	CD2-CE2	6.63	1.49	1.39
9	K	64	GLU	CD-OE2	-6.63	1.18	1.25
4	E	29	PHE	CE1-CZ	6.63	1.50	1.37
6	H	141	TYR	CG-CD2	-6.63	1.30	1.39
10	L	46	VAL	C-O	-6.63	1.10	1.23
6	H	49	VAL	CB-CG2	-6.63	1.39	1.52
1	A	359	LEU	CG-CD2	-6.62	1.27	1.51
1	A	821	ARG	C-O	-6.62	1.10	1.23
1	A	1116	LEU	C-O	-6.62	1.10	1.23
2	B	19	GLU	CD-OE1	6.62	1.32	1.25
4	E	28	TYR	CG-CD2	-6.62	1.30	1.39
5	F	79	ARG	CD-NE	-6.62	1.35	1.46
5	F	106	PRO	CA-C	-6.62	1.39	1.52
6	H	6	PHE	CD2-CE2	6.62	1.52	1.39
1	A	497	THR	N-CA	-6.62	1.33	1.46
2	B	105	SER	CB-OG	6.62	1.50	1.42
2	B	337	ARG	CZ-NH1	-6.62	1.24	1.33
1	A	1002	GLY	CA-C	6.62	1.62	1.51
9	K	7	PHE	CG-CD1	-6.62	1.28	1.38
9	K	18	LYS	C-O	-6.62	1.10	1.23
1	A	376	TYR	CE1-CZ	-6.61	1.29	1.38
1	A	860	LEU	CG-CD2	6.61	1.76	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	550	ASP	CB-CG	6.61	1.65	1.51
2	B	1165	ILE	CA-CB	6.61	1.70	1.54
2	B	1221	SER	N-CA	6.61	1.59	1.46
7	I	94	ASP	CG-OD2	6.61	1.40	1.25
2	B	1151	LEU	N-CA	-6.61	1.33	1.46
4	E	204	THR	CB-CG2	-6.61	1.30	1.52
8	J	63	TYR	CE1-CZ	-6.61	1.29	1.38
9	K	48	ALA	CA-CB	-6.61	1.38	1.52
2	B	1177	HIS	N-CA	6.61	1.59	1.46
6	H	145	ARG	CG-CD	6.61	1.68	1.51
3	C	68	GLY	CA-C	-6.61	1.41	1.51
5	F	114	GLU	C-O	-6.61	1.10	1.23
1	A	840	ARG	CD-NE	6.60	1.57	1.46
6	H	20	TYR	CB-CG	-6.60	1.41	1.51
1	A	1376	THR	CB-CG2	-6.60	1.30	1.52
2	B	281	PRO	N-CA	-6.60	1.36	1.47
1	A	632	VAL	N-CA	6.60	1.59	1.46
7	I	85	PHE	CD1-CE1	-6.60	1.26	1.39
1	A	636	GLU	CD-OE1	-6.60	1.18	1.25
4	E	147	HIS	CA-C	-6.60	1.35	1.52
1	A	1034	GLU	CB-CG	-6.59	1.39	1.52
2	B	766	ARG	CZ-NH2	6.59	1.41	1.33
1	A	1308	THR	C-O	-6.59	1.10	1.23
7	I	30	ARG	CA-C	-6.59	1.35	1.52
10	L	41	SER	N-CA	6.59	1.59	1.46
2	B	626	ILE	C-O	-6.59	1.10	1.23
1	A	243	PRO	CA-CB	-6.59	1.40	1.53
7	I	118	ARG	CB-CG	6.59	1.70	1.52
3	C	20	PHE	CB-CG	-6.58	1.40	1.51
3	C	79	GLN	CA-CB	6.58	1.68	1.53
4	E	152	LYS	CB-CG	6.58	1.70	1.52
2	B	176	SER	C-O	-6.58	1.10	1.23
8	J	6	ARG	CB-CG	6.58	1.70	1.52
1	A	95	PHE	CE2-CZ	-6.58	1.24	1.37
1	A	1136	SER	N-CA	-6.58	1.33	1.46
10	L	66	GLN	CD-NE2	6.58	1.49	1.32
1	A	261	ASP	CB-CG	6.58	1.65	1.51
2	B	1058	LEU	CG-CD1	6.58	1.76	1.51
1	A	977	LYS	CG-CD	6.58	1.74	1.52
2	B	606	LYS	C-O	6.58	1.35	1.23
1	A	9	ALA	CA-C	-6.57	1.35	1.52
1	A	554	PRO	N-CD	-6.57	1.38	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1030	ARG	CB-CG	-6.57	1.34	1.52
8	J	59	LYS	CD-CE	6.57	1.67	1.51
3	C	20	PHE	CD1-CE1	6.57	1.52	1.39
1	A	37	PHE	C-O	-6.57	1.10	1.23
1	A	840	ARG	CB-CG	6.57	1.70	1.52
1	A	914	GLU	CD-OE2	6.57	1.32	1.25
1	A	709	THR	CB-CG2	-6.57	1.30	1.52
1	A	942	PHE	CD1-CE1	-6.56	1.26	1.39
1	A	1154	TYR	CD1-CE1	6.56	1.49	1.39
2	B	1087	PHE	CA-CB	-6.56	1.39	1.53
1	A	1450	LEU	CG-CD1	6.56	1.76	1.51
1	A	572	TRP	CD2-CE3	-6.56	1.30	1.40
7	I	82	GLU	CA-C	6.56	1.70	1.52
1	A	810	PRO	CB-CG	-6.56	1.17	1.50
1	A	892	ALA	C-O	-6.56	1.10	1.23
1	A	1111	MET	C-O	-6.56	1.10	1.23
1	A	461	LYS	CA-CB	-6.55	1.39	1.53
3	C	60	ASP	CB-CG	6.55	1.65	1.51
1	A	747	VAL	CA-CB	-6.55	1.41	1.54
6	H	95	TYR	CD2-CE2	6.55	1.49	1.39
1	A	1277	GLU	N-CA	6.55	1.59	1.46
2	B	486	TYR	CD2-CE2	6.55	1.49	1.39
2	B	566	LEU	C-O	-6.55	1.10	1.23
4	E	114	ASN	N-CA	6.55	1.59	1.46
1	A	560	ILE	C-N	-6.55	1.21	1.34
4	E	103	LYS	C-O	6.55	1.35	1.23
1	A	935	GLN	CG-CD	-6.55	1.35	1.51
2	B	215	GLN	N-CA	-6.55	1.33	1.46
2	B	1220	ARG	CG-CD	6.55	1.68	1.51
2	B	138	GLU	CD-OE2	-6.54	1.18	1.25
2	B	361	LEU	C-N	-6.54	1.21	1.34
2	B	1092	TYR	CD2-CE2	6.54	1.49	1.39
1	A	1121	GLU	CG-CD	6.54	1.61	1.51
2	B	267	ARG	CG-CD	6.54	1.68	1.51
1	A	514	PRO	N-CA	-6.54	1.36	1.47
1	A	1098	VAL	C-N	-6.54	1.21	1.34
4	E	17	ARG	CZ-NH1	6.54	1.41	1.33
1	A	393	ARG	CZ-NH2	6.54	1.41	1.33
2	B	459	TYR	CA-CB	-6.54	1.39	1.53
1	A	1419	ASP	CA-C	-6.54	1.35	1.52
2	B	40	GLU	CA-C	-6.53	1.35	1.52
2	B	118	ARG	C-O	6.53	1.35	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	418	SER	CB-OG	6.53	1.50	1.42
3	C	143	LEU	CA-CB	-6.53	1.38	1.53
3	C	211	ASP	CG-OD1	6.53	1.40	1.25
4	E	77	SER	N-CA	-6.53	1.33	1.46
1	A	877	HIS	N-CA	-6.53	1.33	1.46
1	A	1062	GLU	CB-CG	-6.53	1.39	1.52
1	A	1424	VAL	CA-CB	-6.53	1.41	1.54
3	C	169	LYS	CD-CE	6.53	1.67	1.51
1	A	780	VAL	N-CA	6.53	1.59	1.46
1	A	1053	PHE	CD2-CE2	-6.53	1.26	1.39
1	A	1323	ASP	CB-CG	6.53	1.65	1.51
2	B	1160	VAL	C-O	6.53	1.35	1.23
2	B	1223	ASP	C-N	6.53	1.49	1.34
6	H	79	TRP	CG-CD1	-6.53	1.27	1.36
7	I	121	PHE	CE1-CZ	-6.53	1.25	1.37
2	B	803	LEU	N-CA	-6.52	1.33	1.46
2	B	958	GLN	N-CA	6.52	1.59	1.46
1	A	381	THR	N-CA	-6.51	1.33	1.46
1	A	1035	TYR	CG-CD2	-6.51	1.30	1.39
1	A	750	GLY	CA-C	-6.51	1.41	1.51
1	A	1325	THR	CB-OG1	6.51	1.56	1.43
2	B	654	ARG	CZ-NH1	-6.51	1.24	1.33
2	B	856	PHE	CD2-CE2	-6.51	1.26	1.39
9	K	112	GLN	CB-CG	6.51	1.70	1.52
10	L	30	ILE	CA-CB	-6.51	1.39	1.54
1	A	549	MET	C-O	-6.51	1.10	1.23
3	C	220	ASP	CG-OD1	6.51	1.40	1.25
1	A	188	ASP	N-CA	6.51	1.59	1.46
8	J	51	LEU	C-O	6.51	1.35	1.23
2	B	649	LYS	CB-CG	-6.50	1.34	1.52
2	B	1206	GLU	CG-CD	6.50	1.61	1.51
4	E	92	THR	CB-CG2	6.50	1.73	1.52
8	J	26	GLN	CD-NE2	6.50	1.49	1.32
1	A	493	GLN	CA-CB	-6.50	1.39	1.53
2	B	810	GLU	C-N	-6.50	1.19	1.34
3	C	190	ASP	CB-CG	-6.50	1.38	1.51
1	A	1064	VAL	CB-CG2	-6.50	1.39	1.52
1	A	203	SER	CA-CB	6.50	1.62	1.52
1	A	879	GLU	CD-OE2	-6.50	1.18	1.25
1	A	1203	ASN	CB-CG	-6.50	1.36	1.51
2	B	41	LYS	CD-CE	6.50	1.67	1.51
3	C	3	GLU	N-CA	6.50	1.59	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	135	ARG	N-CA	-6.50	1.33	1.46
6	H	27	GLU	CG-CD	6.50	1.61	1.51
1	A	799	PHE	CG-CD1	-6.50	1.29	1.38
1	A	1443	VAL	CB-CG1	-6.50	1.39	1.52
3	C	192	TRP	CD2-CE2	-6.50	1.33	1.41
2	B	732	SER	CA-C	6.50	1.69	1.52
2	B	356	LEU	C-O	-6.49	1.11	1.23
2	B	879	ARG	N-CA	6.49	1.59	1.46
2	B	1088	GLY	CA-C	-6.49	1.41	1.51
7	I	73	ARG	NE-CZ	6.49	1.41	1.33
1	A	543	LEU	N-CA	-6.49	1.33	1.46
1	A	1211	GLN	CA-C	-6.49	1.36	1.52
4	E	170	LEU	C-O	6.49	1.35	1.23
1	A	1448	GLU	CG-CD	6.49	1.61	1.51
3	C	267	GLN	C-O	6.49	1.35	1.23
4	E	161	LYS	CG-CD	-6.49	1.30	1.52
8	J	22	LEU	N-CA	-6.49	1.33	1.46
1	A	4	GLN	CA-C	6.49	1.69	1.52
2	B	556	THR	C-O	6.49	1.35	1.23
3	C	17	ASN	C-O	-6.49	1.11	1.23
3	C	115	SER	CA-CB	-6.49	1.43	1.52
2	B	446	LEU	CG-CD2	6.48	1.75	1.51
7	I	20	LYS	CG-CD	6.48	1.74	1.52
1	A	1447	GLU	C-O	6.48	1.35	1.23
5	F	74	ILE	C-N	-6.48	1.22	1.34
9	K	82	ASP	CB-CG	6.48	1.65	1.51
1	A	15	LYS	CD-CE	6.48	1.67	1.51
1	A	22	PHE	C-O	6.48	1.35	1.23
1	A	1282	VAL	CA-CB	-6.48	1.41	1.54
2	B	644	GLU	CD-OE2	6.48	1.32	1.25
7	I	101	PHE	CD1-CE1	6.48	1.52	1.39
1	A	75	ASN	CB-CG	6.48	1.66	1.51
1	A	176	LYS	C-O	6.48	1.35	1.23
1	A	23	SER	CA-CB	-6.47	1.43	1.52
1	A	143	LYS	CB-CG	6.47	1.70	1.52
1	A	1223	ASP	CA-CB	6.47	1.68	1.53
2	B	48	LEU	N-CA	-6.47	1.33	1.46
2	B	546	SER	C-O	-6.47	1.11	1.23
2	B	1181	GLU	C-O	6.47	1.35	1.23
4	E	41	ASP	C-O	6.47	1.35	1.23
7	I	101	PHE	CG-CD1	-6.47	1.29	1.38
1	A	641	VAL	C-O	-6.47	1.11	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1078	GLN	CB-CG	6.47	1.70	1.52
2	B	595	ARG	CB-CG	6.47	1.70	1.52
1	A	74	MET	CB-CG	6.47	1.72	1.51
1	A	121	LEU	C-O	-6.47	1.11	1.23
1	A	407	ARG	CG-CD	6.47	1.68	1.51
1	A	918	GLU	CG-CD	6.47	1.61	1.51
2	B	316	PRO	CA-CB	-6.47	1.40	1.53
2	B	664	THR	N-CA	-6.47	1.33	1.46
2	B	1180	PHE	CE2-CZ	-6.47	1.25	1.37
3	C	219	PHE	CB-CG	6.47	1.62	1.51
4	E	194	GLU	CD-OE2	-6.47	1.18	1.25
1	A	810	PRO	C-O	-6.47	1.10	1.23
2	B	183	GLU	CD-OE2	6.47	1.32	1.25
4	E	153	HIS	CA-CB	-6.47	1.39	1.53
1	A	299	HIS	CA-CB	6.46	1.68	1.53
1	A	388	LEU	CG-CD1	-6.46	1.27	1.51
1	A	616	VAL	N-CA	-6.46	1.33	1.46
2	B	870	ILE	CB-CG1	6.46	1.72	1.54
4	E	122	LYS	CA-CB	6.46	1.68	1.53
2	B	879	ARG	CD-NE	6.46	1.57	1.46
2	B	1186	ASP	CA-C	6.46	1.69	1.52
3	C	13	ALA	CA-C	-6.46	1.36	1.52
4	E	129	PRO	CB-CG	6.46	1.82	1.50
3	C	218	PRO	CG-CD	6.46	1.72	1.50
4	E	171	LYS	C-O	-6.46	1.11	1.23
1	A	1132	LYS	CG-CD	6.46	1.74	1.52
1	A	1342	GLU	CD-OE2	6.46	1.32	1.25
1	A	1424	VAL	CB-CG1	-6.46	1.39	1.52
2	B	530	GLY	C-O	6.46	1.33	1.23
7	I	91	ARG	C-O	-6.46	1.11	1.23
2	B	639	ILE	C-N	-6.45	1.19	1.34
10	L	57	LEU	CG-CD2	-6.45	1.27	1.51
2	B	630	ALA	C-O	-6.45	1.11	1.23
1	A	66	LYS	CA-CB	6.45	1.68	1.53
1	A	683	ILE	CA-C	-6.45	1.36	1.52
1	A	479	ASN	C-O	-6.44	1.11	1.23
2	B	1110	PRO	CA-C	6.44	1.65	1.52
1	A	871	ASP	C-O	-6.44	1.11	1.23
2	B	866	TYR	CD1-CE1	6.44	1.49	1.39
3	C	133	ILE	C-O	6.44	1.35	1.23
1	A	520	CYS	CB-SG	-6.44	1.71	1.82
2	B	945	GLU	C-O	6.44	1.35	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	982	SER	CA-C	-6.44	1.36	1.52
1	A	811	GLN	CB-CG	-6.44	1.35	1.52
2	B	231	PRO	CG-CD	6.44	1.71	1.50
9	K	81	TYR	N-CA	6.44	1.59	1.46
9	K	94	ILE	CA-C	-6.44	1.36	1.52
1	A	1068	ALA	CA-C	-6.43	1.36	1.52
1	A	1374	VAL	CB-CG1	-6.43	1.39	1.52
2	B	1096	ARG	NE-CZ	-6.43	1.24	1.33
3	C	44	LEU	C-O	6.43	1.35	1.23
1	A	863	VAL	CB-CG2	6.43	1.66	1.52
1	A	922	ASP	C-O	-6.43	1.11	1.23
1	A	1195	LEU	C-O	-6.43	1.11	1.23
2	B	863	GLU	CB-CG	6.43	1.64	1.52
9	K	30	ALA	CA-C	-6.43	1.36	1.52
1	A	265	LYS	CD-CE	6.43	1.67	1.51
7	I	118	ARG	CA-C	6.43	1.69	1.52
1	A	430	TRP	CG-CD1	-6.42	1.27	1.36
1	A	940	ARG	C-O	-6.42	1.11	1.23
1	A	1326	ARG	CZ-NH2	-6.42	1.24	1.33
3	C	27	LEU	CG-CD1	-6.42	1.28	1.51
1	A	305	ASP	CA-C	6.42	1.69	1.52
2	B	194	GLU	CB-CG	6.42	1.64	1.52
3	C	239	PRO	CG-CD	-6.42	1.29	1.50
5	F	133	VAL	CA-CB	-6.42	1.41	1.54
1	A	896	ARG	NE-CZ	-6.42	1.24	1.33
2	B	866	TYR	CG-CD2	6.42	1.47	1.39
1	A	204	THR	C-O	-6.42	1.11	1.23
1	A	220	THR	CB-OG1	6.42	1.56	1.43
1	A	383	TYR	CB-CG	6.42	1.61	1.51
1	A	724	GLU	CB-CG	6.42	1.64	1.52
2	B	56	ASP	C-O	-6.42	1.11	1.23
2	B	969	ARG	CD-NE	-6.42	1.35	1.46
4	E	33	GLU	CD-OE1	6.42	1.32	1.25
1	A	613	ILE	CA-C	-6.42	1.36	1.52
1	A	1265	ASN	CA-CB	6.41	1.69	1.53
2	B	755	ILE	CB-CG2	-6.41	1.32	1.52
3	C	222	LYS	CG-CD	6.41	1.74	1.52
5	F	98	ALA	CA-CB	-6.41	1.39	1.52
6	H	132	LEU	CA-C	6.41	1.69	1.52
6	H	102	TYR	CD1-CE1	-6.41	1.29	1.39
2	B	667	GLN	CD-NE2	6.41	1.48	1.32
2	B	129	PHE	CE1-CZ	6.41	1.49	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1166	CYS	CA-CB	6.41	1.68	1.53
2	B	1219	ASP	N-CA	6.41	1.59	1.46
5	F	90	ARG	CD-NE	6.41	1.57	1.46
5	F	96	THR	C-O	-6.41	1.11	1.23
6	H	131	ASN	C-O	6.41	1.35	1.23
1	A	575	LYS	CB-CG	-6.40	1.35	1.52
2	B	191	LYS	C-O	-6.40	1.11	1.23
2	B	1154	ALA	N-CA	6.40	1.59	1.46
4	E	43	LYS	C-O	6.40	1.35	1.23
2	B	113	TYR	CD2-CE2	-6.40	1.29	1.39
2	B	351	TYR	CD1-CE1	6.40	1.49	1.39
2	B	878	GLN	CB-CG	6.40	1.69	1.52
1	A	407	ARG	CZ-NH2	6.40	1.41	1.33
1	A	532	ARG	N-CA	-6.40	1.33	1.46
2	B	904	ARG	CD-NE	-6.40	1.35	1.46
4	E	172	GLU	CA-CB	6.40	1.68	1.53
7	I	45	ARG	CZ-NH1	6.40	1.41	1.33
1	A	465	TYR	C-O	-6.39	1.11	1.23
2	B	1138	MET	N-CA	-6.39	1.33	1.46
4	E	46	TYR	CE2-CZ	6.39	1.46	1.38
2	B	775	LYS	N-CA	-6.39	1.33	1.46
1	A	563	PRO	CA-C	-6.39	1.40	1.52
6	H	12	VAL	C-O	6.39	1.35	1.23
2	B	705	MET	CB-CG	-6.39	1.30	1.51
6	H	104	PHE	CG-CD2	6.39	1.48	1.38
2	B	264	SER	CA-CB	6.39	1.62	1.52
1	A	1256	GLU	CA-C	6.39	1.69	1.52
3	C	252	GLN	CD-NE2	6.39	1.48	1.32
1	A	983	ILE	CB-CG2	-6.38	1.33	1.52
1	A	1362	TYR	C-O	-6.38	1.11	1.23
2	B	865	LYS	CA-CB	6.38	1.68	1.53
2	B	1150	ARG	C-O	-6.38	1.11	1.23
4	E	51	GLY	CA-C	6.38	1.62	1.51
1	A	1012	ARG	NE-CZ	6.38	1.41	1.33
1	A	39	GLU	CA-C	6.37	1.69	1.52
2	B	684	LEU	N-CA	-6.37	1.33	1.46
2	B	1039	GLY	C-O	-6.37	1.13	1.23
1	A	942	PHE	C-O	-6.37	1.11	1.23
4	E	63	ASN	CG-OD1	6.37	1.38	1.24
2	B	603	LEU	N-CA	-6.37	1.33	1.46
2	B	868	MET	N-CA	6.37	1.59	1.46
10	L	42	ARG	CG-CD	6.37	1.67	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	67	PHE	CG-CD2	-6.37	1.29	1.38
2	B	730	ARG	CZ-NH1	-6.37	1.24	1.33
7	I	86	PHE	CD1-CE1	6.37	1.51	1.39
1	A	72	GLU	CG-CD	6.37	1.61	1.51
5	F	143	PHE	CG-CD2	-6.36	1.29	1.38
1	A	1255	GLU	CA-C	6.36	1.69	1.52
2	B	274	PRO	CA-CB	6.36	1.66	1.53
2	B	496	ARG	CG-CD	6.36	1.67	1.51
2	B	1222	ARG	CD-NE	-6.36	1.35	1.46
2	B	781	PHE	CD2-CE2	-6.36	1.26	1.39
1	A	748	MET	C-N	-6.36	1.19	1.34
1	A	1381	LEU	C-O	-6.36	1.11	1.23
2	B	37	PHE	CG-CD1	-6.36	1.29	1.38
2	B	887	HIS	CA-C	6.36	1.69	1.52
4	E	195	VAL	N-CA	6.36	1.59	1.46
4	E	106	GLN	CA-CB	6.36	1.68	1.53
7	I	119	THR	CB-CG2	6.35	1.73	1.52
2	B	348	ARG	CA-CB	-6.35	1.40	1.53
8	J	55	ASP	CB-CG	-6.35	1.38	1.51
1	A	425	GLN	CD-NE2	6.35	1.48	1.32
1	A	746	MET	SD-CE	-6.35	1.42	1.77
1	A	842	VAL	CB-CG1	-6.35	1.39	1.52
1	A	867	ILE	C-O	-6.35	1.11	1.23
1	A	917	SER	CB-OG	-6.35	1.33	1.42
1	A	1228	TRP	CG-CD2	6.35	1.54	1.43
5	F	106	PRO	CG-CD	-6.35	1.29	1.50
7	I	78	CYS	CA-CB	6.35	1.68	1.53
1	A	813	PHE	CG-CD2	-6.35	1.29	1.38
2	B	96	TYR	CD1-CE1	6.34	1.48	1.39
2	B	136	THR	CA-C	6.34	1.69	1.52
2	B	810	GLU	CB-CG	6.34	1.64	1.52
3	C	88	CYS	C-O	-6.34	1.11	1.23
1	A	423	ASP	CG-OD1	6.34	1.40	1.25
1	A	1336	MET	C-O	-6.34	1.11	1.23
2	B	998	ASP	CA-CB	-6.34	1.40	1.53
1	A	953	ASN	CG-OD1	6.34	1.37	1.24
1	A	963	ILE	C-O	-6.34	1.11	1.23
2	B	827	ILE	CB-CG2	-6.34	1.33	1.52
1	A	71	GLN	CB-CG	6.34	1.69	1.52
1	A	866	PHE	CE2-CZ	-6.34	1.25	1.37
1	A	606	LEU	C-O	-6.33	1.11	1.23
2	B	39	ARG	CZ-NH2	6.33	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5	GLY	CA-C	6.33	1.61	1.51
8	J	4	PRO	N-CD	-6.33	1.39	1.47
9	K	68	PHE	CA-CB	-6.33	1.40	1.53
4	E	122	LYS	CD-CE	6.33	1.67	1.51
6	H	47	PHE	CE2-CZ	-6.33	1.25	1.37
1	A	940	ARG	NE-CZ	6.33	1.41	1.33
2	B	842	ASN	CG-ND2	-6.33	1.17	1.32
4	E	166	LYS	C-O	6.33	1.35	1.23
1	A	180	LYS	CG-CD	6.32	1.74	1.52
1	A	471	ASN	CB-CG	6.32	1.65	1.51
8	J	58	GLU	CD-OE1	-6.32	1.18	1.25
1	A	1441	PHE	C-O	-6.32	1.11	1.23
1	A	1194	ARG	N-CA	-6.32	1.33	1.46
1	A	593	GLU	CA-C	6.32	1.69	1.52
1	A	777	PHE	CD1-CE1	6.32	1.51	1.39
1	A	572	TRP	CG-CD1	-6.32	1.27	1.36
2	B	882	THR	CB-CG2	6.32	1.73	1.52
9	K	66	PRO	CG-CD	-6.32	1.29	1.50
1	A	70	CYS	CA-CB	6.32	1.67	1.53
1	A	745	GLN	CD-OE1	6.31	1.37	1.24
1	A	825	ILE	CA-CB	-6.31	1.40	1.54
2	B	318	VAL	C-O	6.31	1.35	1.23
4	E	156	LEU	C-O	6.31	1.35	1.23
5	F	123	LYS	CB-CG	6.31	1.69	1.52
1	A	1127	ASP	CB-CG	6.31	1.65	1.51
2	B	562	GLY	CA-C	-6.31	1.41	1.51
4	E	212	ARG	NE-CZ	-6.31	1.24	1.33
1	A	971	PHE	CG-CD2	-6.31	1.29	1.38
2	B	1047	PHE	N-CA	-6.31	1.33	1.46
3	C	228	PHE	N-CA	-6.31	1.33	1.46
5	F	108	PHE	N-CA	-6.31	1.33	1.46
7	I	34	TYR	CA-C	-6.31	1.36	1.52
6	H	30	SER	N-CA	6.31	1.58	1.46
1	A	1241	ARG	C-O	-6.31	1.11	1.23
2	B	105	SER	CA-C	6.31	1.69	1.52
1	A	846	GLU	CD-OE1	6.30	1.32	1.25
1	A	960	ILE	CB-CG1	-6.30	1.36	1.54
6	H	109	LYS	CB-CG	6.30	1.69	1.52
1	A	430	TRP	CD2-CE3	-6.30	1.30	1.40
1	A	556	TRP	CZ2-CH2	-6.30	1.25	1.37
2	B	791	THR	N-CA	-6.30	1.33	1.46
2	B	781	PHE	CA-CB	-6.30	1.40	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	187	LYS	CD-CE	6.30	1.67	1.51
3	C	236	GLY	N-CA	-6.30	1.36	1.46
3	C	180	TYR	CD2-CE2	6.30	1.48	1.39
1	A	110	CYS	CA-CB	6.30	1.67	1.53
1	A	1161	THR	CB-CG2	-6.30	1.31	1.52
2	B	868	MET	CA-CB	6.29	1.67	1.53
3	C	139	GLY	N-CA	6.29	1.55	1.46
7	I	118	ARG	NE-CZ	6.29	1.41	1.33
1	A	10	PRO	CG-CD	6.29	1.71	1.50
1	A	1139	GLU	N-CA	6.29	1.58	1.46
1	A	1280	GLU	CB-CG	6.29	1.64	1.52
3	C	47	ASP	CG-OD2	6.29	1.39	1.25
4	E	195	VAL	CA-CB	-6.29	1.41	1.54
9	K	109	TRP	C-O	6.29	1.35	1.23
1	A	44	THR	CA-C	6.29	1.69	1.52
1	A	208	LEU	CG-CD1	-6.29	1.28	1.51
3	C	105	GLY	CA-C	-6.29	1.41	1.51
1	A	45	GLN	N-CA	6.29	1.58	1.46
1	A	1140	HIS	C-O	-6.29	1.11	1.23
1	A	925	LEU	C-O	-6.29	1.11	1.23
1	A	1339	LEU	CA-CB	-6.29	1.39	1.53
1	A	428	TYR	CD1-CE1	6.29	1.48	1.39
1	A	656	TRP	CZ3-CH2	-6.29	1.29	1.40
1	A	893	PHE	CE2-CZ	-6.29	1.25	1.37
6	H	93	TYR	CG-CD1	6.29	1.47	1.39
10	L	31	CYS	C-O	6.29	1.35	1.23
1	A	498	ARG	CZ-NH2	-6.28	1.24	1.33
1	A	938	LYS	CA-C	-6.28	1.36	1.52
1	A	489	LEU	CA-CB	-6.28	1.39	1.53
5	F	93	ILE	CA-CB	-6.28	1.40	1.54
6	H	127	GLY	CA-C	6.28	1.61	1.51
1	A	711	ARG	N-CA	-6.28	1.33	1.46
1	A	754	SER	CA-CB	6.28	1.62	1.52
5	F	97	ARG	C-O	-6.28	1.11	1.23
6	H	23	VAL	CB-CG2	-6.28	1.39	1.52
1	A	938	LYS	CG-CD	6.27	1.73	1.52
4	E	78	LEU	N-CA	-6.27	1.33	1.46
1	A	100	LYS	CB-CG	-6.27	1.35	1.52
3	C	171	GLY	N-CA	6.27	1.55	1.46
1	A	721	PHE	CG-CD1	-6.27	1.29	1.38
1	A	788	SER	C-O	-6.27	1.11	1.23
1	A	1278	ASN	C-O	-6.27	1.11	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	883	LEU	CB-CG	6.27	1.70	1.52
1	A	127	ALA	C-O	6.26	1.35	1.23
1	A	1074	GLU	CD-OE1	6.26	1.32	1.25
2	B	277	LYS	CD-CE	6.26	1.67	1.51
7	I	73	ARG	CZ-NH1	6.26	1.41	1.33
1	A	1416	ALA	C-O	-6.26	1.11	1.23
2	B	770	GLN	CD-OE1	6.26	1.37	1.24
3	C	245	VAL	CB-CG1	-6.26	1.39	1.52
7	I	53	GLY	C-O	6.26	1.33	1.23
1	A	1287	TYR	CE1-CZ	6.26	1.46	1.38
2	B	367	LEU	CG-CD1	6.26	1.75	1.51
1	A	868	TYR	CG-CD1	-6.26	1.31	1.39
1	A	45	GLN	CA-CB	6.26	1.67	1.53
1	A	927	VAL	C-O	6.26	1.35	1.23
1	A	1050	GLU	C-O	6.26	1.35	1.23
2	B	401	PHE	CE2-CZ	-6.25	1.25	1.37
7	I	92	ARG	CZ-NH2	6.25	1.41	1.33
1	A	36	ARG	CA-C	-6.25	1.36	1.52
1	A	297	GLN	C-O	-6.25	1.11	1.23
2	B	569	TYR	CG-CD1	-6.25	1.31	1.39
2	B	699	GLU	CA-C	-6.25	1.36	1.52
3	C	177	GLU	CG-CD	6.25	1.61	1.51
2	B	961	LEU	C-O	6.25	1.35	1.23
7	I	66	PRO	N-CD	-6.25	1.39	1.47
2	B	1080	LYS	CE-NZ	6.25	1.64	1.49
3	C	268	ASP	CB-CG	6.25	1.64	1.51
4	E	154	ILE	CB-CG2	-6.25	1.33	1.52
8	J	30	LEU	CA-CB	-6.25	1.39	1.53
9	K	66	PRO	CA-CB	-6.25	1.41	1.53
1	A	1203	ASN	CG-OD1	6.25	1.37	1.24
1	A	1332	PHE	CE2-CZ	6.25	1.49	1.37
2	B	866	TYR	CE1-CZ	6.25	1.46	1.38
1	A	698	GLN	CD-OE1	6.25	1.37	1.24
2	B	135	ARG	CD-NE	6.24	1.57	1.46
10	L	68	GLU	N-CA	-6.24	1.33	1.46
2	B	415	GLN	CA-CB	6.24	1.67	1.53
7	I	121	PHE	CD2-CE2	-6.24	1.26	1.39
2	B	132	VAL	C-O	6.24	1.35	1.23
1	A	194	ALA	CA-CB	6.24	1.65	1.52
1	A	407	ARG	NE-CZ	-6.24	1.25	1.33
2	B	1210	MET	N-CA	-6.24	1.33	1.46
1	A	1017	LEU	CA-C	-6.24	1.36	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	594	ALA	CA-C	-6.24	1.36	1.52
5	F	144	GLU	N-CA	-6.24	1.33	1.46
1	A	189	ARG	NE-CZ	6.24	1.41	1.33
2	B	67	SER	CB-OG	6.24	1.50	1.42
1	A	947	PHE	CE2-CZ	-6.23	1.25	1.37
2	B	596	LEU	CG-CD1	-6.23	1.28	1.51
4	E	25	ASP	CB-CG	6.23	1.64	1.51
4	E	154	ILE	C-O	6.23	1.35	1.23
1	A	772	GLY	CA-C	-6.23	1.41	1.51
1	A	1407	GLU	CG-CD	6.23	1.61	1.51
2	B	406	LEU	CA-C	6.23	1.69	1.52
2	B	1215	ARG	C-O	-6.23	1.11	1.23
1	A	1078	GLN	CD-NE2	6.23	1.48	1.32
8	J	55	ASP	N-CA	6.23	1.58	1.46
2	B	575	PRO	CB-CG	-6.23	1.18	1.50
2	B	781	PHE	N-CA	-6.22	1.33	1.46
3	C	192	TRP	CG-CD1	-6.22	1.28	1.36
9	K	55	LYS	C-O	6.22	1.35	1.23
1	A	1206	ASP	CG-OD1	6.22	1.39	1.25
2	B	345	LYS	CB-CG	-6.22	1.35	1.52
2	B	730	ARG	NE-CZ	-6.22	1.25	1.33
4	E	2	ASP	CB-CG	6.22	1.64	1.51
7	I	81	ARG	CZ-NH1	6.22	1.41	1.33
2	B	969	ARG	CB-CG	-6.22	1.35	1.52
1	A	137	ALA	CA-CB	-6.22	1.39	1.52
1	A	1296	GLY	N-CA	6.22	1.55	1.46
8	J	48	ARG	CG-CD	-6.22	1.36	1.51
1	A	50	ILE	N-CA	6.21	1.58	1.46
3	C	181	ASP	C-N	-6.21	1.22	1.34
4	E	99	HIS	N-CA	6.21	1.58	1.46
6	H	141	TYR	CG-CD1	-6.21	1.31	1.39
1	A	1408	ILE	CG1-CD1	6.21	1.93	1.50
3	C	22	LEU	CA-CB	-6.21	1.39	1.53
4	E	167	ARG	CG-CD	6.21	1.67	1.51
3	C	180	TYR	CB-CG	-6.21	1.42	1.51
1	A	540	PHE	CA-CB	-6.21	1.40	1.53
1	A	660	ASN	CA-C	-6.21	1.36	1.52
1	A	1328	TYR	C-O	-6.21	1.11	1.23
2	B	31	TRP	NE1-CE2	-6.21	1.29	1.37
2	B	324	ILE	C-O	-6.21	1.11	1.23
2	B	644	GLU	CA-C	6.21	1.69	1.52
2	B	447	ALA	C-O	6.21	1.35	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	138	GLU	CD-OE1	6.21	1.32	1.25
9	K	70	ARG	CA-CB	-6.21	1.40	1.53
1	A	1067	LEU	CG-CD2	-6.20	1.28	1.51
2	B	667	GLN	C-O	6.20	1.35	1.23
2	B	995	ARG	CZ-NH1	6.20	1.41	1.33
3	C	123	ASN	CG-ND2	6.20	1.48	1.32
1	A	382	PRO	CA-C	-6.20	1.40	1.52
1	A	478	TYR	CD2-CE2	-6.20	1.30	1.39
1	A	1176	LEU	CG-CD2	6.20	1.74	1.51
2	B	586	TRP	CB-CG	-6.20	1.39	1.50
2	B	1021	MET	CG-SD	-6.20	1.65	1.81
4	E	11	ARG	CG-CD	6.20	1.67	1.51
2	B	998	ASP	CB-CG	-6.20	1.38	1.51
2	B	1013	ASN	C-N	-6.20	1.22	1.34
3	C	114	TYR	CG-CD1	-6.20	1.31	1.39
1	A	112	LYS	N-CA	-6.19	1.33	1.46
2	B	547	VAL	CA-CB	-6.19	1.41	1.54
1	A	87	ALA	CA-CB	-6.19	1.39	1.52
1	A	407	ARG	CZ-NH1	6.19	1.41	1.33
1	A	1064	VAL	C-N	6.19	1.44	1.33
2	B	563	MET	SD-CE	-6.19	1.43	1.77
7	I	103	CYS	CB-SG	6.19	1.92	1.82
1	A	527	THR	C-O	-6.19	1.11	1.23
2	B	573	GLN	CB-CG	6.19	1.69	1.52
6	H	96	VAL	CB-CG1	-6.19	1.39	1.52
1	A	1040	GLN	CD-NE2	6.19	1.48	1.32
2	B	201	GLY	C-O	6.19	1.33	1.23
1	A	630	ILE	CG1-CD1	-6.19	1.07	1.50
1	A	95	PHE	CG-CD1	6.18	1.48	1.38
1	A	1153	TYR	CA-CB	-6.18	1.40	1.53
7	I	15	TYR	CG-CD2	-6.18	1.31	1.39
1	A	575	LYS	CG-CD	-6.18	1.31	1.52
1	A	635	ARG	CD-NE	-6.18	1.35	1.46
1	A	649	ILE	CG1-CD1	-6.18	1.07	1.50
1	A	986	ILE	CA-C	-6.18	1.36	1.52
2	B	118	ARG	N-CA	-6.18	1.33	1.46
4	E	72	PHE	CE2-CZ	6.18	1.49	1.37
1	A	722	LEU	C-O	-6.18	1.11	1.23
3	C	219	PHE	C-O	6.18	1.35	1.23
7	I	70	ARG	CZ-NH2	-6.18	1.25	1.33
3	C	230	MET	SD-CE	-6.17	1.43	1.77
7	I	83	ASN	CG-OD1	6.17	1.37	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	THR	N-CA	6.17	1.58	1.46
1	A	233	TRP	CD2-CE2	-6.17	1.33	1.41
6	H	136	LYS	N-CA	6.17	1.58	1.46
7	I	6	PHE	CE1-CZ	-6.17	1.25	1.37
8	J	41	LEU	CA-C	-6.17	1.36	1.52
2	B	951	GLN	CD-NE2	6.17	1.48	1.32
7	I	29	CYS	CB-SG	6.17	1.92	1.82
7	I	120	GLN	C-O	6.17	1.35	1.23
1	A	109	HIS	CA-CB	6.17	1.67	1.53
1	A	705	LYS	CD-CE	6.17	1.66	1.51
6	H	36	CYS	N-CA	6.17	1.58	1.46
2	B	703	ILE	CA-CB	-6.16	1.40	1.54
2	B	410	GLY	C-N	-6.16	1.22	1.34
3	C	254	LYS	CA-C	-6.16	1.36	1.52
1	A	1228	TRP	CA-C	-6.16	1.36	1.52
2	B	1185	CYS	CA-CB	6.16	1.67	1.53
8	J	62	ARG	CA-C	-6.16	1.36	1.52
1	A	1221	LYS	CA-CB	6.16	1.67	1.53
2	B	594	ALA	C-O	-6.16	1.11	1.23
6	H	55	LEU	C-O	-6.16	1.11	1.23
1	A	760	GLN	CG-CD	6.16	1.65	1.51
1	A	829	VAL	CB-CG1	-6.16	1.40	1.52
2	B	512	ARG	CG-CD	-6.16	1.36	1.51
9	K	61	TYR	CB-CG	-6.16	1.42	1.51
1	A	26	GLU	CA-C	-6.16	1.36	1.52
2	B	845	SER	C-N	-6.16	1.19	1.34
3	C	88	CYS	CA-C	-6.16	1.36	1.52
1	A	463	ILE	CB-CG1	-6.15	1.36	1.54
2	B	216	GLU	CD-OE1	6.15	1.32	1.25
3	C	221	TYR	CD1-CE1	6.15	1.48	1.39
4	E	45	LYS	CE-NZ	6.15	1.64	1.49
7	I	24	ARG	CD-NE	6.15	1.56	1.46
1	A	448	PRO	CG-CD	-6.15	1.30	1.50
1	A	1173	HIS	N-CA	6.15	1.58	1.46
4	E	128	PRO	CA-C	6.15	1.65	1.52
2	B	532	ALA	N-CA	6.15	1.58	1.46
3	C	238	ILE	CA-C	-6.15	1.36	1.52
2	B	642	ASP	C-O	6.15	1.35	1.23
3	C	180	TYR	C-O	-6.15	1.11	1.23
6	H	34	ASP	CA-C	6.15	1.69	1.52
2	B	327	ARG	CB-CG	-6.15	1.35	1.52
2	B	241	ARG	CZ-NH1	6.14	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	118	PRO	CA-CB	6.14	1.65	1.53
4	E	212	ARG	CZ-NH1	-6.14	1.25	1.33
2	B	95	ILE	CA-C	-6.14	1.36	1.52
1	A	1113	THR	C-N	-6.14	1.22	1.34
2	B	1183	LYS	CA-C	6.14	1.69	1.52
9	K	46	ILE	CA-CB	-6.14	1.40	1.54
2	B	92	PHE	CD2-CE2	6.14	1.51	1.39
2	B	809	MET	N-CA	-6.13	1.34	1.46
4	E	42	PHE	CD1-CE1	6.13	1.51	1.39
6	H	111	LEU	CA-C	6.13	1.68	1.52
1	A	164	ARG	CB-CG	-6.13	1.35	1.52
2	B	763	GLN	CA-C	-6.13	1.37	1.52
2	B	916	THR	C-O	6.13	1.34	1.23
4	E	119	SER	C-O	6.13	1.34	1.23
7	I	3	THR	CA-C	-6.13	1.37	1.52
4	E	56	LYS	CA-CB	6.13	1.67	1.53
4	E	185	ALA	N-CA	-6.13	1.34	1.46
6	H	106	GLU	CD-OE2	6.13	1.32	1.25
7	I	51	ASN	CG-ND2	6.13	1.48	1.32
1	A	805	LEU	CG-CD1	-6.12	1.29	1.51
2	B	853	SER	CA-CB	-6.12	1.43	1.52
3	C	195	GLN	CD-NE2	6.12	1.48	1.32
2	B	129	PHE	CD2-CE2	-6.12	1.27	1.39
2	B	763	GLN	C-N	-6.12	1.20	1.34
1	A	1238	ILE	N-CA	-6.12	1.34	1.46
2	B	707	PRO	CB-CG	-6.12	1.19	1.50
2	B	966	VAL	C-O	-6.12	1.11	1.23
8	J	6	ARG	CZ-NH1	-6.12	1.25	1.33
1	A	357	PRO	C-O	6.12	1.35	1.23
2	B	591	ARG	CZ-NH1	6.12	1.41	1.33
2	B	781	PHE	CB-CG	-6.12	1.41	1.51
1	A	638	GLY	C-O	-6.11	1.13	1.23
2	B	401	PHE	CG-CD1	-6.11	1.29	1.38
7	I	101	PHE	CE2-CZ	-6.11	1.25	1.37
9	K	12	LEU	N-CA	6.11	1.58	1.46
7	I	93	LYS	C-O	6.11	1.34	1.23
1	A	1014	ALA	C-N	-6.11	1.20	1.34
1	A	629	LEU	C-O	-6.11	1.11	1.23
2	B	568	ASP	CA-CB	6.11	1.67	1.53
2	B	618	ASP	CG-OD1	6.11	1.39	1.25
1	A	585	GLY	N-CA	-6.11	1.36	1.46
6	H	41	ASP	CA-C	-6.11	1.37	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	941	LYS	C-O	6.11	1.34	1.23
3	C	123	ASN	C-N	-6.11	1.20	1.34
3	C	230	MET	C-O	-6.11	1.11	1.23
4	E	208	TYR	CE2-CZ	-6.11	1.30	1.38
1	A	968	GLN	CG-CD	6.10	1.65	1.51
1	A	46	THR	CB-CG2	6.10	1.72	1.52
1	A	603	ASN	CB-CG	-6.10	1.37	1.51
1	A	722	LEU	CG-CD1	-6.10	1.29	1.51
1	A	1134	ILE	C-O	6.10	1.34	1.23
8	J	56	LEU	N-CA	-6.10	1.34	1.46
1	A	286	HIS	CB-CG	6.10	1.61	1.50
1	A	404	TYR	CG-CD2	-6.10	1.31	1.39
3	C	83	SER	CA-CB	-6.10	1.43	1.52
1	A	518	LYS	CE-NZ	-6.10	1.33	1.49
1	A	1005	GLU	C-O	-6.10	1.11	1.23
1	A	133	LYS	CG-CD	6.10	1.73	1.52
2	B	489	SER	C-O	-6.10	1.11	1.23
2	B	1181	GLU	CD-OE2	-6.10	1.19	1.25
1	A	926	GLN	C-O	6.09	1.34	1.23
2	B	512	ARG	CA-C	6.09	1.68	1.52
2	B	1203	LEU	C-N	-6.09	1.20	1.34
7	I	40	SER	CA-C	-6.09	1.37	1.52
7	I	58	VAL	CB-CG1	-6.09	1.40	1.52
1	A	8	SER	CA-CB	6.09	1.62	1.52
1	A	567	LYS	CB-CG	-6.09	1.36	1.52
1	A	748	MET	CG-SD	6.09	1.97	1.81
2	B	306	ASN	CG-ND2	6.09	1.48	1.32
10	L	39	SER	C-O	6.09	1.34	1.23
1	A	504	LEU	CG-CD2	-6.09	1.29	1.51
2	B	70	ILE	CB-CG2	6.09	1.71	1.52
2	B	638	PHE	CD1-CE1	6.09	1.51	1.39
9	K	55	LYS	CB-CG	6.09	1.69	1.52
1	A	880	LYS	N-CA	-6.09	1.34	1.46
1	A	1129	GLU	CA-CB	6.09	1.67	1.53
1	A	1225	PHE	CA-CB	6.09	1.67	1.53
6	H	110	ASP	CB-CG	6.09	1.64	1.51
6	H	110	ASP	CG-OD2	6.09	1.39	1.25
2	B	586	TRP	C-N	-6.08	1.20	1.34
4	E	82	PHE	CE1-CZ	-6.08	1.25	1.37
1	A	19	PHE	CA-CB	-6.08	1.40	1.53
1	A	303	TYR	CB-CG	-6.08	1.42	1.51
1	A	1209	MET	CG-SD	-6.08	1.65	1.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1024	SER	N-CA	-6.08	1.34	1.46
1	A	974	ASP	N-CA	6.08	1.58	1.46
2	B	1146	PHE	CA-C	-6.08	1.37	1.52
2	B	1155	SER	CA-C	6.08	1.68	1.52
3	C	174	ALA	CA-CB	-6.08	1.39	1.52
4	E	7	ARG	CZ-NH2	6.08	1.41	1.33
1	A	16	GLU	C-O	6.08	1.34	1.23
1	A	588	LEU	CG-CD1	-6.08	1.29	1.51
9	K	33	ILE	CB-CG2	-6.07	1.34	1.52
5	F	154	ASP	CG-OD2	6.07	1.39	1.25
7	I	41	PRO	C-N	-6.07	1.20	1.34
1	A	884	ASP	CA-CB	6.07	1.67	1.53
2	B	281	PRO	CB-CG	-6.07	1.19	1.50
2	B	434	ARG	CD-NE	6.07	1.56	1.46
2	B	449	ASN	CG-ND2	6.07	1.48	1.32
1	A	1421	CYS	N-CA	-6.07	1.34	1.46
8	J	36	LEU	CA-C	-6.07	1.37	1.52
2	B	777	ALA	CA-CB	-6.07	1.39	1.52
1	A	84	ILE	CG1-CD1	-6.07	1.08	1.50
1	A	744	LYS	CA-C	-6.07	1.37	1.52
3	C	29	MET	CB-CG	6.07	1.70	1.51
1	A	644	LYS	CA-CB	-6.06	1.40	1.53
1	A	430	TRP	CA-C	-6.06	1.37	1.52
1	A	1108	ALA	CA-C	-6.06	1.37	1.52
1	A	1336	MET	CB-CG	-6.06	1.31	1.51
1	A	1355	VAL	CA-CB	-6.06	1.42	1.54
2	B	306	ASN	CB-CG	6.06	1.65	1.51
2	B	627	PHE	CA-C	-6.06	1.37	1.52
4	E	188	LEU	CA-C	6.06	1.68	1.52
5	F	153	VAL	CB-CG1	6.06	1.65	1.52
9	K	55	LYS	CD-CE	6.06	1.66	1.51
10	L	55	ILE	C-O	6.06	1.34	1.23
1	A	218	ASP	CG-OD2	6.06	1.39	1.25
1	A	1198	ASP	N-CA	6.06	1.58	1.46
6	H	111	LEU	N-CA	6.06	1.58	1.46
1	A	429	GLY	CA-C	6.06	1.61	1.51
2	B	89	GLU	CB-CG	6.06	1.63	1.52
6	H	40	LEU	CG-CD1	-6.06	1.29	1.51
1	A	123	ARG	CZ-NH1	6.06	1.41	1.33
1	A	1141	THR	CB-CG2	-6.06	1.32	1.52
2	B	197	PHE	CE2-CZ	-6.06	1.25	1.37
2	B	1193	GLN	CD-OE1	6.06	1.37	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	87	LEU	C-O	6.06	1.34	1.23
1	A	89	PRO	CA-C	-6.05	1.40	1.52
1	A	370	ILE	CB-CG2	-6.05	1.34	1.52
1	A	404	TYR	CD1-CE1	6.05	1.48	1.39
1	A	519	PRO	N-CA	-6.05	1.36	1.47
1	A	755	PHE	N-CA	-6.05	1.34	1.46
4	E	155	ARG	C-O	6.05	1.34	1.23
7	I	92	ARG	CA-C	6.05	1.68	1.52
1	A	719	VAL	CB-CG2	-6.05	1.40	1.52
1	A	911	SER	C-O	6.05	1.34	1.23
2	B	94	LYS	CA-C	6.05	1.68	1.52
1	A	157	ASP	CA-CB	6.05	1.67	1.53
1	A	207	ILE	CA-CB	6.05	1.68	1.54
2	B	380	TYR	CB-CG	6.05	1.60	1.51
2	B	268	THR	CB-CG2	-6.05	1.32	1.52
3	C	55	THR	C-O	6.04	1.34	1.23
2	B	68	THR	CA-CB	6.04	1.69	1.53
2	B	275	TYR	CZ-OH	-6.04	1.27	1.37
2	B	348	ARG	CZ-NH1	-6.04	1.25	1.33
1	A	758	ILE	CB-CG2	-6.04	1.34	1.52
4	E	46	TYR	CG-CD2	6.04	1.47	1.39
1	A	1121	GLU	CD-OE1	6.04	1.32	1.25
2	B	1156	ASP	CG-OD2	6.04	1.39	1.25
2	B	879	ARG	NE-CZ	6.04	1.41	1.33
2	B	899	ILE	CB-CG1	-6.04	1.37	1.54
6	H	38	LEU	CA-C	-6.04	1.37	1.52
10	L	47	ARG	CB-CG	6.04	1.68	1.52
1	A	777	PHE	CD2-CE2	6.04	1.51	1.39
1	A	1108	ALA	N-CA	-6.04	1.34	1.46
2	B	280	ILE	CA-CB	-6.04	1.41	1.54
2	B	1221	SER	CA-C	6.04	1.68	1.52
4	E	30	ILE	CB-CG2	6.04	1.71	1.52
1	A	1159	ARG	N-CA	6.03	1.58	1.46
2	B	836	GLU	CA-CB	-6.03	1.40	1.53
3	C	175	ALA	CA-CB	-6.03	1.39	1.52
2	B	113	TYR	CG-CD1	-6.03	1.31	1.39
1	A	555	ASP	CA-CB	6.03	1.67	1.53
4	E	23	VAL	CB-CG1	6.03	1.65	1.52
2	B	403	LYS	C-O	-6.03	1.11	1.23
2	B	511	PRO	CA-CB	-6.03	1.41	1.53
5	F	97	ARG	N-CA	-6.03	1.34	1.46
1	A	1128	GLN	CA-C	6.03	1.68	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1197	PRO	CG-CD	-6.03	1.30	1.50
7	I	110	PHE	CD2-CE2	6.03	1.51	1.39
1	A	200	ARG	C-O	-6.02	1.11	1.23
1	A	1333	ILE	CB-CG2	-6.02	1.34	1.52
2	B	24	PRO	CB-CG	-6.02	1.19	1.50
3	C	226	ASP	C-O	-6.02	1.11	1.23
8	J	48	ARG	CB-CG	-6.02	1.36	1.52
1	A	356	ASP	C-N	-6.02	1.22	1.34
2	B	1178	ASN	CB-CG	-6.02	1.37	1.51
4	E	9	ILE	CB-CG2	6.02	1.71	1.52
1	A	192	GLY	C-O	6.02	1.33	1.23
2	B	1043	ASP	CA-C	-6.02	1.37	1.52
1	A	691	LEU	CA-CB	-6.02	1.40	1.53
2	B	551	PRO	CB-CG	-6.01	1.19	1.50
3	C	7	GLN	CG-CD	-6.01	1.37	1.51
9	K	17	SER	CB-OG	6.01	1.50	1.42
9	K	73	LEU	CG-CD2	-6.01	1.29	1.51
1	A	172	PRO	C-O	-6.01	1.11	1.23
1	A	609	ASP	CB-CG	6.01	1.64	1.51
1	A	819	GLY	C-O	-6.01	1.14	1.23
2	B	623	GLU	C-O	-6.01	1.11	1.23
4	E	183	PRO	N-CA	-6.01	1.37	1.47
1	A	1231	ASP	CB-CG	-6.01	1.39	1.51
2	B	124	TYR	CD1-CE1	6.01	1.48	1.39
2	B	700	SER	C-O	-6.01	1.11	1.23
2	B	449	ASN	CG-OD1	6.00	1.37	1.24
1	A	1139	GLU	CA-C	-6.00	1.37	1.52
2	B	259	TYR	CE2-CZ	-6.00	1.30	1.38
2	B	1102	LYS	C-O	6.00	1.34	1.23
6	H	9	ILE	CG1-CD1	6.00	1.91	1.50
1	A	222	LEU	C-O	6.00	1.34	1.23
1	A	731	ARG	CA-C	-6.00	1.37	1.52
1	A	864	ILE	N-CA	-6.00	1.34	1.46
1	A	500	GLU	CD-OE2	6.00	1.32	1.25
1	A	904	THR	C-O	-6.00	1.11	1.23
2	B	310	MET	CB-CG	-6.00	1.32	1.51
9	K	68	PHE	CG-CD1	-6.00	1.29	1.38
1	A	424	ILE	CB-CG2	-6.00	1.34	1.52
1	A	580	VAL	CA-CB	-6.00	1.42	1.54
2	B	49	ASP	C-N	-6.00	1.20	1.34
2	B	854	LEU	C-O	-6.00	1.11	1.23
5	F	97	ARG	CZ-NH2	-6.00	1.25	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	33	GLU	CG-CD	6.00	1.60	1.51
2	B	709	ASP	C-O	-6.00	1.11	1.23
4	E	4	GLU	CG-CD	5.99	1.60	1.51
1	A	457	ALA	C-O	-5.99	1.11	1.23
2	B	1002	THR	CA-C	5.99	1.68	1.52
1	A	62	ASP	CB-CG	5.99	1.64	1.51
2	B	167	ILE	C-O	5.99	1.34	1.23
2	B	428	ILE	CG1-CD1	5.99	1.91	1.50
2	B	902	GLY	C-O	5.99	1.33	1.23
3	C	33	LEU	CG-CD1	-5.99	1.29	1.51
3	C	113	VAL	CB-CG1	-5.99	1.40	1.52
3	C	81	GLU	CG-CD	5.99	1.60	1.51
1	A	1003	LYS	CB-CG	5.99	1.68	1.52
6	H	81	PRO	CG-CD	5.99	1.70	1.50
7	I	69	PRO	N-CA	-5.99	1.37	1.47
8	J	21	TYR	CA-CB	5.99	1.67	1.53
2	B	612	GLU	CG-CD	5.98	1.60	1.51
5	F	150	GLU	CD-OE1	5.98	1.32	1.25
1	A	836	TYR	CA-CB	-5.98	1.40	1.53
2	B	44	VAL	CB-CG2	-5.98	1.40	1.52
2	B	200	GLY	CA-C	-5.98	1.42	1.51
2	B	766	ARG	CB-CG	-5.98	1.36	1.52
2	B	1151	LEU	CG-CD1	-5.98	1.29	1.51
9	K	61	TYR	N-CA	-5.98	1.34	1.46
1	A	1290	LYS	CA-CB	-5.98	1.40	1.53
2	B	435	THR	CA-CB	5.98	1.68	1.53
2	B	633	VAL	CB-CG1	-5.98	1.40	1.52
1	A	233	TRP	CD2-CE3	-5.98	1.31	1.40
1	A	842	VAL	CB-CG2	-5.98	1.40	1.52
2	B	885	MET	CG-SD	5.98	1.96	1.81
2	B	1148	LYS	CG-CD	5.98	1.72	1.52
1	A	762	SER	C-O	-5.97	1.11	1.23
2	B	347	LYS	CE-NZ	5.97	1.64	1.49
4	E	19	VAL	CB-CG2	-5.97	1.40	1.52
5	F	127	GLU	CD-OE1	5.97	1.32	1.25
1	A	153	PRO	C-O	5.97	1.35	1.23
1	A	351	THR	CB-CG2	-5.97	1.32	1.52
1	A	455	MET	N-CA	5.97	1.58	1.46
1	A	526	ASP	CB-CG	5.97	1.64	1.51
1	A	576	GLN	CA-C	-5.97	1.37	1.52
2	B	983	ARG	CD-NE	-5.97	1.36	1.46
2	B	1178	ASN	CG-ND2	5.97	1.47	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1261	LYS	CG-CD	5.97	1.72	1.52
2	B	876	LYS	C-O	-5.97	1.12	1.23
7	I	1	MET	SD-CE	5.97	2.11	1.77
1	A	54	ASN	CB-CG	5.97	1.64	1.51
1	A	386	ASP	CA-CB	5.97	1.67	1.53
1	A	1298	TYR	CB-CG	-5.97	1.42	1.51
2	B	862	GLN	CD-OE1	5.97	1.37	1.24
1	A	626	ASN	CG-ND2	5.97	1.47	1.32
2	B	240	ILE	CA-C	-5.97	1.37	1.52
2	B	626	ILE	CA-CB	-5.97	1.41	1.54
2	B	1004	GLU	C-O	5.97	1.34	1.23
1	A	817	ALA	CA-C	-5.96	1.37	1.52
4	E	42	PHE	CD2-CE2	5.96	1.51	1.39
4	E	122	LYS	CB-CG	5.96	1.68	1.52
2	B	457	LEU	CG-CD2	5.96	1.74	1.51
1	A	206	GLU	CG-CD	5.96	1.60	1.51
1	A	1288	ASP	N-CA	5.96	1.58	1.46
2	B	656	GLY	C-N	5.96	1.47	1.34
2	B	1213	THR	C-O	-5.96	1.12	1.23
8	J	22	LEU	CA-C	5.96	1.68	1.52
6	H	11	GLN	CA-CB	5.96	1.67	1.53
1	A	228	PHE	CE2-CZ	-5.96	1.26	1.37
1	A	801	GLU	CG-CD	-5.96	1.43	1.51
1	A	985	ASP	CA-C	5.96	1.68	1.52
1	A	1019	CYS	CA-CB	-5.96	1.40	1.53
1	A	1265	ASN	CB-CG	5.96	1.64	1.51
7	I	105	SER	N-CA	5.96	1.58	1.46
3	C	267	GLN	CA-CB	5.96	1.67	1.53
1	A	58	LEU	CG-CD2	-5.95	1.29	1.51
1	A	737	LEU	C-O	5.95	1.34	1.23
1	A	1141	THR	CA-CB	-5.95	1.37	1.53
4	E	163	GLU	CD-OE2	-5.95	1.19	1.25
1	A	815	PHE	CD1-CE1	-5.95	1.27	1.39
9	K	30	ALA	C-O	-5.95	1.12	1.23
1	A	65	LEU	CA-CB	5.95	1.67	1.53
1	A	1341	ILE	CA-C	-5.95	1.37	1.52
1	A	624	SER	CB-OG	5.95	1.50	1.42
1	A	918	GLU	N-CA	-5.95	1.34	1.46
1	A	1018	PHE	CE1-CZ	-5.95	1.26	1.37
1	A	615	GLY	C-O	-5.94	1.14	1.23
2	B	1130	PHE	CA-C	-5.94	1.37	1.52
4	E	111	VAL	CA-CB	-5.94	1.42	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	59	VAL	CA-CB	-5.94	1.42	1.54
1	A	614	PHE	CB-CG	-5.94	1.41	1.51
2	B	828	ALA	CA-CB	-5.94	1.40	1.52
9	K	39	ASP	CA-CB	-5.94	1.40	1.53
4	E	32	GLN	C-O	-5.94	1.12	1.23
2	B	1100	ASP	C-O	5.94	1.34	1.23
3	C	251	LEU	C-O	-5.93	1.12	1.23
5	F	86	THR	C-O	-5.93	1.12	1.23
1	A	277	GLU	CG-CD	5.93	1.60	1.51
2	B	591	ARG	CG-CD	5.93	1.66	1.51
2	B	645	SER	C-O	-5.93	1.12	1.23
4	E	191	LYS	C-O	-5.93	1.12	1.23
1	A	209	ASN	CA-C	-5.93	1.37	1.52
1	A	893	PHE	CA-C	-5.93	1.37	1.52
1	A	1093	LYS	CB-CG	5.93	1.68	1.52
1	A	1411	GLU	CD-OE1	5.93	1.32	1.25
1	A	1433	MET	CB-CG	-5.93	1.32	1.51
2	B	336	ARG	C-O	5.93	1.34	1.23
3	C	35	ARG	NE-CZ	-5.93	1.25	1.33
5	F	121	ALA	C-N	-5.93	1.20	1.34
1	A	179	LEU	C-O	5.93	1.34	1.23
1	A	847	ASP	CG-OD2	5.93	1.39	1.25
6	H	104	PHE	CB-CG	5.93	1.61	1.51
1	A	239	LEU	N-CA	-5.92	1.34	1.46
1	A	49	LYS	CB-CG	5.92	1.68	1.52
1	A	141	LEU	N-CA	-5.92	1.34	1.46
2	B	39	ARG	C-O	-5.92	1.12	1.23
2	B	752	ALA	CA-CB	5.92	1.64	1.52
2	B	446	LEU	CA-C	5.92	1.68	1.52
3	C	129	ILE	CB-CG2	5.92	1.71	1.52
2	B	1006	ILE	CB-CG2	-5.92	1.34	1.52
9	K	55	LYS	CG-CD	5.92	1.72	1.52
2	B	598	GLU	CB-CG	5.92	1.63	1.52
2	B	1135	ARG	CZ-NH1	5.92	1.40	1.33
3	C	249	ASP	CG-OD1	5.92	1.39	1.25
1	A	163	SER	CA-C	-5.92	1.37	1.52
1	A	424	ILE	CA-C	-5.92	1.37	1.52
1	A	731	ARG	CG-CD	5.92	1.66	1.51
1	A	737	LEU	CG-CD1	-5.92	1.29	1.51
2	B	643	ASP	CA-C	-5.92	1.37	1.52
2	B	859	TYR	CG-CD2	-5.92	1.31	1.39
4	E	192	ARG	CZ-NH2	5.92	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	110	THR	CA-CB	5.92	1.68	1.53
7	I	70	ARG	CA-CB	-5.92	1.41	1.53
2	B	330	ALA	CA-CB	-5.91	1.40	1.52
3	C	126	GLY	N-CA	5.91	1.54	1.46
1	A	16	GLU	CB-CG	-5.91	1.41	1.52
1	A	167	CYS	CA-CB	5.91	1.67	1.53
1	A	462	VAL	N-CA	5.91	1.58	1.46
2	B	24	PRO	N-CA	-5.91	1.37	1.47
3	C	35	ARG	CB-CG	5.91	1.68	1.52
1	A	1136	SER	C-O	5.91	1.34	1.23
5	F	128	LYS	CG-CD	5.91	1.72	1.52
6	H	86	ASP	CA-CB	5.91	1.67	1.53
2	B	1177	HIS	CB-CG	-5.91	1.39	1.50
1	A	644	LYS	C-O	-5.91	1.12	1.23
1	A	1303	GLU	CG-CD	5.91	1.60	1.51
1	A	883	LEU	N-CA	-5.90	1.34	1.46
2	B	329	THR	CA-CB	-5.90	1.38	1.53
2	B	707	PRO	CA-CB	-5.90	1.41	1.53
2	B	972	LYS	CA-CB	-5.90	1.41	1.53
1	A	805	LEU	CB-CG	-5.90	1.35	1.52
2	B	92	PHE	CA-CB	5.90	1.67	1.53
2	B	708	GLU	CG-CD	5.90	1.60	1.51
2	B	742	GLU	N-CA	-5.90	1.34	1.46
3	C	104	PHE	CB-CG	-5.90	1.41	1.51
1	A	1374	VAL	CA-CB	-5.90	1.42	1.54
3	C	183	TRP	CD2-CE3	-5.90	1.31	1.40
2	B	1171	VAL	CB-CG1	-5.90	1.40	1.52
8	J	43	ARG	CZ-NH1	-5.90	1.25	1.33
1	A	985	ASP	CG-OD1	5.90	1.39	1.25
3	C	201	TRP	CD2-CE2	-5.90	1.34	1.41
1	A	611	GLN	CD-OE1	5.89	1.36	1.24
1	A	821	ARG	N-CA	-5.89	1.34	1.46
1	A	1063	MET	C-O	-5.89	1.12	1.23
1	A	1450	LEU	CB-CG	5.89	1.69	1.52
2	B	205	ILE	CA-CB	-5.89	1.41	1.54
2	B	411	PRO	N-CA	-5.89	1.37	1.47
2	B	916	THR	N-CA	5.89	1.58	1.46
2	B	1181	GLU	CB-CG	5.89	1.63	1.52
1	A	542	GLU	CD-OE1	5.89	1.32	1.25
1	A	912	LEU	C-O	-5.89	1.12	1.23
2	B	128	LEU	CA-CB	-5.89	1.40	1.53
2	B	533	CYS	CA-CB	-5.89	1.41	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	94	LYS	CG-CD	5.89	1.72	1.52
4	E	131	THR	CA-C	-5.89	1.37	1.52
8	J	4	PRO	CG-CD	-5.89	1.31	1.50
2	B	528	PRO	CG-CD	-5.89	1.31	1.50
2	B	576	ASP	CB-CG	5.89	1.64	1.51
1	A	580	VAL	CB-CG1	-5.89	1.40	1.52
2	B	855	PHE	C-O	-5.89	1.12	1.23
6	H	129	TYR	CZ-OH	5.89	1.47	1.37
9	K	15	GLY	CA-C	5.89	1.61	1.51
9	K	70	ARG	C-O	-5.89	1.12	1.23
1	A	1333	ILE	CA-CB	-5.89	1.41	1.54
2	B	814	PHE	CB-CG	-5.89	1.41	1.51
2	B	1109	GLY	C-O	5.89	1.33	1.23
2	B	127	GLY	CA-C	-5.89	1.42	1.51
2	B	315	LYS	CD-CE	5.89	1.66	1.51
8	J	32	GLU	CD-OE1	5.89	1.32	1.25
9	K	96	ASN	CB-CG	5.89	1.64	1.51
1	A	387	ARG	CA-C	5.88	1.68	1.52
1	A	1305	VAL	CA-CB	-5.88	1.42	1.54
2	B	406	LEU	C-O	5.88	1.34	1.23
3	C	187	LYS	CB-CG	-5.88	1.36	1.52
5	F	146	TRP	CD2-CE3	-5.88	1.31	1.40
1	A	976	THR	CB-OG1	5.88	1.55	1.43
9	K	15	GLY	C-O	5.88	1.33	1.23
2	B	489	SER	CA-C	-5.88	1.37	1.52
9	K	28	PRO	C-O	-5.88	1.11	1.23
1	A	701	LEU	CG-CD1	5.88	1.73	1.51
1	A	852	TYR	CD2-CE2	-5.88	1.30	1.39
2	B	996	ARG	C-O	5.88	1.34	1.23
2	B	1108	ARG	C-O	5.88	1.34	1.23
1	A	33	ALA	C-O	-5.88	1.12	1.23
1	A	513	SER	C-O	-5.88	1.12	1.23
2	B	809	MET	CG-SD	5.88	1.96	1.81
2	B	964	VAL	CB-CG2	5.88	1.65	1.52
2	B	1173	ALA	C-O	5.88	1.34	1.23
2	B	415	GLN	CD-OE1	5.88	1.36	1.24
1	A	133	LYS	CA-CB	-5.87	1.41	1.53
1	A	1255	GLU	CB-CG	5.87	1.63	1.52
1	A	1440	ALA	C-O	5.87	1.34	1.23
2	B	18	PHE	CA-C	5.87	1.68	1.52
2	B	231	PRO	CB-CG	5.87	1.79	1.50
2	B	437	GLU	N-CA	5.87	1.58	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	108	PHE	CA-CB	-5.87	1.41	1.53
1	A	738	LYS	CD-CE	5.87	1.66	1.51
1	A	799	PHE	CE2-CZ	-5.87	1.26	1.37
2	B	203	PHE	CD1-CE1	-5.87	1.27	1.39
2	B	581	PHE	CD2-CE2	-5.87	1.27	1.39
4	E	14	ARG	CZ-NH2	-5.87	1.25	1.33
3	C	102	GLN	CA-C	-5.87	1.37	1.52
4	E	161	LYS	CB-CG	-5.87	1.36	1.52
2	B	519	TRP	CE2-CZ2	-5.87	1.29	1.39
4	E	162	ARG	CZ-NH2	5.87	1.40	1.33
2	B	251	ILE	CA-CB	5.87	1.68	1.54
4	E	23	VAL	N-CA	-5.87	1.34	1.46
8	J	62	ARG	CG-CD	-5.87	1.37	1.51
1	A	214	ILE	C-O	5.86	1.34	1.23
9	K	90	ALA	CA-CB	-5.86	1.40	1.52
1	A	381	THR	C-O	-5.86	1.12	1.23
1	A	1070	GLN	CB-CG	-5.86	1.36	1.52
2	B	652	LYS	CG-CD	5.86	1.72	1.52
2	B	847	ASP	CB-CG	5.86	1.64	1.51
4	E	192	ARG	CG-CD	5.86	1.66	1.51
10	L	32	ALA	C-O	5.86	1.34	1.23
2	B	1029	CYS	CA-C	5.86	1.68	1.52
3	C	79	GLN	C-N	-5.86	1.20	1.34
6	H	21	ASN	CA-C	-5.86	1.37	1.52
1	A	1035	TYR	CB-CG	-5.86	1.42	1.51
1	A	940	ARG	CZ-NH1	-5.86	1.25	1.33
2	B	1048	THR	CA-C	-5.86	1.37	1.52
3	C	70	ILE	CA-C	-5.86	1.37	1.52
4	E	20	LYS	CB-CG	5.86	1.68	1.52
2	B	422	LYS	CD-CE	5.85	1.65	1.51
6	H	84	ALA	C-N	5.85	1.43	1.33
1	A	945	GLU	CG-CD	5.85	1.60	1.51
1	A	1053	PHE	CE2-CZ	-5.85	1.26	1.37
3	C	56	THR	C-O	-5.85	1.12	1.23
3	C	214	ASN	CG-OD1	5.85	1.36	1.24
6	H	79	TRP	CA-CB	-5.85	1.41	1.53
3	C	169	LYS	CA-CB	-5.85	1.41	1.53
2	B	833	TYR	C-O	-5.85	1.12	1.23
1	A	273	ASN	CG-ND2	5.84	1.47	1.32
1	A	646	PHE	CG-CD2	-5.84	1.29	1.38
2	B	478	GLY	N-CA	5.84	1.54	1.46
2	B	1165	ILE	CA-C	5.84	1.68	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	84	ALA	C-O	5.84	1.34	1.23
6	H	86	ASP	CB-CG	5.84	1.64	1.51
9	K	58	PHE	CE2-CZ	5.84	1.48	1.37
1	A	1109	LYS	CE-NZ	5.84	1.63	1.49
2	B	497	ARG	CZ-NH2	5.84	1.40	1.33
2	B	1158	PHE	CE1-CZ	5.84	1.48	1.37
3	C	87	PHE	C-O	-5.84	1.12	1.23
10	L	26	THR	C-O	5.84	1.34	1.23
2	B	511	PRO	CA-C	-5.84	1.41	1.52
1	A	666	ILE	CA-CB	-5.83	1.41	1.54
1	A	831	THR	CB-OG1	5.83	1.54	1.43
2	B	100	PRO	CB-CG	-5.83	1.20	1.50
2	B	1171	VAL	CB-CG2	-5.83	1.40	1.52
5	F	106	PRO	CB-CG	5.83	1.79	1.50
1	A	941	LYS	N-CA	-5.83	1.34	1.46
1	A	1315	GLU	C-N	-5.83	1.20	1.34
2	B	182	SER	CB-OG	-5.83	1.34	1.42
2	B	345	LYS	CG-CD	5.83	1.72	1.52
7	I	23	ASN	CG-ND2	5.83	1.47	1.32
2	B	550	ASP	CA-C	-5.83	1.37	1.52
1	A	149	GLU	CA-C	-5.83	1.37	1.52
4	E	202	SER	CA-CB	-5.83	1.44	1.52
9	K	35	PHE	C-O	-5.83	1.12	1.23
2	B	203	PHE	CB-CG	-5.83	1.41	1.51
4	E	152	LYS	CG-CD	5.83	1.72	1.52
2	B	809	MET	CA-C	-5.83	1.37	1.52
2	B	835	GLN	CD-OE1	-5.83	1.11	1.24
6	H	34	ASP	C-O	5.83	1.34	1.23
1	A	491	VAL	C-O	-5.82	1.12	1.23
2	B	766	ARG	NE-CZ	-5.82	1.25	1.33
4	E	11	ARG	CB-CG	5.82	1.68	1.52
4	E	79	TRP	CD2-CE3	5.82	1.49	1.40
1	A	986	ILE	C-O	-5.82	1.12	1.23
1	A	1118	VAL	N-CA	-5.82	1.34	1.46
1	A	220	THR	CA-C	-5.82	1.37	1.52
1	A	432	VAL	C-O	-5.82	1.12	1.23
2	B	811	TYR	CA-CB	5.82	1.66	1.53
1	A	93	VAL	C-N	-5.82	1.22	1.33
2	B	205	ILE	CG1-CD1	-5.82	1.10	1.50
2	B	1178	ASN	C-O	5.82	1.34	1.23
1	A	298	PHE	CE2-CZ	5.82	1.48	1.37
1	A	850	VAL	C-O	-5.82	1.12	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1057	VAL	CB-CG1	-5.82	1.40	1.52
7	I	9	ASP	CG-OD2	5.82	1.38	1.25
1	A	742	ASN	CB-CG	-5.82	1.37	1.51
2	B	365	THR	CB-CG2	-5.82	1.33	1.52
2	B	1048	THR	C-O	-5.82	1.12	1.23
2	B	1154	ALA	C-N	5.82	1.47	1.34
3	C	230	MET	CB-CG	5.82	1.70	1.51
6	H	79	TRP	CZ2-CH2	-5.82	1.26	1.37
1	A	1063	MET	CG-SD	-5.81	1.66	1.81
2	B	557	PHE	N-CA	-5.81	1.34	1.46
4	E	33	GLU	CD-OE2	5.81	1.32	1.25
4	E	102	GLU	C-O	5.81	1.34	1.23
1	A	403	LYS	N-CA	-5.81	1.34	1.46
1	A	826	ASP	CG-OD2	5.81	1.38	1.25
2	B	778	MET	CB-CG	-5.81	1.32	1.51
4	E	14	ARG	CA-CB	-5.81	1.41	1.53
1	A	508	PRO	CG-CD	5.81	1.69	1.50
2	B	370	PHE	CE1-CZ	5.81	1.48	1.37
6	H	124	ARG	NE-CZ	-5.81	1.25	1.33
10	L	28	LYS	CA-C	5.81	1.68	1.52
1	A	600	PRO	CA-C	-5.81	1.41	1.52
4	E	138	ALA	C-O	-5.81	1.12	1.23
8	J	6	ARG	C-O	5.81	1.34	1.23
2	B	1211	ASN	N-CA	5.81	1.57	1.46
1	A	1141	THR	C-O	5.80	1.34	1.23
1	A	1263	ILE	CB-CG2	-5.80	1.34	1.52
1	A	1368	MET	SD-CE	-5.80	1.45	1.77
2	B	283	VAL	CA-CB	-5.80	1.42	1.54
2	B	572	HIS	C-O	-5.80	1.12	1.23
3	C	178	PHE	CB-CG	-5.80	1.41	1.51
1	A	734	GLU	CB-CG	5.80	1.63	1.52
2	B	112	LEU	C-O	-5.80	1.12	1.23
2	B	804	GLY	N-CA	5.80	1.54	1.46
2	B	1175	LEU	N-CA	5.80	1.57	1.46
2	B	628	THR	C-O	5.80	1.34	1.23
3	C	52	GLU	CA-CB	5.80	1.66	1.53
3	C	61	GLU	CD-OE2	-5.80	1.19	1.25
6	H	121	LEU	C-O	5.80	1.34	1.23
1	A	964	ILE	CG1-CD1	-5.80	1.10	1.50
1	A	1449	SER	C-O	5.80	1.34	1.23
3	C	170	TRP	CE2-CZ2	-5.80	1.29	1.39
6	H	133	ASN	C-O	5.80	1.34	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	24	LEU	CA-CB	-5.80	1.40	1.53
9	K	66	PRO	N-CA	-5.80	1.37	1.47
1	A	1119	TYR	CE1-CZ	-5.79	1.31	1.38
4	E	52	ARG	CD-NE	5.79	1.56	1.46
1	A	563	PRO	C-O	-5.79	1.11	1.23
1	A	977	LYS	CD-CE	5.79	1.65	1.51
1	A	1222	ASN	CA-C	5.79	1.68	1.52
2	B	865	LYS	CE-NZ	-5.79	1.34	1.49
4	E	21	GLU	CA-CB	-5.79	1.41	1.53
1	A	418	SER	CA-CB	-5.79	1.44	1.52
1	A	1206	ASP	C-O	5.79	1.34	1.23
2	B	33	VAL	C-O	-5.79	1.12	1.23
2	B	822	ASN	C-O	-5.79	1.12	1.23
4	E	186	LEU	C-N	-5.79	1.20	1.34
2	B	940	PRO	N-CD	-5.79	1.39	1.47
2	B	1079	LYS	CA-C	-5.79	1.38	1.52
9	K	20	LYS	CB-CG	5.79	1.68	1.52
1	A	248	PRO	CA-C	5.79	1.64	1.52
1	A	1195	LEU	C-N	-5.79	1.20	1.34
3	C	87	PHE	CA-CB	-5.79	1.41	1.53
6	H	29	ALA	CA-CB	-5.79	1.40	1.52
1	A	1242	VAL	CA-CB	-5.79	1.42	1.54
2	B	177	LYS	C-O	5.79	1.34	1.23
2	B	1186	ASP	C-O	5.79	1.34	1.23
7	I	50	THR	CA-C	-5.79	1.38	1.52
1	A	1071	SER	N-CA	-5.78	1.34	1.46
2	B	1176	ASN	CG-ND2	5.78	1.47	1.32
1	A	1034	GLU	CA-CB	-5.78	1.41	1.53
1	A	1359	ASP	CA-C	-5.78	1.38	1.52
1	A	996	ASN	CA-C	5.78	1.68	1.52
2	B	1011	ILE	CA-CB	5.78	1.68	1.54
7	I	9	ASP	CB-CG	5.78	1.63	1.51
1	A	244	PRO	CA-C	5.78	1.64	1.52
1	A	568	PRO	N-CD	-5.78	1.39	1.47
1	A	940	ARG	CA-CB	-5.78	1.41	1.53
1	A	1070	GLN	N-CA	-5.78	1.34	1.46
1	A	1236	LEU	CA-C	-5.78	1.38	1.52
1	A	1446	ASP	CG-OD2	5.78	1.38	1.25
1	A	1100	ARG	CB-CG	5.78	1.68	1.52
2	B	641	GLU	CB-CG	5.78	1.63	1.52
8	J	8	PHE	CB-CG	-5.78	1.41	1.51
3	C	67	LEU	CG-CD1	-5.77	1.30	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	104	LEU	CG-CD2	-5.77	1.30	1.51
1	A	326	ARG	CD-NE	5.77	1.56	1.46
1	A	380	VAL	CA-CB	-5.77	1.42	1.54
1	A	698	GLN	CD-NE2	5.77	1.47	1.32
1	A	1227	ILE	CA-C	-5.77	1.38	1.52
6	H	16	ASP	CG-OD2	5.77	1.38	1.25
1	A	874	ASP	CB-CG	5.77	1.63	1.51
2	B	345	LYS	CA-CB	-5.77	1.41	1.53
2	B	1099	VAL	C-O	-5.77	1.12	1.23
1	A	393	ARG	CA-C	-5.77	1.38	1.52
1	A	1223	ASP	N-CA	5.77	1.57	1.46
2	B	934	LYS	C-O	5.77	1.34	1.23
7	I	43	VAL	CA-C	-5.77	1.38	1.52
1	A	519	PRO	C-O	-5.77	1.11	1.23
4	E	212	ARG	CD-NE	-5.77	1.36	1.46
1	A	968	GLN	CB-CG	-5.76	1.36	1.52
1	A	1162	VAL	N-CA	-5.76	1.34	1.46
6	H	18	GLY	C-O	-5.76	1.14	1.23
8	J	27	GLU	CG-CD	5.76	1.60	1.51
1	A	537	ARG	CG-CD	-5.76	1.37	1.51
1	A	919	ILE	CA-CB	5.76	1.68	1.54
1	A	443	LEU	CA-C	-5.76	1.38	1.52
1	A	471	ASN	CG-ND2	-5.76	1.18	1.32
2	B	307	ASP	CB-CG	-5.76	1.39	1.51
1	A	1030	ARG	CZ-NH2	-5.76	1.25	1.33
2	B	30	SER	CA-CB	-5.76	1.44	1.52
1	A	769	SER	CA-CB	-5.76	1.44	1.52
1	A	1363	VAL	C-O	5.76	1.34	1.23
1	A	180	LYS	CE-NZ	5.76	1.63	1.49
1	A	1332	PHE	N-CA	-5.76	1.34	1.46
2	B	400	HIS	CB-CG	-5.76	1.39	1.50
3	C	260	LEU	CG-CD1	5.76	1.73	1.51
1	A	650	GLN	CD-NE2	-5.75	1.18	1.32
1	A	652	VAL	N-CA	-5.75	1.34	1.46
1	A	711	ARG	C-O	-5.75	1.12	1.23
9	K	44	ASN	C-O	5.75	1.34	1.23
1	A	1100	ARG	CZ-NH1	-5.75	1.25	1.33
2	B	232	SER	CA-CB	-5.75	1.44	1.52
2	B	282	ILE	CA-CB	-5.75	1.41	1.54
3	C	142	VAL	CA-CB	-5.75	1.42	1.54
1	A	1060	PRO	N-CD	-5.75	1.39	1.47
7	I	39	GLY	C-O	5.75	1.32	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	GLY	N-CA	5.75	1.54	1.46
1	A	736	ASN	C-N	-5.75	1.20	1.34
1	A	764	CYS	CA-CB	-5.75	1.41	1.53
2	B	221	ASN	CG-ND2	5.75	1.47	1.32
1	A	84	ILE	CB-CG2	-5.75	1.35	1.52
1	A	105	CYS	N-CA	5.75	1.57	1.46
1	A	845	LEU	CG-CD2	-5.75	1.30	1.51
2	B	411	PRO	CB-CG	-5.75	1.21	1.50
2	B	846	ILE	C-O	5.75	1.34	1.23
2	B	304	ASP	CG-OD2	5.75	1.38	1.25
2	B	518	HIS	CA-CB	-5.75	1.41	1.53
2	B	1173	ALA	CA-CB	-5.75	1.40	1.52
4	E	61	GLN	CA-CB	5.75	1.66	1.53
4	E	89	GLY	C-O	5.75	1.32	1.23
3	C	3	GLU	CA-CB	-5.74	1.41	1.53
3	C	177	GLU	C-O	-5.74	1.12	1.23
7	I	121	PHE	CD1-CE1	-5.74	1.27	1.39
2	B	281	PRO	N-CD	-5.74	1.39	1.47
2	B	972	LYS	CE-NZ	5.74	1.63	1.49
3	C	267	GLN	CD-OE1	5.74	1.36	1.24
7	I	121	PHE	CG-CD2	-5.74	1.30	1.38
2	B	696	GLU	CB-CG	5.74	1.63	1.52
2	B	907	GLY	CA-C	5.74	1.61	1.51
9	K	34	THR	CA-C	-5.74	1.38	1.52
2	B	430	ARG	NE-CZ	5.74	1.40	1.33
3	C	170	TRP	CD2-CE2	-5.74	1.34	1.41
4	E	133	GLU	C-O	5.74	1.34	1.23
2	B	20	ASP	N-CA	5.74	1.57	1.46
1	A	120	GLU	CD-OE2	5.74	1.31	1.25
2	B	351	TYR	CZ-OH	5.74	1.47	1.37
10	L	63	ARG	CA-CB	5.73	1.66	1.53
1	A	1072	ILE	C-O	-5.73	1.12	1.23
1	A	1349	TYR	C-N	-5.73	1.20	1.34
2	B	350	GLN	CD-OE1	5.73	1.36	1.24
3	C	34	ARG	CZ-NH2	5.73	1.40	1.33
3	C	263	THR	C-O	-5.73	1.12	1.23
9	K	88	LYS	CB-CG	5.73	1.68	1.52
2	B	839	MET	C-O	-5.73	1.12	1.23
2	B	1168	LEU	N-CA	5.73	1.57	1.46
1	A	179	LEU	CA-CB	5.72	1.67	1.53
1	A	727	ASP	CA-CB	-5.72	1.41	1.53
1	A	1283	VAL	CB-CG1	-5.72	1.40	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	868	MET	CB-CG	5.72	1.69	1.51
2	B	1051	THR	N-CA	-5.72	1.34	1.46
6	H	13	SER	CB-OG	5.72	1.49	1.42
2	B	738	PHE	C-O	5.72	1.34	1.23
2	B	884	ARG	CB-CG	5.72	1.68	1.52
2	B	1045	SER	C-N	-5.72	1.23	1.34
3	C	166	GLU	CB-CG	5.72	1.63	1.52
1	A	32	VAL	CB-CG1	5.72	1.64	1.52
2	B	1192	TYR	CE1-CZ	-5.72	1.31	1.38
1	A	635	ARG	C-O	-5.72	1.12	1.23
1	A	738	LYS	N-CA	-5.72	1.34	1.46
3	C	29	MET	SD-CE	5.72	2.09	1.77
9	K	89	ASN	CB-CG	5.72	1.64	1.51
1	A	619	LYS	CD-CE	5.71	1.65	1.51
1	A	900	ASP	C-O	5.71	1.34	1.23
2	B	104	GLU	C-O	5.71	1.34	1.23
2	B	417	PHE	CB-CG	-5.71	1.41	1.51
2	B	768	THR	CB-CG2	-5.71	1.33	1.52
2	B	851	PHE	C-O	-5.71	1.12	1.23
3	C	192	TRP	CZ3-CH2	5.71	1.49	1.40
1	A	468	PHE	CB-CG	-5.71	1.41	1.51
2	B	240	ILE	CA-CB	-5.71	1.41	1.54
3	C	168	ALA	C-O	-5.71	1.12	1.23
1	A	664	THR	C-O	-5.71	1.12	1.23
2	B	996	ARG	NE-CZ	-5.71	1.25	1.33
1	A	608	ILE	CB-CG2	-5.71	1.35	1.52
3	C	166	GLU	CD-OE1	5.71	1.31	1.25
4	E	106	GLN	CD-NE2	5.71	1.47	1.32
1	A	261	ASP	N-CA	5.71	1.57	1.46
2	B	621	GLU	CD-OE1	-5.71	1.19	1.25
4	E	164	LEU	CA-C	-5.71	1.38	1.52
1	A	1197	LEU	CA-CB	-5.71	1.40	1.53
2	B	1031	LEU	CA-CB	-5.71	1.40	1.53
2	B	1163	CYS	C-N	-5.71	1.22	1.33
3	C	104	PHE	CD1-CE1	5.71	1.50	1.39
1	A	385	ILE	C-O	-5.70	1.12	1.23
1	A	1442	ASP	CA-C	-5.70	1.38	1.52
3	C	259	LEU	CG-CD2	-5.70	1.30	1.51
4	E	87	SER	CB-OG	5.70	1.49	1.42
1	A	761	MET	CA-C	-5.70	1.38	1.52
2	B	747	MET	CB-CG	-5.70	1.33	1.51
1	A	100	LYS	N-CA	5.70	1.57	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ARG	CD-NE	5.70	1.56	1.46
2	B	627	PHE	CA-CB	-5.70	1.41	1.53
1	A	1299	VAL	CB-CG2	-5.69	1.40	1.52
9	K	97	LYS	C-O	-5.69	1.12	1.23
1	A	729	ALA	CA-CB	-5.69	1.40	1.52
3	C	170	TRP	CZ2-CH2	-5.69	1.26	1.37
2	B	411	PRO	CA-CB	-5.69	1.42	1.53
2	B	875	GLU	CD-OE1	5.69	1.31	1.25
1	A	962	ARG	CB-CG	5.69	1.68	1.52
3	C	149	LYS	CE-NZ	5.69	1.63	1.49
1	A	1217	LYS	C-O	5.69	1.34	1.23
2	B	89	GLU	C-O	5.69	1.34	1.23
2	B	286	PHE	CE2-CZ	5.69	1.48	1.37
2	B	557	PHE	CE1-CZ	5.69	1.48	1.37
2	B	848	ARG	NE-CZ	-5.69	1.25	1.33
2	B	1192	TYR	CE2-CZ	-5.68	1.31	1.38
6	H	19	ARG	CD-NE	5.68	1.56	1.46
1	A	1303	GLU	CD-OE2	5.68	1.31	1.25
2	B	289	LEU	CA-CB	-5.68	1.40	1.53
2	B	555	ILE	CA-CB	-5.68	1.41	1.54
6	H	105	GLU	CG-CD	5.68	1.60	1.51
6	H	115	TYR	CE1-CZ	-5.68	1.31	1.38
9	K	73	LEU	CA-CB	-5.68	1.40	1.53
1	A	893	PHE	CA-CB	-5.68	1.41	1.53
2	B	202	TYR	CE1-CZ	-5.68	1.31	1.38
2	B	595	ARG	C-O	-5.68	1.12	1.23
4	E	67	GLU	CB-CG	5.68	1.62	1.52
4	E	161	LYS	CA-CB	-5.68	1.41	1.53
6	H	96	VAL	N-CA	-5.68	1.34	1.46
2	B	324	ILE	CA-CB	-5.68	1.41	1.54
2	B	370	PHE	CD1-CE1	5.68	1.50	1.39
2	B	1135	ARG	N-CA	-5.68	1.34	1.46
2	B	1206	GLU	CD-OE2	5.68	1.31	1.25
1	A	126	LEU	C-O	5.67	1.34	1.23
1	A	407	ARG	CA-CB	-5.67	1.41	1.53
1	A	511	ILE	CA-C	-5.67	1.38	1.52
1	A	1263	ILE	CA-CB	5.67	1.68	1.54
1	A	884	ASP	CG-OD1	5.67	1.38	1.25
2	B	217	ARG	CZ-NH1	-5.67	1.25	1.33
3	C	265	MET	CG-SD	5.67	1.95	1.81
4	E	183	PRO	CA-C	-5.67	1.41	1.52
5	F	72	LYS	CG-CD	5.67	1.71	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	97	LYS	CD-CE	5.67	1.65	1.51
2	B	687	GLU	CG-CD	5.67	1.60	1.51
2	B	734	HIS	CA-C	5.67	1.67	1.52
5	F	120	ILE	N-CA	-5.67	1.35	1.46
1	A	722	LEU	CA-C	-5.67	1.38	1.52
1	A	878	ILE	CB-CG1	-5.67	1.38	1.54
1	A	954	TRP	CA-CB	-5.67	1.41	1.53
6	H	78	SER	CB-OG	-5.67	1.34	1.42
1	A	63	ARG	NE-CZ	5.67	1.40	1.33
1	A	1411	GLU	CB-CG	5.67	1.62	1.52
2	B	743	ILE	N-CA	-5.67	1.35	1.46
1	A	1326	ARG	CB-CG	-5.67	1.37	1.52
2	B	667	GLN	CB-CG	5.67	1.67	1.52
3	C	131	HIS	C-N	-5.67	1.23	1.34
1	A	380	VAL	CB-CG1	-5.66	1.41	1.52
1	A	826	ASP	C-O	-5.66	1.12	1.23
2	B	710	LEU	CG-CD2	-5.66	1.30	1.51
4	E	35	VAL	CB-CG2	-5.66	1.41	1.52
10	L	27	LEU	CG-CD1	5.66	1.72	1.51
2	B	538	ASN	C-O	-5.66	1.12	1.23
1	A	133	LYS	CB-CG	5.66	1.67	1.52
1	A	451	HIS	N-CA	-5.66	1.35	1.46
2	B	231	PRO	CA-C	5.66	1.64	1.52
2	B	370	PHE	CA-CB	5.66	1.66	1.53
2	B	602	THR	CB-CG2	-5.66	1.33	1.52
9	K	14	GLU	CD-OE2	5.66	1.31	1.25
9	K	36	GLU	CD-OE1	5.66	1.31	1.25
1	A	28	ARG	CB-CG	5.66	1.67	1.52
1	A	38	PRO	N-CD	-5.66	1.40	1.47
1	A	369	SER	C-O	5.66	1.34	1.23
1	A	618	GLU	CA-CB	-5.66	1.41	1.53
1	A	896	ARG	CA-C	-5.66	1.38	1.52
2	B	272	THR	CA-C	-5.66	1.38	1.52
2	B	620	ARG	NE-CZ	-5.66	1.25	1.33
1	A	406	ILE	CB-CG2	5.66	1.70	1.52
4	E	127	ILE	C-O	5.66	1.34	1.23
1	A	215	SER	CB-OG	-5.66	1.34	1.42
1	A	397	ASN	N-CA	-5.66	1.35	1.46
2	B	310	MET	CA-CB	-5.66	1.41	1.53
2	B	914	LYS	CB-CG	-5.65	1.37	1.52
3	C	254	LYS	CD-CE	-5.65	1.37	1.51
10	L	43	THR	N-CA	5.65	1.57	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	21	GLU	C-O	-5.65	1.12	1.23
2	B	404	LYS	CG-CD	5.65	1.71	1.52
2	B	697	GLU	N-CA	5.65	1.57	1.46
2	B	792	MET	CA-C	-5.65	1.38	1.52
2	B	914	LYS	CA-CB	-5.65	1.41	1.53
3	C	54	ASN	CG-ND2	5.65	1.47	1.32
7	I	105	SER	CA-CB	5.65	1.61	1.52
1	A	527	THR	CB-OG1	5.65	1.54	1.43
1	A	713	SER	CA-CB	-5.65	1.44	1.52
2	B	889	THR	C-O	-5.65	1.12	1.23
1	A	614	PHE	CD2-CE2	-5.65	1.27	1.39
1	A	298	PHE	CD2-CE2	5.65	1.50	1.39
1	A	376	TYR	CD1-CE1	-5.65	1.30	1.39
2	B	959	ASP	CA-C	5.65	1.67	1.52
3	C	129	ILE	CA-C	-5.65	1.38	1.52
7	I	6	PHE	CD2-CE2	5.65	1.50	1.39
1	A	177	ASP	C-O	5.64	1.34	1.23
1	A	571	LEU	CG-CD1	-5.64	1.30	1.51
2	B	255	GLN	CG-CD	5.64	1.64	1.51
2	B	980	PHE	CE2-CZ	-5.64	1.26	1.37
2	B	1000	PRO	N-CA	-5.64	1.37	1.47
2	B	1095	LEU	CB-CG	-5.64	1.36	1.52
3	C	111	THR	CB-OG1	5.64	1.54	1.43
7	I	59	VAL	CB-CG1	-5.64	1.41	1.52
7	I	98	VAL	C-O	5.64	1.34	1.23
1	A	1239	ARG	NE-CZ	-5.64	1.25	1.33
1	A	1379	GLY	C-O	5.64	1.32	1.23
2	B	593	PRO	C-O	-5.64	1.11	1.23
2	B	787	VAL	N-CA	-5.64	1.35	1.46
2	B	859	TYR	CB-CG	-5.64	1.43	1.51
7	I	86	PHE	CD2-CE2	5.64	1.50	1.39
8	J	51	LEU	CA-CB	-5.64	1.40	1.53
2	B	104	GLU	CA-C	5.64	1.67	1.52
7	I	86	PHE	CG-CD2	5.64	1.47	1.38
2	B	1018	PRO	N-CD	-5.64	1.40	1.47
1	A	965	GLN	C-O	-5.64	1.12	1.23
2	B	254	LEU	CG-CD1	-5.64	1.30	1.51
1	A	363	GLN	CA-C	-5.63	1.38	1.52
1	A	363	GLN	CB-CG	-5.63	1.37	1.52
6	H	25	ARG	CZ-NH2	-5.63	1.25	1.33
9	K	81	TYR	CD1-CE1	-5.63	1.30	1.39
2	B	377	PHE	CG-CD1	-5.63	1.30	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	107	GLY	CA-C	5.63	1.60	1.51
2	B	185	THR	CA-C	-5.63	1.38	1.52
2	B	551	PRO	CA-CB	-5.63	1.42	1.53
2	B	822	ASN	CA-C	-5.63	1.38	1.52
1	A	77	CYS	C-O	5.63	1.34	1.23
1	A	542	GLU	C-O	-5.63	1.12	1.23
1	A	574	GLY	CA-C	-5.63	1.42	1.51
2	B	436	VAL	CB-CG1	5.63	1.64	1.52
2	B	712	PRO	CB-CG	5.63	1.78	1.50
10	L	27	LEU	N-CA	5.63	1.57	1.46
1	A	1282	VAL	C-O	-5.63	1.12	1.23
9	K	43	GLY	CA-C	5.62	1.60	1.51
1	A	155	GLU	CB-CG	5.62	1.62	1.52
1	A	408	ASP	C-O	5.62	1.34	1.23
1	A	961	ARG	CZ-NH1	5.62	1.40	1.33
1	A	366	VAL	CA-CB	-5.62	1.43	1.54
1	A	527	THR	N-CA	-5.62	1.35	1.46
1	A	700	ASN	CB-CG	-5.62	1.38	1.51
1	A	880	LYS	CE-NZ	5.62	1.63	1.49
1	A	1449	SER	CA-CB	5.62	1.61	1.52
2	B	250	PHE	CA-C	5.62	1.67	1.52
2	B	367	LEU	CA-CB	5.62	1.66	1.53
2	B	1028	GLU	CG-CD	5.62	1.60	1.51
1	A	105	CYS	C-O	-5.62	1.12	1.23
1	A	482	PHE	CD1-CE1	5.62	1.50	1.39
1	A	1168	GLU	CD-OE1	5.62	1.31	1.25
4	E	95	THR	CA-CB	5.62	1.68	1.53
1	A	827	THR	N-CA	-5.62	1.35	1.46
4	E	46	TYR	CA-CB	-5.62	1.41	1.53
1	A	836	TYR	CD2-CE2	-5.62	1.30	1.39
6	H	21	ASN	C-O	-5.62	1.12	1.23
2	B	187	SER	CA-CB	-5.62	1.44	1.52
2	B	417	PHE	C-O	5.62	1.34	1.23
2	B	982	SER	CB-OG	-5.61	1.34	1.42
5	F	116	ASP	C-N	-5.61	1.23	1.34
7	I	17	ARG	CZ-NH1	5.61	1.40	1.33
1	A	717	ASN	CB-CG	-5.61	1.38	1.51
10	L	41	SER	C-O	5.61	1.34	1.23
1	A	795	GLU	C-N	-5.61	1.21	1.34
2	B	45	SER	CB-OG	5.61	1.49	1.42
2	B	1139	ILE	CA-CB	-5.61	1.42	1.54
5	F	75	PRO	CA-C	-5.61	1.41	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	77	LYS	CG-CD	5.61	1.71	1.52
1	A	838	GLN	N-CA	-5.61	1.35	1.46
2	B	321	GLY	C-O	5.61	1.32	1.23
1	A	77	CYS	CB-SG	5.60	1.91	1.82
1	A	1214	GLU	CA-CB	5.60	1.66	1.53
2	B	683	SER	CB-OG	5.60	1.49	1.42
1	A	583	PRO	N-CD	-5.60	1.40	1.47
2	B	33	VAL	CB-CG1	-5.60	1.41	1.52
2	B	535	LEU	CG-CD2	-5.60	1.31	1.51
2	B	976	ILE	C-O	-5.60	1.12	1.23
4	E	6	GLU	CG-CD	5.60	1.60	1.51
6	H	34	ASP	CA-CB	5.60	1.66	1.53
9	K	74	ARG	C-O	5.60	1.33	1.23
1	A	810	PRO	CA-C	5.60	1.64	1.52
7	I	69	PRO	CA-C	-5.60	1.41	1.52
1	A	237	THR	CA-CB	-5.60	1.38	1.53
1	A	392	VAL	CB-CG2	5.60	1.64	1.52
1	A	1426	GLU	CB-CG	5.60	1.62	1.52
2	B	1091	TYR	CE2-CZ	-5.60	1.31	1.38
4	E	18	THR	CB-OG1	5.60	1.54	1.43
7	I	22	ASN	CG-OD1	5.60	1.36	1.24
3	C	184	ASN	CB-CG	5.60	1.64	1.51
1	A	404	TYR	CD2-CE2	5.59	1.47	1.39
1	A	820	GLY	C-N	-5.59	1.21	1.34
1	A	855	THR	C-O	-5.59	1.12	1.23
2	B	821	GLN	CB-CG	-5.59	1.37	1.52
6	H	17	PRO	C-O	-5.59	1.12	1.23
6	H	43	ASN	C-O	-5.59	1.12	1.23
2	B	382	ILE	N-CA	-5.59	1.35	1.46
3	C	154	LYS	C-O	-5.59	1.12	1.23
3	C	179	GLU	CA-C	-5.59	1.38	1.52
1	A	5	GLN	CD-NE2	5.59	1.46	1.32
1	A	711	ARG	CB-CG	5.59	1.67	1.52
4	E	148	GLU	CA-C	-5.59	1.38	1.52
9	K	65	HIS	C-N	-5.59	1.23	1.34
1	A	917	SER	CA-C	-5.59	1.38	1.52
2	B	773	MET	N-CA	-5.59	1.35	1.46
1	A	1241	ARG	CZ-NH1	5.59	1.40	1.33
2	B	189	LEU	C-O	5.59	1.33	1.23
2	B	1065	GLN	N-CA	5.59	1.57	1.46
2	B	1168	LEU	CA-C	-5.59	1.38	1.52
3	C	156	THR	CA-C	-5.59	1.38	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	104	ASN	CG-ND2	5.59	1.46	1.32
9	K	97	LYS	CE-NZ	5.58	1.63	1.49
1	A	55	ASP	CG-OD2	5.58	1.38	1.25
1	A	1019	CYS	CA-C	-5.58	1.38	1.52
2	B	116	GLU	C-N	-5.58	1.21	1.34
2	B	240	ILE	C-O	-5.58	1.12	1.23
2	B	771	SER	C-O	-5.58	1.12	1.23
5	F	122	MET	C-O	5.58	1.33	1.23
1	A	434	ARG	CZ-NH2	5.58	1.40	1.33
2	B	999	MET	CA-C	-5.58	1.38	1.52
3	C	91	HIS	CA-CB	5.58	1.66	1.53
1	A	770	VAL	CA-CB	-5.58	1.43	1.54
4	E	155	ARG	CB-CG	-5.58	1.37	1.52
1	A	87	ALA	C-N	-5.58	1.21	1.34
1	A	843	LYS	CA-CB	5.58	1.66	1.53
2	B	287	ARG	NE-CZ	-5.58	1.25	1.33
2	B	573	GLN	CD-OE1	5.58	1.36	1.24
2	B	1100	ASP	CG-OD1	5.58	1.38	1.25
4	E	73	PRO	CB-CG	5.58	1.77	1.50
1	A	1047	SER	C-O	5.58	1.33	1.23
2	B	128	LEU	N-CA	-5.58	1.35	1.46
1	A	117	GLU	CA-C	-5.57	1.38	1.52
1	A	687	LYS	CA-C	5.57	1.67	1.52
1	A	1062	GLU	C-O	5.57	1.33	1.23
1	A	1103	GLU	CD-OE1	5.57	1.31	1.25
2	B	1130	PHE	CG-CD1	-5.57	1.30	1.38
1	A	80	HIS	CG-CD2	5.57	1.45	1.35
2	B	615	MET	N-CA	-5.57	1.35	1.46
2	B	185	THR	CB-CG2	5.57	1.70	1.52
2	B	1110	PRO	N-CA	5.57	1.56	1.47
7	I	72	ASP	CG-OD2	5.57	1.38	1.25
1	A	486	GLU	CG-CD	5.57	1.60	1.51
1	A	859	SER	CA-CB	-5.57	1.44	1.52
1	A	915	SER	C-N	-5.57	1.23	1.33
1	A	1080	THR	C-O	5.57	1.33	1.23
3	C	183	TRP	C-O	-5.57	1.12	1.23
4	E	40	GLU	CG-CD	5.56	1.60	1.51
1	A	813	PHE	C-N	-5.56	1.21	1.34
1	A	935	GLN	CA-CB	-5.56	1.41	1.53
2	B	609	ILE	CB-CG2	-5.56	1.35	1.52
3	C	148	ARG	CZ-NH1	5.56	1.40	1.33
1	A	109	HIS	CB-CG	5.56	1.60	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	465	ASN	CG-ND2	5.56	1.46	1.32
1	A	436	ILE	CB-CG2	5.56	1.70	1.52
1	A	771	GLU	CB-CG	5.56	1.62	1.52
2	B	209	GLU	CA-CB	-5.56	1.41	1.53
2	B	994	TYR	CB-CG	5.56	1.59	1.51
1	A	1062	GLU	CD-OE2	5.56	1.31	1.25
3	C	247	GLY	N-CA	-5.56	1.37	1.46
1	A	1024	SER	CA-C	-5.56	1.38	1.52
2	B	1076	HIS	N-CA	-5.56	1.35	1.46
1	A	453	MET	CG-SD	-5.55	1.66	1.81
1	A	1307	GLU	CB-CG	-5.55	1.41	1.52
2	B	540	SER	C-O	-5.55	1.12	1.23
2	B	691	GLU	CB-CG	-5.55	1.41	1.52
1	A	1357	ALA	C-O	5.55	1.33	1.23
2	B	855	PHE	CB-CG	-5.55	1.42	1.51
2	B	1099	VAL	CA-CB	-5.55	1.43	1.54
1	A	539	THR	CB-CG2	-5.55	1.34	1.52
1	A	622	VAL	CA-C	-5.55	1.38	1.52
9	K	71	PHE	C-O	5.55	1.33	1.23
1	A	69	THR	C-N	5.55	1.46	1.34
1	A	93	VAL	CB-CG1	5.55	1.64	1.52
1	A	782	ARG	C-O	-5.55	1.12	1.23
1	A	933	TYR	CD2-CE2	5.55	1.47	1.39
2	B	818	PRO	CG-CD	-5.55	1.32	1.50
1	A	1220	PHE	CG-CD1	-5.54	1.30	1.38
1	A	1289	ARG	CZ-NH1	-5.54	1.25	1.33
9	K	100	ALA	N-CA	-5.54	1.35	1.46
1	A	187	LYS	N-CA	5.54	1.57	1.46
1	A	206	GLU	CB-CG	5.54	1.62	1.52
1	A	770	VAL	C-O	-5.54	1.12	1.23
2	B	299	GLU	CG-CD	5.54	1.60	1.51
3	C	97	VAL	CB-CG1	-5.54	1.41	1.52
4	E	212	ARG	CZ-NH2	5.54	1.40	1.33
1	A	107	CYS	CB-SG	5.54	1.91	1.82
4	E	82	PHE	CG-CD1	5.54	1.47	1.38
1	A	1114	PRO	C-O	-5.54	1.12	1.23
2	B	319	GLU	CB-CG	5.54	1.62	1.52
1	A	685	GLU	CB-CG	5.54	1.62	1.52
1	A	110	CYS	C-O	5.54	1.33	1.23
1	A	121	LEU	CG-CD2	5.54	1.72	1.51
3	C	156	THR	C-O	-5.54	1.12	1.23
1	A	434	ARG	NE-CZ	-5.53	1.25	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1104	ILE	C-O	-5.53	1.12	1.23
3	C	147	LEU	CA-C	-5.53	1.38	1.52
1	A	1241	ARG	CG-CD	5.53	1.65	1.51
1	A	750	GLY	C-N	-5.53	1.21	1.34
1	A	1283	VAL	CA-CB	-5.53	1.43	1.54
1	A	1350	LYS	N-CA	-5.53	1.35	1.46
1	A	1367	HIS	C-O	-5.53	1.12	1.23
1	A	1435	PRO	CA-C	-5.53	1.41	1.52
2	B	165	VAL	N-CA	5.53	1.57	1.46
2	B	352	ALA	CA-C	-5.53	1.38	1.52
2	B	608	ASP	CB-CG	5.53	1.63	1.51
2	B	491	THR	N-CA	-5.53	1.35	1.46
2	B	106	ASP	CA-CB	5.53	1.66	1.53
2	B	466	TRP	CZ3-CH2	-5.53	1.31	1.40
4	E	181	ALA	CA-C	-5.53	1.38	1.52
7	I	119	THR	CA-CB	5.53	1.67	1.53
2	B	43	LEU	CA-CB	-5.53	1.41	1.53
4	E	33	GLU	CG-CD	5.53	1.60	1.51
7	I	6	PHE	CD1-CE1	5.53	1.50	1.39
7	I	90	GLN	C-O	-5.53	1.12	1.23
7	I	96	SER	CB-OG	5.53	1.49	1.42
2	B	431	TYR	CE2-CZ	5.52	1.45	1.38
1	A	241	VAL	C-O	-5.52	1.12	1.23
1	A	411	ASP	CG-OD1	5.52	1.38	1.25
1	A	1111	MET	SD-CE	-5.52	1.47	1.77
3	C	123	ASN	C-O	-5.52	1.12	1.23
7	I	97	MET	C-O	5.52	1.33	1.23
1	A	799	PHE	CE1-CZ	-5.52	1.26	1.37
1	A	1025	ARG	NE-CZ	-5.52	1.25	1.33
7	I	41	PRO	C-O	-5.52	1.12	1.23
2	B	766	ARG	CD-NE	5.52	1.55	1.46
10	L	49	LYS	CA-C	5.52	1.67	1.52
1	A	413	ILE	CB-CG1	-5.52	1.38	1.54
2	B	308	TRP	CG-CD2	-5.52	1.34	1.43
2	B	1212	ILE	CA-CB	-5.52	1.42	1.54
4	E	173	SER	CB-OG	5.52	1.49	1.42
2	B	95	ILE	CA-CB	-5.52	1.42	1.54
3	C	206	ASN	C-O	-5.52	1.12	1.23
1	A	137	ALA	C-O	5.51	1.33	1.23
1	A	442	VAL	CB-CG1	-5.51	1.41	1.52
1	A	1217	LYS	CA-CB	-5.51	1.41	1.53
2	B	767	ASN	N-CA	-5.51	1.35	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1129	ARG	CZ-NH2	5.51	1.40	1.33
3	C	111	THR	CB-CG2	5.51	1.70	1.52
4	E	85	GLU	CB-CG	5.51	1.62	1.52
2	B	299	GLU	CD-OE2	5.51	1.31	1.25
9	K	49	GLU	C-O	-5.51	1.12	1.23
1	A	997	LEU	CA-C	-5.51	1.38	1.52
2	B	542	MET	CA-CB	5.51	1.66	1.53
2	B	1185	CYS	CA-C	5.51	1.67	1.52
9	K	73	LEU	CB-CG	-5.51	1.36	1.52
1	A	586	ILE	CB-CG2	-5.51	1.35	1.52
1	A	1308	THR	N-CA	-5.51	1.35	1.46
2	B	728	ARG	CZ-NH2	5.51	1.40	1.33
2	B	999	MET	CG-SD	5.51	1.95	1.81
7	I	94	ASP	CG-OD1	5.51	1.38	1.25
1	A	120	GLU	CA-CB	5.50	1.66	1.53
1	A	498	ARG	N-CA	-5.50	1.35	1.46
1	A	833	GLU	C-O	5.50	1.33	1.23
1	A	1021	LEU	N-CA	-5.50	1.35	1.46
4	E	35	VAL	N-CA	-5.50	1.35	1.46
2	B	276	ILE	CG1-CD1	-5.50	1.12	1.50
2	B	664	THR	CB-CG2	-5.50	1.34	1.52
3	C	15	LYS	CA-CB	5.50	1.66	1.53
6	H	115	TYR	CB-CG	-5.50	1.43	1.51
8	J	8	PHE	CE2-CZ	-5.50	1.26	1.37
1	A	159	THR	CA-CB	5.50	1.67	1.53
1	A	219	PHE	CB-CG	-5.50	1.42	1.51
1	A	635	ARG	CZ-NH2	5.50	1.40	1.33
1	A	660	ASN	CB-CG	-5.50	1.38	1.51
1	A	1063	MET	CA-C	5.50	1.67	1.52
1	A	1274	ARG	N-CA	5.50	1.57	1.46
1	A	1329	THR	N-CA	-5.50	1.35	1.46
4	E	71	LYS	CG-CD	5.50	1.71	1.52
5	F	148	VAL	N-CA	-5.50	1.35	1.46
1	A	755	PHE	C-O	5.50	1.33	1.23
1	A	432	VAL	CA-CB	-5.50	1.43	1.54
4	E	74	ASP	CB-CG	-5.50	1.40	1.51
7	I	43	VAL	CA-CB	-5.50	1.43	1.54
1	A	228	PHE	C-O	5.50	1.33	1.23
2	B	617	ARG	CG-CD	5.50	1.65	1.51
2	B	684	LEU	CA-CB	-5.50	1.41	1.53
1	A	470	LEU	N-CA	-5.49	1.35	1.46
1	A	482	PHE	CG-CD1	-5.49	1.30	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	524	VAL	C-O	-5.49	1.12	1.23
1	A	994	GLN	N-CA	-5.49	1.35	1.46
1	A	1105	LEU	N-CA	-5.49	1.35	1.46
1	A	1354	ASN	C-O	-5.49	1.12	1.23
2	B	174	LEU	C-N	-5.49	1.21	1.34
4	E	172	GLU	CB-CG	5.49	1.62	1.52
1	A	790	ASP	CA-CB	-5.49	1.41	1.53
2	B	951	GLN	CD-OE1	5.49	1.36	1.24
9	K	91	CYS	CA-C	5.49	1.67	1.52
1	A	66	LYS	N-CA	5.49	1.57	1.46
3	C	11	ARG	C-N	-5.49	1.21	1.34
1	A	349	ALA	CA-C	-5.49	1.38	1.52
1	A	143	LYS	C-O	5.49	1.33	1.23
1	A	482	PHE	C-O	-5.49	1.12	1.23
2	B	906	SER	CB-OG	5.49	1.49	1.42
5	F	78	GLN	CD-NE2	5.49	1.46	1.32
1	A	412	ARG	N-CA	-5.48	1.35	1.46
2	B	1030	LEU	CA-CB	-5.48	1.41	1.53
1	A	193	ASP	CA-C	5.48	1.67	1.52
1	A	352	VAL	CB-CG2	5.48	1.64	1.52
2	B	554	ILE	CA-CB	-5.48	1.42	1.54
2	B	744	HIS	N-CA	5.48	1.57	1.46
3	C	27	LEU	C-O	-5.48	1.12	1.23
5	F	145	ASP	C-O	5.48	1.33	1.23
1	A	1358	SER	CA-CB	5.48	1.61	1.52
2	B	887	HIS	CB-CG	5.48	1.59	1.50
3	C	182	PRO	N-CD	-5.48	1.40	1.47
4	E	38	PRO	CA-C	-5.48	1.41	1.52
1	A	517	ASN	CB-CG	5.48	1.63	1.51
2	B	1162	ILE	CB-CG1	-5.48	1.38	1.54
4	E	52	ARG	CA-CB	5.48	1.66	1.53
9	K	50	LEU	CA-CB	-5.48	1.41	1.53
2	B	418	LYS	CA-C	-5.48	1.38	1.52
2	B	707	PRO	C-N	-5.47	1.21	1.34
9	K	114	LEU	CB-CG	5.47	1.68	1.52
1	A	828	ALA	C-O	5.47	1.33	1.23
1	A	1199	ARG	C-O	5.47	1.33	1.23
1	A	1239	ARG	CD-NE	5.47	1.55	1.46
1	A	1408	ILE	CA-CB	-5.47	1.42	1.54
1	A	142	CYS	C-O	5.47	1.33	1.23
4	E	205	SER	C-O	-5.47	1.12	1.23
7	I	85	PHE	CG-CD1	-5.47	1.30	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	502	SER	CA-C	-5.47	1.38	1.52
1	A	840	ARG	CA-C	-5.47	1.38	1.52
1	A	842	VAL	CA-CB	-5.47	1.43	1.54
2	B	38	PHE	CE1-CZ	-5.47	1.26	1.37
2	B	590	HIS	CA-CB	-5.47	1.42	1.53
1	A	943	LEU	N-CA	-5.47	1.35	1.46
8	J	63	TYR	CD2-CE2	-5.47	1.31	1.39
1	A	55	ASP	CA-C	-5.46	1.38	1.52
2	B	126	SER	CA-CB	-5.46	1.44	1.52
2	B	899	ILE	C-O	-5.46	1.12	1.23
3	C	14	SER	CA-CB	-5.46	1.44	1.52
4	E	104	ASN	CB-CG	5.46	1.63	1.51
4	E	160	GLU	CD-OE2	5.46	1.31	1.25
7	I	9	ASP	C-O	5.46	1.33	1.23
1	A	1041	ALA	N-CA	-5.46	1.35	1.46
1	A	1289	ARG	CA-C	-5.46	1.38	1.52
2	B	954	VAL	CA-CB	5.46	1.66	1.54
2	B	983	ARG	C-O	5.46	1.33	1.23
1	A	839	ARG	CZ-NH1	5.46	1.40	1.33
4	E	169	ARG	CA-C	5.46	1.67	1.52
8	J	31	ASP	CG-OD1	5.46	1.38	1.25
1	A	377	PRO	N-CA	-5.46	1.38	1.47
2	B	726	ALA	C-O	-5.46	1.12	1.23
2	B	513	GLN	CD-NE2	5.46	1.46	1.32
3	C	117	ASP	N-CA	-5.46	1.35	1.46
1	A	388	LEU	CB-CG	-5.46	1.36	1.52
1	A	1286	LYS	CD-CE	5.46	1.64	1.51
2	B	436	VAL	N-CA	5.46	1.57	1.46
4	E	184	VAL	CB-CG1	-5.46	1.41	1.52
2	B	1008	PRO	CA-C	-5.45	1.42	1.52
3	C	233	GLU	CB-CG	5.45	1.62	1.52
1	A	1270	ASN	CB-CG	5.45	1.63	1.51
2	B	97	VAL	CB-CG2	-5.45	1.41	1.52
5	F	109	VAL	CB-CG1	-5.45	1.41	1.52
1	A	277	GLU	CD-OE1	5.45	1.31	1.25
1	A	1325	THR	CA-CB	-5.45	1.39	1.53
3	C	210	GLU	C-O	-5.45	1.12	1.23
2	B	113	TYR	CD1-CE1	-5.45	1.31	1.39
3	C	117	ASP	CA-CB	-5.45	1.42	1.53
1	A	649	ILE	N-CA	-5.45	1.35	1.46
2	B	177	LYS	CG-CD	5.45	1.71	1.52
3	C	136	ASP	N-CA	-5.45	1.35	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	441	PRO	CA-CB	-5.44	1.42	1.53
1	A	439	ASN	C-O	-5.44	1.13	1.23
4	E	68	SER	CA-CB	-5.44	1.44	1.52
9	K	29	ASN	CG-ND2	5.44	1.46	1.32
1	A	49	LYS	CA-C	5.44	1.67	1.52
2	B	195	CYS	C-N	-5.44	1.24	1.34
2	B	769	TYR	CE1-CZ	-5.44	1.31	1.38
7	I	61	ASP	CB-CG	5.44	1.63	1.51
10	L	69	ALA	N-CA	5.44	1.57	1.46
2	B	212	LEU	CB-CG	5.44	1.68	1.52
2	B	417	PHE	CG-CD2	-5.44	1.30	1.38
1	A	285	PRO	C-O	-5.44	1.12	1.23
2	B	1047	PHE	CB-CG	-5.44	1.42	1.51
9	K	5	ASP	CG-OD1	5.44	1.37	1.25
2	B	186	GLU	N-CA	5.44	1.57	1.46
2	B	564	GLU	CG-CD	5.44	1.60	1.51
4	E	208	TYR	CA-C	-5.44	1.38	1.52
8	J	64	ASN	CG-ND2	5.44	1.46	1.32
1	A	1435	PRO	N-CA	-5.43	1.38	1.47
3	C	18	VAL	CB-CG1	-5.43	1.41	1.52
1	A	104	GLU	C-O	5.43	1.33	1.23
3	C	223	ALA	CA-C	-5.43	1.38	1.52
5	F	106	PRO	CA-CB	-5.43	1.42	1.53
9	K	84	LYS	N-CA	-5.43	1.35	1.46
2	B	908	GLU	CA-CB	5.43	1.65	1.53
1	A	138	ILE	CA-C	5.43	1.67	1.52
1	A	189	ARG	C-O	5.43	1.33	1.23
2	B	120	ARG	CZ-NH2	5.43	1.40	1.33
7	I	107	SER	C-O	5.43	1.33	1.23
2	B	638	PHE	CB-CG	-5.43	1.42	1.51
2	B	1026	LEU	CG-CD1	-5.43	1.31	1.51
2	B	1221	SER	CB-OG	5.43	1.49	1.42
4	E	72	PHE	CG-CD1	5.43	1.46	1.38
2	B	189	LEU	CB-CG	-5.42	1.36	1.52
2	B	532	ALA	CA-C	-5.42	1.38	1.52
3	C	13	ALA	C-N	-5.42	1.21	1.34
3	C	59	ALA	C-O	-5.42	1.13	1.23
3	C	90	ASP	C-O	-5.42	1.13	1.23
2	B	620	ARG	CD-NE	-5.42	1.37	1.46
2	B	1149	GLU	C-N	-5.42	1.21	1.34
5	F	128	LYS	CA-C	-5.42	1.38	1.52
1	A	756	ILE	CB-CG2	-5.42	1.36	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	813	PHE	CA-CB	-5.42	1.42	1.53
1	A	959	ASN	CG-OD1	-5.42	1.12	1.24
2	B	228	LYS	CE-NZ	5.42	1.62	1.49
2	B	405	ARG	NE-CZ	-5.42	1.26	1.33
2	B	595	ARG	CA-C	-5.42	1.38	1.52
2	B	811	TYR	CD2-CE2	5.42	1.47	1.39
6	H	41	ASP	CG-OD1	5.42	1.37	1.25
6	H	128	ASN	CG-ND2	5.42	1.46	1.32
1	A	1126	ALA	CA-C	5.42	1.67	1.52
1	A	1340	GLY	C-O	-5.42	1.15	1.23
3	C	261	ALA	CA-CB	-5.42	1.41	1.52
9	K	58	PHE	C-O	5.42	1.33	1.23
1	A	559	VAL	CA-CB	-5.42	1.43	1.54
2	B	784	ASN	CG-ND2	5.42	1.46	1.32
1	A	40	THR	C-O	5.41	1.33	1.23
1	A	47	ARG	CG-CD	5.41	1.65	1.51
1	A	787	PHE	CA-CB	-5.41	1.42	1.53
2	B	652	LYS	C-O	5.41	1.33	1.23
4	E	36	GLU	CB-CG	5.41	1.62	1.52
1	A	386	ASP	CB-CG	5.41	1.63	1.51
1	A	759	ALA	C-N	-5.41	1.21	1.34
1	A	1009	ASN	CB-CG	5.41	1.63	1.51
6	H	115	TYR	CG-CD1	-5.41	1.32	1.39
2	B	20	ASP	CB-CG	5.41	1.63	1.51
2	B	187	SER	N-CA	-5.41	1.35	1.46
2	B	361	LEU	CA-C	-5.41	1.38	1.52
2	B	629	ASP	C-N	-5.41	1.21	1.34
2	B	209	GLU	CD-OE1	-5.40	1.19	1.25
2	B	394	ASP	CG-OD1	5.40	1.37	1.25
1	A	1105	LEU	C-O	-5.40	1.13	1.23
1	A	1407	GLU	CD-OE1	5.40	1.31	1.25
2	B	708	GLU	N-CA	-5.40	1.35	1.46
1	A	997	LEU	C-O	-5.40	1.13	1.23
3	C	234	SER	N-CA	-5.40	1.35	1.46
5	F	79	ARG	CZ-NH2	-5.40	1.26	1.33
7	I	50	THR	C-O	-5.40	1.13	1.23
1	A	265	LYS	CE-NZ	5.40	1.62	1.49
1	A	1446	ASP	CG-OD1	5.40	1.37	1.25
2	B	328	GLU	C-N	-5.40	1.21	1.34
4	E	79	TRP	CZ2-CH2	5.40	1.47	1.37
2	B	326	ASP	N-CA	-5.40	1.35	1.46
2	B	357	GLN	CG-CD	-5.40	1.38	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	994	TYR	CZ-OH	5.40	1.47	1.37
3	C	138	GLU	C-O	5.40	1.33	1.23
1	A	420	ARG	CZ-NH2	-5.39	1.26	1.33
1	A	423	ASP	CG-OD2	5.39	1.37	1.25
1	A	1301	GLU	CA-CB	5.39	1.65	1.53
3	C	170	TRP	C-N	-5.39	1.23	1.33
1	A	551	TYR	CD2-CE2	-5.39	1.31	1.39
5	F	79	ARG	CZ-NH1	-5.39	1.26	1.33
6	H	6	PHE	CA-CB	-5.39	1.42	1.53
1	A	1012	ARG	CD-NE	5.39	1.55	1.46
2	B	597	MET	CB-CG	-5.39	1.34	1.51
2	B	757	PRO	N-CA	-5.39	1.38	1.47
3	C	110	THR	CA-C	-5.39	1.39	1.52
1	A	537	ARG	N-CA	5.39	1.57	1.46
7	I	75	CYS	CB-SG	-5.39	1.73	1.81
1	A	404	TYR	CE1-CZ	-5.39	1.31	1.38
1	A	1055	ARG	CZ-NH2	5.39	1.40	1.33
2	B	896	ASP	C-O	-5.39	1.13	1.23
1	A	47	ARG	CB-CG	5.38	1.67	1.52
1	A	263	THR	C-O	5.38	1.33	1.23
1	A	525	GLN	CD-OE1	5.38	1.35	1.24
1	A	940	ARG	CD-NE	-5.38	1.37	1.46
2	B	847	ASP	CG-OD2	5.38	1.37	1.25
2	B	868	MET	CA-C	5.38	1.67	1.52
2	B	914	LYS	CE-NZ	5.38	1.62	1.49
7	I	86	PHE	N-CA	-5.38	1.35	1.46
1	A	1274	ARG	CB-CG	-5.38	1.38	1.52
1	A	1405	THR	CA-C	5.38	1.67	1.52
2	B	1068	GLY	N-CA	-5.38	1.38	1.46
6	H	137	GLN	CD-NE2	5.38	1.46	1.32
1	A	944	ARG	CG-CD	5.38	1.65	1.51
2	B	102	VAL	CB-CG1	-5.38	1.41	1.52
2	B	1034	VAL	CB-CG1	-5.38	1.41	1.52
4	E	16	PHE	CA-C	-5.38	1.39	1.52
1	A	1003	LYS	CE-NZ	5.38	1.62	1.49
5	F	103	MET	N-CA	-5.38	1.35	1.46
3	C	60	ASP	CA-C	-5.38	1.39	1.52
1	A	987	VAL	C-O	5.37	1.33	1.23
2	B	1147	LEU	CG-CD2	-5.37	1.31	1.51
5	F	81	THR	C-O	-5.37	1.13	1.23
6	H	118	PHE	CG-CD1	5.37	1.46	1.38
1	A	425	GLN	CD-OE1	5.37	1.35	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	528	LEU	CG-CD1	-5.37	1.31	1.51
1	A	669	THR	C-O	5.37	1.33	1.23
2	B	342	GLY	C-O	5.37	1.32	1.23
7	I	43	VAL	CB-CG2	-5.37	1.41	1.52
1	A	748	MET	CB-CG	5.37	1.68	1.51
2	B	1103	ILE	N-CA	5.37	1.57	1.46
4	E	64	PRO	N-CD	-5.37	1.40	1.47
2	B	775	LYS	CD-CE	-5.37	1.37	1.51
3	C	9	LYS	C-O	-5.37	1.13	1.23
4	E	211	TYR	C-O	5.37	1.33	1.23
2	B	569	TYR	CA-CB	5.37	1.65	1.53
6	H	126	GLU	C-O	5.37	1.33	1.23
1	A	237	THR	CB-CG2	5.36	1.70	1.52
1	A	1173	HIS	CA-CB	5.36	1.65	1.53
1	A	1288	ASP	CB-CG	5.36	1.63	1.51
2	B	279	ASP	CG-OD1	5.36	1.37	1.25
2	B	305	VAL	CB-CG2	5.36	1.64	1.52
2	B	629	ASP	C-O	-5.36	1.13	1.23
2	B	848	ARG	CG-CD	5.36	1.65	1.51
4	E	143	ASN	C-O	-5.36	1.13	1.23
1	A	1383	SER	N-CA	-5.36	1.35	1.46
2	B	1224	PHE	CA-C	5.36	1.66	1.52
1	A	1176	LEU	CG-CD1	5.36	1.71	1.51
1	A	1254	ALA	C-O	5.36	1.33	1.23
1	A	1423	GLY	C-N	-5.36	1.21	1.34
2	B	217	ARG	CD-NE	-5.36	1.37	1.46
1	A	561	PRO	CB-CG	-5.36	1.23	1.50
1	A	467	THR	C-O	-5.36	1.13	1.23
4	E	175	LEU	C-N	-5.36	1.24	1.34
6	H	86	ASP	N-CA	5.36	1.57	1.46
9	K	64	GLU	CD-OE1	5.36	1.31	1.25
1	A	1307	GLU	CG-CD	5.36	1.59	1.51
2	B	578	THR	C-O	-5.36	1.13	1.23
2	B	802	PRO	CA-C	-5.36	1.42	1.52
6	H	50	ALA	CA-CB	5.36	1.63	1.52
1	A	419	LYS	CB-CG	5.35	1.67	1.52
9	K	67	PHE	CD1-CE1	-5.35	1.28	1.39
1	A	789	LYS	CG-CD	-5.35	1.34	1.52
2	B	1129	ARG	C-O	5.35	1.33	1.23
3	C	256	ALA	N-CA	-5.35	1.35	1.46
1	A	1159	ARG	CA-CB	5.35	1.65	1.53
2	B	124	TYR	CZ-OH	-5.35	1.28	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	10	PHE	CB-CG	5.35	1.60	1.51
1	A	42	ASP	CB-CG	5.35	1.62	1.51
1	A	969	GLN	CB-CG	5.35	1.67	1.52
2	B	762	ASN	CG-OD1	-5.35	1.12	1.24
6	H	87	ARG	NE-CZ	5.35	1.40	1.33
7	I	34	TYR	CB-CG	5.35	1.59	1.51
10	L	67	PHE	CD2-CE2	-5.35	1.28	1.39
1	A	175	ARG	CG-CD	5.35	1.65	1.51
1	A	81	PHE	CG-CD2	-5.34	1.30	1.38
1	A	1023	ARG	CA-CB	-5.34	1.42	1.53
2	B	190	TYR	CA-CB	-5.34	1.42	1.53
4	E	2	ASP	C-O	5.34	1.33	1.23
4	E	165	LEU	C-O	5.34	1.33	1.23
1	A	160	GLN	CA-C	-5.34	1.39	1.52
1	A	244	PRO	C-O	5.34	1.33	1.23
1	A	514	PRO	CB-CG	-5.34	1.23	1.50
2	B	643	ASP	CG-OD2	5.34	1.37	1.25
2	B	826	ALA	N-CA	-5.34	1.35	1.46
1	A	1435	PRO	CB-CG	-5.34	1.23	1.50
2	B	705	MET	CA-C	-5.34	1.39	1.52
7	I	44	TYR	CA-CB	5.34	1.65	1.53
1	A	530	GLY	N-CA	-5.34	1.38	1.46
6	H	87	ARG	CA-CB	5.34	1.65	1.53
7	I	109	ILE	CA-CB	5.34	1.67	1.54
1	A	973	ILE	CB-CG2	5.33	1.69	1.52
2	B	109	THR	CB-OG1	5.33	1.53	1.43
2	B	180	TYR	N-CA	-5.33	1.35	1.46
3	C	156	THR	CA-CB	-5.33	1.39	1.53
1	A	811	GLN	N-CA	-5.33	1.35	1.46
2	B	1110	PRO	CA-CB	5.33	1.64	1.53
4	E	196	VAL	N-CA	5.33	1.57	1.46
2	B	521	LEU	C-O	-5.33	1.13	1.23
2	B	397	ASP	CB-CG	5.33	1.62	1.51
1	A	76	GLU	C-O	5.33	1.33	1.23
1	A	116	ASP	C-O	-5.33	1.13	1.23
1	A	733	ALA	C-O	-5.33	1.13	1.23
1	A	1156	PRO	C-O	5.33	1.33	1.23
2	B	1059	LEU	N-CA	-5.33	1.35	1.46
2	B	344	LYS	CE-NZ	5.33	1.62	1.49
2	B	1193	GLN	CD-NE2	5.33	1.46	1.32
3	C	168	ALA	CA-CB	-5.33	1.41	1.52
1	A	1001	ARG	N-CA	-5.32	1.35	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1335	ILE	CB-CG2	-5.32	1.36	1.52
2	B	340	ALA	N-CA	-5.32	1.35	1.46
2	B	750	GLY	C-O	-5.32	1.15	1.23
3	C	187	LYS	CA-CB	-5.32	1.42	1.53
1	A	559	VAL	CB-CG1	5.32	1.64	1.52
2	B	999	MET	C-O	-5.32	1.13	1.23
1	A	148	CYS	N-CA	5.32	1.56	1.46
1	A	326	ARG	CA-C	5.32	1.66	1.52
1	A	545	GLN	C-O	-5.32	1.13	1.23
1	A	1279	ILE	CA-C	-5.32	1.39	1.52
2	B	166	PHE	CD2-CE2	-5.32	1.28	1.39
2	B	851	PHE	CG-CD1	-5.32	1.30	1.38
10	L	62	LYS	CG-CD	5.32	1.70	1.52
1	A	135	PHE	CD2-CE2	-5.32	1.28	1.39
7	I	18	GLU	C-O	5.32	1.33	1.23
9	K	6	ARG	CB-CG	-5.32	1.38	1.52
2	B	996	ARG	CA-CB	-5.32	1.42	1.53
2	B	92	PHE	N-CA	5.31	1.56	1.46
2	B	1129	ARG	NE-CZ	5.31	1.40	1.33
2	B	1161	HIS	CG-CD2	5.31	1.44	1.35
3	C	104	PHE	CA-C	-5.31	1.39	1.52
4	E	158	SER	N-CA	-5.31	1.35	1.46
5	F	112	GLU	CB-CG	-5.31	1.42	1.52
9	K	106	GLU	C-O	5.31	1.33	1.23
1	A	662	PHE	CG-CD1	-5.31	1.30	1.38
2	B	66	ASP	CB-CG	5.31	1.62	1.51
2	B	587	HIS	CB-CG	-5.31	1.40	1.50
1	A	99	ILE	CA-CB	-5.31	1.42	1.54
1	A	814	PHE	CG-CD1	-5.31	1.30	1.38
1	A	1130	GLN	CA-CB	5.31	1.65	1.53
2	B	230	ALA	CA-C	5.31	1.66	1.52
2	B	958	GLN	CA-C	5.31	1.66	1.52
2	B	1211	ASN	CG-OD1	-5.31	1.12	1.24
7	I	4	PHE	CE1-CZ	5.31	1.47	1.37
9	K	10	PHE	CE2-CZ	-5.31	1.27	1.37
2	B	804	GLY	C-N	-5.31	1.21	1.34
2	B	830	TYR	CB-CG	5.31	1.59	1.51
8	J	46	CYS	CB-SG	5.31	1.91	1.82
1	A	1070	GLN	C-O	-5.31	1.13	1.23
1	A	1122	PRO	CG-CD	5.31	1.68	1.50
2	B	825	VAL	N-CA	-5.31	1.35	1.46
2	B	838	SER	N-CA	-5.31	1.35	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	263	GLY	CA-C	5.30	1.60	1.51
2	B	758	PHE	C-O	-5.30	1.13	1.23
2	B	1050	ILE	C-N	-5.30	1.21	1.34
3	C	215	GLU	CD-OE2	5.30	1.31	1.25
4	E	17	ARG	CG-CD	5.30	1.65	1.51
10	L	40	LEU	CA-CB	5.30	1.66	1.53
1	A	532	ARG	CZ-NH2	5.30	1.40	1.33
1	A	1305	VAL	CB-CG2	5.30	1.64	1.52
2	B	851	PHE	CE2-CZ	-5.30	1.27	1.37
3	C	34	ARG	CD-NE	-5.30	1.37	1.46
4	E	170	LEU	CG-CD1	-5.30	1.32	1.51
1	A	902	LEU	CG-CD2	-5.30	1.32	1.51
1	A	1164	PRO	C-O	5.30	1.33	1.23
2	B	416	LEU	CA-C	-5.30	1.39	1.52
4	E	101	GLN	CD-NE2	5.30	1.46	1.32
1	A	1281	ARG	CD-NE	5.30	1.55	1.46
2	B	191	LYS	CE-NZ	5.30	1.62	1.49
2	B	627	PHE	CG-CD1	-5.30	1.30	1.38
6	H	119	GLY	C-O	5.30	1.32	1.23
1	A	391	LEU	CG-CD2	-5.29	1.32	1.51
2	B	325	GLN	CA-CB	-5.29	1.42	1.53
2	B	1153	GLU	CB-CG	5.29	1.62	1.52
6	H	2	SER	CB-OG	5.29	1.49	1.42
1	A	180	LYS	CD-CE	5.29	1.64	1.51
1	A	465	TYR	CZ-OH	5.29	1.46	1.37
1	A	981	LEU	C-N	-5.29	1.21	1.34
4	E	9	ILE	CA-CB	5.29	1.67	1.54
4	E	12	LEU	CB-CG	5.29	1.68	1.52
1	A	1288	ASP	C-O	5.29	1.33	1.23
2	B	254	LEU	N-CA	-5.29	1.35	1.46
3	C	209	TYR	CB-CG	5.29	1.59	1.51
9	K	50	LEU	CA-C	-5.29	1.39	1.52
1	A	1314	SER	CA-C	-5.29	1.39	1.52
4	E	60	PHE	CE1-CZ	5.29	1.47	1.37
1	A	200	ARG	CZ-NH1	5.29	1.40	1.33
1	A	511	ILE	C-O	-5.29	1.13	1.23
1	A	785	PRO	N-CD	-5.29	1.40	1.47
1	A	937	VAL	CB-CG2	-5.29	1.41	1.52
2	B	827	ILE	CB-CG1	-5.29	1.39	1.54
2	B	896	ASP	CA-C	-5.29	1.39	1.52
3	C	57	VAL	CA-C	5.29	1.66	1.52
7	I	28	GLU	CA-C	-5.29	1.39	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	14	VAL	C-N	-5.29	1.23	1.33
9	K	16	GLU	CB-CG	5.29	1.62	1.52
2	B	510	LYS	C-N	-5.29	1.24	1.34
2	B	561	TRP	C-N	-5.29	1.23	1.33
2	B	948	ILE	CB-CG1	-5.29	1.39	1.54
2	B	1074	ASN	C-N	-5.29	1.23	1.33
7	I	17	ARG	CD-NE	5.29	1.55	1.46
1	A	129	LYS	CD-CE	5.28	1.64	1.51
1	A	591	PHE	CA-C	-5.28	1.39	1.52
2	B	136	THR	N-CA	5.28	1.56	1.46
2	B	165	VAL	CA-CB	5.28	1.65	1.54
2	B	353	LYS	CD-CE	5.28	1.64	1.51
1	A	911	SER	N-CA	5.28	1.56	1.46
3	C	145	CYS	N-CA	-5.28	1.35	1.46
7	I	36	GLU	CD-OE2	5.28	1.31	1.25
3	C	125	MET	C-O	5.28	1.33	1.23
1	A	383	TYR	CG-CD1	-5.28	1.32	1.39
7	I	51	ASN	CA-C	-5.28	1.39	1.52
1	A	720	ARG	CA-CB	5.28	1.65	1.53
2	B	134	LYS	CD-CE	5.28	1.64	1.51
2	B	418	LYS	CE-NZ	5.28	1.62	1.49
2	B	961	LEU	CB-CG	5.28	1.67	1.52
2	B	1146	PHE	CD2-CE2	-5.28	1.28	1.39
3	C	200	GLU	CG-CD	-5.28	1.44	1.51
4	E	79	TRP	C-N	-5.28	1.22	1.34
6	H	41	ASP	C-O	-5.28	1.13	1.23
6	H	130	ARG	CA-C	5.28	1.66	1.52
1	A	1322	ILE	N-CA	5.28	1.56	1.46
2	B	313	MET	SD-CE	-5.28	1.48	1.77
2	B	485	ARG	NE-CZ	-5.28	1.26	1.33
2	B	742	GLU	CD-OE1	-5.28	1.19	1.25
4	E	15	ALA	N-CA	-5.28	1.35	1.46
4	E	58	MET	CG-SD	5.28	1.94	1.81
4	E	178	ILE	CB-CG2	5.28	1.69	1.52
1	A	599	SER	C-N	-5.27	1.24	1.34
1	A	644	LYS	CD-CE	5.27	1.64	1.51
1	A	1427	ASN	N-CA	-5.27	1.35	1.46
2	B	24	PRO	CA-CB	-5.27	1.43	1.53
2	B	312	GLU	CA-CB	-5.27	1.42	1.53
2	B	965	LYS	C-O	-5.27	1.13	1.23
1	A	65	LEU	C-O	5.27	1.33	1.23
1	A	356	ASP	CB-CG	-5.27	1.40	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1108	ARG	N-CA	5.27	1.56	1.46
9	K	17	SER	N-CA	5.27	1.56	1.46
1	A	653	VAL	C-N	-5.26	1.22	1.34
1	A	937	VAL	CA-CB	-5.26	1.43	1.54
7	I	81	ARG	CG-CD	5.26	1.65	1.51
1	A	854	ASN	N-CA	5.26	1.56	1.46
1	A	1267	MET	SD-CE	-5.26	1.48	1.77
1	A	198	GLU	CG-CD	5.26	1.59	1.51
1	A	499	ALA	CA-C	-5.26	1.39	1.52
2	B	385	LEU	CA-C	-5.26	1.39	1.52
2	B	554	ILE	C-O	-5.26	1.13	1.23
4	E	184	VAL	CB-CG2	5.26	1.63	1.52
7	I	36	GLU	CD-OE1	5.26	1.31	1.25
2	B	118	ARG	CZ-NH2	5.26	1.39	1.33
2	B	611	PRO	CB-CG	-5.26	1.23	1.50
3	C	199	LYS	N-CA	5.26	1.56	1.46
4	E	31	THR	CA-CB	5.26	1.67	1.53
7	I	25	LEU	CG-CD2	-5.26	1.32	1.51
1	A	736	ASN	N-CA	-5.26	1.35	1.46
2	B	950	ASP	C-N	-5.26	1.22	1.34
6	H	137	GLN	CD-OE1	5.26	1.35	1.24
1	A	991	LYS	CD-CE	5.25	1.64	1.51
2	B	974	PRO	N-CD	-5.25	1.40	1.47
2	B	1156	ASP	CG-OD1	5.25	1.37	1.25
1	A	905	ASP	CA-CB	-5.25	1.42	1.53
9	K	83	PRO	C-O	-5.25	1.12	1.23
2	B	261	ARG	NE-CZ	5.25	1.39	1.33
2	B	310	MET	SD-CE	-5.25	1.48	1.77
2	B	646	LEU	N-CA	5.25	1.56	1.46
2	B	692	TYR	CD2-CE2	-5.25	1.31	1.39
2	B	835	GLN	CB-CG	5.25	1.66	1.52
1	A	95	PHE	CD2-CE2	5.25	1.49	1.39
2	B	1025	HIS	CG-ND1	-5.25	1.27	1.38
1	A	458	HIS	C-O	5.25	1.33	1.23
2	B	61	ASP	CG-OD1	5.25	1.37	1.25
4	E	84	ASP	CB-CG	5.25	1.62	1.51
5	F	97	ARG	CZ-NH1	5.25	1.39	1.33
1	A	185	TRP	CE3-CZ3	-5.25	1.29	1.38
1	A	782	ARG	CB-CG	-5.25	1.38	1.52
1	A	810	PRO	C-N	-5.25	1.22	1.34
2	B	268	THR	N-CA	-5.25	1.35	1.46
2	B	976	ILE	CA-C	-5.25	1.39	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1150	ARG	CG-CD	-5.25	1.38	1.51
8	J	13	VAL	CB-CG1	-5.25	1.41	1.52
4	E	60	PHE	CD2-CE2	5.25	1.49	1.39
1	A	998	LEU	C-O	-5.24	1.13	1.23
1	A	1014	ALA	CA-CB	-5.24	1.41	1.52
1	A	1155	ASP	N-CA	5.24	1.56	1.46
2	B	622	LYS	CG-CD	5.24	1.70	1.52
3	C	84	ARG	CZ-NH1	-5.24	1.26	1.33
4	E	178	ILE	CA-C	5.24	1.66	1.52
6	H	37	LYS	CG-CD	5.24	1.70	1.52
1	A	434	ARG	CZ-NH1	5.24	1.39	1.33
2	B	890	TYR	CD1-CE1	5.24	1.47	1.39
4	E	24	LYS	CA-CB	-5.24	1.42	1.53
1	A	233	TRP	CG-CD1	-5.24	1.29	1.36
2	B	387	LEU	N-CA	-5.24	1.35	1.46
2	B	557	PHE	CE2-CZ	-5.24	1.27	1.37
2	B	1027	ILE	C-N	-5.24	1.22	1.34
2	B	29	ASP	CG-OD1	5.24	1.37	1.25
2	B	1091	TYR	C-O	-5.24	1.13	1.23
9	K	105	PHE	CD1-CE1	-5.24	1.28	1.39
1	A	472	LEU	CG-CD1	-5.24	1.32	1.51
1	A	1018	PHE	CB-CG	-5.24	1.42	1.51
2	B	1084	GLN	C-O	-5.24	1.13	1.23
2	B	131	ASP	CA-CB	5.23	1.65	1.53
2	B	956	THR	CA-CB	-5.23	1.39	1.53
10	L	47	ARG	C-O	-5.23	1.13	1.23
1	A	87	ALA	N-CA	-5.23	1.35	1.46
1	A	772	GLY	C-O	-5.23	1.15	1.23
6	H	95	TYR	C-N	-5.23	1.22	1.34
1	A	163	SER	N-CA	5.23	1.56	1.46
1	A	400	PRO	N-CA	-5.23	1.38	1.47
1	A	893	PHE	CD1-CE1	-5.23	1.28	1.39
1	A	1066	VAL	CA-CB	-5.23	1.43	1.54
1	A	630	ILE	CB-CG2	-5.23	1.36	1.52
2	B	1095	LEU	C-O	5.23	1.33	1.23
1	A	1095	THR	CA-C	-5.23	1.39	1.52
4	E	6	GLU	CD-OE2	5.23	1.31	1.25
5	F	90	ARG	NE-CZ	-5.23	1.26	1.33
7	I	27	PHE	CA-CB	-5.23	1.42	1.53
9	K	69	ALA	CA-C	-5.23	1.39	1.52
2	B	580	VAL	CA-C	-5.23	1.39	1.52
3	C	144	ILE	CB-CG1	-5.23	1.39	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	171	LYS	CG-CD	5.23	1.70	1.52
1	A	939	ASP	CB-CG	5.22	1.62	1.51
6	H	104	PHE	CA-CB	5.22	1.65	1.53
1	A	411	ASP	N-CA	5.22	1.56	1.46
1	A	1445	ILE	CA-CB	-5.22	1.42	1.54
4	E	70	SER	N-CA	-5.22	1.35	1.46
4	E	188	LEU	N-CA	-5.22	1.35	1.46
7	I	67	THR	CA-C	-5.22	1.39	1.52
1	A	1278	ASN	C-N	-5.22	1.22	1.34
2	B	191	LYS	CA-C	-5.22	1.39	1.52
9	K	84	LYS	CD-CE	5.22	1.64	1.51
1	A	448	PRO	N-CA	-5.22	1.38	1.47
1	A	649	ILE	C-O	5.22	1.33	1.23
1	A	787	PHE	N-CA	-5.22	1.35	1.46
1	A	1310	GLY	C-O	-5.22	1.15	1.23
2	B	301	ILE	CB-CG2	-5.22	1.36	1.52
2	B	756	ILE	C-N	-5.22	1.24	1.34
2	B	1106	ARG	N-CA	5.22	1.56	1.46
3	C	244	VAL	C-O	5.22	1.33	1.23
5	F	131	PRO	CB-CG	-5.22	1.23	1.50
1	A	108	MET	SD-CE	-5.22	1.48	1.77
1	A	614	PHE	C-O	-5.22	1.13	1.23
2	B	657	HIS	C-N	-5.22	1.22	1.34
3	C	100	THR	C-O	5.22	1.33	1.23
1	A	998	LEU	CG-CD2	-5.22	1.32	1.51
1	A	1289	ARG	CB-CG	-5.22	1.38	1.52
2	B	68	THR	CB-CG2	5.22	1.69	1.52
2	B	120	ARG	CD-NE	5.22	1.55	1.46
1	A	441	PRO	CB-CG	-5.21	1.23	1.50
1	A	1157	ASP	CG-OD1	5.21	1.37	1.25
1	A	1340	GLY	CA-C	-5.21	1.43	1.51
2	B	573	GLN	N-CA	5.21	1.56	1.46
6	H	129	TYR	CG-CD1	5.21	1.46	1.39
4	E	186	LEU	C-O	-5.21	1.13	1.23
9	K	27	ALA	CA-CB	5.21	1.63	1.52
2	B	103	ASN	CA-CB	5.21	1.66	1.53
2	B	535	LEU	N-CA	-5.21	1.35	1.46
4	E	91	LYS	C-O	5.21	1.33	1.23
1	A	860	LEU	C-O	-5.21	1.13	1.23
9	K	84	LYS	CG-CD	5.21	1.70	1.52
10	L	49	LYS	CE-NZ	5.21	1.62	1.49
1	A	600	PRO	CB-CG	5.21	1.75	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	936	LEU	CA-CB	-5.21	1.41	1.53
1	A	993	LEU	C-O	-5.21	1.13	1.23
2	B	298	LEU	N-CA	-5.21	1.35	1.46
2	B	882	THR	C-O	5.21	1.33	1.23
6	H	25	ARG	CA-C	5.21	1.66	1.52
6	H	103	LYS	CA-C	-5.21	1.39	1.52
9	K	72	LYS	CD-CE	5.21	1.64	1.51
1	A	602	ASP	C-O	-5.21	1.13	1.23
2	B	344	LYS	C-O	5.21	1.33	1.23
2	B	483	LEU	CA-CB	-5.21	1.41	1.53
9	K	112	GLN	CD-NE2	5.21	1.45	1.32
1	A	1232	ASN	CA-C	5.20	1.66	1.52
2	B	1044	ALA	N-CA	5.20	1.56	1.46
1	A	233	TRP	CA-CB	5.20	1.65	1.53
1	A	1341	ILE	CB-CG2	-5.20	1.36	1.52
4	E	125	PRO	CG-CD	5.20	1.67	1.50
4	E	147	HIS	CG-ND1	-5.20	1.27	1.38
1	A	248	PRO	N-CD	5.20	1.55	1.47
1	A	962	ARG	C-O	-5.20	1.13	1.23
2	B	137	TYR	N-CA	5.20	1.56	1.46
1	A	868	TYR	CA-CB	-5.20	1.42	1.53
1	A	951	GLU	CB-CG	-5.20	1.42	1.52
2	B	431	TYR	C-O	5.20	1.33	1.23
2	B	658	ILE	N-CA	-5.20	1.35	1.46
2	B	819	ALA	N-CA	-5.20	1.35	1.46
3	C	266	ASP	CA-C	5.20	1.66	1.52
1	A	371	ALA	CA-CB	-5.19	1.41	1.52
6	H	80	ARG	CZ-NH2	5.19	1.39	1.33
1	A	868	TYR	CB-CG	5.19	1.59	1.51
1	A	1027	ALA	N-CA	-5.19	1.35	1.46
1	A	1360	GLY	C-O	5.19	1.31	1.23
2	B	1073	TYR	CB-CG	5.19	1.59	1.51
1	A	190	ALA	CA-C	5.19	1.66	1.52
2	B	1066	SER	CB-OG	5.19	1.49	1.42
3	C	148	ARG	C-O	5.19	1.33	1.23
6	H	79	TRP	CD2-CE2	-5.19	1.35	1.41
1	A	377	PRO	CB-CG	-5.19	1.24	1.50
2	B	310	MET	CG-SD	-5.19	1.67	1.81
2	B	380	TYR	C-O	-5.19	1.13	1.23
2	B	858	SER	N-CA	5.19	1.56	1.46
4	E	148	GLU	CG-CD	-5.19	1.44	1.51
1	A	866	PHE	C-O	5.19	1.33	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	961	ARG	C-O	-5.19	1.13	1.23
2	B	959	ASP	CA-CB	5.19	1.65	1.53
2	B	1035	ALA	CA-CB	-5.19	1.41	1.52
1	A	718	VAL	CA-CB	-5.19	1.43	1.54
1	A	811	GLN	CD-OE1	5.19	1.35	1.24
3	C	201	TRP	CG-CD2	-5.19	1.34	1.43
1	A	76	GLU	CG-CD	5.18	1.59	1.51
1	A	711	ARG	CZ-NH2	-5.18	1.26	1.33
1	A	1305	VAL	C-N	-5.18	1.22	1.34
2	B	553	PRO	N-CD	-5.18	1.40	1.47
2	B	763	GLN	CB-CG	-5.18	1.38	1.52
2	B	1132	GLU	N-CA	-5.18	1.35	1.46
1	A	1426	GLU	CD-OE2	5.18	1.31	1.25
2	B	573	GLN	CD-NE2	5.18	1.45	1.32
2	B	1215	ARG	CD-NE	5.18	1.55	1.46
2	B	879	ARG	CB-CG	5.18	1.66	1.52
5	F	151	LEU	N-CA	5.18	1.56	1.46
6	H	33	GLN	CB-CG	5.18	1.66	1.52
1	A	21	LEU	CA-CB	-5.18	1.41	1.53
1	A	377	PRO	N-CD	-5.18	1.40	1.47
1	A	396	PRO	CA-C	-5.18	1.42	1.52
2	B	678	GLU	N-CA	5.18	1.56	1.46
10	L	47	ARG	CZ-NH2	5.18	1.39	1.33
3	C	115	SER	CB-OG	-5.18	1.35	1.42
2	B	235	SER	CA-C	-5.18	1.39	1.52
4	E	108	GLY	N-CA	-5.18	1.38	1.46
1	A	69	THR	C-O	5.17	1.33	1.23
1	A	1098	VAL	CA-CB	-5.17	1.43	1.54
2	B	384	ARG	CG-CD	5.17	1.64	1.51
3	C	160	LYS	CG-CD	5.17	1.70	1.52
1	A	874	ASP	CA-C	-5.17	1.39	1.52
1	A	984	LYS	CD-CE	5.17	1.64	1.51
1	A	1287	TYR	CB-CG	-5.17	1.43	1.51
1	A	22	PHE	CA-CB	-5.17	1.42	1.53
1	A	556	TRP	CB-CG	-5.17	1.41	1.50
1	A	560	ILE	C-O	-5.17	1.13	1.23
6	H	132	LEU	CB-CG	5.17	1.67	1.52
2	B	791	THR	CA-CB	-5.17	1.40	1.53
1	A	19	PHE	CB-CG	5.17	1.60	1.51
1	A	191	THR	C-O	5.17	1.33	1.23
2	B	463	THR	C-O	5.17	1.33	1.23
6	H	52	GLN	CD-OE1	5.17	1.35	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	110	ASP	N-CA	5.17	1.56	1.46
6	H	126	GLU	CD-OE2	5.17	1.31	1.25
1	A	596	THR	CA-C	-5.17	1.39	1.52
1	A	1368	MET	CG-SD	5.17	1.94	1.81
2	B	116	GLU	CB-CG	5.17	1.61	1.52
1	A	1104	ILE	CA-CB	-5.17	1.43	1.54
2	B	306	ASN	CG-OD1	5.16	1.35	1.24
2	B	529	GLU	CB-CG	5.16	1.61	1.52
4	E	180	ARG	CD-NE	5.16	1.55	1.46
1	A	408	ASP	N-CA	-5.16	1.36	1.46
2	B	213	ILE	N-CA	-5.16	1.36	1.46
1	A	194	ALA	N-CA	5.16	1.56	1.46
1	A	694	THR	C-O	5.16	1.33	1.23
2	B	244	LEU	CA-C	5.16	1.66	1.52
3	C	174	ALA	N-CA	-5.16	1.36	1.46
1	A	129	LYS	C-O	5.16	1.33	1.23
1	A	1243	VAL	CB-CG1	5.16	1.63	1.52
2	B	42	GLY	C-O	5.16	1.31	1.23
2	B	401	PHE	CA-C	-5.16	1.39	1.52
2	B	733	HIS	CB-CG	5.16	1.59	1.50
1	A	25	GLU	CA-CB	-5.16	1.42	1.53
1	A	438	ASP	CG-OD2	5.16	1.37	1.25
1	A	730	GLY	C-O	-5.16	1.15	1.23
1	A	1304	TRP	CA-C	-5.16	1.39	1.52
2	B	299	GLU	C-O	-5.16	1.13	1.23
2	B	978	ASP	CB-CG	5.16	1.62	1.51
8	J	60	PHE	C-O	5.16	1.33	1.23
9	K	54	ARG	CG-CD	5.16	1.64	1.51
3	C	214	ASN	C-O	5.15	1.33	1.23
9	K	58	PHE	CG-CD2	5.15	1.46	1.38
1	A	1212	VAL	CA-CB	-5.15	1.44	1.54
2	B	103	ASN	CG-ND2	5.15	1.45	1.32
2	B	1015	HIS	C-O	-5.15	1.13	1.23
4	E	183	PRO	N-CD	-5.15	1.40	1.47
10	L	38	LEU	CG-CD2	5.15	1.71	1.51
1	A	658	LEU	CA-CB	-5.15	1.42	1.53
3	C	117	ASP	C-O	5.15	1.33	1.23
1	A	137	ALA	CA-C	5.15	1.66	1.52
3	C	146	LYS	CG-CD	5.15	1.70	1.52
7	I	104	LEU	C-O	-5.15	1.13	1.23
1	A	1332	PHE	CA-CB	-5.15	1.42	1.53
1	A	1342	GLU	CG-CD	5.15	1.59	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1448	GLU	CB-CG	5.15	1.61	1.52
2	B	343	ILE	CB-CG2	-5.15	1.36	1.52
2	B	1057	LYS	CB-CG	5.15	1.66	1.52
3	C	203	GLN	CG-CD	-5.15	1.39	1.51
4	E	198	ILE	C-N	-5.15	1.22	1.34
8	J	50	ILE	CB-CG2	5.15	1.68	1.52
1	A	124	GLN	CB-CG	5.14	1.66	1.52
2	B	859	TYR	CE2-CZ	-5.14	1.31	1.38
2	B	989	THR	CA-CB	-5.14	1.40	1.53
3	C	132	PRO	CA-C	-5.14	1.42	1.52
6	H	103	LYS	C-O	-5.14	1.13	1.23
1	A	347	PHE	CA-C	-5.14	1.39	1.52
1	A	376	TYR	CB-CG	-5.14	1.44	1.51
2	B	304	ASP	CG-OD1	5.14	1.37	1.25
2	B	567	GLU	CA-C	5.14	1.66	1.52
8	J	53	HIS	CG-CD2	-5.14	1.27	1.35
9	K	3	ALA	N-CA	5.14	1.56	1.46
1	A	907	THR	CB-CG2	-5.14	1.35	1.52
2	B	490	SER	CA-CB	5.14	1.60	1.52
1	A	224	PHE	CD1-CE1	-5.14	1.28	1.39
1	A	800	VAL	CB-CG2	-5.14	1.42	1.52
1	A	983	ILE	C-O	-5.14	1.13	1.23
4	E	114	ASN	CB-CG	-5.14	1.39	1.51
6	H	144	ILE	CB-CG2	-5.14	1.36	1.52
9	K	92	ASN	CA-CB	5.14	1.66	1.53
1	A	538	ASP	CB-CG	-5.14	1.41	1.51
1	A	1044	TRP	CE2-CZ2	-5.14	1.31	1.39
2	B	454	THR	CA-CB	-5.14	1.40	1.53
2	B	828	ALA	C-O	-5.14	1.13	1.23
4	E	13	TRP	C-O	5.14	1.33	1.23
2	B	187	SER	C-O	5.13	1.33	1.23
2	B	265	SER	CA-C	5.13	1.66	1.52
2	B	992	ILE	CB-CG1	-5.13	1.39	1.54
2	B	771	SER	CA-C	-5.13	1.39	1.52
2	B	1186	ASP	CG-OD1	5.13	1.37	1.25
7	I	115	LYS	C-O	5.13	1.33	1.23
1	A	1060	PRO	CB-CG	-5.13	1.24	1.50
2	B	466	TRP	C-N	5.13	1.42	1.33
4	E	81	GLU	CD-OE2	5.13	1.31	1.25
2	B	995	ARG	N-CA	5.13	1.56	1.46
1	A	471	ASN	CA-CB	5.13	1.66	1.53
2	B	61	ASP	N-CA	-5.13	1.36	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	796	LEU	CG-CD2	-5.13	1.32	1.51
4	E	172	GLU	CD-OE1	-5.13	1.20	1.25
6	H	22	LYS	CD-CE	5.13	1.64	1.51
4	E	129	PRO	CA-C	5.12	1.63	1.52
1	A	387	ARG	C-O	5.12	1.33	1.23
1	A	523	ILE	N-CA	-5.12	1.36	1.46
1	A	983	ILE	C-N	-5.12	1.22	1.34
2	B	509	ALA	C-O	5.12	1.33	1.23
6	H	57	VAL	N-CA	5.12	1.56	1.46
9	K	47	ARG	N-CA	-5.12	1.36	1.46
10	L	56	LEU	C-O	-5.12	1.13	1.23
2	B	40	GLU	N-CA	-5.12	1.36	1.46
2	B	523	CYS	C-O	-5.12	1.13	1.23
2	B	964	VAL	CB-CG1	-5.12	1.42	1.52
4	E	65	THR	CB-OG1	5.12	1.53	1.43
1	A	1004	ASN	CA-C	5.12	1.66	1.52
1	A	1440	ALA	CA-C	5.12	1.66	1.52
2	B	395	GLN	CB-CG	-5.12	1.38	1.52
2	B	1180	PHE	CD1-CE1	-5.12	1.29	1.39
6	H	137	GLN	CB-CG	5.12	1.66	1.52
1	A	213	HIS	C-O	5.12	1.33	1.23
1	A	490	HIS	N-CA	-5.12	1.36	1.46
1	A	756	ILE	N-CA	5.12	1.56	1.46
2	B	357	GLN	C-O	-5.12	1.13	1.23
2	B	1128	LEU	CG-CD1	-5.12	1.32	1.51
1	A	364	VAL	C-N	-5.12	1.23	1.33
2	B	60	GLN	N-CA	-5.12	1.36	1.46
2	B	809	MET	C-N	-5.12	1.22	1.34
2	B	1069	PHE	CD1-CE1	5.12	1.49	1.39
3	C	249	ASP	CA-CB	5.12	1.65	1.53
5	F	94	LEU	CA-C	-5.12	1.39	1.52
1	A	929	LEU	N-CA	-5.11	1.36	1.46
9	K	32	VAL	C-O	5.11	1.33	1.23
1	A	1164	PRO	CB-CG	5.11	1.75	1.50
2	B	1052	VAL	CB-CG1	-5.11	1.42	1.52
8	J	54	VAL	N-CA	-5.11	1.36	1.46
1	A	786	HIS	CB-CG	-5.11	1.40	1.50
1	A	866	PHE	CG-CD2	-5.11	1.31	1.38
1	A	1314	SER	N-CA	-5.11	1.36	1.46
4	E	73	PRO	N-CD	5.11	1.55	1.47
1	A	942	PHE	CG-CD2	-5.11	1.31	1.38
1	A	1045	VAL	CB-CG2	-5.11	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	325	GLN	CD-NE2	5.11	1.45	1.32
7	I	102	VAL	N-CA	5.11	1.56	1.46
2	B	1008	PRO	N-CA	-5.11	1.38	1.47
1	A	1079	MET	CG-SD	5.11	1.94	1.81
2	B	177	LYS	CD-CE	5.11	1.64	1.51
5	F	119	ARG	CA-C	-5.11	1.39	1.52
9	K	97	LYS	CA-C	-5.11	1.39	1.52
1	A	1148	ILE	C-O	-5.10	1.13	1.23
2	B	1143	ALA	C-O	-5.10	1.13	1.23
1	A	743	VAL	CA-CB	-5.10	1.44	1.54
3	C	236	GLY	CA-C	-5.10	1.43	1.51
1	A	47	ARG	CA-C	5.10	1.66	1.52
1	A	91	PHE	CE2-CZ	-5.10	1.27	1.37
2	B	679	TYR	CG-CD1	-5.10	1.32	1.39
2	B	800	GLN	CB-CG	-5.10	1.38	1.52
2	B	1128	LEU	CA-C	5.10	1.66	1.52
3	C	103	ALA	CA-CB	-5.10	1.41	1.52
1	A	771	GLU	C-O	-5.10	1.13	1.23
2	B	451	LYS	CB-CG	5.10	1.66	1.52
2	B	789	MET	SD-CE	5.10	2.06	1.77
2	B	860	MET	CA-CB	-5.10	1.42	1.53
2	B	869	SER	CB-OG	5.10	1.48	1.42
3	C	191	TYR	N-CA	-5.10	1.36	1.46
1	A	36	ARG	CD-NE	5.10	1.55	1.46
2	B	402	GLY	N-CA	-5.10	1.38	1.46
2	B	602	THR	CB-OG1	5.10	1.53	1.43
1	A	562	THR	CB-CG2	5.09	1.69	1.52
1	A	597	LEU	CA-C	-5.09	1.39	1.52
9	K	61	TYR	CA-C	-5.09	1.39	1.52
2	B	1088	GLY	C-O	-5.09	1.15	1.23
4	E	181	ALA	C-O	5.09	1.33	1.23
5	F	78	GLN	CB-CG	5.09	1.66	1.52
2	B	634	TYR	CD1-CE1	-5.09	1.31	1.39
2	B	856	PHE	CE1-CZ	-5.09	1.27	1.37
4	E	149	LEU	CG-CD1	-5.09	1.33	1.51
1	A	432	VAL	CB-CG1	-5.09	1.42	1.52
2	B	709	ASP	N-CA	-5.09	1.36	1.46
2	B	895	ASP	CA-CB	5.09	1.65	1.53
3	C	138	GLU	CA-C	-5.09	1.39	1.52
2	B	55	VAL	CB-CG1	-5.09	1.42	1.52
2	B	1174	LYS	CE-NZ	5.09	1.61	1.49
10	L	60	ARG	NE-CZ	5.09	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1152	ILE	CA-CB	-5.08	1.43	1.54
2	B	188	ASP	C-O	5.08	1.33	1.23
2	B	306	ASN	N-CA	5.08	1.56	1.46
2	B	722	ASP	CA-CB	5.08	1.65	1.53
8	J	23	ASN	CG-OD1	5.08	1.35	1.24
9	K	63	VAL	C-O	5.08	1.33	1.23
1	A	120	GLU	CA-C	5.08	1.66	1.52
1	A	397	ASN	C-O	5.08	1.33	1.23
1	A	661	GLY	C-O	-5.08	1.15	1.23
3	C	113	VAL	CB-CG2	-5.08	1.42	1.52
2	B	32	ALA	CA-C	-5.08	1.39	1.52
2	B	527	THR	CA-CB	-5.08	1.40	1.53
10	L	50	ASP	N-CA	5.08	1.56	1.46
1	A	943	LEU	C-O	-5.08	1.13	1.23
2	B	137	TYR	CA-CB	5.08	1.65	1.53
2	B	730	ARG	N-CA	-5.08	1.36	1.46
2	B	1013	ASN	C-O	-5.08	1.13	1.23
2	B	1199	ALA	C-O	5.08	1.32	1.23
3	C	48	SER	CB-OG	5.08	1.48	1.42
8	J	38	ARG	CA-C	-5.08	1.39	1.52
2	B	193	LYS	CE-NZ	5.08	1.61	1.49
2	B	581	PHE	CG-CD2	-5.08	1.31	1.38
2	B	1139	ILE	CB-CG2	-5.08	1.37	1.52
10	L	37	LYS	C-O	-5.08	1.13	1.23
1	A	1421	CYS	CB-SG	5.08	1.90	1.82
2	B	362	PRO	CA-CB	-5.08	1.43	1.53
3	C	191	TYR	CZ-OH	5.08	1.46	1.37
4	E	104	ASN	CG-ND2	5.08	1.45	1.32
1	A	521	MET	CA-C	-5.07	1.39	1.52
2	B	798	TYR	CE2-CZ	5.07	1.45	1.38
3	C	4	GLU	CB-CG	5.07	1.61	1.52
2	B	1075	GLY	CA-C	5.07	1.59	1.51
2	B	1198	TYR	CG-CD2	5.07	1.45	1.39
1	A	37	PHE	CG-CD1	5.07	1.46	1.38
1	A	387	ARG	CZ-NH1	-5.07	1.26	1.33
1	A	944	ARG	CZ-NH1	-5.07	1.26	1.33
2	B	214	ALA	N-CA	-5.07	1.36	1.46
2	B	326	ASP	CA-CB	-5.07	1.42	1.53
2	B	1210	MET	CA-C	-5.07	1.39	1.52
1	A	1164	PRO	CA-CB	5.07	1.63	1.53
2	B	557	PHE	CA-CB	-5.07	1.42	1.53
4	E	137	GLU	CG-CD	5.07	1.59	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195	ASP	C-N	5.07	1.45	1.34
2	B	557	PHE	CG-CD2	5.07	1.46	1.38
3	C	70	ILE	CB-CG1	5.07	1.68	1.54
9	K	52	ASN	N-CA	-5.07	1.36	1.46
1	A	716	ASP	CG-OD2	5.07	1.36	1.25
2	B	31	TRP	C-N	-5.07	1.22	1.34
2	B	815	ARG	C-O	-5.07	1.13	1.23
2	B	963	PHE	CD1-CE1	-5.07	1.29	1.39
6	H	91	ASP	CG-OD1	5.07	1.36	1.25
8	J	38	ARG	NE-CZ	5.07	1.39	1.33
1	A	814	PHE	C-O	-5.06	1.13	1.23
1	A	1368	MET	C-O	-5.06	1.13	1.23
1	A	599	SER	C-O	-5.06	1.13	1.23
2	B	225	VAL	CA-CB	-5.06	1.44	1.54
2	B	247	GLY	C-O	5.06	1.31	1.23
3	C	183	TRP	NE1-CE2	-5.06	1.30	1.37
4	E	49	SER	C-O	5.06	1.32	1.23
4	E	61	GLN	CG-CD	-5.06	1.39	1.51
5	F	150	GLU	CA-C	-5.06	1.39	1.52
6	H	87	ARG	CA-C	5.06	1.66	1.52
8	J	8	PHE	CG-CD1	-5.06	1.31	1.38
7	I	48	LEU	CA-CB	-5.06	1.42	1.53
2	B	327	ARG	CA-CB	-5.06	1.42	1.53
1	A	1038	THR	C-O	-5.06	1.13	1.23
1	A	1220	PHE	CE2-CZ	-5.06	1.27	1.37
5	F	136	ARG	C-O	-5.06	1.13	1.23
10	L	60	ARG	CB-CG	5.06	1.66	1.52
3	C	217	ASP	CG-OD1	5.06	1.36	1.25
1	A	14	VAL	CA-C	-5.05	1.39	1.52
1	A	119	ASN	CB-CG	5.05	1.62	1.51
2	B	519	TRP	CZ2-CH2	5.05	1.47	1.37
2	B	535	LEU	CG-CD1	-5.05	1.33	1.51
2	B	653	VAL	C-O	5.05	1.32	1.23
1	A	483	ASP	N-CA	5.05	1.56	1.46
2	B	89	GLU	N-CA	5.05	1.56	1.46
2	B	435	THR	C-O	5.05	1.32	1.23
6	H	34	ASP	CG-OD2	5.05	1.36	1.25
2	B	1135	ARG	CD-NE	-5.05	1.37	1.46
6	H	105	GLU	CD-OE1	5.05	1.31	1.25
1	A	47	ARG	N-CA	5.05	1.56	1.46
5	F	116	ASP	N-CA	5.05	1.56	1.46
1	A	1103	GLU	CG-CD	5.05	1.59	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	27	GLU	CB-CG	5.05	1.61	1.52
9	K	83	PRO	CA-CB	-5.05	1.43	1.53
7	I	81	ARG	CA-C	5.04	1.66	1.52
1	A	19	PHE	CE1-CZ	-5.04	1.27	1.37
2	B	199	MET	CG-SD	5.04	1.94	1.81
2	B	1095	LEU	CG-CD2	-5.04	1.33	1.51
6	H	35	GLN	CA-CB	5.04	1.65	1.53
1	A	212	LYS	CD-CE	5.04	1.63	1.51
2	B	38	PHE	CE2-CZ	-5.04	1.27	1.37
2	B	869	SER	CA-C	5.04	1.66	1.52
4	E	194	GLU	CB-CG	5.04	1.61	1.52
1	A	1042	PHE	CG-CD2	-5.04	1.31	1.38
1	A	913	LEU	CG-CD2	-5.04	1.33	1.51
6	H	7	ASP	CB-CG	5.04	1.62	1.51
1	A	19	PHE	C-O	-5.04	1.13	1.23
1	A	447	GLN	CG-CD	-5.04	1.39	1.51
1	A	677	ARG	CG-CD	5.04	1.64	1.51
1	A	877	HIS	CA-CB	-5.04	1.42	1.53
3	C	42	PRO	CA-C	-5.04	1.42	1.52
1	A	553	VAL	CA-CB	-5.03	1.44	1.54
1	A	721	PHE	C-O	5.03	1.32	1.23
1	A	751	SER	C-O	-5.03	1.13	1.23
1	A	1242	VAL	N-CA	-5.03	1.36	1.46
3	C	206	ASN	CB-CG	-5.03	1.39	1.51
1	A	1320	PRO	N-CD	-5.03	1.40	1.47
4	E	94	LYS	CD-CE	5.03	1.63	1.51
10	L	61	THR	CB-OG1	-5.03	1.33	1.43
1	A	1038	THR	CB-OG1	-5.03	1.33	1.43
1	A	1365	TYR	CA-C	-5.03	1.39	1.52
2	B	350	GLN	CB-CG	5.03	1.66	1.52
2	B	430	ARG	CG-CD	5.03	1.64	1.51
4	E	166	LYS	CD-CE	5.03	1.63	1.51
8	J	2	ILE	C-O	-5.03	1.13	1.23
1	A	99	ILE	N-CA	-5.03	1.36	1.46
1	A	1106	ASN	C-N	-5.03	1.22	1.34
2	B	611	PRO	C-O	-5.03	1.13	1.23
6	H	145	ARG	CZ-NH1	5.03	1.39	1.33
2	B	321	GLY	CA-C	5.02	1.59	1.51
1	A	14	VAL	CB-CG1	-5.02	1.42	1.52
1	A	1331	SER	CB-OG	5.02	1.48	1.42
2	B	1220	ARG	NE-CZ	5.02	1.39	1.33
1	A	361	LEU	C-O	-5.02	1.13	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	468	PHE	CD1-CE1	5.02	1.49	1.39
1	A	743	VAL	CB-CG2	5.02	1.63	1.52
2	B	1030	LEU	C-O	-5.02	1.13	1.23
1	A	836	TYR	CB-CG	5.02	1.59	1.51
1	A	1351	GLU	CD-OE1	5.02	1.31	1.25
2	B	712	PRO	C-O	5.02	1.33	1.23
1	A	84	ILE	CB-CG1	-5.02	1.40	1.54
1	A	1327	ILE	CA-CB	5.02	1.66	1.54
2	B	734	HIS	CB-CG	5.02	1.59	1.50
8	J	52	THR	CB-CG2	-5.02	1.35	1.52
9	K	25	THR	CB-CG2	5.02	1.69	1.52
1	A	248	PRO	CA-CB	5.02	1.63	1.53
4	E	97	VAL	CA-CB	-5.01	1.44	1.54
4	E	113	GLN	CD-NE2	5.01	1.45	1.32
1	A	1239	ARG	N-CA	-5.01	1.36	1.46
1	A	1281	ARG	N-CA	5.01	1.56	1.46
2	B	1146	PHE	CD1-CE1	-5.01	1.29	1.39
6	H	116	TYR	CD1-CE1	-5.01	1.31	1.39
1	A	495	GLU	CG-CD	-5.01	1.44	1.51
1	A	858	ASN	N-CA	5.01	1.56	1.46
1	A	1067	LEU	CB-CG	-5.01	1.38	1.52
3	C	220	ASP	C-O	5.01	1.32	1.23
7	I	42	LEU	C-O	-5.01	1.13	1.23
2	B	343	ILE	CG1-CD1	5.01	1.85	1.50
6	H	128	ASN	CG-OD1	5.01	1.34	1.24
1	A	41	MET	SD-CE	5.01	2.05	1.77
1	A	1339	LEU	N-CA	-5.01	1.36	1.46
2	B	498	THR	CA-CB	5.01	1.66	1.53
2	B	858	SER	CA-CB	-5.01	1.45	1.52
3	C	24	ASN	CB-CG	5.01	1.62	1.51
3	C	266	ASP	CG-OD2	5.00	1.36	1.25
1	A	206	GLU	CA-C	-5.00	1.40	1.52
2	B	660	LYS	CD-CE	-5.00	1.38	1.51
6	H	135	LEU	CG-CD1	5.00	1.70	1.51
8	J	21	TYR	CD2-CE2	5.00	1.46	1.39
1	A	347	PHE	C-O	-5.00	1.13	1.23
2	B	812	LEU	N-CA	-5.00	1.36	1.46

All (3046) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1064	VAL	CA-C-O	-35.84	44.85	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	136	ARG	NE-CZ-NH1	-34.13	103.24	120.30
1	A	774	ARG	NE-CZ-NH1	32.04	136.32	120.30
1	A	1064	VAL	O-C-N	-31.34	69.93	123.20
1	A	821	ARG	NE-CZ-NH2	-29.52	105.54	120.30
1	A	469	ARG	NE-CZ-NH2	-29.20	105.70	120.30
2	B	807	ARG	NE-CZ-NH2	-28.69	105.95	120.30
1	A	896	ARG	NE-CZ-NH2	-28.14	106.23	120.30
2	B	1150	ARG	NE-CZ-NH1	-28.10	106.25	120.30
1	A	1241	ARG	NE-CZ-NH2	-27.64	106.48	120.30
2	B	496	ARG	NE-CZ-NH1	27.12	133.86	120.30
10	L	70	ARG	NE-CZ-NH1	26.97	133.79	120.30
1	A	1064	VAL	CA-C-N	-26.09	64.02	116.20
2	B	995	ARG	NE-CZ-NH2	-25.98	107.31	120.30
8	J	43	ARG	NE-CZ-NH2	25.79	133.19	120.30
9	K	47	ARG	NE-CZ-NH2	-24.58	108.01	120.30
4	E	11	ARG	NE-CZ-NH1	-24.38	108.11	120.30
1	A	774	ARG	NE-CZ-NH2	-24.16	108.22	120.30
1	A	469	ARG	NE-CZ-NH1	24.13	132.37	120.30
2	B	1135	ARG	NE-CZ-NH2	-23.82	108.39	120.30
8	J	43	ARG	NE-CZ-NH1	-23.64	108.48	120.30
2	B	983	ARG	NE-CZ-NH1	23.57	132.09	120.30
8	J	2	ILE	CG1-CB-CG2	-22.83	61.18	111.40
1	A	1100	ARG	NE-CZ-NH1	22.32	131.46	120.30
2	B	106	ASP	CB-CG-OD2	22.14	138.23	118.30
1	A	1135	ARG	NE-CZ-NH1	-22.05	109.28	120.30
2	B	620	ARG	NE-CZ-NH2	-22.04	109.28	120.30
9	K	47	ARG	NE-CZ-NH1	21.88	131.24	120.30
3	C	35	ARG	NE-CZ-NH2	-21.74	109.43	120.30
2	B	601	ARG	NE-CZ-NH1	-21.57	109.51	120.30
1	A	806	ARG	NE-CZ-NH1	-21.56	109.52	120.30
2	B	983	ARG	NE-CZ-NH2	-21.42	109.59	120.30
2	B	604	ARG	NE-CZ-NH1	21.18	130.89	120.30
1	A	1241	ARG	NE-CZ-NH1	21.14	130.87	120.30
9	K	6	ARG	NE-CZ-NH2	-21.03	109.78	120.30
2	B	604	ARG	NE-CZ-NH2	-20.69	109.95	120.30
1	A	85	ASP	CB-CG-OD1	-20.33	100.01	118.30
1	A	1064	VAL	CB-CA-C	19.50	148.46	111.40
1	A	188	ASP	CB-CG-OD2	19.37	135.74	118.30
1	A	434	ARG	NE-CZ-NH2	-19.25	110.67	120.30
2	B	839	MET	CG-SD-CE	-19.20	69.48	100.20
3	C	66	ARG	NE-CZ-NH1	-19.07	110.77	120.30
2	B	241	ARG	NE-CZ-NH2	-19.03	110.78	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	136	ARG	NE-CZ-NH2	18.98	129.79	120.30
2	B	909	ASP	CB-CG-OD2	18.90	135.31	118.30
2	B	106	ASP	CB-CG-OD1	-18.78	101.40	118.30
6	H	77	ARG	NE-CZ-NH1	18.71	129.66	120.30
1	A	801	GLU	OE1-CD-OE2	18.47	145.47	123.30
2	B	848	ARG	NE-CZ-NH1	-18.43	111.08	120.30
2	B	1043	ASP	CB-CG-OD1	-18.42	101.72	118.30
3	C	136	ASP	CB-CG-OD2	18.38	134.84	118.30
1	A	1006	ILE	CG1-CB-CG2	-18.33	71.07	111.40
1	A	940	ARG	NE-CZ-NH1	18.12	129.36	120.30
2	B	1049	ASP	CB-CG-OD1	17.92	134.43	118.30
2	B	497	ARG	NE-CZ-NH2	-17.90	111.35	120.30
7	I	61	ASP	CB-CG-OD2	17.80	134.32	118.30
5	F	97	ARG	NE-CZ-NH2	-17.55	111.53	120.30
1	A	1064	VAL	C-N-CA	-17.48	85.59	122.30
8	J	7	CYS	CA-CB-SG	17.48	145.46	114.00
2	B	1043	ASP	CB-CG-OD2	17.31	133.88	118.30
10	L	68	GLU	OE1-CD-OE2	-17.21	102.65	123.30
1	A	1336	MET	CG-SD-CE	17.08	127.52	100.20
4	E	25	ASP	CB-CG-OD2	17.04	133.63	118.30
1	A	590	ARG	NE-CZ-NH2	-16.96	111.82	120.30
1	A	407	ARG	NE-CZ-NH2	-16.91	111.84	120.30
2	B	1150	ARG	NH1-CZ-NH2	16.75	137.82	119.40
6	H	41	ASP	CB-CG-OD1	16.70	133.33	118.30
9	K	24	ASP	CB-CG-OD2	16.66	133.30	118.30
2	B	711	GLU	OE1-CD-OE2	-16.59	103.39	123.30
1	A	434	ARG	NE-CZ-NH1	16.51	128.56	120.30
7	I	81	ARG	NE-CZ-NH1	16.48	128.54	120.30
1	A	1064	VAL	N-CA-CB	-16.21	75.83	111.50
8	J	1	MET	CG-SD-CE	-16.16	74.34	100.20
1	A	1442	ASP	CB-CG-OD1	-16.11	103.80	118.30
7	I	81	ARG	NE-CZ-NH2	-16.05	112.27	120.30
1	A	416	ARG	NE-CZ-NH2	-16.02	112.29	120.30
3	C	127	ARG	NE-CZ-NH1	15.84	128.22	120.30
2	B	198	ASP	CB-CG-OD1	15.82	132.53	118.30
2	B	326	ASP	CB-CG-OD2	15.80	132.52	118.30
9	K	6	ARG	NE-CZ-NH1	15.80	128.20	120.30
2	B	760	ASP	CB-CG-OD2	15.79	132.51	118.30
4	E	24	LYS	CD-CE-NZ	-15.73	75.52	111.70
9	K	114	LEU	CB-CG-CD2	15.71	137.70	111.00
2	B	654	ARG	NE-CZ-NH1	-15.69	112.45	120.30
3	C	16	ASP	CB-CG-OD1	-15.65	104.22	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	76	ASP	CB-CG-OD2	-15.59	104.27	118.30
1	A	420	ARG	NE-CZ-NH1	15.58	128.09	120.30
2	B	1010	LEU	CB-CG-CD1	-15.51	84.63	111.00
1	A	605	MET	CG-SD-CE	-15.47	75.45	100.20
2	B	620	ARG	NH1-CZ-NH2	15.41	136.35	119.40
7	I	91	ARG	NE-CZ-NH2	-15.33	112.64	120.30
4	E	212	ARG	NE-CZ-NH2	-15.32	112.64	120.30
1	A	826	ASP	CB-CG-OD2	15.22	132.00	118.30
1	A	206	GLU	OE1-CD-OE2	15.21	141.55	123.30
2	B	391	ASP	CB-CG-OD2	15.15	131.94	118.30
2	B	249	ARG	NE-CZ-NH1	15.09	127.85	120.30
3	C	35	ARG	NE-CZ-NH1	15.05	127.83	120.30
7	I	70	ARG	NE-CZ-NH2	-15.02	112.79	120.30
9	K	22	ASP	CB-CG-OD1	15.00	131.80	118.30
1	A	130	ASP	CB-CG-OD1	14.89	131.70	118.30
7	I	106	CYS	CA-CB-SG	14.89	140.80	114.00
1	A	1422	ARG	NE-CZ-NH2	14.88	127.74	120.30
8	J	62	ARG	NE-CZ-NH1	14.87	127.74	120.30
1	A	1442	ASP	CB-CG-OD2	14.82	131.64	118.30
2	B	747	MET	CG-SD-CE	-14.65	76.75	100.20
3	C	165	LYS	CD-CE-NZ	14.64	145.37	111.70
1	A	151	ASP	CB-CG-OD2	14.63	131.47	118.30
1	A	557	ASP	CB-CG-OD2	14.54	131.38	118.30
1	A	387	ARG	NE-CZ-NH1	14.53	127.57	120.30
8	J	38	ARG	NE-CZ-NH1	14.52	127.56	120.30
7	I	54	GLU	OE1-CD-OE2	14.51	140.71	123.30
2	B	373	ARG	NE-CZ-NH2	-14.46	113.07	120.30
2	B	807	ARG	NE-CZ-NH1	14.43	127.52	120.30
2	B	995	ARG	NE-CZ-NH1	14.39	127.50	120.30
4	E	204	THR	CA-CB-CG2	14.39	132.55	112.40
1	A	446	ARG	NE-CZ-NH2	-14.36	113.12	120.30
2	B	646	LEU	CB-CG-CD2	14.35	135.39	111.00
1	A	884	ASP	CB-CG-OD1	-14.33	105.40	118.30
1	A	814	PHE	CG-CD2-CE2	-14.25	105.12	120.80
1	A	857	ARG	NE-CZ-NH2	14.25	127.42	120.30
7	I	61	ASP	CB-CG-OD1	-14.24	105.48	118.30
3	C	34	ARG	NE-CZ-NH2	-14.23	113.19	120.30
2	B	1129	ARG	NE-CZ-NH2	-14.21	113.19	120.30
1	A	590	ARG	NE-CZ-NH1	14.20	127.40	120.30
6	H	130	ARG	NE-CZ-NH1	-14.14	113.23	120.30
1	A	771	GLU	OE1-CD-OE2	14.12	140.25	123.30
1	A	1269	GLU	OE1-CD-OE2	14.07	140.18	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	962	ARG	NE-CZ-NH1	14.06	127.33	120.30
1	A	782	ARG	NE-CZ-NH1	14.03	127.31	120.30
2	B	294	ASP	CB-CG-OD2	14.01	130.91	118.30
2	B	188	ASP	CB-CG-OD2	13.83	130.75	118.30
8	J	49	MET	CG-SD-CE	-13.79	78.14	100.20
1	A	821	ARG	NE-CZ-NH1	13.76	127.18	120.30
4	E	14	ARG	NE-CZ-NH2	-13.75	113.43	120.30
10	L	68	GLU	CG-CD-OE1	13.73	145.75	118.30
3	C	47	ASP	CB-CG-OD1	-13.72	105.95	118.30
1	A	949	ASP	CB-CG-OD2	13.71	130.64	118.30
2	B	485	ARG	NE-CZ-NH2	-13.67	113.47	120.30
2	B	552	MET	CG-SD-CE	13.65	122.05	100.20
2	B	790	ASP	CB-CG-OD1	13.62	130.56	118.30
2	B	198	ASP	CB-CG-OD2	-13.62	106.04	118.30
1	A	618	GLU	OE1-CD-OE2	13.57	139.59	123.30
2	B	883	LEU	CA-CB-CG	13.54	146.44	115.30
6	H	40	LEU	CB-CG-CD2	13.50	133.95	111.00
7	I	75	CYS	CA-CB-SG	13.49	138.29	114.00
1	A	874	ASP	CB-CG-OD1	-13.43	106.22	118.30
2	B	758	PHE	CD1-CE1-CZ	-13.37	104.06	120.10
9	K	1	MET	CG-SD-CE	13.34	121.54	100.20
4	E	55	ARG	NE-CZ-NH2	13.34	126.97	120.30
2	B	635	ARG	NE-CZ-NH1	13.31	126.95	120.30
2	B	118	ARG	NE-CZ-NH1	13.30	126.95	120.30
2	B	967	ARG	NE-CZ-NH1	-13.27	113.67	120.30
1	A	782	ARG	NE-CZ-NH2	-13.23	113.69	120.30
1	A	42	ASP	CB-CG-OD2	13.22	130.20	118.30
3	C	84	ARG	NE-CZ-NH2	13.20	126.90	120.30
4	E	81	GLU	OE1-CD-OE2	13.17	139.10	123.30
8	J	62	ARG	NE-CZ-NH2	-13.16	113.72	120.30
1	A	720	ARG	NE-CZ-NH2	13.13	126.87	120.30
1	A	761	MET	CG-SD-CE	13.13	121.21	100.20
1	A	884	ASP	CB-CG-OD2	13.12	130.10	118.30
1	A	962	ARG	NE-CZ-NH2	-13.10	113.75	120.30
4	E	167	ARG	NE-CZ-NH1	-13.09	113.75	120.30
7	I	24	ARG	NE-CZ-NH1	-13.03	113.79	120.30
1	A	812	GLU	OE1-CD-OE2	-12.97	107.73	123.30
1	A	70	CYS	CA-CB-SG	12.95	137.31	114.00
1	A	850	VAL	CG1-CB-CG2	-12.91	90.24	110.90
4	E	11	ARG	NH1-CZ-NH2	12.90	133.59	119.40
3	C	143	LEU	CB-CG-CD2	-12.84	89.17	111.00
4	E	52	ARG	NE-CZ-NH1	12.82	126.71	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	66	ARG	NE-CZ-NH2	12.77	126.69	120.30
2	B	1159	ARG	NE-CZ-NH2	-12.76	113.92	120.30
3	C	86	CYS	CA-CB-SG	12.76	136.97	114.00
4	E	208	TYR	CG-CD1-CE1	12.74	131.50	121.30
7	I	43	VAL	N-CA-CB	-12.70	83.56	111.50
2	B	1050	ILE	CG1-CB-CG2	-12.62	83.64	111.40
5	F	81	THR	N-CA-CB	-12.60	86.36	110.30
1	A	53	LEU	CA-CB-CG	12.55	144.18	115.30
1	A	826	ASP	CB-CG-OD1	-12.56	107.00	118.30
1	A	748	MET	CG-SD-CE	12.54	120.27	100.20
7	I	92	ARG	NE-CZ-NH1	-12.47	114.06	120.30
1	A	1264	GLU	OE1-CD-OE2	-12.46	108.35	123.30
2	B	996	ARG	NE-CZ-NH2	-12.45	114.08	120.30
2	B	1159	ARG	NE-CZ-NH1	12.44	126.52	120.30
2	B	788	ARG	NE-CZ-NH1	12.43	126.52	120.30
10	L	44	ASP	CB-CG-OD2	-12.42	107.12	118.30
8	J	6	ARG	NE-CZ-NH2	12.42	126.51	120.30
1	A	1207	LEU	CB-CG-CD1	-12.39	89.93	111.00
2	B	511	PRO	N-CD-CG	-12.36	84.66	103.20
1	A	1018	PHE	CB-CG-CD1	12.34	129.44	120.80
8	J	25	LEU	CB-CG-CD2	-12.33	90.03	111.00
1	A	752	LYS	CD-CE-NZ	12.33	140.06	111.70
2	B	498	THR	N-CA-CB	-12.28	86.97	110.30
2	B	895	ASP	CB-CG-OD2	12.23	129.31	118.30
1	A	107	CYS	CA-CB-SG	12.23	136.01	114.00
2	B	1185	CYS	CA-CB-SG	12.21	135.99	114.00
1	A	949	ASP	N-CA-CB	-12.20	88.64	110.60
6	H	110	ASP	CB-CG-OD2	12.18	129.26	118.30
1	A	538	ASP	CB-CA-C	-12.13	86.14	110.40
2	B	1019	SER	CB-CA-C	-12.12	87.06	110.10
10	L	70	ARG	NE-CZ-NH2	-12.11	114.25	120.30
2	B	391	ASP	OD1-CG-OD2	-12.11	100.29	123.30
2	B	833	TYR	CB-CG-CD1	12.06	128.24	121.00
5	F	90	ARG	NE-CZ-NH2	-12.04	114.28	120.30
2	B	801	LYS	CD-CE-NZ	-12.03	84.02	111.70
1	A	459	ARG	NE-CZ-NH1	12.03	126.31	120.30
5	F	85	MET	CG-SD-CE	-12.02	80.97	100.20
1	A	1223	ASP	CB-CG-OD1	11.90	129.01	118.30
1	A	353	ILE	CG1-CB-CG2	-11.87	85.29	111.40
2	B	620	ARG	NE-CZ-NH1	-11.87	114.37	120.30
5	F	92	ARG	NE-CZ-NH1	11.86	126.23	120.30
2	B	591	ARG	NE-CZ-NH2	-11.86	114.37	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	392	ARG	NE-CZ-NH2	-11.83	114.38	120.30
3	C	16	ASP	CB-CG-OD2	11.79	128.91	118.30
1	A	814	PHE	CB-CG-CD1	-11.78	112.55	120.80
4	E	52	ARG	NE-CZ-NH2	-11.78	114.41	120.30
10	L	44	ASP	CB-CG-OD1	11.67	128.80	118.30
1	A	1043	ASP	CB-CG-OD2	11.66	128.79	118.30
2	B	1096	ARG	NE-CZ-NH1	-11.66	114.47	120.30
4	E	208	TYR	CB-CG-CD1	11.66	128.00	121.00
2	B	884	ARG	NE-CZ-NH1	11.65	126.13	120.30
1	A	93	VAL	CB-CA-C	-11.65	89.27	111.40
6	H	135	LEU	CB-CG-CD2	11.64	130.80	111.00
1	A	1119	TYR	CD1-CE1-CZ	11.63	130.26	119.80
3	C	26	ASP	CB-CG-OD2	-11.63	107.83	118.30
1	A	157	ASP	CB-CG-OD1	11.61	128.75	118.30
9	K	73	LEU	CB-CG-CD1	-11.61	91.27	111.00
2	B	963	PHE	CB-CA-C	-11.57	87.26	110.40
1	A	790	ASP	CB-CG-OD1	11.55	128.70	118.30
2	B	652	LYS	CD-CE-NZ	11.50	138.15	111.70
1	A	1349	TYR	CZ-CE2-CD2	11.49	130.14	119.80
2	B	496	ARG	NH1-CZ-NH2	-11.48	106.77	119.40
1	A	894	GLU	OE1-CD-OE2	-11.47	109.53	123.30
2	B	853	SER	CB-CA-C	-11.45	88.34	110.10
2	B	256	VAL	CG1-CB-CG2	-11.44	92.60	110.90
1	A	1285	MET	CG-SD-CE	11.43	118.49	100.20
4	E	201	LYS	CD-CE-NZ	-11.43	85.41	111.70
6	H	92	ASP	CB-CG-OD1	11.43	128.58	118.30
2	B	978	ASP	CB-CG-OD2	11.36	128.52	118.30
1	A	416	ARG	NE-CZ-NH1	11.34	125.97	120.30
1	A	830	LYS	CB-CA-C	-11.33	87.75	110.40
1	A	1032	LEU	CB-CG-CD1	-11.31	91.78	111.00
4	E	208	TYR	CZ-CE2-CD2	11.30	129.97	119.80
1	A	716	ASP	CB-CG-OD2	-11.30	108.13	118.30
2	B	394	ASP	CB-CG-OD1	-11.30	108.13	118.30
1	A	616	VAL	CG1-CB-CG2	-11.29	92.83	110.90
6	H	135	LEU	CA-CB-CG	11.26	141.20	115.30
1	A	326	ARG	NE-CZ-NH1	11.26	125.93	120.30
7	I	113	ASP	CB-CG-OD2	11.25	128.42	118.30
2	B	56	ASP	CB-CG-OD1	-11.20	108.22	118.30
1	A	1438	THR	N-CA-CB	-11.18	89.06	110.30
1	A	174	ILE	CG1-CB-CG2	-11.18	86.81	111.40
1	A	1081	LEU	CB-CG-CD2	11.16	129.97	111.00
1	A	567	LYS	CD-CE-NZ	11.14	137.33	111.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	419	THR	OG1-CB-CG2	-11.14	84.38	110.00
1	A	537	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	A	949	ASP	CB-CG-OD1	-11.12	108.30	118.30
7	I	30	ARG	NE-CZ-NH1	-11.11	114.75	120.30
3	C	160	LYS	CD-CE-NZ	11.08	137.19	111.70
2	B	654	ARG	NE-CZ-NH2	11.08	125.84	120.30
2	B	963	PHE	CB-CG-CD2	-11.02	113.09	120.80
9	K	114	LEU	CA-CB-CG	10.99	140.58	115.30
2	B	768	THR	CA-CB-CG2	-10.98	97.02	112.40
1	A	163	SER	N-CA-CB	10.97	126.96	110.50
9	K	53	ASP	CB-CG-OD2	10.96	128.17	118.30
2	B	40	GLU	OE1-CD-OE2	10.95	136.44	123.30
7	I	45	ARG	NE-CZ-NH1	-10.94	114.83	120.30
2	B	120	ARG	NE-CZ-NH1	-10.94	114.83	120.30
1	A	982	THR	N-CA-CB	-10.89	89.61	110.30
1	A	1271	ILE	CG1-CB-CG2	-10.87	87.48	111.40
1	A	151	ASP	OD1-CG-OD2	-10.87	102.65	123.30
2	B	1166	CYS	CA-CB-SG	10.85	133.54	114.00
10	L	27	LEU	CA-CB-CG	10.84	140.23	115.30
1	A	1257	ASP	CB-CG-OD1	-10.84	108.55	118.30
4	E	16	PHE	CB-CG-CD2	-10.83	113.22	120.80
1	A	389	THR	OG1-CB-CG2	-10.79	85.18	110.00
2	B	1135	ARG	NE-CZ-NH1	10.79	125.70	120.30
7	I	18	GLU	OE1-CD-OE2	10.77	136.23	123.30
1	A	466	SER	CB-CA-C	-10.75	89.67	110.10
1	A	1204	ASP	CB-CG-OD2	10.75	127.98	118.30
2	B	1127	GLY	N-CA-C	10.74	139.94	113.10
4	E	212	ARG	CD-NE-CZ	10.72	138.62	123.60
7	I	109	ILE	CG1-CB-CG2	-10.67	87.94	111.40
3	C	191	TYR	CD1-CE1-CZ	-10.65	110.22	119.80
2	B	655	LYS	CD-CE-NZ	10.65	136.19	111.70
1	A	681	GLU	OE1-CD-OE2	10.63	136.06	123.30
2	B	416	LEU	CA-CB-CG	-10.63	90.85	115.30
9	K	83	PRO	N-CD-CG	-10.63	87.26	103.20
1	A	1318	THR	N-CA-CB	-10.61	90.14	110.30
1	A	923	LEU	CB-CG-CD1	-10.59	92.99	111.00
2	B	563	MET	CG-SD-CE	10.59	117.15	100.20
8	J	42	LYS	CD-CE-NZ	10.59	136.06	111.70
1	A	170	THR	OG1-CB-CG2	-10.59	85.65	110.00
1	A	985	ASP	CB-CG-OD2	-10.58	108.78	118.30
1	A	656	TRP	CD1-NE1-CE2	-10.57	99.48	109.00
2	B	137	TYR	CA-CB-CG	10.57	133.48	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	48	CYS	CA-CB-SG	10.54	132.97	114.00
1	A	897	TYR	CZ-CE2-CD2	10.53	129.28	119.80
2	B	241	ARG	NE-CZ-NH1	10.53	125.56	120.30
1	A	544	ASP	CB-CG-OD1	10.52	127.77	118.30
1	A	1450	LEU	CB-CG-CD2	10.50	128.85	111.00
1	A	771	GLU	CG-CD-OE1	-10.49	97.31	118.30
2	B	1136	ASP	CB-CG-OD2	10.48	127.73	118.30
1	A	909	ASP	CB-CG-OD2	-10.47	108.88	118.30
2	B	1077	THR	N-CA-CB	-10.47	90.40	110.30
3	C	220	ASP	CB-CG-OD1	10.46	127.72	118.30
4	E	50	MET	CG-SD-CE	10.46	116.94	100.20
2	B	999	MET	CG-SD-CE	-10.45	83.48	100.20
5	F	135	ARG	NE-CZ-NH2	10.45	125.53	120.30
1	A	992	ASP	CB-CG-OD2	10.44	127.70	118.30
2	B	605	ARG	NE-CZ-NH2	10.44	125.52	120.30
3	C	155	LEU	CB-CA-C	-10.42	90.40	110.20
5	F	97	ARG	NE-CZ-NH1	10.42	125.51	120.30
8	J	22	LEU	N-CA-CB	-10.42	89.56	110.40
2	B	642	ASP	CB-CG-OD1	10.41	127.67	118.30
1	A	1062	GLU	CB-CA-C	-10.40	89.59	110.40
2	B	397	ASP	CB-CG-OD2	10.40	127.66	118.30
7	I	7	CYS	CA-CB-SG	10.40	132.72	114.00
2	B	539	LEU	CB-CG-CD2	10.39	128.67	111.00
1	A	423	ASP	CB-CG-OD1	10.39	127.65	118.30
1	A	1376	THR	N-CA-CB	-10.37	90.59	110.30
3	C	53	THR	OG1-CB-CG2	-10.37	86.16	110.00
2	B	680	THR	N-CA-CB	-10.36	90.61	110.30
1	A	419	LYS	CD-CE-NZ	-10.34	87.92	111.70
1	A	305	ASP	CB-CG-OD2	10.34	127.60	118.30
2	B	841	MET	CG-SD-CE	10.33	116.73	100.20
1	A	85	ASP	CB-CG-OD2	10.33	127.60	118.30
1	A	708	MET	N-CA-CB	-10.32	92.03	110.60
2	B	852	ARG	NE-CZ-NH1	10.31	125.45	120.30
1	A	1417	GLU	OE1-CD-OE2	-10.29	110.95	123.30
8	J	21	TYR	CB-CG-CD1	10.27	127.16	121.00
1	A	1263	ILE	CG1-CB-CG2	-10.26	88.83	111.40
1	A	117	GLU	OE1-CD-OE2	10.26	135.61	123.30
2	B	327	ARG	NE-CZ-NH2	-10.22	115.19	120.30
3	C	29	MET	CG-SD-CE	10.21	116.54	100.20
2	B	394	ASP	CB-CG-OD2	10.20	127.48	118.30
1	A	450	LEU	CB-CG-CD1	-10.19	93.68	111.00
4	E	118	PRO	N-CD-CG	10.18	118.47	103.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	18	VAL	CB-CA-C	-10.18	92.06	111.40
2	B	852	ARG	NH1-CZ-NH2	-10.17	108.21	119.40
6	H	45	GLU	OE1-CD-OE2	10.17	135.50	123.30
3	C	93	ASP	CB-CG-OD2	10.16	127.44	118.30
1	A	96	ILE	CG1-CB-CG2	-10.14	89.10	111.40
1	A	1267	MET	CG-SD-CE	-10.11	84.02	100.20
1	A	391	LEU	CB-CG-CD2	-10.11	93.81	111.00
4	E	25	ASP	OD1-CG-OD2	-10.10	104.12	123.30
1	A	110	CYS	CA-CB-SG	10.08	132.15	114.00
1	A	1257	ASP	CB-CG-OD2	10.07	127.36	118.30
7	I	24	ARG	NH1-CZ-NH2	10.05	130.46	119.40
2	B	217	ARG	CG-CD-NE	-10.04	90.72	111.80
1	A	438	ASP	CB-CG-OD2	10.03	127.32	118.30
3	C	211	ASP	CB-CG-OD2	-10.02	109.28	118.30
2	B	940	PRO	N-CD-CG	-10.01	88.19	103.20
1	A	12	ARG	NE-CZ-NH2	-10.00	115.30	120.30
2	B	138	GLU	OE1-CD-OE2	-10.00	111.30	123.30
3	C	127	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	A	821	ARG	CG-CD-NE	-9.99	90.81	111.80
2	B	642	ASP	N-CA-C	-9.99	84.03	111.00
1	A	59	GLY	N-CA-C	9.98	138.06	113.10
2	B	284	ILE	CG1-CB-CG2	-9.96	89.48	111.40
3	C	226	ASP	CB-CG-OD2	9.96	127.26	118.30
2	B	598	GLU	OE1-CD-OE2	-9.93	111.39	123.30
2	B	1069	PHE	CB-CG-CD1	9.93	127.75	120.80
1	A	1228	TRP	CB-CA-C	-9.90	90.59	110.40
2	B	170	LEU	CB-CG-CD1	-9.90	94.17	111.00
4	E	98	ILE	CG1-CB-CG2	-9.90	89.63	111.40
1	A	600	PRO	N-CD-CG	-9.89	88.36	103.20
1	A	1289	ARG	NE-CZ-NH1	-9.89	115.36	120.30
1	A	909	ASP	CB-CG-OD1	9.88	127.19	118.30
1	A	1411	GLU	OE1-CD-OE2	-9.87	111.46	123.30
2	B	272	THR	OG1-CB-CG2	-9.86	87.32	110.00
2	B	709	ASP	CB-CG-OD2	9.86	127.17	118.30
2	B	632	ARG	NE-CZ-NH2	-9.85	115.38	120.30
1	A	1001	ARG	CG-CD-NE	-9.84	91.13	111.80
1	A	407	ARG	NH1-CZ-NH2	9.83	130.22	119.40
1	A	549	MET	CG-SD-CE	9.83	115.93	100.20
8	J	13	VAL	CG1-CB-CG2	-9.83	95.17	110.90
2	B	391	ASP	CB-CG-OD1	9.82	127.14	118.30
2	B	996	ARG	NH1-CZ-NH2	9.82	130.21	119.40
8	J	3	VAL	CB-CA-C	-9.79	92.80	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	464	PRO	O-C-N	-9.78	107.05	122.70
2	B	579	ARG	NE-CZ-NH1	-9.76	115.42	120.30
1	A	546	VAL	CG1-CB-CG2	-9.75	95.30	110.90
2	B	983	ARG	CA-CB-CG	9.74	134.84	113.40
1	A	350	ARG	NE-CZ-NH2	-9.74	115.43	120.30
7	I	31	THR	N-CA-CB	-9.74	91.80	110.30
3	C	9	LYS	CD-CE-NZ	9.73	134.09	111.70
1	A	1027	ALA	N-CA-CB	-9.71	96.50	110.10
6	H	7	ASP	CB-CG-OD2	9.71	127.04	118.30
1	A	1290	LYS	CD-CE-NZ	9.71	134.03	111.70
2	B	705	MET	CG-SD-CE	-9.69	84.69	100.20
1	A	1100	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	A	980	ASP	CB-CG-OD1	-9.67	109.60	118.30
3	C	44	LEU	CB-CG-CD1	-9.65	94.60	111.00
7	I	35	VAL	CA-CB-CG2	-9.65	96.43	110.90
10	L	40	LEU	CB-CG-CD2	9.64	127.39	111.00
4	E	163	GLU	OE1-CD-OE2	-9.64	111.73	123.30
1	A	1231	ASP	CB-CG-OD1	-9.64	109.63	118.30
1	A	1326	ARG	NE-CZ-NH2	9.64	125.12	120.30
1	A	1284	MET	CA-CB-CG	-9.63	96.93	113.30
1	A	393	ARG	NE-CZ-NH1	-9.62	115.49	120.30
1	A	516	SER	N-CA-CB	-9.61	96.08	110.50
3	C	175	ALA	N-CA-CB	-9.61	96.65	110.10
2	B	368	GLU	C-N-CA	-9.61	102.13	122.30
2	B	100	PRO	N-CD-CG	-9.60	88.81	103.20
1	A	222	LEU	CB-CG-CD2	9.57	127.28	111.00
10	L	42	ARG	NE-CZ-NH1	9.57	125.09	120.30
8	J	61	LEU	CB-CG-CD2	9.57	127.26	111.00
6	H	86	ASP	CB-CG-OD2	9.55	126.89	118.30
2	B	728	ARG	NE-CZ-NH1	-9.54	115.53	120.30
1	A	420	ARG	NE-CZ-NH2	-9.53	115.54	120.30
1	A	1239	ARG	N-CA-CB	-9.52	93.46	110.60
2	B	966	VAL	CG1-CB-CG2	-9.52	95.67	110.90
1	A	268	ASP	CB-CG-OD1	9.52	126.87	118.30
1	A	899	VAL	CG1-CB-CG2	-9.51	95.68	110.90
2	B	488	TYR	CB-CG-CD2	-9.51	115.30	121.00
4	E	202	SER	CB-CA-C	-9.50	92.06	110.10
1	A	386	ASP	CB-CG-OD1	9.49	126.84	118.30
8	J	29	GLU	OE1-CD-OE2	9.49	134.69	123.30
1	A	555	ASP	CB-CG-OD2	9.49	126.84	118.30
1	A	613	ILE	CG1-CB-CG2	-9.49	90.53	111.40
2	B	768	THR	CA-CB-OG1	9.47	128.89	109.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	725	ALA	CB-CA-C	-9.45	95.93	110.10
1	A	1023	ARG	NE-CZ-NH2	9.44	125.02	120.30
2	B	1041	GLU	OE1-CD-OE2	9.43	134.62	123.30
4	E	16	PHE	CB-CG-CD1	9.43	127.40	120.80
1	A	914	GLU	OE1-CD-OE2	9.43	134.61	123.30
2	B	89	GLU	OE1-CD-OE2	-9.43	111.99	123.30
1	A	305	ASP	CB-CG-OD1	9.42	126.78	118.30
7	I	24	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	A	1001	ARG	NE-CZ-NH1	-9.42	115.59	120.30
1	A	459	ARG	NE-CZ-NH2	-9.41	115.59	120.30
1	A	446	ARG	NH1-CZ-NH2	9.40	129.74	119.40
2	B	1183	LYS	N-CA-C	-9.39	85.63	111.00
1	A	1274	ARG	NE-CZ-NH2	-9.39	115.60	120.30
2	B	174	LEU	CB-CG-CD2	9.38	126.95	111.00
9	K	70	ARG	NE-CZ-NH1	-9.36	115.62	120.30
4	E	1	MET	CG-SD-CE	9.34	115.14	100.20
1	A	620	LYS	CD-CE-NZ	9.34	133.17	111.70
2	B	165	VAL	CB-CA-C	-9.34	93.66	111.40
2	B	434	ARG	NE-CZ-NH1	9.33	124.97	120.30
7	I	35	VAL	CB-CA-C	-9.33	93.68	111.40
1	A	399	HIS	C-N-CD	-9.32	100.09	120.60
3	C	266	ASP	CB-CG-OD1	-9.31	109.92	118.30
1	A	305	ASP	OD1-CG-OD2	-9.31	105.62	123.30
3	C	190	ASP	CB-CG-OD1	9.30	126.67	118.30
2	B	860	MET	CB-CA-C	-9.30	91.81	110.40
1	A	230	ARG	NE-CZ-NH2	-9.29	115.66	120.30
2	B	1049	ASP	OD1-CG-OD2	-9.29	105.66	123.30
2	B	29	ASP	CB-CG-OD2	-9.27	109.95	118.30
1	A	1109	LYS	CB-CA-C	9.26	128.93	110.40
7	I	91	ARG	NE-CZ-NH1	9.26	124.93	120.30
2	B	619	ILE	CG1-CB-CG2	-9.26	91.03	111.40
1	A	199	LEU	CA-CB-CG	9.25	136.58	115.30
3	C	183	TRP	C-N-CA	-9.25	98.57	121.70
2	B	124	TYR	CB-CG-CD2	9.23	126.54	121.00
2	B	1219	ASP	CB-CG-OD2	9.23	126.60	118.30
2	B	336	ARG	NE-CZ-NH1	-9.22	115.69	120.30
9	K	23	PRO	N-CD-CG	-9.21	89.39	103.20
2	B	996	ARG	NE-CZ-NH1	-9.21	115.69	120.30
1	A	218	ASP	CB-CG-OD2	-9.21	110.02	118.30
1	A	925	LEU	CB-CG-CD1	-9.20	95.35	111.00
3	C	180	TYR	CG-CD2-CE2	9.20	128.66	121.30
2	B	628	THR	OG1-CB-CG2	-9.19	88.87	110.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1367	HIS	CA-CB-CG	-9.18	97.99	113.60
1	A	1012	ARG	CG-CD-NE	-9.16	92.56	111.80
6	H	41	ASP	OD1-CG-OD2	-9.16	105.89	123.30
1	A	1192	LEU	CB-CG-CD1	-9.16	95.43	111.00
1	A	408	ASP	CB-CG-OD2	9.15	126.54	118.30
1	A	1025	ARG	NE-CZ-NH1	-9.15	115.72	120.30
2	B	1156	ASP	CB-CG-OD2	9.14	126.53	118.30
1	A	905	ASP	CB-CG-OD1	-9.14	110.08	118.30
1	A	914	GLU	CG-CD-OE2	-9.14	100.03	118.30
2	B	497	ARG	NH1-CZ-NH2	9.12	129.44	119.40
1	A	781	ASP	CB-CG-OD1	9.11	126.50	118.30
2	B	639	ILE	CA-CB-CG1	9.12	128.32	111.00
3	C	15	LYS	CG-CD-CE	9.11	139.24	111.90
1	A	1422	ARG	NH1-CZ-NH2	-9.11	109.38	119.40
1	A	268	ASP	CB-CG-OD2	9.10	126.49	118.30
9	K	10	PHE	CB-CG-CD2	9.10	127.17	120.80
1	A	731	ARG	NE-CZ-NH2	-9.10	115.75	120.30
2	B	249	ARG	NE-CZ-NH2	-9.09	115.75	120.30
2	B	1097	HIS	CB-CG-ND1	-9.09	100.49	123.20
1	A	386	ASP	CB-CG-OD2	-9.07	110.13	118.30
2	B	381	MET	CG-SD-CE	-9.07	85.68	100.20
1	A	1139	GLU	OE1-CD-OE2	-9.05	112.44	123.30
1	A	1284	MET	CG-SD-CE	-9.05	85.72	100.20
1	A	206	GLU	CG-CD-OE1	-9.05	100.21	118.30
7	I	84	VAL	N-CA-CB	-9.04	91.61	111.50
1	A	28	ARG	NE-CZ-NH2	-9.03	115.78	120.30
2	B	691	GLU	CA-CB-CG	9.02	133.25	113.40
2	B	1094	ARG	NE-CZ-NH2	9.02	124.81	120.30
3	C	136	ASP	CB-CG-OD1	-9.02	110.18	118.30
1	A	193	ASP	CB-CG-OD1	9.02	126.41	118.30
8	J	17	LYS	CD-CE-NZ	-9.02	90.97	111.70
1	A	728	LYS	CD-CE-NZ	9.01	132.42	111.70
2	B	394	ASP	N-CA-CB	-9.01	94.39	110.60
2	B	336	ARG	CB-CA-C	-9.00	92.39	110.40
1	A	896	ARG	NH1-CZ-NH2	8.99	129.29	119.40
3	C	185	LYS	CD-CE-NZ	-8.99	91.01	111.70
1	A	268	ASP	OD1-CG-OD2	-8.99	106.22	123.30
1	A	481	ASP	CB-CG-OD1	8.99	126.39	118.30
2	B	95	ILE	CG1-CB-CG2	-8.99	91.63	111.40
3	C	163	ILE	CA-CB-CG2	8.99	128.88	110.90
1	A	1194	ARG	NE-CZ-NH2	8.98	124.79	120.30
2	B	367	LEU	CB-CG-CD2	8.98	126.26	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	350	ARG	NE-CZ-NH1	8.95	124.78	120.30
2	B	316	PRO	N-CD-CG	-8.95	89.78	103.20
1	A	32	VAL	CG1-CB-CG2	-8.95	96.59	110.90
2	B	384	ARG	NE-CZ-NH2	-8.94	115.83	120.30
2	B	1129	ARG	NE-CZ-NH1	8.92	124.76	120.30
3	C	251	LEU	CB-CG-CD1	-8.91	95.85	111.00
2	B	90	ILE	CB-CA-C	-8.89	93.81	111.60
1	A	739	ASP	CB-CG-OD2	8.89	126.30	118.30
3	C	26	ASP	CB-CG-OD1	8.89	126.30	118.30
1	A	1417	GLU	CG-CD-OE1	8.88	136.07	118.30
6	H	107	VAL	N-CA-C	-8.89	87.01	111.00
1	A	1239	ARG	CD-NE-CZ	-8.88	111.16	123.60
2	B	602	THR	CA-CB-CG2	-8.88	99.96	112.40
6	H	19	ARG	NE-CZ-NH2	-8.88	115.86	120.30
10	L	40	LEU	CB-CA-C	8.88	127.07	110.20
8	J	48	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	A	1365	TYR	CG-CD1-CE1	-8.86	114.21	121.30
1	A	927	VAL	CA-CB-CG2	-8.85	97.62	110.90
7	I	4	PHE	CB-CG-CD1	-8.85	114.61	120.80
4	E	98	ILE	CB-CA-C	8.84	129.27	111.60
9	K	17	SER	CB-CA-C	-8.83	93.32	110.10
9	K	61	TYR	CZ-CE2-CD2	8.82	127.74	119.80
10	L	42	ARG	NE-CZ-NH2	8.82	124.71	120.30
1	A	1146	VAL	N-CA-CB	-8.82	92.11	111.50
4	E	163	GLU	CG-CD-OE1	8.82	135.93	118.30
1	A	53	LEU	CB-CG-CD1	8.81	125.98	111.00
2	B	969	ARG	NE-CZ-NH2	8.80	124.70	120.30
2	B	1150	ARG	NE-CZ-NH2	-8.81	115.90	120.30
2	B	737	THR	CA-CB-CG2	-8.80	100.08	112.40
1	A	1348	LEU	CB-CG-CD1	-8.79	96.05	111.00
2	B	644	GLU	N-CA-CB	-8.76	94.83	110.60
2	B	909	ASP	OD1-CG-OD2	-8.75	106.68	123.30
2	B	1099	VAL	CB-CA-C	-8.74	94.78	111.40
2	B	797	TYR	CZ-CE2-CD2	8.74	127.67	119.80
1	A	719	VAL	CA-CB-CG1	-8.74	97.79	110.90
10	L	64	LEU	CB-CG-CD1	8.74	125.86	111.00
1	A	1161	THR	OG1-CB-CG2	-8.74	89.91	110.00
6	H	132	LEU	CA-CB-CG	8.74	135.40	115.30
7	I	118	ARG	CA-CB-CG	8.73	132.62	113.40
3	C	92	CYS	N-CA-CB	-8.73	94.88	110.60
1	A	1215	ARG	NE-CZ-NH2	-8.73	115.94	120.30
2	B	364	ILE	CA-CB-CG1	-8.71	94.45	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1078	GLY	N-CA-C	8.71	134.87	113.10
5	F	150	GLU	N-CA-CB	-8.71	94.92	110.60
1	A	980	ASP	CB-CG-OD2	8.71	126.14	118.30
1	A	325	ILE	CG1-CB-CG2	-8.69	92.28	111.40
2	B	416	LEU	CB-CA-C	-8.69	93.69	110.20
2	B	598	GLU	N-CA-CB	8.68	126.22	110.60
6	H	110	ASP	CB-CG-OD1	-8.67	110.49	118.30
1	A	1055	ARG	NE-CZ-NH1	8.66	124.63	120.30
7	I	55	THR	CA-CB-CG2	8.66	124.52	112.40
1	A	1164	PRO	N-CD-CG	8.65	116.18	103.20
4	E	212	ARG	NE-CZ-NH1	8.65	124.62	120.30
2	B	303	TYR	CB-CG-CD2	-8.65	115.81	121.00
2	B	320	ASP	CB-CG-OD1	8.64	126.08	118.30
1	A	1259	MET	CG-SD-CE	8.63	114.01	100.20
2	B	914	LYS	CB-CA-C	-8.63	93.14	110.40
5	F	92	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	A	164	ARG	NE-CZ-NH2	-8.63	115.98	120.30
4	E	93	MET	CG-SD-CE	-8.63	86.39	100.20
4	E	208	TYR	CD1-CG-CD2	-8.62	108.42	117.90
6	H	114	VAL	CG1-CB-CG2	-8.62	97.11	110.90
2	B	697	GLU	OE1-CD-OE2	8.61	133.63	123.30
2	B	1006	ILE	CG1-CB-CG2	-8.61	92.45	111.40
1	A	720	ARG	CG-CD-NE	8.59	129.84	111.80
3	C	100	THR	OG1-CB-CG2	-8.59	90.25	110.00
9	K	39	ASP	CB-CG-OD1	8.59	126.03	118.30
1	A	50	ILE	CB-CA-C	-8.59	94.43	111.60
1	A	188	ASP	OD1-CG-OD2	-8.59	106.98	123.30
2	B	1064	TYR	CG-CD2-CE2	8.59	128.17	121.30
4	E	197	LYS	CB-CA-C	-8.58	93.23	110.40
7	I	13	MET	N-CA-CB	-8.58	95.15	110.60
1	A	974	ASP	N-CA-CB	8.58	126.04	110.60
1	A	1320	PRO	N-CD-CG	-8.58	90.33	103.20
2	B	959	ASP	CB-CG-OD2	8.58	126.02	118.30
2	B	745	PRO	N-CD-CG	-8.57	90.35	103.20
3	C	36	VAL	CG1-CB-CG2	-8.57	97.19	110.90
9	K	32	VAL	CG1-CB-CG2	-8.57	97.19	110.90
1	A	1036	ARG	NE-CZ-NH2	-8.56	116.02	120.30
6	H	117	SER	CB-CA-C	-8.56	93.83	110.10
1	A	1345	ARG	NE-CZ-NH2	-8.56	116.02	120.30
6	H	40	LEU	CB-CG-CD1	-8.56	96.46	111.00
7	I	45	ARG	CB-CA-C	-8.55	93.31	110.40
1	A	1313	LEU	CB-CG-CD1	-8.54	96.48	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	127	GLY	N-CA-C	8.53	134.42	113.10
2	B	268	THR	N-CA-CB	-8.52	94.11	110.30
2	B	405	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	A	557	ASP	C-N-CA	-8.52	104.42	122.30
2	B	131	ASP	N-CA-C	-8.51	88.01	111.00
1	A	296	LEU	CB-CG-CD1	-8.50	96.54	111.00
2	B	552	MET	CA-CB-CG	8.50	127.75	113.30
3	C	191	TYR	CZ-CE2-CD2	8.50	127.45	119.80
10	L	29	TYR	CB-CG-CD1	8.50	126.10	121.00
1	A	833	GLU	CG-CD-OE1	8.50	135.29	118.30
2	B	980	PHE	CG-CD2-CE2	8.49	130.14	120.80
10	L	34	CYS	CA-CB-SG	-8.49	98.72	114.00
1	A	1371	LEU	CB-CG-CD1	-8.48	96.58	111.00
3	C	38	ILE	CG1-CB-CG2	-8.48	92.73	111.40
1	A	655	PHE	CB-CG-CD1	8.48	126.73	120.80
2	B	564	GLU	OE1-CD-OE2	8.48	133.47	123.30
1	A	486	GLU	OE1-CD-OE2	-8.47	113.13	123.30
1	A	1280	GLU	CA-C-N	8.47	135.83	117.20
7	I	113	ASP	OD1-CG-OD2	-8.46	107.22	123.30
10	L	70	ARG	N-CA-C	8.46	133.84	111.00
2	B	564	GLU	CG-CD-OE2	-8.45	101.41	118.30
1	A	635	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	A	565	ILE	CG1-CB-CG2	-8.43	92.85	111.40
2	B	997	GLU	CA-CB-CG	-8.43	94.85	113.40
1	A	1280	GLU	O-C-N	-8.42	109.23	122.70
1	A	1226	VAL	CB-CA-C	-8.41	95.42	111.40
1	A	413	ILE	CG1-CB-CG2	-8.40	92.92	111.40
1	A	472	LEU	CB-CG-CD1	8.40	125.28	111.00
9	K	87	LEU	CB-CG-CD2	8.40	125.28	111.00
1	A	1135	ARG	NH1-CZ-NH2	8.39	128.63	119.40
9	K	61	TYR	CB-CG-CD1	8.39	126.04	121.00
6	H	85	GLY	N-CA-C	8.39	134.08	113.10
10	L	42	ARG	NH1-CZ-NH2	-8.38	110.18	119.40
1	A	1012	ARG	NE-CZ-NH1	8.38	124.49	120.30
2	B	992	ILE	CG1-CB-CG2	-8.38	92.98	111.40
3	C	84	ARG	NH1-CZ-NH2	-8.37	110.19	119.40
2	B	1094	ARG	NE-CZ-NH1	-8.37	116.12	120.30
2	B	1160	VAL	CB-CA-C	-8.37	95.50	111.40
1	A	557	ASP	O-C-N	-8.36	109.00	123.20
1	A	424	ILE	CG1-CB-CG2	-8.35	93.02	111.40
1	A	1193	LEU	CB-CG-CD2	-8.35	96.80	111.00
6	H	142	LEU	CB-CG-CD2	-8.35	96.80	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1005	GLY	N-CA-C	8.35	133.97	113.10
7	I	74	GLU	CA-CB-CG	8.35	131.76	113.40
1	A	326	ARG	CA-CB-CG	8.34	131.75	113.40
2	B	978	ASP	CB-CG-OD1	-8.33	110.80	118.30
1	A	1062	GLU	CA-CB-CG	8.33	131.72	113.40
1	A	1334	ASP	CB-CG-OD1	8.32	125.79	118.30
2	B	1139	ILE	O-C-N	-8.31	109.40	122.70
1	A	995	GLU	OE1-CD-OE2	8.31	133.27	123.30
1	A	804	TYR	CG-CD2-CE2	8.31	127.94	121.30
1	A	1356	ILE	CG1-CB-CG2	-8.31	93.13	111.40
8	J	43	ARG	CG-CD-NE	-8.30	94.36	111.80
2	B	894	ASP	CB-CG-OD1	8.30	125.77	118.30
1	A	731	ARG	NE-CZ-NH1	-8.30	116.15	120.30
5	F	82	THR	CB-CA-C	-8.30	89.19	111.60
2	B	981	ALA	N-CA-CB	-8.29	98.49	110.10
1	A	137	ALA	N-CA-CB	-8.29	98.49	110.10
1	A	896	ARG	NE-CZ-NH1	8.29	124.44	120.30
2	B	637	LEU	CB-CG-CD1	-8.29	96.91	111.00
1	A	601	LYS	CD-CE-NZ	-8.29	92.64	111.70
1	A	1362	TYR	CZ-CE2-CD2	8.28	127.25	119.80
1	A	649	ILE	CA-CB-CG1	8.28	126.73	111.00
1	A	1080	THR	CA-CB-CG2	8.27	123.98	112.40
8	J	44	TYR	CZ-CE2-CD2	8.27	127.24	119.80
3	C	29	MET	CA-CB-CG	8.27	127.35	113.30
1	A	629	LEU	CB-CG-CD2	-8.26	96.95	111.00
1	A	1273	LEU	CB-CG-CD1	8.25	125.03	111.00
2	B	135	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	A	652	VAL	CG1-CB-CG2	-8.25	97.70	110.90
2	B	605	ARG	NE-CZ-NH1	-8.24	116.18	120.30
4	E	78	LEU	CB-CG-CD2	8.24	125.01	111.00
4	E	167	ARG	NH1-CZ-NH2	8.24	128.46	119.40
3	C	154	LYS	CD-CE-NZ	8.23	130.64	111.70
8	J	8	PHE	CB-CG-CD1	8.23	126.56	120.80
9	K	50	LEU	CA-CB-CG	-8.23	96.38	115.30
2	B	758	PHE	CG-CD1-CE1	8.21	129.83	120.80
3	C	229	TYR	CB-CG-CD2	8.21	125.92	121.00
1	A	636	GLU	OE1-CD-OE2	-8.20	113.46	123.30
2	B	488	TYR	CB-CG-CD1	8.19	125.92	121.00
2	B	1009	ASP	CB-CG-OD1	8.19	125.67	118.30
1	A	393	ARG	NE-CZ-NH2	8.18	124.39	120.30
8	J	1	MET	N-CA-CB	-8.18	95.87	110.60
4	E	17	ARG	NE-CZ-NH2	8.18	124.39	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	123	LEU	CA-CB-CG	-8.18	96.50	115.30
1	A	151	ASP	CB-CG-OD1	8.17	125.65	118.30
1	A	609	ASP	CB-CG-OD2	8.17	125.65	118.30
2	B	345	LYS	CD-CE-NZ	8.16	130.48	111.70
2	B	910	VAL	CG1-CB-CG2	-8.15	97.86	110.90
9	K	7	PHE	CB-CG-CD1	-8.14	115.10	120.80
1	A	84	ILE	CG1-CB-CG2	-8.13	93.51	111.40
3	C	86	CYS	N-CA-CB	8.13	125.23	110.60
2	B	709	ASP	CB-CG-OD1	-8.12	110.99	118.30
3	C	265	MET	CG-SD-CE	-8.12	87.20	100.20
1	A	1436	ILE	CG1-CB-CG2	-8.12	93.53	111.40
1	A	532	ARG	NE-CZ-NH2	-8.12	116.24	120.30
7	I	102	VAL	CG1-CB-CG2	-8.12	97.91	110.90
2	B	261	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	A	36	ARG	CG-CD-NE	8.11	128.83	111.80
1	A	666	ILE	CG1-CB-CG2	8.11	129.24	111.40
1	A	1017	LEU	CB-CG-CD2	-8.10	97.22	111.00
2	B	1075	GLY	N-CA-C	8.10	133.36	113.10
2	B	666	TYR	CB-CG-CD1	8.10	125.86	121.00
1	A	352	VAL	CG1-CB-CG2	-8.09	97.95	110.90
1	A	1239	ARG	CB-CA-C	8.09	126.58	110.40
9	K	47	ARG	CG-CD-NE	8.09	128.79	111.80
6	H	81	PRO	N-CD-CG	-8.08	91.08	103.20
10	L	69	ALA	CB-CA-C	-8.08	97.98	110.10
1	A	199	LEU	CB-CG-CD1	8.07	124.72	111.00
5	F	110	ASP	CB-CG-OD2	-8.07	111.04	118.30
6	H	82	PRO	N-CA-C	-8.07	91.12	112.10
1	A	885	THR	OG1-CB-CG2	-8.06	91.47	110.00
2	B	911	ILE	CG1-CB-CG2	-8.05	93.69	111.40
6	H	102	TYR	CG-CD1-CE1	8.05	127.74	121.30
1	A	243	PRO	N-CD-CG	-8.05	91.13	103.20
1	A	279	LEU	CB-CG-CD1	8.05	124.68	111.00
2	B	434	ARG	CG-CD-NE	8.05	128.70	111.80
2	B	550	ASP	CB-CG-OD2	-8.04	111.06	118.30
4	E	125	PRO	N-CA-C	-8.04	91.21	112.10
2	B	1055	ILE	CA-CB-CG1	8.03	126.26	111.00
1	A	793	SER	N-CA-CB	-8.02	98.47	110.50
2	B	942	ARG	CB-CA-C	-8.02	94.35	110.40
1	A	596	THR	CB-CA-C	-8.02	89.94	111.60
2	B	1183	LYS	CA-CB-CG	8.02	131.05	113.40
4	E	128	PRO	N-CD-CG	8.02	115.23	103.20
1	A	475	THR	N-CA-CB	-8.02	95.07	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	34	ASP	CB-CG-OD2	8.02	125.51	118.30
7	I	14	LEU	CB-CG-CD1	-8.01	97.38	111.00
1	A	126	LEU	CB-CG-CD1	-8.01	97.39	111.00
2	B	542	MET	CG-SD-CE	-8.01	87.39	100.20
2	B	936	ASP	CB-CG-OD1	8.01	125.50	118.30
2	B	51	PHE	CB-CG-CD1	-8.00	115.20	120.80
1	A	374	LEU	CB-CG-CD2	8.00	124.60	111.00
1	A	834	THR	OG1-CB-CG2	-7.99	91.61	110.00
5	F	125	LEU	CB-CG-CD1	-7.99	97.42	111.00
3	C	95	CYS	CA-CB-SG	7.99	128.38	114.00
1	A	1385	THR	N-CA-C	7.98	132.55	111.00
3	C	66	ARG	CD-NE-CZ	-7.98	112.42	123.60
1	A	1234	GLU	CA-CB-CG	7.98	130.96	113.40
2	B	1183	LYS	CB-CA-C	7.98	126.36	110.40
8	J	2	ILE	CB-CG1-CD1	-7.98	91.55	113.90
1	A	885	THR	CA-CB-CG2	7.98	123.57	112.40
2	B	227	LYS	CD-CE-NZ	7.98	130.05	111.70
1	A	588	LEU	CB-CG-CD1	-7.97	97.44	111.00
2	B	341	LEU	CB-CG-CD1	7.96	124.54	111.00
1	A	1373	ASP	CB-CG-OD2	7.96	125.47	118.30
3	C	266	ASP	CB-CG-OD2	7.96	125.47	118.30
9	K	94	ILE	CG1-CB-CG2	-7.96	93.89	111.40
1	A	907	THR	CB-CA-C	-7.96	90.12	111.60
1	A	79	GLY	N-CA-C	-7.95	93.22	113.10
1	A	1062	GLU	OE1-CD-OE2	7.95	132.84	123.30
5	F	114	GLU	CA-C-N	7.95	134.69	117.20
2	B	24	PRO	N-CD-CG	-7.95	91.28	103.20
6	H	102	TYR	CD1-CE1-CZ	-7.95	112.65	119.80
1	A	302	THR	OG1-CB-CG2	-7.94	91.74	110.00
4	E	28	TYR	CB-CG-CD2	7.94	125.76	121.00
2	B	1083	ALA	CB-CA-C	-7.93	98.20	110.10
3	C	182	PRO	N-CD-CG	-7.93	91.31	103.20
8	J	48	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	A	791	ASP	CB-CG-OD2	-7.92	111.17	118.30
2	B	1052	VAL	CG1-CB-CG2	-7.91	98.24	110.90
9	K	20	LYS	CD-CE-NZ	7.91	129.89	111.70
8	J	24	LEU	CB-CA-C	-7.91	95.18	110.20
1	A	466	SER	N-CA-C	7.90	132.34	111.00
1	A	1029	ARG	NE-CZ-NH1	-7.90	116.35	120.30
1	A	1176	LEU	CB-CG-CD2	7.90	124.44	111.00
1	A	944	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	1230	GLU	OE1-CD-OE2	7.90	132.78	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	672	ASP	CB-CG-OD2	7.90	125.41	118.30
2	B	809	MET	CG-SD-CE	-7.90	87.56	100.20
1	A	622	VAL	CA-CB-CG1	7.89	122.74	110.90
6	H	87	ARG	CA-CB-CG	7.89	130.77	113.40
6	H	63	LEU	CB-CA-C	7.89	125.19	110.20
1	A	1030	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	535	THR	N-CA-CB	-7.88	95.33	110.30
1	A	731	ARG	NH1-CZ-NH2	7.87	128.06	119.40
2	B	911	ILE	N-CA-CB	-7.87	92.70	110.80
2	B	886	LYS	CD-CE-NZ	7.86	129.79	111.70
2	B	212	LEU	CD1-CG-CD2	-7.86	86.92	110.50
2	B	424	LEU	CA-CB-CG	-7.85	97.24	115.30
1	A	1362	TYR	CB-CG-CD2	-7.85	116.29	121.00
1	A	806	ARG	NH1-CZ-NH2	7.84	128.03	119.40
1	A	555	ASP	OD1-CG-OD2	-7.84	108.41	123.30
1	A	1349	TYR	CG-CD1-CE1	7.84	127.57	121.30
7	I	8	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	A	396	PRO	N-CD-CG	-7.83	91.46	103.20
2	B	976	ILE	CG1-CB-CG2	-7.82	94.19	111.40
1	A	460	VAL	CG1-CB-CG2	-7.82	98.39	110.90
1	A	1154	TYR	CD1-CE1-CZ	-7.82	112.76	119.80
2	B	892	LYS	CD-CE-NZ	7.81	129.67	111.70
3	C	210	GLU	O-C-N	-7.81	110.21	122.70
4	E	211	TYR	CB-CG-CD1	7.81	125.69	121.00
2	B	337	ARG	CG-CD-NE	-7.80	95.42	111.80
2	B	368	GLU	CA-CB-CG	7.79	130.54	113.40
2	B	370	PHE	CB-CA-C	7.79	125.97	110.40
10	L	58	LYS	O-C-N	-7.79	110.24	122.70
1	A	1056	SER	N-CA-CB	-7.79	98.82	110.50
1	A	1357	ALA	CB-CA-C	-7.78	98.42	110.10
2	B	792	MET	CG-SD-CE	-7.78	87.75	100.20
1	A	379	VAL	CG1-CB-CG2	-7.78	98.45	110.90
2	B	426	LYS	CD-CE-NZ	7.77	129.58	111.70
4	E	142	VAL	CG1-CB-CG2	-7.77	98.46	110.90
10	L	57	LEU	N-CA-C	7.77	131.99	111.00
1	A	944	ARG	NE-CZ-NH2	7.77	124.18	120.30
1	A	1112	LYS	CD-CE-NZ	7.77	129.57	111.70
4	E	103	LYS	N-CA-CB	7.77	124.58	110.60
9	K	82	ASP	CB-CG-OD2	7.77	125.29	118.30
1	A	295	LEU	CB-CA-C	-7.76	95.45	110.20
1	A	279	LEU	CA-CB-CG	7.76	133.15	115.30
1	A	1192	LEU	CB-CA-C	-7.76	95.45	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	353	LYS	CD-CE-NZ	7.76	129.55	111.70
6	H	112	ILE	CG1-CB-CG2	-7.76	94.33	111.40
1	A	728	LYS	N-CA-CB	7.75	124.56	110.60
2	B	303	TYR	CZ-CE2-CD2	7.75	126.77	119.80
8	J	34	THR	OG1-CB-CG2	-7.74	92.19	110.00
2	B	942	ARG	CG-CD-NE	-7.74	95.54	111.80
1	A	687	LYS	CD-CE-NZ	7.74	129.50	111.70
1	A	840	ARG	CD-NE-CZ	7.74	134.43	123.60
1	A	266	LEU	CB-CG-CD1	-7.73	97.85	111.00
1	A	984	LYS	CA-CB-CG	7.73	130.41	113.40
4	E	147	HIS	CG-CD2-NE2	-7.73	94.52	109.20
1	A	940	ARG	NH1-CZ-NH2	-7.72	110.90	119.40
2	B	214	ALA	N-CA-CB	-7.72	99.30	110.10
1	A	843	LYS	CB-CG-CD	7.71	131.65	111.60
2	B	898	LEU	CB-CG-CD2	7.71	124.11	111.00
1	A	1289	ARG	NE-CZ-NH2	7.71	124.16	120.30
3	C	252	GLN	CB-CA-C	7.70	125.80	110.40
9	K	74	ARG	NE-CZ-NH1	-7.70	116.45	120.30
4	E	28	TYR	CD1-CE1-CZ	7.70	126.73	119.80
2	B	969	ARG	CD-NE-CZ	-7.70	112.82	123.60
1	A	571	LEU	CB-CG-CD1	-7.70	97.91	111.00
1	A	1233	ASP	CB-CG-OD2	7.70	125.23	118.30
2	B	916	THR	N-CA-C	7.70	131.78	111.00
1	A	908	LEU	CB-CG-CD2	-7.69	97.93	111.00
4	E	62	ALA	N-CA-CB	-7.69	99.34	110.10
2	B	847	ASP	CB-CG-OD1	-7.68	111.38	118.30
2	B	637	LEU	CB-CG-CD2	7.67	124.03	111.00
1	A	1196	GLU	CG-CD-OE2	-7.66	102.97	118.30
7	I	44	TYR	CB-CG-CD2	7.66	125.59	121.00
7	I	100	PHE	CB-CG-CD1	7.66	126.16	120.80
1	A	185	TRP	CD1-NE1-CE2	-7.65	102.11	109.00
1	A	887	GLY	C-N-CA	-7.65	106.23	122.30
7	I	72	ASP	CB-CG-OD1	7.65	125.19	118.30
2	B	578	THR	CA-CB-CG2	-7.65	101.69	112.40
1	A	291	GLU	OE1-CD-OE2	-7.65	114.12	123.30
1	A	1122	PRO	C-N-CA	-7.65	106.24	122.30
1	A	1418	LEU	CB-CA-C	-7.64	95.68	110.20
6	H	135	LEU	CB-CG-CD1	-7.64	98.01	111.00
2	B	113	TYR	CB-CG-CD1	-7.64	116.42	121.00
2	B	568	ASP	CB-CG-OD1	7.63	125.17	118.30
9	K	5	ASP	CB-CG-OD1	-7.63	111.43	118.30
1	A	1211	GLN	N-CA-CB	7.63	124.34	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	979	LYS	CB-CA-C	-7.63	95.15	110.40
2	B	653	VAL	CB-CA-C	-7.62	96.92	111.40
5	F	109	VAL	CG1-CB-CG2	-7.62	98.71	110.90
7	I	93	LYS	CA-CB-CG	7.62	130.16	113.40
1	A	123	ARG	NE-CZ-NH1	7.62	124.11	120.30
2	B	1097	HIS	CB-CA-C	7.62	125.63	110.40
1	A	706	HIS	N-CA-CB	7.61	124.30	110.60
1	A	646	PHE	C-N-CA	-7.61	106.33	122.30
2	B	962	LYS	N-CA-C	-7.61	90.47	111.00
1	A	686	ALA	N-CA-CB	7.60	120.74	110.10
2	B	378	LEU	CB-CG-CD1	-7.60	98.08	111.00
2	B	646	LEU	CB-CA-C	-7.59	95.77	110.20
1	A	504	LEU	N-CA-CB	-7.58	95.23	110.40
1	A	576	GLN	CB-CA-C	-7.58	95.25	110.40
3	C	193	TYR	CD1-CE1-CZ	7.58	126.62	119.80
3	C	3	GLU	OE1-CD-OE2	7.57	132.39	123.30
1	A	1328	TYR	CB-CG-CD1	7.57	125.54	121.00
9	K	32	VAL	CA-CB-CG1	7.56	122.25	110.90
1	A	186	LYS	CD-CE-NZ	7.56	129.09	111.70
6	H	19	ARG	CG-CD-NE	7.56	127.68	111.80
7	I	27	PHE	CB-CG-CD1	7.56	126.09	120.80
1	A	792	TYR	CG-CD1-CE1	7.56	127.35	121.30
2	B	625	LYS	CD-CE-NZ	-7.56	94.32	111.70
3	C	111	THR	CA-CB-CG2	-7.56	101.82	112.40
1	A	1371	LEU	CB-CG-CD2	7.55	123.84	111.00
9	K	62	LYS	CB-CA-C	-7.55	95.30	110.40
1	A	870	GLU	CG-CD-OE1	-7.55	103.20	118.30
3	C	183	TRP	CA-C-N	7.55	133.81	117.20
1	A	711	ARG	NE-CZ-NH1	7.55	124.07	120.30
2	B	261	ARG	NE-CZ-NH2	-7.55	116.53	120.30
4	E	154	ILE	CB-CA-C	-7.55	96.50	111.60
1	A	578	LEU	CB-CG-CD1	-7.55	98.17	111.00
1	A	907	THR	CA-CB-CG2	7.54	122.96	112.40
3	C	202	PRO	O-C-N	7.54	134.77	122.70
1	A	948	VAL	N-CA-CB	-7.54	94.91	111.50
1	A	525	GLN	CG-CD-OE1	7.54	136.67	121.60
2	B	408	LEU	CB-CG-CD2	-7.54	98.19	111.00
1	A	790	ASP	OD1-CG-OD2	-7.53	108.99	123.30
1	A	1062	GLU	CG-CD-OE1	-7.53	103.23	118.30
2	B	1190	ASP	CB-CG-OD2	7.53	125.08	118.30
8	J	55	ASP	CB-CG-OD1	7.53	125.08	118.30
1	A	144	THR	CA-CB-CG2	7.53	122.94	112.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	GLU	O-C-N	7.53	135.99	123.20
6	H	142	LEU	CA-CB-CG	-7.52	98.00	115.30
2	B	1042	GLY	CA-C-O	-7.52	107.06	120.60
1	A	290	GLU	OE1-CD-OE2	7.52	132.32	123.30
2	B	1096	ARG	NH1-CZ-NH2	7.52	127.67	119.40
1	A	239	LEU	CB-CG-CD2	7.51	123.76	111.00
1	A	559	VAL	CA-CB-CG2	-7.50	99.64	110.90
1	A	1377	THR	CB-CA-C	-7.50	91.35	111.60
3	C	94	LYS	CA-CB-CG	7.49	129.88	113.40
1	A	1136	SER	CB-CA-C	7.49	124.33	110.10
2	B	595	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	A	412	ARG	CD-NE-CZ	-7.49	113.12	123.60
2	B	580	VAL	CG1-CB-CG2	-7.49	98.92	110.90
3	C	35	ARG	CD-NE-CZ	7.49	134.08	123.60
2	B	616	ILE	CG1-CB-CG2	-7.48	94.94	111.40
2	B	587	HIS	O-C-N	-7.48	110.48	123.20
2	B	642	ASP	CB-CA-C	7.48	125.36	110.40
1	A	1385	THR	N-CA-CB	-7.48	96.09	110.30
1	A	404	TYR	CD1-CE1-CZ	7.47	126.53	119.80
2	B	289	LEU	C-N-CA	-7.47	106.61	122.30
3	C	123	ASN	O-C-N	-7.47	110.74	122.70
4	E	149	LEU	CB-CG-CD1	7.47	123.70	111.00
5	F	115	THR	OG1-CB-CG2	-7.47	92.81	110.00
7	I	9	ASP	CB-CG-OD1	-7.47	111.58	118.30
10	L	57	LEU	CB-CG-CD1	-7.47	98.30	111.00
1	A	537	ARG	CB-CG-CD	7.47	131.01	111.60
2	B	513	GLN	CA-CB-CG	7.46	129.82	113.40
4	E	111	VAL	CG1-CB-CG2	7.46	122.83	110.90
6	H	63	LEU	CA-CB-CG	7.46	132.45	115.30
7	I	17	ARG	N-CA-CB	7.46	124.02	110.60
3	C	156	THR	CA-CB-CG2	-7.45	101.97	112.40
1	A	603	ASN	N-CA-CB	-7.45	97.19	110.60
1	A	1377	THR	N-CA-CB	7.45	124.46	110.30
3	C	113	VAL	CG1-CB-CG2	-7.44	98.99	110.90
7	I	4	PHE	N-CA-C	7.44	131.09	111.00
2	B	956	THR	CB-CA-C	-7.44	91.51	111.60
2	B	385	LEU	CB-CG-CD1	-7.44	98.35	111.00
2	B	1081	LEU	CB-CG-CD2	7.44	123.64	111.00
2	B	38	PHE	CB-CG-CD1	-7.44	115.59	120.80
3	C	3	GLU	CA-CB-CG	-7.43	97.04	113.40
4	E	181	ALA	N-CA-CB	-7.43	99.69	110.10
1	A	592	ASP	CB-CG-OD2	-7.43	111.61	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1202	MET	CG-SD-CE	7.43	112.08	100.20
1	A	111	GLY	CA-C-N	-7.42	100.86	117.20
2	B	124	TYR	CD1-CG-CD2	-7.42	109.73	117.90
1	A	112	LYS	CD-CE-NZ	-7.42	94.63	111.70
2	B	836	GLU	O-C-N	7.42	134.57	122.70
2	B	807	ARG	CG-CD-NE	-7.42	96.23	111.80
2	B	1154	ALA	N-CA-CB	7.42	120.48	110.10
3	C	93	ASP	CB-CG-OD1	-7.42	111.63	118.30
2	B	186	GLU	OE1-CD-OE2	7.42	132.20	123.30
2	B	827	ILE	CG1-CB-CG2	-7.41	95.09	111.40
2	B	405	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	A	678	GLU	OE1-CD-OE2	-7.41	114.41	123.30
4	E	5	ASN	N-CA-CB	7.40	123.93	110.60
1	A	1349	TYR	CE1-CZ-CE2	-7.40	107.96	119.80
1	A	1197	LEU	CB-CG-CD2	-7.40	98.42	111.00
2	B	942	ARG	NE-CZ-NH2	-7.40	116.60	120.30
2	B	89	GLU	N-CA-C	7.39	130.95	111.00
2	B	398	ARG	CB-CA-C	-7.39	95.62	110.40
9	K	57	LEU	CB-CG-CD1	-7.38	98.46	111.00
2	B	635	ARG	NH1-CZ-NH2	-7.38	111.29	119.40
1	A	102	VAL	CG1-CB-CG2	-7.37	99.11	110.90
2	B	601	ARG	NH1-CZ-NH2	7.37	127.50	119.40
2	B	644	GLU	C-N-CA	-7.37	103.29	121.70
2	B	57	TYR	CD1-CE1-CZ	7.36	126.43	119.80
1	A	683	ILE	CG1-CB-CG2	-7.36	95.21	111.40
3	C	119	VAL	CA-CB-CG1	-7.36	99.86	110.90
7	I	16	PRO	CA-N-CD	-7.35	101.20	111.50
1	A	1154	TYR	N-CA-C	-7.35	91.15	111.00
2	B	1017	ILE	CA-CB-CG1	-7.35	97.04	111.00
1	A	1134	ILE	CA-CB-CG2	-7.34	96.21	110.90
2	B	124	TYR	CZ-CE2-CD2	7.34	126.41	119.80
1	A	1014	ALA	CA-C-O	7.33	135.50	120.10
2	B	416	LEU	N-CA-CB	7.33	125.07	110.40
1	A	1077	THR	CA-C-N	7.33	133.33	117.20
1	A	588	LEU	N-CA-CB	-7.33	95.75	110.40
2	B	838	SER	N-CA-CB	-7.32	99.52	110.50
1	A	302	THR	CA-CB-CG2	7.32	122.65	112.40
2	B	844	SER	N-CA-CB	-7.31	99.53	110.50
2	B	1132	GLU	OE1-CD-OE2	-7.31	114.52	123.30
2	B	303	TYR	CB-CG-CD1	7.31	125.39	121.00
2	B	587	HIS	CA-C-N	7.31	130.82	116.20
6	H	136	LYS	CD-CE-NZ	7.31	128.51	111.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	519	PRO	N-CD-CG	7.31	114.16	103.20
1	A	495	GLU	CA-CB-CG	7.30	129.47	113.40
2	B	1026	LEU	CB-CG-CD1	-7.30	98.58	111.00
2	B	961	LEU	CB-CG-CD1	7.30	123.41	111.00
2	B	56	ASP	O-C-N	-7.30	111.02	122.70
2	B	735	ALA	O-C-N	7.30	134.38	122.70
3	C	255	VAL	CG1-CB-CG2	-7.30	99.22	110.90
4	E	66	GLU	CA-CB-CG	7.30	129.45	113.40
10	L	25	ALA	N-CA-CB	7.29	120.31	110.10
2	B	63	ILE	O-C-N	-7.29	111.03	122.70
3	C	62	PHE	CZ-CE2-CD2	-7.29	111.35	120.10
3	C	70	ILE	CB-CA-C	-7.29	97.03	111.60
1	A	695	LYS	CD-CE-NZ	7.28	128.45	111.70
4	E	176	PRO	CB-CA-C	-7.28	93.79	112.00
7	I	5	ARG	CG-CD-NE	7.28	127.08	111.80
1	A	206	GLU	CB-CA-C	-7.28	95.85	110.40
1	A	394	ASN	CB-CA-C	-7.28	95.85	110.40
1	A	895	LYS	N-CA-CB	7.28	123.70	110.60
2	B	377	PHE	CB-CG-CD1	-7.28	115.71	120.80
1	A	1332	PHE	CB-CG-CD2	-7.27	115.71	120.80
2	B	830	TYR	CD1-CE1-CZ	7.27	126.34	119.80
2	B	567	GLU	O-C-N	-7.27	111.07	122.70
1	A	1299	VAL	N-CA-CB	-7.25	95.54	111.50
2	B	500	THR	CA-CB-CG2	-7.25	102.24	112.40
6	H	126	GLU	OE1-CD-OE2	-7.25	114.59	123.30
1	A	682	THR	CA-CB-CG2	-7.25	102.25	112.40
1	A	925	LEU	CB-CG-CD2	7.25	123.33	111.00
2	B	788	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	A	367	PRO	N-CD-CG	7.25	114.07	103.20
1	A	694	THR	OG1-CB-CG2	-7.25	93.33	110.00
2	B	258	LEU	CB-CG-CD1	7.25	123.32	111.00
1	A	96	ILE	CA-CB-CG1	7.24	124.76	111.00
2	B	569	TYR	CZ-CE2-CD2	7.24	126.32	119.80
1	A	497	THR	N-CA-CB	-7.24	96.54	110.30
2	B	666	TYR	CG-CD2-CE2	7.24	127.09	121.30
2	B	680	THR	CA-CB-CG2	7.24	122.54	112.40
1	A	912	LEU	N-CA-CB	7.24	124.88	110.40
6	H	130	ARG	NH1-CZ-NH2	7.24	127.36	119.40
1	A	1316	VAL	CB-CA-C	-7.23	97.66	111.40
1	A	911	SER	O-C-N	7.23	134.27	122.70
2	B	828	ALA	N-CA-CB	-7.23	99.97	110.10
3	C	205	LYS	N-CA-CB	7.23	123.62	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	596	THR	CA-CB-CG2	-7.23	102.28	112.40
2	B	933	SER	CB-CA-C	7.23	123.83	110.10
2	B	711	GLU	CB-CA-C	-7.22	95.95	110.40
4	E	14	ARG	C-N-CA	-7.22	103.64	121.70
8	J	7	CYS	CB-CA-C	-7.22	95.95	110.40
1	A	364	VAL	CG1-CB-CG2	-7.22	99.35	110.90
1	A	1280	GLU	CG-CD-OE2	7.22	132.74	118.30
2	B	642	ASP	N-CA-CB	7.22	123.59	110.60
2	B	532	ALA	N-CA-CB	7.22	120.20	110.10
2	B	936	ASP	OD1-CG-OD2	-7.21	109.60	123.30
4	E	192	ARG	CD-NE-CZ	7.21	133.69	123.60
6	H	26	ILE	CB-CA-C	-7.21	97.18	111.60
2	B	212	LEU	CB-CG-CD2	7.21	123.25	111.00
1	A	11	LEU	CD1-CG-CD2	-7.21	88.88	110.50
2	B	666	TYR	CE1-CZ-OH	7.21	139.56	120.10
2	B	935	ARG	CD-NE-CZ	7.21	133.69	123.60
4	E	74	ASP	CB-CG-OD1	-7.20	111.82	118.30
1	A	148	CYS	CA-CB-SG	7.20	126.96	114.00
1	A	852	TYR	CB-CG-CD2	-7.20	116.68	121.00
1	A	470	LEU	CB-CA-C	-7.19	96.53	110.20
6	H	111	LEU	CA-CB-CG	7.19	131.84	115.30
10	L	58	LYS	N-CA-C	7.19	130.40	111.00
9	K	56	VAL	CG1-CB-CG2	-7.18	99.41	110.90
4	E	177	ARG	NE-CZ-NH2	7.18	123.89	120.30
2	B	945	GLU	CG-CD-OE2	-7.18	103.95	118.30
1	A	1000	LEU	CB-CG-CD2	-7.17	98.81	111.00
6	H	34	ASP	CB-CG-OD1	-7.17	111.85	118.30
2	B	56	ASP	CA-C-N	7.17	132.97	117.20
2	B	618	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	A	1012	ARG	CA-CB-CG	7.16	129.16	113.40
7	I	81	ARG	CA-C-O	7.16	135.15	120.10
4	E	66	GLU	N-CA-CB	7.16	123.49	110.60
1	A	555	ASP	CB-CG-OD1	7.16	124.74	118.30
6	H	11	GLN	CB-CA-C	-7.16	96.08	110.40
2	B	1156	ASP	OD1-CG-OD2	-7.16	109.70	123.30
9	K	74	ARG	CG-CD-NE	-7.16	96.77	111.80
2	B	872	GLU	OE1-CD-OE2	-7.16	114.71	123.30
8	J	7	CYS	N-CA-CB	7.16	123.48	110.60
10	L	67	PHE	CB-CG-CD2	7.16	125.81	120.80
9	K	6	ARG	N-CA-CB	-7.15	97.72	110.60
1	A	283	GLY	N-CA-C	-7.15	95.22	113.10
10	L	63	ARG	NE-CZ-NH2	7.15	123.88	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1223	ASP	C-N-CA	7.15	139.57	121.70
7	I	1	MET	CA-CB-CG	7.15	125.45	113.30
2	B	522	VAL	N-CA-CB	-7.14	95.80	111.50
1	A	704	ALA	C-N-CA	-7.13	103.87	121.70
2	B	626	ILE	N-CA-CB	-7.13	94.39	110.80
1	A	944	ARG	NH1-CZ-NH2	-7.13	111.56	119.40
10	L	28	LYS	CD-CE-NZ	7.13	128.09	111.70
1	A	1018	PHE	CG-CD1-CE1	7.13	128.64	120.80
4	E	46	TYR	CB-CG-CD2	7.13	125.28	121.00
1	A	1242	VAL	CG1-CB-CG2	-7.12	99.50	110.90
5	F	79	ARG	CA-CB-CG	7.12	129.07	113.40
1	A	164	ARG	NE-CZ-NH1	7.12	123.86	120.30
3	C	260	LEU	CB-CG-CD2	7.12	123.10	111.00
1	A	61	ILE	N-CA-C	-7.12	91.78	111.00
2	B	37	PHE	CD1-CE1-CZ	7.11	128.63	120.10
1	A	770	VAL	CG1-CB-CG2	-7.11	99.52	110.90
1	A	878	ILE	N-CA-CB	-7.11	94.45	110.80
3	C	125	MET	CG-SD-CE	7.11	111.58	100.20
1	A	153	PRO	C-N-CA	-7.11	103.93	121.70
3	C	254	LYS	CD-CE-NZ	-7.11	95.35	111.70
5	F	79	ARG	CB-CG-CD	-7.11	93.12	111.60
1	A	1241	ARG	CD-NE-CZ	7.10	133.54	123.60
10	L	61	THR	CA-CB-CG2	7.10	122.34	112.40
1	A	634	THR	CA-CB-CG2	-7.10	102.46	112.40
2	B	936	ASP	CB-CG-OD2	7.10	124.69	118.30
1	A	277	GLU	CA-CB-CG	7.09	129.01	113.40
2	B	56	ASP	CB-CG-OD2	7.09	124.69	118.30
2	B	183	GLU	OE1-CD-OE2	-7.08	114.80	123.30
1	A	179	LEU	CB-CG-CD1	7.08	123.04	111.00
1	A	360	GLU	CA-CB-CG	7.08	128.98	113.40
2	B	568	ASP	CB-CG-OD2	7.08	124.67	118.30
3	C	89	GLU	N-CA-C	-7.08	91.88	111.00
2	B	483	LEU	CB-CG-CD2	7.08	123.03	111.00
6	H	126	GLU	CG-CD-OE1	7.08	132.46	118.30
2	B	312	GLU	OE1-CD-OE2	7.07	131.79	123.30
1	A	65	LEU	CA-CB-CG	7.07	131.56	115.30
2	B	408	LEU	N-CA-CB	-7.07	96.26	110.40
1	A	868	TYR	CB-CG-CD1	7.07	125.24	121.00
1	A	982	THR	CA-CB-CG2	7.06	122.29	112.40
1	A	821	ARG	NH1-CZ-NH2	7.06	127.17	119.40
1	A	1134	ILE	CG1-CB-CG2	-7.06	95.86	111.40
1	A	941	LYS	CD-CE-NZ	-7.06	95.46	111.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	495	LEU	CB-CG-CD1	7.06	123.00	111.00
1	A	936	LEU	CB-CG-CD1	7.05	122.99	111.00
2	B	355	ILE	CA-CB-CG1	7.04	124.38	111.00
1	A	962	ARG	O-C-N	-7.04	111.44	122.70
2	B	858	SER	CA-CB-OG	-7.04	92.20	111.20
1	A	1066	VAL	CA-CB-CG2	-7.04	100.34	110.90
2	B	855	PHE	CB-CG-CD1	7.04	125.73	120.80
1	A	1191	TRP	CD1-NE1-CE2	-7.03	102.67	109.00
2	B	571	PRO	N-CD-CG	-7.03	92.65	103.20
1	A	62	ASP	CB-CG-OD2	7.03	124.63	118.30
1	A	196	GLU	OE1-CD-OE2	7.03	131.74	123.30
2	B	129	PHE	CB-CG-CD2	-7.03	115.88	120.80
2	B	434	ARG	CA-CB-CG	7.03	128.87	113.40
1	A	36	ARG	NE-CZ-NH1	7.03	123.81	120.30
2	B	365	THR	N-CA-C	-7.03	92.03	111.00
5	F	108	PHE	CB-CG-CD1	-7.02	115.88	120.80
7	I	53	GLY	N-CA-C	7.02	130.65	113.10
3	C	183	TRP	O-C-N	-7.02	111.47	122.70
1	A	1426	GLU	OE1-CD-OE2	-7.02	114.88	123.30
2	B	630	ALA	CB-CA-C	-7.01	99.58	110.10
2	B	373	ARG	CB-CG-CD	7.01	129.83	111.60
1	A	1276	VAL	CA-CB-CG2	-7.01	100.39	110.90
4	E	195	VAL	CG1-CB-CG2	-7.01	99.69	110.90
2	B	852	ARG	N-CA-CB	-7.00	97.99	110.60
2	B	1220	ARG	NE-CZ-NH1	7.00	123.80	120.30
3	C	239	PRO	CA-CB-CG	-7.00	90.70	104.00
9	K	19	LEU	CB-CG-CD1	-7.00	99.10	111.00
1	A	830	LYS	N-CA-CB	7.00	123.20	110.60
3	C	268	ASP	CB-CG-OD2	7.00	124.60	118.30
1	A	727	ASP	CB-CG-OD2	7.00	124.60	118.30
8	J	44	TYR	CB-CG-CD1	7.00	125.20	121.00
7	I	52	ILE	CA-C-N	-6.99	102.22	116.20
8	J	1	MET	CA-CB-CG	6.99	125.19	113.30
2	B	766	ARG	NE-CZ-NH1	-6.99	116.80	120.30
1	A	130	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	A	305	ASP	N-CA-C	6.99	129.87	111.00
2	B	565	PRO	N-CD-CG	6.99	113.68	103.20
2	B	547	VAL	CG1-CB-CG2	6.99	122.08	110.90
3	C	47	ASP	CB-CG-OD2	6.99	124.59	118.30
6	H	27	GLU	OE1-CD-OE2	-6.99	114.92	123.30
1	A	295	LEU	CA-CB-CG	6.98	131.36	115.30
2	B	879	ARG	CG-CD-NE	6.97	126.44	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	ASP	CB-CG-OD2	6.97	124.57	118.30
1	A	269	ILE	CG1-CB-CG2	-6.96	96.08	111.40
2	B	568	ASP	OD1-CG-OD2	-6.96	110.07	123.30
2	B	986	GLN	CA-CB-CG	-6.96	98.08	113.40
7	I	34	TYR	CZ-CE2-CD2	6.96	126.07	119.80
2	B	791	THR	OG1-CB-CG2	-6.96	93.98	110.00
2	B	351	TYR	CG-CD2-CE2	6.96	126.87	121.30
6	H	104	PHE	O-C-N	-6.96	111.57	122.70
1	A	1284	MET	N-CA-C	-6.96	92.22	111.00
1	A	856	THR	N-CA-CB	-6.95	97.09	110.30
1	A	1259	MET	N-CA-C	-6.95	92.22	111.00
2	B	768	THR	O-C-N	-6.95	111.57	122.70
4	E	196	VAL	CG1-CB-CG2	-6.95	99.77	110.90
7	I	82	GLU	OE1-CD-OE2	-6.95	114.96	123.30
2	B	31	TRP	O-C-N	-6.95	111.58	122.70
2	B	510	LYS	CB-CG-CD	-6.95	93.53	111.60
2	B	553	PRO	N-CD-CG	-6.95	92.78	103.20
6	H	146	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	A	189	ARG	NE-CZ-NH2	6.95	123.77	120.30
2	B	267	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	A	226	GLU	CG-CD-OE2	6.95	132.19	118.30
1	A	1119	TYR	CG-CD1-CE1	-6.94	115.75	121.30
2	B	499	ASN	CB-CA-C	-6.94	96.52	110.40
3	C	196	ASP	CB-CA-C	-6.94	96.52	110.40
2	B	137	TYR	CB-CG-CD1	6.94	125.16	121.00
6	H	59	ILE	CB-CA-C	-6.94	97.72	111.60
6	H	19	ARG	NH1-CZ-NH2	6.93	127.03	119.40
1	A	983	ILE	CG1-CB-CG2	-6.93	96.16	111.40
5	F	152	ILE	CG1-CB-CG2	-6.93	96.16	111.40
8	J	30	LEU	CB-CG-CD1	6.93	122.77	111.00
1	A	512	VAL	CA-CB-CG1	6.92	121.28	110.90
1	A	566	ILE	CB-CA-C	-6.92	97.76	111.60
2	B	814	PHE	CG-CD2-CE2	-6.92	113.19	120.80
6	H	77	ARG	CD-NE-CZ	6.92	133.28	123.60
1	A	702	LEU	CB-CG-CD2	6.91	122.75	111.00
1	A	90	VAL	N-CA-CB	-6.91	96.31	111.50
6	H	80	ARG	N-CA-C	-6.91	92.36	111.00
1	A	34	LYS	CD-CE-NZ	6.90	127.58	111.70
3	C	99	LEU	CB-CG-CD1	-6.90	99.27	111.00
5	F	112	GLU	OE1-CD-OE2	6.90	131.58	123.30
3	C	33	LEU	CB-CA-C	6.90	123.31	110.20
2	B	798	TYR	CB-CG-CD2	6.90	125.14	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	195	GLN	N-CA-CB	6.90	123.01	110.60
1	A	442	VAL	CB-CA-C	-6.89	98.30	111.40
1	A	1108	ALA	CB-CA-C	-6.89	99.76	110.10
2	B	908	GLU	CG-CD-OE1	-6.89	104.51	118.30
2	B	529	GLU	OE1-CD-OE2	6.89	131.57	123.30
2	B	1062	HIS	CB-CA-C	-6.89	96.62	110.40
2	B	622	LYS	CA-CB-CG	6.89	128.56	113.40
2	B	536	VAL	CG1-CB-CG2	-6.89	99.88	110.90
2	B	1219	ASP	OD1-CG-OD2	-6.89	110.22	123.30
8	J	26	GLN	CB-CA-C	6.89	124.17	110.40
2	B	962	LYS	CD-CE-NZ	6.88	127.53	111.70
2	B	903	VAL	CA-CB-CG2	-6.88	100.58	110.90
2	B	712	PRO	N-CD-CG	-6.88	92.88	103.20
1	A	1153	TYR	CG-CD2-CE2	6.88	126.80	121.30
2	B	479	VAL	CG1-CB-CG2	-6.88	99.89	110.90
2	B	1021	MET	CG-SD-CE	-6.88	89.19	100.20
2	B	966	VAL	CA-CB-CG2	-6.87	100.59	110.90
1	A	722	LEU	CB-CG-CD1	6.87	122.67	111.00
1	A	864	ILE	CG1-CB-CG2	-6.87	96.29	111.40
1	A	1166	ASP	N-CA-C	-6.87	92.46	111.00
1	A	1153	TYR	CD1-CE1-CZ	6.87	125.98	119.80
3	C	34	ARG	NH1-CZ-NH2	6.87	126.95	119.40
1	A	1323	ASP	CB-CG-OD2	6.86	124.48	118.30
3	C	81	GLU	CB-CA-C	-6.86	96.68	110.40
1	A	412	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	A	696	GLU	CG-CD-OE2	6.86	132.01	118.30
2	B	270	LYS	CD-CE-NZ	-6.86	95.93	111.70
10	L	27	LEU	CB-CG-CD2	6.85	122.65	111.00
1	A	1351	GLU	OE1-CD-OE2	6.85	131.51	123.30
2	B	598	GLU	CB-CG-CD	6.84	132.68	114.20
2	B	354	ASP	CB-CG-OD1	6.84	124.46	118.30
2	B	1083	ALA	N-CA-CB	-6.84	100.52	110.10
1	A	659	HIS	N-CA-CB	-6.84	98.30	110.60
2	B	188	ASP	CB-CG-OD1	-6.84	112.15	118.30
1	A	361	LEU	CB-CA-C	-6.83	97.22	110.20
1	A	913	LEU	CB-CG-CD1	-6.83	99.39	111.00
2	B	501	PRO	CA-C-O	-6.83	103.81	120.20
3	C	101	LEU	CB-CG-CD2	6.83	122.61	111.00
8	J	45	CYS	CA-CB-SG	6.82	126.28	114.00
1	A	974	ASP	CB-CG-OD2	-6.82	112.16	118.30
7	I	27	PHE	CG-CD1-CE1	6.82	128.30	120.80
2	B	338	GLY	CA-C-O	-6.82	108.32	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	135	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	A	1274	ARG	NH1-CZ-NH2	6.82	126.90	119.40
1	A	37	PHE	CB-CG-CD2	-6.82	116.03	120.80
4	E	82	PHE	CG-CD2-CE2	-6.81	113.31	120.80
2	B	1169	MET	CG-SD-CE	6.80	111.09	100.20
2	B	29	ASP	CB-CG-OD1	6.80	124.42	118.30
2	B	690	VAL	N-CA-CB	-6.80	96.53	111.50
2	B	778	MET	CG-SD-CE	6.80	111.08	100.20
1	A	893	PHE	CD1-CG-CD2	-6.80	109.46	118.30
1	A	925	LEU	CA-CB-CG	-6.80	99.66	115.30
4	E	197	LYS	N-CA-C	-6.80	92.64	111.00
1	A	155	GLU	CA-CB-CG	6.79	128.35	113.40
4	E	20	LYS	CA-CB-CG	6.79	128.34	113.40
10	L	65	VAL	CB-CA-C	-6.79	98.50	111.40
1	A	154	SER	CB-CA-C	6.79	122.99	110.10
2	B	138	GLU	CG-CD-OE1	6.79	131.87	118.30
4	E	14	ARG	NE-CZ-NH1	6.79	123.69	120.30
7	I	24	ARG	CB-CA-C	-6.79	96.83	110.40
2	B	429	PHE	O-C-N	-6.78	111.85	122.70
2	B	1106	ARG	CD-NE-CZ	6.78	133.09	123.60
2	B	620	ARG	CG-CD-NE	-6.78	97.56	111.80
2	B	694	ASP	CB-CG-OD2	6.78	124.40	118.30
1	A	948	VAL	CG1-CB-CG2	-6.78	100.05	110.90
1	A	814	PHE	CZ-CE2-CD2	6.78	128.23	120.10
2	B	884	ARG	CB-CG-CD	6.77	129.20	111.60
10	L	56	LEU	N-CA-CB	-6.77	96.86	110.40
4	E	77	SER	N-CA-C	-6.77	92.73	111.00
8	J	21	TYR	CG-CD1-CE1	6.77	126.72	121.30
1	A	239	LEU	CA-CB-CG	6.76	130.86	115.30
1	A	857	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	A	1129	GLU	CA-CB-CG	6.76	128.28	113.40
1	A	238	CYS	CA-CB-SG	-6.76	101.83	114.00
10	L	70	ARG	NH1-CZ-NH2	-6.76	111.96	119.40
2	B	962	LYS	CG-CD-CE	6.76	132.17	111.90
2	B	987	LYS	CD-CE-NZ	-6.75	96.18	111.70
1	A	475	THR	CA-CB-CG2	6.74	121.84	112.40
8	J	6	ARG	NE-CZ-NH1	-6.74	116.93	120.30
2	B	351	TYR	CB-CG-CD2	6.74	125.04	121.00
2	B	69	LEU	CB-CG-CD1	6.74	122.45	111.00
1	A	72	GLU	N-CA-C	6.74	129.18	111.00
5	F	77	ASP	C-N-CA	-6.73	104.86	121.70
1	A	362	ASP	CB-CG-OD2	6.73	124.36	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1370	LEU	CD1-CG-CD2	-6.73	90.31	110.50
2	B	650	GLU	CG-CD-OE1	-6.73	104.84	118.30
2	B	260	GLY	N-CA-C	-6.73	96.28	113.10
1	A	9	ALA	N-CA-C	-6.72	92.84	111.00
2	B	944	THR	O-C-N	6.72	133.46	122.70
4	E	190	LEU	O-C-N	6.72	133.46	122.70
3	C	11	ARG	CB-CA-C	-6.72	96.95	110.40
1	A	895	LYS	CD-CE-NZ	-6.72	96.24	111.70
1	A	740	LEU	CB-CG-CD1	6.72	122.42	111.00
2	B	764	SER	N-CA-CB	-6.72	100.42	110.50
10	L	63	ARG	C-N-CA	-6.71	104.91	121.70
5	F	97	ARG	N-CA-CB	-6.71	98.52	110.60
1	A	918	GLU	OE1-CD-OE2	-6.71	115.25	123.30
7	I	70	ARG	CD-NE-CZ	-6.71	114.20	123.60
1	A	129	LYS	N-CA-CB	-6.71	98.52	110.60
1	A	1136	SER	N-CA-C	-6.71	92.88	111.00
3	C	79	GLN	O-C-N	-6.71	111.97	122.70
2	B	954	VAL	CB-CA-C	-6.71	98.66	111.40
3	C	88	CYS	CA-CB-SG	6.70	126.06	114.00
2	B	333	PHE	CB-CG-CD1	6.70	125.49	120.80
1	A	867	ILE	CG1-CB-CG2	-6.70	96.66	111.40
2	B	328	GLU	N-CA-CB	6.70	122.66	110.60
2	B	1201	LYS	CD-CE-NZ	-6.70	96.30	111.70
4	E	121	MET	CB-CG-SD	6.70	132.49	112.40
3	C	10	ILE	CB-CA-C	-6.70	98.21	111.60
2	B	684	LEU	CB-CG-CD1	-6.69	99.63	111.00
2	B	1155	SER	CA-CB-OG	6.69	129.26	111.20
9	K	42	LEU	CB-CG-CD1	-6.69	99.63	111.00
2	B	202	TYR	CD1-CE1-CZ	6.68	125.82	119.80
2	B	452	THR	OG1-CB-CG2	-6.68	94.63	110.00
3	C	262	LEU	CB-CG-CD2	-6.68	99.64	111.00
1	A	455	MET	CG-SD-CE	-6.68	89.51	100.20
1	A	151	ASP	N-CA-C	-6.68	92.97	111.00
2	B	1134	GLU	CG-CD-OE1	6.68	131.66	118.30
2	B	1161	HIS	CB-CA-C	6.68	123.76	110.40
2	B	97	VAL	N-CA-C	-6.68	92.97	111.00
1	A	34	LYS	O-C-N	-6.68	112.02	122.70
7	I	55	THR	N-CA-CB	-6.68	97.62	110.30
1	A	947	PHE	CD1-CE1-CZ	6.67	128.11	120.10
1	A	1424	VAL	CG1-CB-CG2	6.67	121.58	110.90
7	I	75	CYS	CB-CA-C	-6.67	97.05	110.40
2	B	216	GLU	OE1-CD-OE2	6.67	131.30	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	37	GLU	CB-CA-C	-6.67	97.07	110.40
6	H	23	VAL	CA-CB-CG2	-6.67	100.90	110.90
1	A	1258	HIS	N-CA-CB	6.66	122.59	110.60
1	A	504	LEU	CA-CB-CG	6.66	130.61	115.30
1	A	570	PRO	N-CD-CG	-6.66	93.21	103.20
2	B	482	VAL	CB-CA-C	-6.66	98.75	111.40
1	A	57	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	547	LEU	CB-CG-CD2	-6.65	99.69	111.00
2	B	741	CYS	CA-CB-SG	6.65	125.97	114.00
2	B	811	TYR	CG-CD1-CE1	-6.65	115.98	121.30
10	L	25	ALA	O-C-N	6.65	133.34	122.70
10	L	54	ARG	N-CA-C	6.65	128.95	111.00
7	I	63	GLY	O-C-N	-6.65	112.06	122.70
2	B	387	LEU	CA-CB-CG	6.65	130.59	115.30
7	I	17	ARG	CB-CG-CD	6.65	128.88	111.60
2	B	948	ILE	CG1-CB-CG2	-6.64	96.78	111.40
1	A	1154	TYR	CE1-CZ-OH	-6.64	102.16	120.10
2	B	223	VAL	CB-CA-C	-6.64	98.78	111.40
4	E	9	ILE	CG1-CB-CG2	-6.64	96.79	111.40
1	A	1318	THR	CA-CB-CG2	6.64	121.70	112.40
1	A	1417	GLU	CA-CB-CG	6.64	128.01	113.40
1	A	4	GLN	CB-CA-C	6.64	123.67	110.40
1	A	856	THR	OG1-CB-CG2	-6.64	94.74	110.00
1	A	1166	ASP	CB-CG-OD2	-6.64	112.33	118.30
2	B	497	ARG	CG-CD-NE	-6.64	97.86	111.80
1	A	436	ILE	CG1-CB-CG2	-6.63	96.81	111.40
4	E	113	GLN	N-CA-CB	6.63	122.54	110.60
2	B	599	THR	OG1-CB-CG2	-6.63	94.74	110.00
1	A	1301	GLU	OE1-CD-OE2	6.63	131.26	123.30
9	K	75	ILE	CA-CB-CG1	6.63	123.60	111.00
1	A	12	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	A	695	LYS	N-CA-CB	-6.63	98.67	110.60
2	B	122	LEU	CB-CG-CD1	-6.63	99.73	111.00
5	F	122	MET	CG-SD-CE	6.63	110.80	100.20
1	A	1077	THR	O-C-N	-6.62	112.10	122.70
4	E	198	ILE	CG1-CB-CG2	-6.62	96.83	111.40
1	A	946	VAL	CB-CA-C	-6.62	98.82	111.40
2	B	131	ASP	CB-CG-OD2	6.62	124.26	118.30
7	I	113	ASP	CB-CG-OD1	6.62	124.26	118.30
1	A	1111	MET	N-CA-CB	-6.62	98.69	110.60
1	A	970	THR	OG1-CB-CG2	-6.62	94.78	110.00
7	I	10	CYS	N-CA-C	6.62	128.86	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	125	LEU	N-CA-C	-6.61	93.15	111.00
1	A	469	ARG	CG-CD-NE	-6.61	97.93	111.80
1	A	793	SER	CB-CA-C	-6.61	97.55	110.10
2	B	310	MET	CG-SD-CE	6.61	110.77	100.20
6	H	37	LYS	O-C-N	6.61	133.27	122.70
1	A	1302	PRO	O-C-N	6.60	133.27	122.70
3	C	169	LYS	CD-CE-NZ	-6.60	96.51	111.70
1	A	98	LYS	CG-CD-CE	-6.60	92.10	111.90
2	B	166	PHE	CB-CG-CD1	-6.60	116.18	120.80
2	B	1166	CYS	N-CA-CB	-6.60	98.72	110.60
3	C	211	ASP	OD1-CG-OD2	6.60	135.83	123.30
2	B	373	ARG	NE-CZ-NH1	6.59	123.60	120.30
2	B	567	GLU	CB-CA-C	6.59	123.59	110.40
2	B	661	LEU	CB-CG-CD2	6.59	122.21	111.00
3	C	247	GLY	CA-C-O	-6.59	108.74	120.60
1	A	904	THR	CA-CB-CG2	-6.58	103.19	112.40
1	A	1365	TYR	CB-CG-CD2	-6.58	117.05	121.00
2	B	698	GLU	CG-CD-OE1	6.58	131.46	118.30
8	J	27	GLU	OE1-CD-OE2	6.58	131.20	123.30
1	A	877	HIS	CG-ND1-CE1	6.58	117.41	108.20
3	C	121	VAL	CA-CB-CG2	-6.58	101.03	110.90
1	A	1135	ARG	CG-CD-NE	-6.58	97.99	111.80
1	A	149	GLU	OE1-CD-OE2	6.57	131.19	123.30
1	A	1138	ILE	CG1-CB-CG2	-6.57	96.95	111.40
2	B	559	SER	CA-CB-OG	-6.57	93.46	111.20
2	B	833	TYR	CD1-CG-CD2	-6.57	110.67	117.90
6	H	63	LEU	CA-C-O	6.57	133.90	120.10
1	A	531	ILE	CG1-CB-CG2	-6.57	96.95	111.40
2	B	963	PHE	CD1-CG-CD2	6.57	126.84	118.30
4	E	215	MET	N-CA-C	6.57	128.73	111.00
7	I	83	ASN	CB-CA-C	-6.57	97.27	110.40
1	A	804	TYR	CB-CG-CD1	6.56	124.94	121.00
3	C	70	ILE	CA-CB-CG1	6.56	123.46	111.00
6	H	84	ALA	C-N-CA	6.56	136.07	122.30
1	A	1127	ASP	CB-CG-OD1	-6.55	112.40	118.30
1	A	1243	VAL	N-CA-C	-6.55	93.31	111.00
3	C	202	PRO	CA-C-O	-6.55	104.47	120.20
5	F	123	LYS	CD-CE-NZ	-6.55	96.63	111.70
2	B	633	VAL	CG1-CB-CG2	-6.55	100.42	110.90
2	B	1223	ASP	CB-CG-OD2	6.55	124.20	118.30
7	I	109	ILE	CB-CG1-CD1	-6.55	95.56	113.90
2	B	217	ARG	CB-CG-CD	6.55	128.62	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	THR	CB-CA-C	-6.54	93.93	111.60
2	B	329	THR	OG1-CB-CG2	-6.54	94.95	110.00
1	A	833	GLU	CG-CD-OE2	-6.54	105.22	118.30
2	B	532	ALA	O-C-N	6.54	133.16	122.70
3	C	201	TRP	CD1-NE1-CE2	-6.54	103.12	109.00
3	C	219	PHE	CZ-CE2-CD2	6.53	127.94	120.10
2	B	459	TYR	O-C-N	-6.53	112.25	122.70
1	A	446	ARG	NE-CZ-NH1	-6.53	117.04	120.30
1	A	592	ASP	CB-CG-OD1	6.53	124.17	118.30
1	A	1119	TYR	CG-CD2-CE2	6.53	126.52	121.30
2	B	642	ASP	CA-C-N	-6.53	102.84	117.20
2	B	789	MET	CG-SD-CE	-6.53	89.75	100.20
1	A	1153	TYR	CG-CD1-CE1	-6.53	116.08	121.30
3	C	238	ILE	CG1-CB-CG2	-6.53	97.05	111.40
1	A	813	PHE	CD1-CE1-CZ	6.52	127.93	120.10
1	A	842	VAL	O-C-N	-6.52	112.27	122.70
6	H	146	ARG	CD-NE-CZ	6.52	132.73	123.60
2	B	802	PRO	CA-C-O	-6.51	104.56	120.20
2	B	589	VAL	CB-CA-C	6.51	123.77	111.40
4	E	112	TYR	OH-CZ-CE2	6.51	137.68	120.10
1	A	106	VAL	CG1-CB-CG2	-6.51	100.49	110.90
2	B	1162	ILE	CG1-CB-CG2	-6.51	97.08	111.40
3	C	11	ARG	NE-CZ-NH2	6.51	123.55	120.30
7	I	1	MET	CG-SD-CE	6.51	110.61	100.20
1	A	635	ARG	N-CA-CB	6.50	122.31	110.60
7	I	13	MET	CG-SD-CE	-6.50	89.79	100.20
2	B	942	ARG	CA-CB-CG	6.50	127.70	113.40
9	K	5	ASP	CB-CA-C	-6.50	97.40	110.40
1	A	591	PHE	CG-CD1-CE1	6.50	127.95	120.80
2	B	650	GLU	OE1-CD-OE2	6.50	131.10	123.30
2	B	629	ASP	CB-CG-OD2	6.50	124.15	118.30
3	C	263	THR	CA-CB-CG2	6.50	121.50	112.40
9	K	13	GLY	N-CA-C	-6.50	96.86	113.10
1	A	1433	MET	N-CA-CB	6.49	122.29	110.60
2	B	1134	GLU	CG-CD-OE2	-6.49	105.31	118.30
2	B	710	LEU	CB-CG-CD1	-6.49	99.97	111.00
9	K	93	SER	N-CA-CB	6.49	120.23	110.50
2	B	1095	LEU	CB-CA-C	-6.49	97.87	110.20
4	E	23	VAL	CG1-CB-CG2	-6.49	100.52	110.90
1	A	1108	ALA	O-C-N	6.49	133.08	122.70
1	A	203	SER	N-CA-CB	6.49	120.23	110.50
3	C	230	MET	N-CA-C	6.49	128.51	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	194	GLU	OE1-CD-OE2	-6.49	115.52	123.30
2	B	1018	PRO	CA-C-O	-6.48	104.64	120.20
1	A	86	LEU	CB-CG-CD2	6.48	122.01	111.00
2	B	1212	ILE	CG1-CB-CG2	-6.48	97.15	111.40
2	B	267	ARG	N-CA-CB	-6.48	98.94	110.60
1	A	793	SER	CA-CB-OG	6.47	128.68	111.20
2	B	975	GLN	CB-CA-C	-6.47	97.46	110.40
4	E	180	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	1269	GLU	CG-CD-OE2	-6.47	105.36	118.30
1	A	1221	LYS	CD-CE-NZ	6.47	126.58	111.70
2	B	92	PHE	N-CA-CB	6.47	122.24	110.60
2	B	530	GLY	N-CA-C	6.47	129.27	113.10
1	A	541	ILE	CB-CA-C	-6.47	98.67	111.60
4	E	109	ILE	CB-CA-C	-6.47	98.67	111.60
4	E	200	ARG	NE-CZ-NH1	-6.46	117.07	120.30
10	L	64	LEU	CB-CG-CD2	-6.46	100.01	111.00
1	A	244	PRO	N-CD-CG	-6.46	93.51	103.20
4	E	114	ASN	N-CA-CB	6.46	122.23	110.60
7	I	100	PHE	CG-CD1-CE1	6.46	127.91	120.80
7	I	109	ILE	CA-CB-CG1	6.46	123.28	111.00
4	E	159	ASP	CB-CG-OD1	6.46	124.11	118.30
1	A	1043	ASP	OD1-CG-OD2	-6.46	111.03	123.30
9	K	35	PHE	CB-CG-CD2	6.45	125.32	120.80
1	A	607	ILE	CA-C-O	-6.45	106.55	120.10
4	E	75	MET	CG-SD-CE	-6.45	89.88	100.20
8	J	6	ARG	CG-CD-NE	-6.45	98.25	111.80
2	B	275	TYR	CZ-CE2-CD2	-6.45	113.99	119.80
1	A	960	ILE	CG1-CB-CG2	-6.45	97.22	111.40
3	C	51	VAL	CG1-CB-CG2	-6.44	100.59	110.90
1	A	636	GLU	CG-CD-OE2	6.43	131.17	118.30
1	A	434	ARG	CG-CD-NE	-6.43	98.29	111.80
3	C	172	PRO	CB-CA-C	-6.43	95.92	112.00
1	A	1418	LEU	CB-CG-CD1	6.43	121.93	111.00
2	B	987	LYS	CB-CA-C	-6.43	97.54	110.40
6	H	19	ARG	NE-CZ-NH1	-6.43	117.09	120.30
1	A	65	LEU	CB-CG-CD2	6.42	121.92	111.00
4	E	159	ASP	CB-CG-OD2	-6.42	112.52	118.30
6	H	143	LEU	CB-CG-CD1	6.42	121.92	111.00
10	L	63	ARG	CG-CD-NE	6.42	125.28	111.80
4	E	207	ARG	CG-CD-NE	-6.42	98.32	111.80
3	C	181	ASP	CB-CG-OD2	6.42	124.08	118.30
3	C	23	SER	N-CA-C	-6.42	93.68	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	THR	CA-CB-CG2	6.42	121.38	112.40
1	A	870	GLU	OE1-CD-OE2	6.41	131.00	123.30
3	C	124	LEU	CB-CA-C	-6.41	98.01	110.20
9	K	10	PHE	CB-CG-CD1	-6.41	116.31	120.80
9	K	24	ASP	OD1-CG-OD2	-6.41	111.11	123.30
6	H	77	ARG	NH1-CZ-NH2	-6.41	112.35	119.40
2	B	61	ASP	CB-CG-OD2	-6.41	112.53	118.30
3	C	125	MET	CB-CG-SD	6.41	131.62	112.40
2	B	380	TYR	CB-CG-CD2	6.41	124.84	121.00
2	B	463	THR	OG1-CB-CG2	-6.41	95.27	110.00
2	B	1202	LEU	CB-CG-CD2	6.40	121.88	111.00
1	A	186	LYS	CB-CG-CD	6.40	128.24	111.60
1	A	563	PRO	O-C-N	-6.40	112.47	122.70
1	A	1212	VAL	CA-CB-CG1	-6.39	101.31	110.90
2	B	790	ASP	OD1-CG-OD2	-6.39	111.16	123.30
2	B	368	GLU	N-CA-CB	6.39	122.09	110.60
2	B	1037	LEU	CB-CG-CD1	6.38	121.86	111.00
2	B	1177	HIS	N-CA-CB	6.38	122.09	110.60
2	B	1212	ILE	CA-CB-CG1	-6.38	98.87	111.00
3	C	124	LEU	N-CA-C	6.38	128.22	111.00
2	B	1064	TYR	CB-CG-CD1	6.37	124.82	121.00
1	A	1445	ILE	O-C-N	6.37	132.90	122.70
6	H	106	GLU	CB-CA-C	6.37	123.14	110.40
1	A	1223	ASP	N-CA-CB	6.37	122.07	110.60
10	L	50	ASP	CB-CG-OD1	6.37	124.03	118.30
1	A	868	TYR	CG-CD1-CE1	-6.37	116.21	121.30
2	B	1033	LYS	CD-CE-NZ	-6.37	97.06	111.70
7	I	73	ARG	NE-CZ-NH2	-6.36	117.12	120.30
2	B	1019	SER	C-N-CA	-6.36	105.80	121.70
3	C	241	ASP	CB-CG-OD1	-6.36	112.58	118.30
1	A	361	LEU	CB-CG-CD2	-6.36	100.19	111.00
1	A	1064	VAL	CG1-CB-CG2	-6.36	100.73	110.90
2	B	665	GLU	CA-CB-CG	6.36	127.39	113.40
1	A	170	THR	N-CA-C	-6.35	93.84	111.00
4	E	73	PRO	CA-C-O	-6.35	104.95	120.20
1	A	557	ASP	CB-CG-OD1	-6.35	112.59	118.30
1	A	868	TYR	CD1-CE1-CZ	6.35	125.52	119.80
1	A	1303	GLU	OE1-CD-OE2	6.35	130.92	123.30
2	B	228	LYS	CB-CG-CD	6.35	128.11	111.60
2	B	268	THR	OG1-CB-CG2	-6.35	95.40	110.00
3	C	241	ASP	CB-CG-OD2	6.34	124.01	118.30
9	K	22	ASP	CB-CG-OD2	-6.34	112.59	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	472	LEU	CA-CB-CG	-6.34	100.71	115.30
2	B	678	GLU	CB-CG-CD	6.34	131.33	114.20
2	B	641	GLU	OE1-CD-OE2	-6.34	115.69	123.30
2	B	621	GLU	CG-CD-OE2	6.34	130.98	118.30
1	A	541	ILE	CG1-CB-CG2	-6.34	97.46	111.40
1	A	396	PRO	CA-C-O	-6.34	104.99	120.20
2	B	710	LEU	CB-CG-CD2	6.34	121.77	111.00
2	B	815	ARG	NE-CZ-NH1	-6.34	117.13	120.30
2	B	711	GLU	CA-CB-CG	6.33	127.33	113.40
3	C	172	PRO	O-C-N	6.33	132.83	122.70
4	E	21	GLU	CB-CA-C	-6.33	97.73	110.40
1	A	1275	GLY	CA-C-N	-6.33	103.27	117.20
7	I	44	TYR	CD1-CE1-CZ	6.33	125.50	119.80
1	A	214	ILE	O-C-N	6.33	132.83	122.70
1	A	230	ARG	N-CA-CB	-6.33	99.21	110.60
2	B	994	TYR	CZ-CE2-CD2	6.33	125.50	119.80
9	K	14	GLU	CB-CA-C	6.33	123.05	110.40
2	B	666	TYR	CB-CG-CD2	-6.33	117.20	121.00
4	E	78	LEU	N-CA-CB	-6.32	97.76	110.40
1	A	123	ARG	N-CA-CB	6.32	121.97	110.60
1	A	956	LEU	CB-CG-CD1	6.32	121.74	111.00
1	A	1409	LEU	CB-CG-CD2	-6.32	100.26	111.00
2	B	739	THR	CA-CB-CG2	-6.32	103.56	112.40
1	A	725	ALA	N-CA-C	6.32	128.05	111.00
2	B	50	SER	CB-CA-C	-6.32	98.10	110.10
3	C	240	VAL	CB-CA-C	-6.31	99.41	111.40
1	A	1004	ASN	N-CA-C	6.31	128.04	111.00
1	A	1005	GLU	CG-CD-OE2	-6.31	105.68	118.30
2	B	477	ALA	N-CA-CB	6.31	118.93	110.10
1	A	751	SER	N-CA-CB	-6.31	101.04	110.50
2	B	1061	GLU	CG-CD-OE2	-6.31	105.69	118.30
2	B	390	LEU	CB-CG-CD1	-6.31	100.28	111.00
6	H	38	LEU	CB-CA-C	-6.31	98.22	110.20
1	A	173	THR	CA-CB-CG2	-6.30	103.57	112.40
1	A	659	HIS	CB-CG-ND1	-6.30	107.44	123.20
2	B	111	ALA	CB-CA-C	-6.30	100.64	110.10
2	B	870	ILE	CB-CG1-CD1	6.30	131.55	113.90
2	B	680	THR	OG1-CB-CG2	-6.30	95.51	110.00
7	I	31	THR	C-N-CA	6.30	137.45	121.70
2	B	357	GLN	CB-CA-C	-6.30	97.80	110.40
2	B	459	TYR	CA-C-N	6.30	131.06	117.20
9	K	79	GLU	CA-CB-CG	6.30	127.26	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1214	GLU	O-C-N	6.30	132.78	122.70
2	B	944	THR	CA-C-N	-6.29	103.35	117.20
2	B	957	ASN	N-CA-CB	-6.29	99.27	110.60
2	B	1152	MET	CG-SD-CE	-6.29	90.13	100.20
4	E	65	THR	C-N-CA	-6.29	105.97	121.70
2	B	97	VAL	CG1-CB-CG2	-6.29	100.83	110.90
2	B	225	VAL	CG1-CB-CG2	-6.29	100.83	110.90
10	L	55	ILE	CB-CA-C	-6.29	99.02	111.60
7	I	59	VAL	O-C-N	-6.29	112.64	122.70
1	A	947	PHE	CE1-CZ-CE2	-6.29	108.69	120.00
2	B	664	THR	OG1-CB-CG2	-6.29	95.55	110.00
7	I	98	VAL	CA-C-O	-6.29	106.90	120.10
1	A	836	TYR	CB-CG-CD2	6.28	124.77	121.00
2	B	116	GLU	OE1-CD-OE2	6.28	130.84	123.30
7	I	81	ARG	CD-NE-CZ	6.28	132.40	123.60
2	B	807	ARG	NH1-CZ-NH2	6.28	126.31	119.40
3	C	186	LEU	CB-CG-CD1	-6.28	100.32	111.00
1	A	536	LEU	CB-CG-CD1	6.28	121.68	111.00
1	A	843	LYS	CB-CA-C	6.28	122.96	110.40
2	B	646	LEU	N-CA-C	6.28	127.96	111.00
2	B	1086	PHE	N-CA-C	-6.28	94.04	111.00
10	L	40	LEU	CA-CB-CG	6.28	129.74	115.30
9	K	70	ARG	CD-NE-CZ	-6.28	114.81	123.60
9	K	53	ASP	OD1-CG-OD2	-6.28	111.37	123.30
1	A	1208	THR	CA-CB-OG1	6.28	122.18	109.00
1	A	1275	GLY	N-CA-C	-6.27	97.42	113.10
2	B	525	ALA	N-CA-C	6.27	127.93	111.00
1	A	1192	LEU	CB-CG-CD2	6.27	121.66	111.00
2	B	46	GLN	CA-CB-CG	-6.27	99.61	113.40
1	A	852	TYR	CA-C-O	-6.27	106.94	120.10
1	A	968	GLN	CA-CB-CG	-6.26	99.62	113.40
1	A	1113	THR	N-CA-CB	-6.26	98.40	110.30
2	B	1103	ILE	N-CA-CB	6.26	125.21	110.80
7	I	29	CYS	CA-CB-SG	6.26	125.28	114.00
2	B	477	ALA	O-C-N	-6.26	112.55	123.20
1	A	571	LEU	CB-CG-CD2	6.26	121.64	111.00
6	H	107	VAL	CB-CA-C	6.26	123.30	111.40
4	E	7	ARG	CG-CD-NE	6.26	124.94	111.80
1	A	49	LYS	CD-CE-NZ	6.26	126.09	111.70
1	A	610	GLY	O-C-N	6.25	132.69	122.70
1	A	915	SER	C-N-CA	-6.25	109.18	122.30
2	B	378	LEU	CB-CG-CD2	-6.25	100.38	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	386	LEU	CB-CG-CD2	-6.25	100.38	111.00
1	A	1141	THR	OG1-CB-CG2	-6.25	95.64	110.00
7	I	16	PRO	O-C-N	6.24	132.69	122.70
1	A	272	ALA	N-CA-CB	6.24	118.84	110.10
1	A	566	ILE	O-C-N	6.24	132.68	122.70
8	J	63	TYR	CB-CG-CD1	6.24	124.74	121.00
1	A	100	LYS	CD-CE-NZ	6.24	126.05	111.70
1	A	1225	PHE	CD1-CE1-CZ	-6.24	112.62	120.10
2	B	284	ILE	CA-CB-CG1	6.23	122.84	111.00
2	B	1194	ILE	CB-CA-C	-6.23	99.13	111.60
2	B	1129	ARG	CG-CD-NE	-6.23	98.71	111.80
1	A	176	LYS	CD-CE-NZ	6.23	126.03	111.70
2	B	105	SER	CA-CB-OG	6.23	128.02	111.20
7	I	82	GLU	CG-CD-OE1	6.23	130.76	118.30
1	A	226	GLU	CG-CD-OE1	-6.23	105.84	118.30
1	A	1242	VAL	N-CA-CB	-6.23	97.80	111.50
2	B	118	ARG	CB-CG-CD	6.23	127.79	111.60
2	B	273	LEU	CB-CA-C	-6.23	98.37	110.20
2	B	1224	PHE	CB-CG-CD2	6.23	125.16	120.80
4	E	17	ARG	CA-C-O	6.22	133.17	120.10
5	F	135	ARG	CG-CD-NE	-6.22	98.73	111.80
1	A	188	ASP	CB-CA-C	6.22	122.84	110.40
1	A	153	PRO	N-CD-CG	6.22	112.53	103.20
8	J	39	LEU	CB-CG-CD1	6.22	121.58	111.00
2	B	798	TYR	CE1-CZ-CE2	-6.22	109.85	119.80
6	H	136	LYS	CA-CB-CG	6.22	127.08	113.40
2	B	324	ILE	CG1-CB-CG2	-6.22	97.72	111.40
2	B	277	LYS	N-CA-CB	-6.22	99.41	110.60
1	A	107	CYS	N-CA-C	-6.21	94.22	111.00
1	A	619	LYS	CA-CB-CG	6.21	127.07	113.40
2	B	739	THR	CB-CA-C	-6.21	94.82	111.60
1	A	86	LEU	CB-CG-CD1	-6.21	100.45	111.00
2	B	595	ARG	NH1-CZ-NH2	-6.21	112.57	119.40
1	A	670	ILE	CA-CB-CG2	-6.21	98.49	110.90
2	B	1183	LYS	CG-CD-CE	6.20	130.51	111.90
8	J	2	ILE	CB-CA-C	-6.20	99.20	111.60
2	B	239	GLU	CB-CA-C	6.20	122.80	110.40
2	B	327	ARG	NH1-CZ-NH2	6.20	126.22	119.40
2	B	1175	LEU	CB-CG-CD1	-6.20	100.46	111.00
2	B	1203	LEU	CA-C-O	6.20	133.12	120.10
1	A	146	MET	N-CA-CB	-6.20	99.44	110.60
2	B	724	ASP	CB-CG-OD1	-6.20	112.72	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1103	GLU	CB-CA-C	6.20	122.79	110.40
1	A	649	ILE	CG1-CB-CG2	-6.19	97.78	111.40
2	B	509	ALA	CB-CA-C	6.19	119.39	110.10
2	B	1098	MET	CG-SD-CE	6.19	110.11	100.20
7	I	41	PRO	CA-CB-CG	-6.19	92.23	104.00
2	B	964	VAL	CA-CB-CG2	-6.19	101.61	110.90
2	B	101	MET	CB-CA-C	-6.19	98.02	110.40
3	C	248	ILE	CB-CG1-CD1	-6.19	96.58	113.90
3	C	143	LEU	CB-CG-CD1	6.18	121.51	111.00
1	A	446	ARG	CG-CD-NE	6.18	124.78	111.80
4	E	44	ALA	CA-C-N	-6.18	103.60	117.20
5	F	120	ILE	CA-CB-CG1	6.18	122.75	111.00
1	A	13	THR	CA-CB-CG2	-6.18	103.75	112.40
1	A	264	PHE	O-C-N	-6.18	112.81	122.70
1	A	799	PHE	CD1-CE1-CZ	6.18	127.52	120.10
1	A	938	LYS	O-C-N	6.18	132.59	122.70
1	A	980	ASP	CB-CA-C	-6.18	98.05	110.40
2	B	817	LEU	CB-CG-CD2	-6.18	100.50	111.00
4	E	162	ARG	CB-CG-CD	6.18	127.66	111.60
3	C	16	ASP	N-CA-CB	-6.17	99.48	110.60
1	A	777	PHE	CZ-CE2-CD2	6.17	127.51	120.10
2	B	1108	ARG	N-CA-C	6.17	127.66	111.00
3	C	263	THR	N-CA-CB	-6.17	98.59	110.30
6	H	86	ASP	CB-CA-C	6.17	122.73	110.40
2	B	634	TYR	CB-CG-CD2	6.16	124.69	121.00
4	E	201	LYS	N-CA-CB	-6.16	99.52	110.60
1	A	897	TYR	CG-CD2-CE2	-6.16	116.38	121.30
1	A	703	THR	CA-CB-CG2	-6.16	103.78	112.40
4	E	147	HIS	CB-CG-CD2	6.16	149.88	130.80
1	A	145	LYS	CD-CE-NZ	6.15	125.85	111.70
1	A	1326	ARG	NH1-CZ-NH2	-6.15	112.64	119.40
2	B	593	PRO	C-N-CA	-6.15	106.33	121.70
1	A	1204	ASP	OD1-CG-OD2	-6.15	111.62	123.30
8	J	61	LEU	CA-CB-CG	-6.15	101.16	115.30
1	A	776	ALA	CB-CA-C	-6.14	100.88	110.10
3	C	4	GLU	CG-CD-OE2	-6.14	106.01	118.30
3	C	205	LYS	CA-CB-CG	-6.14	99.88	113.40
1	A	122	MET	CG-SD-CE	6.14	110.03	100.20
2	B	392	ARG	NE-CZ-NH1	6.14	123.37	120.30
8	J	62	ARG	CG-CD-NE	-6.14	98.90	111.80
1	A	514	PRO	N-CA-CB	-6.14	95.85	102.60
2	B	57	TYR	CB-CG-CD2	6.14	124.68	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	194	GLU	OE1-CD-OE2	6.14	130.66	123.30
1	A	679	ILE	CG1-CB-CG2	-6.13	97.91	111.40
3	C	14	SER	O-C-N	-6.13	112.89	122.70
1	A	577	ILE	CG1-CB-CG2	-6.13	97.91	111.40
2	B	396	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	A	1342	GLU	OE1-CD-OE2	6.13	130.65	123.30
2	B	168	GLY	CA-C-N	-6.13	103.72	117.20
3	C	219	PHE	O-C-N	6.12	132.50	122.70
6	H	25	ARG	CG-CD-NE	-6.12	98.94	111.80
8	J	63	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	A	814	PHE	CG-CD1-CE1	6.12	127.53	120.80
1	A	889	SER	CB-CA-C	-6.12	98.47	110.10
2	B	28	GLU	OE1-CD-OE2	6.12	130.65	123.30
2	B	1093	GLN	N-CA-CB	-6.12	99.58	110.60
1	A	1281	ARG	NE-CZ-NH2	6.12	123.36	120.30
2	B	197	PHE	CB-CG-CD2	6.12	125.08	120.80
4	E	26	ARG	NE-CZ-NH2	6.12	123.36	120.30
4	E	107	THR	CA-CB-CG2	-6.12	103.83	112.40
2	B	1035	ALA	N-CA-CB	6.12	118.66	110.10
8	J	21	TYR	CD1-CG-CD2	-6.12	111.17	117.90
1	A	978	PRO	CB-CG-CD	-6.11	82.66	106.50
8	J	55	ASP	CA-C-N	-6.11	103.75	117.20
1	A	354	SER	CA-CB-OG	6.11	127.69	111.20
2	B	204	ILE	CA-CB-CG2	-6.11	98.69	110.90
2	B	905	VAL	CA-CB-CG2	6.11	120.06	110.90
2	B	935	ARG	NE-CZ-NH2	6.11	123.35	120.30
1	A	439	ASN	O-C-N	-6.11	112.93	122.70
2	B	1030	LEU	CB-CG-CD2	-6.11	100.62	111.00
1	A	1103	GLU	N-CA-CB	-6.10	99.62	110.60
1	A	1206	ASP	CB-CG-OD1	6.10	123.79	118.30
2	B	1097	HIS	CA-CB-CG	-6.10	103.23	113.60
4	E	153	HIS	O-C-N	-6.10	112.95	122.70
2	B	501	PRO	O-C-N	6.09	132.45	122.70
1	A	226	GLU	N-CA-CB	6.09	121.56	110.60
1	A	873	MET	CB-CG-SD	6.09	130.66	112.40
5	F	84	TYR	N-CA-CB	-6.09	99.64	110.60
1	A	724	GLU	CB-CA-C	6.09	122.58	110.40
2	B	177	LYS	CD-CE-NZ	6.09	125.70	111.70
2	B	915	THR	OG1-CB-CG2	-6.09	96.00	110.00
1	A	1313	LEU	CB-CG-CD2	-6.08	100.66	111.00
2	B	848	ARG	NH1-CZ-NH2	6.08	126.09	119.40
2	B	583	ASN	C-N-CA	-6.08	109.53	122.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	PHE	CB-CG-CD2	6.08	125.06	120.80
2	B	1182	CYS	CA-CB-SG	6.08	124.94	114.00
2	B	1202	LEU	CB-CG-CD1	-6.08	100.67	111.00
1	A	438	ASP	N-CA-CB	-6.08	99.66	110.60
1	A	946	VAL	CA-CB-CG2	-6.08	101.79	110.90
2	B	833	TYR	CD1-CE1-CZ	6.08	125.27	119.80
1	A	985	ASP	OD1-CG-OD2	6.07	134.84	123.30
3	C	4	GLU	CA-C-N	-6.07	104.05	116.20
5	F	154	ASP	CB-CG-OD1	6.07	123.77	118.30
2	B	1109	GLY	N-CA-C	6.07	128.28	113.10
2	B	1156	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	493	GLN	CB-CG-CD	6.07	127.38	111.60
8	J	21	TYR	N-CA-C	-6.07	94.61	111.00
1	A	392	VAL	CA-CB-CG1	-6.07	101.80	110.90
1	A	1281	ARG	CB-CA-C	-6.07	98.27	110.40
2	B	1028	GLU	CB-CA-C	-6.07	98.27	110.40
1	A	920	LEU	CB-CG-CD1	-6.06	100.69	111.00
9	K	20	LYS	CB-CG-CD	6.06	127.36	111.60
1	A	1297	GLU	OE1-CD-OE2	-6.06	116.03	123.30
2	B	833	TYR	CA-C-O	-6.06	107.38	120.10
1	A	608	ILE	CA-CB-CG1	6.06	122.51	111.00
2	B	1103	ILE	CG1-CB-CG2	-6.06	98.08	111.40
4	E	43	LYS	CD-CE-NZ	6.06	125.63	111.70
1	A	1267	MET	C-N-CA	-6.05	106.56	121.70
10	L	48	CYS	N-CA-CB	-6.05	99.70	110.60
1	A	456	MET	CG-SD-CE	-6.05	90.52	100.20
1	A	1210	GLY	O-C-N	6.05	132.38	122.70
8	J	24	LEU	N-CA-CB	6.05	122.50	110.40
2	B	708	GLU	OE1-CD-OE2	6.05	130.56	123.30
1	A	1237	ILE	CG1-CB-CG2	-6.05	98.10	111.40
2	B	40	GLU	CG-CD-OE2	-6.05	106.21	118.30
9	K	46	ILE	CA-CB-CG1	6.05	122.49	111.00
2	B	553	PRO	CA-N-CD	6.04	120.16	111.70
2	B	696	GLU	CG-CD-OE1	-6.04	106.21	118.30
2	B	972	LYS	CD-CE-NZ	-6.04	97.80	111.70
4	E	90	VAL	CG1-CB-CG2	6.04	120.57	110.90
1	A	1055	ARG	CG-CD-NE	-6.04	99.12	111.80
2	B	1215	ARG	NE-CZ-NH2	-6.04	117.28	120.30
3	C	110	THR	O-C-N	6.04	132.36	122.70
2	B	980	PHE	CB-CG-CD2	6.04	125.02	120.80
3	C	66	ARG	CB-CG-CD	6.04	127.29	111.60
7	I	96	SER	CA-CB-OG	6.04	127.50	111.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	840	ARG	CG-CD-NE	-6.03	99.13	111.80
2	B	712	PRO	N-CA-C	6.03	127.79	112.10
2	B	307	ASP	CB-CG-OD1	-6.03	112.87	118.30
6	H	102	TYR	N-CA-CB	-6.03	99.75	110.60
9	K	110	ASN	CB-CA-C	6.03	122.46	110.40
9	K	47	ARG	C-N-CA	-6.03	106.63	121.70
2	B	876	LYS	CD-CE-NZ	6.03	125.56	111.70
1	A	987	VAL	CA-CB-CG2	-6.02	101.86	110.90
9	K	85	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	A	1219	THR	OG1-CB-CG2	-6.02	96.15	110.00
3	C	124	LEU	CB-CG-CD2	-6.02	100.77	111.00
2	B	1136	ASP	OD1-CG-OD2	-6.02	111.86	123.30
2	B	1156	ASP	N-CA-CB	6.02	121.43	110.60
8	J	14	VAL	O-C-N	-6.02	112.97	123.20
4	E	208	TYR	CE1-CZ-CE2	-6.02	110.17	119.80
1	A	416	ARG	N-CA-CB	6.02	121.43	110.60
1	A	770	VAL	CA-CB-CG1	-6.02	101.88	110.90
4	E	112	TYR	CD1-CE1-CZ	6.01	125.21	119.80
1	A	600	PRO	CA-N-CD	6.01	120.12	111.70
2	B	446	LEU	CB-CG-CD1	6.01	121.22	111.00
1	A	465	TYR	O-C-N	-6.01	113.08	122.70
1	A	999	VAL	CG1-CB-CG2	6.01	120.52	110.90
1	A	1334	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	1194	ARG	CB-CA-C	-6.01	98.38	110.40
4	E	110	PHE	CB-CA-C	-6.01	98.39	110.40
2	B	1185	CYS	N-CA-C	-6.00	94.79	111.00
9	K	114	LEU	N-CA-CB	6.00	122.41	110.40
9	K	74	ARG	CB-CG-CD	6.00	127.21	111.60
7	I	65	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	693	VAL	CA-CB-CG1	-6.00	101.90	110.90
1	A	1282	VAL	CB-CA-C	-6.00	100.00	111.40
4	E	106	GLN	N-CA-C	-6.00	94.81	111.00
7	I	2	THR	CA-CB-CG2	-6.00	104.00	112.40
9	K	48	ALA	O-C-N	6.00	132.30	122.70
2	B	245	GLU	CA-CB-CG	6.00	126.59	113.40
6	H	117	SER	O-C-N	6.00	132.29	122.70
10	L	27	LEU	N-CA-C	6.00	127.19	111.00
4	E	71	LYS	CB-CG-CD	6.00	127.19	111.60
1	A	145	LYS	CB-CA-C	-5.99	98.41	110.40
1	A	684	ALA	CB-CA-C	5.99	119.09	110.10
2	B	850	LEU	CB-CG-CD2	-5.99	100.81	111.00
6	H	10	PHE	CB-CG-CD1	5.99	125.00	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1301	GLU	N-CA-CB	5.99	121.39	110.60
2	B	391	ASP	N-CA-CB	5.99	121.39	110.60
2	B	1185	CYS	CB-CA-C	5.99	122.38	110.40
4	E	137	GLU	OE1-CD-OE2	5.99	130.49	123.30
1	A	346	ASP	CA-C-N	5.99	130.38	117.20
1	A	218	ASP	OD1-CG-OD2	5.99	134.68	123.30
2	B	190	TYR	CB-CG-CD2	5.99	124.59	121.00
2	B	981	ALA	N-CA-C	5.99	127.17	111.00
2	B	106	ASP	N-CA-CB	-5.99	99.83	110.60
2	B	788	ARG	CA-CB-CG	5.99	126.57	113.40
2	B	1106	ARG	NE-CZ-NH1	-5.99	117.31	120.30
9	K	47	ARG	O-C-N	-5.98	113.13	122.70
1	A	598	LEU	CA-CB-CG	5.98	129.06	115.30
2	B	1061	GLU	OE1-CD-OE2	5.98	130.48	123.30
9	K	73	LEU	CA-CB-CG	5.98	129.05	115.30
1	A	553	VAL	CA-CB-CG2	5.98	119.86	110.90
2	B	621	GLU	OE1-CD-OE2	-5.98	116.13	123.30
1	A	878	ILE	CB-CG1-CD1	-5.97	97.17	113.90
2	B	1193	GLN	N-CA-CB	-5.97	99.85	110.60
2	B	399	ASP	N-CA-CB	-5.97	99.85	110.60
2	B	982	SER	CA-C-O	-5.96	107.57	120.10
2	B	1023	VAL	N-CA-CB	-5.96	98.38	111.50
3	C	25	VAL	CB-CA-C	-5.96	100.07	111.40
5	F	133	VAL	CG1-CB-CG2	-5.96	101.36	110.90
1	A	815	PHE	CB-CG-CD1	5.96	124.97	120.80
1	A	42	ASP	CB-CG-OD1	-5.96	112.93	118.30
1	A	853	ASP	CB-CG-OD2	5.96	123.67	118.30
10	L	58	LYS	CA-C-N	5.96	130.32	117.20
1	A	1287	TYR	CB-CG-CD2	-5.96	117.42	121.00
3	C	123	ASN	CB-CA-C	5.96	122.32	110.40
1	A	482	PHE	CB-CG-CD2	5.96	124.97	120.80
2	B	18	PHE	CB-CA-C	5.96	122.31	110.40
1	A	913	LEU	O-C-N	-5.95	113.17	122.70
2	B	535	LEU	CB-CG-CD2	5.95	121.12	111.00
8	J	55	ASP	CB-CG-OD2	-5.95	112.94	118.30
7	I	92	ARG	CG-CD-NE	-5.95	99.30	111.80
1	A	359	LEU	CB-CA-C	-5.95	98.89	110.20
3	C	136	ASP	OD1-CG-OD2	-5.95	112.00	123.30
8	J	17	LYS	C-N-CA	-5.95	106.82	121.70
9	K	64	GLU	CG-CD-OE1	5.95	130.20	118.30
9	K	78	THR	CB-CA-C	-5.95	95.53	111.60
1	A	375	THR	CA-CB-CG2	-5.95	104.07	112.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	884	ARG	NE-CZ-NH2	-5.95	117.33	120.30
3	C	229	TYR	N-CA-C	5.95	127.05	111.00
4	E	45	LYS	CD-CE-NZ	5.95	125.38	111.70
1	A	538	ASP	CB-CG-OD1	-5.94	112.95	118.30
1	A	886	ILE	CG1-CB-CG2	-5.94	98.33	111.40
1	A	961	ARG	CD-NE-CZ	5.94	131.92	123.60
1	A	861	GLY	O-C-N	-5.94	113.20	122.70
4	E	187	TYR	CD1-CE1-CZ	5.94	125.15	119.80
1	A	1284	MET	CB-CG-SD	5.94	130.22	112.40
1	A	1406	VAL	CA-C-N	-5.94	104.14	117.20
2	B	48	LEU	CB-CG-CD1	5.94	121.10	111.00
2	B	589	VAL	N-CA-CB	-5.94	98.44	111.50
4	E	182	ASP	CB-CA-C	-5.94	98.53	110.40
2	B	42	GLY	N-CA-C	5.93	127.94	113.10
1	A	93	VAL	CA-C-N	-5.93	104.33	116.20
1	A	890	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	882	SER	CA-CB-OG	-5.93	95.19	111.20
4	E	215	MET	CB-CA-C	-5.93	98.54	110.40
1	A	619	LYS	CB-CG-CD	5.93	127.02	111.60
1	A	1153	TYR	CB-CG-CD2	5.93	124.56	121.00
9	K	12	LEU	N-CA-C	-5.93	94.99	111.00
1	A	606	LEU	CA-CB-CG	-5.93	101.67	115.30
1	A	945	GLU	OE1-CD-OE2	5.93	130.41	123.30
1	A	1030	ARG	NH1-CZ-NH2	-5.93	112.88	119.40
2	B	365	THR	OG1-CB-CG2	-5.93	96.37	110.00
4	E	168	TYR	CB-CG-CD2	5.93	124.56	121.00
7	I	3	THR	O-C-N	5.93	132.18	122.70
7	I	78	CYS	CA-CB-SG	5.93	124.67	114.00
1	A	868	TYR	CZ-CE2-CD2	-5.92	114.47	119.80
1	A	1129	GLU	CB-CA-C	5.92	122.25	110.40
2	B	1146	PHE	CB-CG-CD1	5.92	124.94	120.80
4	E	91	LYS	CA-CB-CG	5.92	126.42	113.40
9	K	111	LEU	CD1-CG-CD2	5.92	128.25	110.50
1	A	177	ASP	N-CA-C	-5.91	95.03	111.00
1	A	295	LEU	N-CA-C	-5.91	95.03	111.00
2	B	292	ILE	CG1-CB-CG2	-5.91	98.39	111.40
4	E	118	PRO	CB-CG-CD	-5.91	83.44	106.50
6	H	102	TYR	CA-C-O	5.91	132.51	120.10
2	B	189	LEU	CB-CG-CD2	-5.91	100.95	111.00
1	A	934	LYS	N-CA-CB	5.91	121.24	110.60
1	A	995	GLU	CA-CB-CG	5.91	126.39	113.40
1	A	1349	TYR	CG-CD2-CE2	-5.90	116.58	121.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	14	SER	N-CA-C	-5.90	95.07	111.00
1	A	938	LYS	CG-CD-CE	-5.90	94.21	111.90
7	I	106	CYS	CB-CA-C	-5.90	98.61	110.40
1	A	412	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	1353	TYR	CG-CD2-CE2	5.89	126.02	121.30
2	B	346	GLU	OE1-CD-OE2	-5.89	116.22	123.30
2	B	1083	ALA	C-N-CA	-5.89	106.96	121.70
1	A	157	ASP	OD1-CG-OD2	-5.89	112.10	123.30
1	A	164	ARG	CD-NE-CZ	5.89	131.85	123.60
2	B	326	ASP	CB-CG-OD1	-5.89	113.00	118.30
5	F	112	GLU	CA-CB-CG	-5.89	100.44	113.40
1	A	121	LEU	CA-CB-CG	5.89	128.85	115.30
1	A	1025	ARG	NE-CZ-NH2	5.89	123.25	120.30
7	I	54	GLU	CG-CD-OE2	-5.89	106.52	118.30
4	E	209	ALA	CB-CA-C	-5.89	101.27	110.10
1	A	1154	TYR	CA-C-O	-5.89	107.74	120.10
7	I	107	SER	CA-C-N	-5.89	104.25	117.20
1	A	1100	ARG	NH1-CZ-NH2	-5.88	112.93	119.40
1	A	912	LEU	O-C-N	-5.88	113.29	122.70
4	E	147	HIS	ND1-CG-CD2	-5.88	97.77	106.00
2	B	973	ILE	CG1-CB-CG2	-5.88	98.47	111.40
1	A	1005	GLU	CG-CD-OE1	5.88	130.05	118.30
8	J	25	LEU	CA-CB-CG	5.88	128.82	115.30
3	C	96	SER	N-CA-CB	-5.88	101.69	110.50
9	K	11	LEU	CB-CA-C	-5.88	99.04	110.20
1	A	1307	GLU	OE1-CD-OE2	-5.87	116.25	123.30
2	B	164	LYS	CA-C-N	5.87	130.12	117.20
2	B	97	VAL	CB-CA-C	5.87	122.56	111.40
3	C	99	LEU	CB-CG-CD2	5.87	120.98	111.00
6	H	126	GLU	N-CA-C	-5.87	95.15	111.00
1	A	696	GLU	CB-CA-C	5.87	122.14	110.40
2	B	43	LEU	CA-CB-CG	-5.87	101.81	115.30
2	B	589	VAL	O-C-N	-5.87	113.31	122.70
7	I	99	LEU	CB-CG-CD2	-5.87	101.03	111.00
1	A	1188	GLN	CB-CA-C	-5.86	98.67	110.40
2	B	125	SER	CB-CA-C	5.86	121.24	110.10
2	B	353	LYS	N-CA-CB	5.86	121.15	110.60
9	K	51	LEU	CB-CG-CD1	-5.86	101.03	111.00
2	B	855	PHE	CD1-CG-CD2	-5.86	110.68	118.30
7	I	15	TYR	CA-CB-CG	5.86	124.53	113.40
3	C	161	LYS	CD-CE-NZ	5.86	125.17	111.70
1	A	901	LEU	CB-CG-CD2	5.86	120.96	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	35	ARG	CG-CD-NE	-5.86	99.50	111.80
3	C	79	GLN	CA-CB-CG	5.86	126.28	113.40
6	H	103	LYS	CB-CG-CD	5.85	126.82	111.60
7	I	92	ARG	CA-C-N	-5.85	104.33	117.20
2	B	264	SER	CB-CA-C	5.85	121.22	110.10
1	A	236	LEU	CA-C-N	-5.85	104.33	117.20
9	K	113	THR	CA-CB-CG2	-5.85	104.21	112.40
2	B	1067	ARG	NE-CZ-NH1	5.85	123.22	120.30
2	B	1153	GLU	CG-CD-OE1	-5.85	106.61	118.30
1	A	1128	GLN	O-C-N	-5.84	113.35	122.70
2	B	635	ARG	CG-CD-NE	-5.84	99.53	111.80
1	A	922	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	448	PRO	CA-C-O	-5.84	106.19	120.20
2	B	305	VAL	CG1-CB-CG2	5.84	120.24	110.90
1	A	664	THR	N-CA-CB	5.84	121.39	110.30
1	A	121	LEU	CB-CG-CD1	5.84	120.92	111.00
1	A	1031	VAL	CB-CA-C	-5.84	100.31	111.40
1	A	131	SER	CB-CA-C	5.83	121.19	110.10
1	A	1280	GLU	CG-CD-OE1	-5.83	106.63	118.30
2	B	582	VAL	CG1-CB-CG2	-5.83	101.57	110.90
1	A	740	LEU	CB-CA-C	-5.83	99.12	110.20
1	A	824	LEU	CD1-CG-CD2	-5.83	93.00	110.50
1	A	1097	GLY	CA-C-O	-5.83	110.11	120.60
2	B	451	LYS	CA-C-N	5.83	130.02	117.20
2	B	967	ARG	N-CA-CB	-5.83	100.11	110.60
2	B	1007	VAL	N-CA-CB	-5.83	98.68	111.50
2	B	885	MET	CG-SD-CE	5.83	109.52	100.20
2	B	1054	GLY	O-C-N	5.83	132.02	122.70
1	A	50	ILE	N-CA-C	5.83	126.73	111.00
1	A	1018	PHE	CG-CD2-CE2	5.83	127.21	120.80
1	A	1025	ARG	N-CA-CB	5.83	121.09	110.60
2	B	1002	THR	OG1-CB-CG2	-5.83	96.60	110.00
2	B	1020	ARG	CA-CB-CG	5.82	126.21	113.40
5	F	149	GLU	N-CA-CB	5.82	121.08	110.60
2	B	666	TYR	OH-CZ-CE2	-5.82	104.38	120.10
2	B	1087	PHE	CB-CG-CD1	-5.82	116.72	120.80
1	A	109	HIS	CB-CA-C	5.82	122.04	110.40
3	C	252	GLN	N-CA-C	-5.82	95.29	111.00
1	A	764	CYS	CA-CB-SG	5.82	124.47	114.00
2	B	59	LEU	N-CA-C	-5.82	95.30	111.00
2	B	429	PHE	N-CA-CB	-5.81	100.14	110.60
1	A	980	ASP	N-CA-C	5.81	126.69	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1063	MET	O-C-N	-5.81	113.40	122.70
1	A	740	LEU	CB-CG-CD2	-5.81	101.12	111.00
1	A	962	ARG	CG-CD-NE	-5.81	99.60	111.80
4	E	149	LEU	CA-CB-CG	5.81	128.66	115.30
1	A	174	ILE	N-CA-C	-5.81	95.32	111.00
1	A	514	PRO	CA-CB-CG	5.81	115.83	104.80
1	A	664	THR	CB-CA-C	-5.80	95.93	111.60
1	A	1172	LEU	CB-CA-C	-5.80	99.17	110.20
4	E	47	CYS	N-CA-C	5.80	126.67	111.00
2	B	89	GLU	CG-CD-OE1	5.80	129.90	118.30
2	B	1146	PHE	CD1-CE1-CZ	5.80	127.06	120.10
10	L	70	ARG	N-CA-CB	-5.80	100.17	110.60
1	A	957	PRO	N-CA-C	-5.79	97.03	112.10
1	A	1081	LEU	CB-CG-CD1	-5.79	101.15	111.00
3	C	80	LEU	O-C-N	-5.79	113.43	122.70
5	F	119	ARG	O-C-N	5.79	131.97	122.70
1	A	364	VAL	CA-CB-CG2	5.79	119.59	110.90
2	B	954	VAL	CG1-CB-CG2	-5.79	101.63	110.90
1	A	1345	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	896	ARG	CD-NE-CZ	-5.79	115.50	123.60
2	B	297	ILE	CA-CB-CG1	5.79	122.00	111.00
1	A	14	VAL	CA-C-N	5.79	129.93	117.20
2	B	512	ARG	CA-CB-CG	5.79	126.13	113.40
1	A	209	ASN	N-CA-CB	5.78	121.01	110.60
1	A	877	HIS	ND1-CE1-NE2	-5.78	97.17	109.90
1	A	1350	LYS	N-CA-CB	-5.78	100.19	110.60
6	H	107	VAL	CA-CB-CG1	5.78	119.57	110.90
2	B	1064	TYR	CB-CG-CD2	-5.78	117.53	121.00
7	I	117	LYS	CD-CE-NZ	5.78	125.00	111.70
10	L	69	ALA	CA-C-N	-5.78	104.48	117.20
1	A	986	ILE	CG1-CB-CG2	-5.78	98.69	111.40
3	C	3	GLU	C-N-CA	5.78	136.14	121.70
4	E	87	SER	N-CA-C	-5.78	95.40	111.00
6	H	120	GLY	N-CA-C	5.78	127.54	113.10
1	A	817	ALA	CB-CA-C	-5.78	101.44	110.10
2	B	483	LEU	CA-CB-CG	5.78	128.58	115.30
1	A	883	LEU	N-CA-C	-5.77	95.41	111.00
10	L	68	GLU	CB-CG-CD	5.77	129.78	114.20
4	E	28	TYR	CD1-CG-CD2	-5.77	111.55	117.90
3	C	195	GLN	CA-CB-CG	5.77	126.09	113.40
9	K	36	GLU	OE1-CD-OE2	5.77	130.22	123.30
1	A	814	PHE	CB-CG-CD2	5.77	124.84	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	705	MET	CA-CB-CG	5.77	123.10	113.30
2	B	1101	ASP	OD1-CG-OD2	-5.77	112.34	123.30
1	A	1295	THR	OG1-CB-CG2	-5.76	96.74	110.00
2	B	210	LYS	CD-CE-NZ	5.76	124.96	111.70
2	B	854	LEU	CB-CG-CD1	-5.76	101.20	111.00
2	B	305	VAL	CB-CA-C	-5.76	100.45	111.40
6	H	111	LEU	CB-CG-CD1	5.76	120.80	111.00
10	L	29	TYR	CZ-CE2-CD2	5.76	124.99	119.80
9	K	87	LEU	CA-CB-CG	5.76	128.55	115.30
1	A	616	VAL	N-CA-CB	-5.76	98.83	111.50
1	A	1274	ARG	CB-CA-C	-5.76	98.88	110.40
1	A	376	TYR	CD1-CE1-CZ	5.76	124.98	119.80
1	A	748	MET	CB-CG-SD	-5.76	95.13	112.40
1	A	801	GLU	CG-CD-OE1	-5.76	106.79	118.30
1	A	1110	ASN	CA-C-O	5.76	132.19	120.10
2	B	117	ALA	C-N-CA	-5.76	107.31	121.70
6	H	103	LYS	CB-CA-C	5.76	121.91	110.40
5	F	87	LYS	CD-CE-NZ	-5.75	98.46	111.70
1	A	56	PRO	O-C-N	5.75	131.91	122.70
1	A	1195	LEU	CB-CG-CD2	-5.75	101.22	111.00
3	C	24	ASN	CB-CA-C	-5.75	98.89	110.40
3	C	249	ASP	CB-CG-OD1	-5.75	113.12	118.30
4	E	193	GLY	CA-C-O	-5.75	110.24	120.60
5	F	72	LYS	C-N-CA	5.75	136.08	121.70
10	L	63	ARG	CB-CA-C	5.75	121.90	110.40
2	B	58	THR	CA-CB-CG2	-5.75	104.35	112.40
1	A	220	THR	CA-CB-CG2	-5.75	104.35	112.40
1	A	719	VAL	CA-CB-CG2	5.75	119.52	110.90
2	B	265	SER	CA-CB-OG	5.75	126.72	111.20
2	B	662	MET	CG-SD-CE	-5.75	91.01	100.20
8	J	4	PRO	N-CD-CG	-5.75	94.58	103.20
1	A	1309	ASP	CB-CA-C	-5.74	98.91	110.40
8	J	34	THR	CA-CB-CG2	-5.74	104.36	112.40
1	A	1235	LYS	CD-CE-NZ	5.74	124.91	111.70
2	B	61	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	1141	THR	CA-CB-CG2	-5.74	104.36	112.40
1	A	1299	VAL	CB-CA-C	5.74	122.31	111.40
2	B	754	SER	O-C-N	-5.74	113.52	122.70
1	A	1274	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	A	787	PHE	CD1-CG-CD2	-5.74	110.84	118.30
4	E	156	LEU	CA-C-N	-5.74	104.58	117.20
1	A	70	CYS	N-CA-CB	5.73	120.92	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1243	VAL	N-CA-CB	-5.73	98.88	111.50
4	E	105	PHE	CB-CG-CD1	-5.73	116.79	120.80
1	A	922	ASP	CB-CG-OD2	-5.73	113.14	118.30
2	B	336	ARG	NH1-CZ-NH2	5.73	125.71	119.40
2	B	1135	ARG	NH1-CZ-NH2	5.73	125.71	119.40
2	B	251	ILE	CA-CB-CG2	5.73	122.36	110.90
3	C	161	LYS	CA-CB-CG	5.73	126.00	113.40
5	F	97	ARG	CB-CG-CD	5.73	126.50	111.60
1	A	850	VAL	O-C-N	-5.73	113.53	122.70
10	L	26	THR	CA-C-N	-5.73	104.60	117.20
1	A	981	LEU	CB-CG-CD2	-5.72	101.27	111.00
1	A	111	GLY	CA-C-O	5.72	130.90	120.60
5	F	117	PRO	CA-N-CD	-5.72	103.49	111.50
5	F	114	GLU	CA-C-O	-5.72	108.08	120.10
1	A	129	LYS	CB-CG-CD	5.72	126.47	111.60
1	A	416	ARG	CG-CD-NE	-5.72	99.79	111.80
1	A	724	GLU	OE1-CD-OE2	5.72	130.16	123.30
2	B	539	LEU	CA-CB-CG	-5.72	102.14	115.30
9	K	6	ARG	CD-NE-CZ	5.72	131.61	123.60
1	A	1198	ASP	CB-CA-C	-5.72	98.96	110.40
2	B	233	PRO	N-CD-CG	5.72	111.78	103.20
1	A	940	ARG	CG-CD-NE	-5.71	99.80	111.80
1	A	1311	VAL	N-CA-CB	-5.71	98.93	111.50
1	A	498	ARG	NE-CZ-NH2	5.71	123.16	120.30
6	H	126	GLU	CA-CB-CG	5.71	125.97	113.40
7	I	98	VAL	CA-CB-CG2	-5.71	102.33	110.90
9	K	78	THR	N-CA-CB	5.71	121.15	110.30
3	C	143	LEU	N-CA-CB	-5.71	98.98	110.40
1	A	29	ALA	N-CA-C	5.71	126.41	111.00
2	B	1153	GLU	OE1-CD-OE2	5.71	130.15	123.30
1	A	1262	LYS	CA-CB-CG	5.71	125.96	113.40
1	A	685	GLU	N-CA-CB	-5.71	100.33	110.60
10	L	41	SER	N-CA-CB	5.70	119.06	110.50
2	B	709	ASP	N-CA-C	-5.70	95.61	111.00
3	C	11	ARG	NH1-CZ-NH2	-5.70	113.13	119.40
4	E	80	VAL	CB-CA-C	-5.70	100.57	111.40
9	K	6	ARG	CG-CD-NE	-5.70	99.83	111.80
2	B	945	GLU	OE1-CD-OE2	5.70	130.14	123.30
4	E	53	PRO	C-N-CA	-5.70	107.46	121.70
4	E	179	GLN	CB-CG-CD	-5.70	96.78	111.60
2	B	354	ASP	CB-CG-OD2	-5.70	113.17	118.30
7	I	27	PHE	N-CA-C	5.70	126.38	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1274	ARG	CA-CB-CG	-5.70	100.87	113.40
1	A	122	MET	CA-CB-CG	5.69	122.98	113.30
1	A	162	VAL	CA-CB-CG1	-5.69	102.36	110.90
2	B	202	TYR	CZ-CE2-CD2	-5.69	114.68	119.80
2	B	811	TYR	CD1-CE1-CZ	5.69	124.92	119.80
3	C	171	GLY	N-CA-C	5.69	127.33	113.10
2	B	1203	LEU	O-C-N	-5.69	113.60	122.70
4	E	50	MET	CB-CA-C	5.69	121.77	110.40
1	A	716	ASP	OD1-CG-OD2	5.69	134.10	123.30
1	A	810	PRO	N-CD-CG	-5.68	94.67	103.20
1	A	1374	VAL	CA-CB-CG2	-5.68	102.37	110.90
2	B	1165	ILE	CA-CB-CG1	5.68	121.80	111.00
1	A	787	PHE	CB-CG-CD2	5.68	124.78	120.80
1	A	671	ALA	CB-CA-C	-5.68	101.58	110.10
1	A	1135	ARG	CD-NE-CZ	5.68	131.55	123.60
1	A	709	THR	N-CA-CB	-5.68	99.51	110.30
3	C	77	ILE	C-N-CA	-5.68	107.51	121.70
6	H	56	THR	N-CA-C	-5.68	95.67	111.00
7	I	115	LYS	N-CA-C	-5.68	95.67	111.00
1	A	1383	SER	CB-CA-C	-5.67	99.32	110.10
3	C	57	VAL	N-CA-CB	-5.67	99.02	111.50
3	C	178	PHE	N-CA-CB	-5.67	100.39	110.60
8	J	47	ARG	NE-CZ-NH2	-5.67	117.46	120.30
2	B	266	ALA	C-N-CA	-5.67	107.52	121.70
9	K	106	GLU	CB-CA-C	5.67	121.74	110.40
3	C	267	GLN	N-CA-C	5.67	126.31	111.00
1	A	936	LEU	CD1-CG-CD2	-5.67	93.50	110.50
3	C	134	ILE	CG1-CB-CG2	-5.67	98.93	111.40
6	H	55	LEU	CB-CG-CD1	5.67	120.64	111.00
8	J	36	LEU	C-N-CA	-5.67	107.53	121.70
1	A	993	LEU	CA-CB-CG	5.67	128.33	115.30
2	B	322	PHE	CB-CG-CD1	5.67	124.77	120.80
7	I	106	CYS	C-N-CA	5.67	135.87	121.70
1	A	879	GLU	OE1-CD-OE2	5.67	130.10	123.30
4	E	47	CYS	N-CA-CB	-5.67	100.40	110.60
4	E	49	SER	N-CA-C	5.67	126.30	111.00
1	A	35	ILE	N-CA-C	5.66	126.29	111.00
1	A	1133	LEU	CB-CG-CD2	-5.66	101.38	111.00
2	B	644	GLU	CB-CG-CD	-5.66	98.91	114.20
2	B	833	TYR	CA-C-N	5.66	129.65	117.20
2	B	239	GLU	OE1-CD-OE2	-5.66	116.51	123.30
6	H	44	VAL	CG1-CB-CG2	5.66	119.95	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	938	LYS	CB-CA-C	-5.65	99.09	110.40
1	A	1278	ASN	N-CA-C	5.65	126.26	111.00
2	B	1064	TYR	CG-CD1-CE1	-5.65	116.78	121.30
4	E	28	TYR	CE1-CZ-CE2	-5.65	110.76	119.80
4	E	135	PHE	CB-CG-CD2	5.65	124.76	120.80
1	A	492	PRO	O-C-N	5.65	131.74	122.70
3	C	20	PHE	CB-CG-CD1	-5.65	116.84	120.80
1	A	415	LEU	C-N-CA	-5.65	107.58	121.70
2	B	693	ILE	CG1-CB-CG2	-5.65	98.98	111.40
6	H	52	GLN	CA-C-N	5.65	129.62	117.20
2	B	51	PHE	CZ-CE2-CD2	-5.65	113.33	120.10
1	A	474	VAL	O-C-N	-5.64	113.67	122.70
1	A	656	TRP	CG-CD1-NE1	5.64	115.74	110.10
2	B	1224	PHE	CA-C-O	-5.64	108.25	120.10
5	F	107	VAL	C-N-CA	-5.64	107.59	121.70
9	K	39	ASP	OD1-CG-OD2	-5.64	112.58	123.30
1	A	418	SER	N-CA-CB	5.64	118.96	110.50
2	B	35	SER	CB-CA-C	-5.64	99.39	110.10
2	B	407	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	1292	PRO	N-CD-CG	5.64	111.66	103.20
1	A	266	LEU	CA-CB-CG	5.64	128.26	115.30
1	A	1218	GLN	O-C-N	5.64	131.72	122.70
1	A	898	ARG	NE-CZ-NH1	5.63	123.12	120.30
6	H	139	ASN	N-CA-C	-5.63	95.78	111.00
2	B	888	GLY	CA-C-O	-5.63	110.46	120.60
9	K	92	ASN	CB-CA-C	5.63	121.66	110.40
2	B	651	LEU	CB-CG-CD1	5.63	120.57	111.00
3	C	70	ILE	CA-CB-CG2	-5.63	99.64	110.90
3	C	200	GLU	OE1-CD-OE2	5.63	130.05	123.30
4	E	148	GLU	N-CA-CB	5.63	120.73	110.60
1	A	612	ILE	CG1-CB-CG2	-5.63	99.02	111.40
2	B	731	VAL	N-CA-C	-5.63	95.81	111.00
9	K	91	CYS	N-CA-CB	-5.63	100.47	110.60
1	A	156	ASP	CB-CG-OD2	5.62	123.36	118.30
2	B	477	ALA	CB-CA-C	5.62	118.54	110.10
1	A	891	ALA	N-CA-CB	-5.62	102.23	110.10
2	B	938	SER	CB-CA-C	5.62	120.78	110.10
1	A	116	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	1081	LEU	CA-CB-CG	5.62	128.22	115.30
2	B	1148	LYS	CA-CB-CG	5.62	125.76	113.40
3	C	153	LEU	N-CA-CB	-5.62	99.16	110.40
7	I	65	ASP	CB-CG-OD1	-5.62	113.24	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1271	ILE	CA-CB-CG2	-5.62	99.67	110.90
2	B	90	ILE	N-CA-C	5.62	126.16	111.00
1	A	126	LEU	O-C-N	5.61	131.68	122.70
1	A	808	LEU	N-CA-CB	-5.61	99.17	110.40
1	A	978	PRO	CA-CB-CG	-5.61	93.34	104.00
2	B	131	ASP	CA-C-N	-5.61	104.85	117.20
1	A	1327	ILE	CG1-CB-CG2	-5.61	99.06	111.40
2	B	360	PHE	N-CA-CB	-5.61	100.50	110.60
6	H	53	ASP	CB-CG-OD2	5.61	123.35	118.30
8	J	28	ASP	N-CA-CB	5.61	120.70	110.60
1	A	1429	ILE	CG1-CB-CG2	-5.61	99.06	111.40
6	H	141	TYR	CZ-CE2-CD2	5.61	124.85	119.80
2	B	1167	GLY	N-CA-C	5.61	127.11	113.10
1	A	66	LYS	CA-CB-CG	5.60	125.72	113.40
10	L	26	THR	O-C-N	5.60	131.66	122.70
10	L	53	HIS	N-CA-C	5.60	126.13	111.00
2	B	823	ALA	CB-CA-C	-5.60	101.70	110.10
6	H	53	ASP	CB-CA-C	-5.60	99.20	110.40
1	A	1107	VAL	CA-CB-CG1	-5.60	102.50	110.90
1	A	1111	MET	O-C-N	-5.60	113.74	122.70
7	I	45	ARG	CA-CB-CG	5.60	125.72	113.40
7	I	118	ARG	CD-NE-CZ	5.60	131.44	123.60
2	B	727	LYS	N-CA-C	-5.60	95.89	111.00
1	A	434	ARG	CD-NE-CZ	5.59	131.43	123.60
1	A	1227	ILE	CG1-CB-CG2	-5.59	99.09	111.40
2	B	276	ILE	CA-CB-CG2	-5.59	99.71	110.90
4	E	154	ILE	CG1-CB-CG2	-5.59	99.09	111.40
2	B	110	HIS	O-C-N	-5.59	113.75	122.70
1	A	121	LEU	O-C-N	-5.59	113.75	122.70
2	B	408	LEU	CB-CG-CD1	-5.59	101.50	111.00
2	B	1025	HIS	ND1-CE1-NE2	-5.59	97.60	109.90
2	B	1081	LEU	CD1-CG-CD2	-5.59	93.73	110.50
7	I	106	CYS	N-CA-CB	-5.59	100.53	110.60
10	L	55	ILE	CG1-CB-CG2	-5.59	99.10	111.40
2	B	517	THR	N-CA-CB	5.59	120.92	110.30
1	A	99	ILE	CA-CB-CG2	-5.59	99.73	110.90
2	B	446	LEU	CB-CA-C	5.59	120.81	110.20
2	B	595	ARG	NE-CZ-NH2	5.59	123.09	120.30
2	B	1193	GLN	O-C-N	-5.59	113.76	122.70
4	E	16	PHE	CB-CA-C	5.59	121.57	110.40
7	I	76	PRO	N-CA-C	5.59	126.62	112.10
9	K	94	ILE	N-CA-C	-5.58	95.92	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	ARG	CD-NE-CZ	5.58	131.42	123.60
1	A	579	SER	N-CA-CB	5.58	118.88	110.50
3	C	241	ASP	CB-CA-C	-5.58	99.24	110.40
1	A	270	LEU	CB-CG-CD2	5.58	120.48	111.00
1	A	846	GLU	N-CA-CB	-5.58	100.56	110.60
2	B	1011	ILE	CB-CG1-CD1	-5.58	98.29	113.90
1	A	1351	GLU	CG-CD-OE2	-5.58	107.15	118.30
3	C	82	TYR	CG-CD2-CE2	5.58	125.76	121.30
9	K	87	LEU	CB-CG-CD1	-5.58	101.52	111.00
2	B	393	LYS	CD-CE-NZ	-5.57	98.88	111.70
2	B	487	THR	N-CA-CB	-5.57	99.71	110.30
4	E	94	LYS	CD-CE-NZ	-5.57	98.88	111.70
2	B	807	ARG	CB-CA-C	-5.57	99.26	110.40
1	A	55	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	A	977	LYS	CB-CA-C	5.57	121.54	110.40
2	B	244	LEU	CB-CG-CD1	-5.57	101.53	111.00
1	A	65	LEU	CB-CA-C	5.57	120.78	110.20
2	B	57	TYR	CA-C-N	5.57	129.45	117.20
2	B	539	LEU	CB-CG-CD1	-5.56	101.55	111.00
2	B	855	PHE	CG-CD1-CE1	5.56	126.92	120.80
3	C	42	PRO	CA-N-CD	5.56	119.48	111.70
1	A	358	ASN	N-CA-CB	5.56	120.61	110.60
1	A	1208	THR	CB-CA-C	-5.56	96.59	111.60
2	B	387	LEU	CB-CG-CD1	-5.56	101.55	111.00
2	B	514	LEU	CB-CG-CD2	-5.56	101.55	111.00
6	H	88	SER	N-CA-C	5.56	126.01	111.00
1	A	1151	GLU	OE1-CD-OE2	-5.56	116.63	123.30
10	L	25	ALA	C-N-CA	5.56	135.59	121.70
1	A	1343	ALA	C-N-CA	-5.55	110.64	122.30
2	B	380	TYR	CG-CD2-CE2	5.55	125.74	121.30
1	A	1239	ARG	CG-CD-NE	-5.55	100.14	111.80
1	A	3	GLY	CA-C-N	-5.55	104.99	117.20
2	B	552	MET	O-C-N	-5.55	110.55	121.10
3	C	58	LEU	N-CA-CB	-5.55	99.30	110.40
1	A	370	ILE	CG1-CB-CG2	-5.55	99.19	111.40
1	A	661	GLY	CA-C-O	-5.55	110.61	120.60
2	B	131	ASP	N-CA-CB	5.55	120.59	110.60
2	B	392	ARG	CD-NE-CZ	-5.55	115.83	123.60
2	B	1172	ILE	CG1-CB-CG2	-5.55	99.19	111.40
8	J	43	ARG	N-CA-C	5.55	125.98	111.00
1	A	503	GLN	O-C-N	-5.55	113.83	122.70
6	H	7	ASP	OD1-CG-OD2	-5.55	112.76	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	17	ASN	CB-CA-C	-5.54	99.31	110.40
1	A	961	ARG	NE-CZ-NH1	-5.54	117.53	120.30
2	B	166	PHE	N-CA-CB	-5.54	100.63	110.60
2	B	598	GLU	CG-CD-OE2	5.54	129.38	118.30
2	B	910	VAL	CA-CB-CG2	-5.54	102.59	110.90
8	J	36	LEU	CB-CG-CD1	-5.54	101.58	111.00
9	K	96	ASN	N-CA-CB	5.54	120.57	110.60
2	B	27	ALA	O-C-N	-5.54	113.84	122.70
1	A	976	THR	CA-CB-CG2	-5.54	104.65	112.40
1	A	870	GLU	N-CA-CB	5.54	120.56	110.60
4	E	168	TYR	CD1-CE1-CZ	5.54	124.78	119.80
6	H	129	TYR	CB-CG-CD1	-5.54	117.68	121.00
2	B	1215	ARG	NE-CZ-NH1	5.53	123.07	120.30
3	C	190	ASP	CB-CG-OD2	-5.53	113.32	118.30
10	L	29	TYR	CD1-CG-CD2	-5.53	111.81	117.90
1	A	918	GLU	CA-CB-CG	5.53	125.57	113.40
2	B	893	LEU	CB-CG-CD2	5.53	120.40	111.00
9	K	12	LEU	CB-CG-CD1	5.53	120.40	111.00
1	A	352	VAL	CA-CB-CG1	5.53	119.19	110.90
1	A	590	ARG	N-CA-CB	-5.53	100.65	110.60
1	A	1191	TRP	CG-CD1-NE1	5.53	115.63	110.10
4	E	71	LYS	CB-CA-C	-5.53	99.34	110.40
2	B	389	ALA	N-CA-CB	-5.53	102.36	110.10
2	B	955	THR	CB-CA-C	-5.53	96.67	111.60
9	K	41	THR	CA-CB-CG2	-5.53	104.66	112.40
1	A	1033	GLN	CA-C-N	5.53	129.36	117.20
1	A	1295	THR	CB-CA-C	-5.53	96.68	111.60
2	B	413	LEU	CB-CA-C	-5.53	99.70	110.20
3	C	18	VAL	CA-C-N	5.53	129.35	117.20
3	C	22	LEU	CB-CA-C	-5.52	99.70	110.20
2	B	635	ARG	CA-CB-CG	5.52	125.55	113.40
1	A	922	ASP	O-C-N	-5.52	113.87	122.70
1	A	383	TYR	CD1-CE1-CZ	5.52	124.77	119.80
2	B	1138	MET	O-C-N	-5.52	113.87	122.70
6	H	110	ASP	C-N-CA	5.52	135.49	121.70
1	A	1196	GLU	OE1-CD-OE2	5.51	129.92	123.30
4	E	206	GLY	CA-C-O	-5.51	110.67	120.60
1	A	1362	TYR	CB-CG-CD1	5.51	124.31	121.00
2	B	1067	ARG	CB-CG-CD	5.51	125.93	111.60
2	B	1072	MET	CG-SD-CE	5.51	109.02	100.20
1	A	147	VAL	CG1-CB-CG2	-5.51	102.08	110.90
1	A	921	GLY	N-CA-C	5.51	126.88	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	249	ARG	CD-NE-CZ	5.51	131.32	123.60
3	C	258	ILE	CA-CB-CG1	-5.51	100.53	111.00
6	H	87	ARG	CD-NE-CZ	5.51	131.31	123.60
1	A	590	ARG	CA-C-N	5.51	129.32	117.20
1	A	1221	LYS	CA-CB-CG	5.51	125.52	113.40
2	B	611	PRO	CA-N-CD	-5.51	103.79	111.50
2	B	855	PHE	CA-C-O	-5.51	108.54	120.10
3	C	192	TRP	O-C-N	-5.51	113.89	122.70
4	E	38	PRO	O-C-N	5.50	131.51	122.70
1	A	934	LYS	CD-CE-NZ	-5.50	99.04	111.70
2	B	689	LEU	N-CA-CB	-5.50	99.39	110.40
2	B	1106	ARG	CA-CB-CG	5.50	125.51	113.40
1	A	917	SER	CA-CB-OG	-5.50	96.36	111.20
1	A	1139	GLU	CB-CA-C	-5.50	99.40	110.40
2	B	36	ALA	CB-CA-C	5.50	118.35	110.10
4	E	46	TYR	CB-CG-CD1	-5.50	117.70	121.00
10	L	26	THR	C-N-CA	5.50	135.44	121.70
2	B	579	ARG	NH1-CZ-NH2	5.50	125.44	119.40
1	A	868	TYR	CG-CD2-CE2	5.49	125.69	121.30
1	A	1406	VAL	O-C-N	5.49	131.49	122.70
3	C	246	ARG	NE-CZ-NH1	5.49	123.05	120.30
7	I	14	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	A	373	THR	N-CA-CB	-5.49	99.87	110.30
2	B	95	ILE	CB-CA-C	-5.49	100.62	111.60
2	B	414	ALA	CB-CA-C	5.49	118.33	110.10
2	B	531	GLN	C-N-CA	-5.49	107.98	121.70
2	B	1011	ILE	CA-CB-CG1	5.49	121.43	111.00
3	C	72	LEU	CB-CG-CD1	-5.49	101.67	111.00
2	B	57	TYR	O-C-N	-5.49	113.92	122.70
2	B	806	THR	N-CA-CB	-5.49	99.88	110.30
3	C	163	ILE	CB-CA-C	5.49	122.57	111.60
4	E	47	CYS	CA-CB-SG	-5.49	104.13	114.00
1	A	797	LYS	CD-CE-NZ	-5.48	99.09	111.70
4	E	5	ASN	N-CA-C	-5.48	96.20	111.00
1	A	1307	GLU	CG-CD-OE1	5.48	129.26	118.30
2	B	192	LEU	CB-CG-CD2	5.48	120.32	111.00
2	B	905	VAL	CA-CB-CG1	-5.48	102.68	110.90
3	C	87	PHE	CE1-CZ-CE2	-5.48	110.14	120.00
2	B	776	GLN	O-C-N	-5.48	113.94	122.70
1	A	372	LYS	CD-CE-NZ	-5.47	99.11	111.70
1	A	618	GLU	CG-CD-OE1	-5.47	107.35	118.30
1	A	1239	ARG	CB-CG-CD	5.47	125.83	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	609	ASP	CB-CG-OD1	-5.47	113.38	118.30
2	B	722	ASP	CB-CG-OD1	5.47	123.22	118.30
2	B	1094	ARG	CB-CG-CD	5.47	125.83	111.60
1	A	1221	LYS	N-CA-CB	5.47	120.45	110.60
1	A	346	ASP	CB-CG-OD1	5.47	123.22	118.30
2	B	1198	TYR	CZ-CE2-CD2	-5.47	114.88	119.80
7	I	100	PHE	CZ-CE2-CD2	5.47	126.66	120.10
2	B	852	ARG	NE-CZ-NH2	5.47	123.03	120.30
2	B	1021	MET	N-CA-CB	-5.47	100.76	110.60
1	A	205	GLU	CB-CA-C	5.47	121.33	110.40
2	B	941	LEU	CA-CB-CG	-5.47	102.73	115.30
1	A	374	LEU	CB-CA-C	-5.46	99.82	110.20
1	A	1077	THR	CA-CB-CG2	5.46	120.05	112.40
6	H	126	GLU	CB-CA-C	-5.46	99.47	110.40
1	A	1010	ALA	CA-C-N	-5.46	105.18	117.20
2	B	900	ALA	CB-CA-C	-5.46	101.91	110.10
2	B	990	ILE	CB-CA-C	-5.46	100.67	111.60
2	B	1223	ASP	O-C-N	5.46	131.44	122.70
2	B	1018	PRO	CA-C-N	5.46	129.22	117.20
8	J	48	ARG	CD-NE-CZ	5.46	131.25	123.60
9	K	35	PHE	CB-CG-CD1	-5.46	116.98	120.80
2	B	303	TYR	CD1-CE1-CZ	-5.46	114.89	119.80
9	K	107	THR	CA-CB-CG2	5.46	120.05	112.40
10	L	32	ALA	CA-C-N	-5.46	105.19	117.20
1	A	731	ARG	N-CA-CB	-5.46	100.77	110.60
1	A	1440	ALA	N-CA-CB	-5.46	102.46	110.10
2	B	347	LYS	CD-CE-NZ	5.46	124.25	111.70
2	B	432	MET	CA-CB-CG	5.46	122.58	113.30
1	A	792	TYR	CG-CD2-CE2	-5.46	116.94	121.30
1	A	1405	THR	N-CA-C	5.46	125.73	111.00
1	A	1409	LEU	CB-CG-CD1	5.46	120.27	111.00
2	B	790	ASP	CB-CA-C	5.46	121.31	110.40
5	F	94	LEU	C-N-CA	-5.46	110.84	122.30
1	A	603	ASN	CB-CA-C	-5.46	99.49	110.40
1	A	1287	TYR	CB-CG-CD1	5.46	124.27	121.00
1	A	1260	LEU	O-C-N	-5.45	113.97	122.70
2	B	952	VAL	N-CA-C	-5.45	96.27	111.00
3	C	11	ARG	CA-CB-CG	5.45	125.39	113.40
1	A	1337	GLU	O-C-N	5.45	131.42	122.70
9	K	45	LEU	CB-CA-C	5.45	120.55	110.20
2	B	903	VAL	CB-CA-C	-5.45	101.05	111.40
2	B	982	SER	O-C-N	5.45	131.42	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	50	GLU	CB-CG-CD	5.45	128.91	114.20
1	A	938	LYS	N-CA-CB	5.45	120.40	110.60
1	A	1039	LYS	CA-C-N	-5.45	105.22	117.20
2	B	736	THR	OG1-CB-CG2	-5.45	97.48	110.00
4	E	155	ARG	N-CA-CB	-5.44	100.80	110.60
1	A	1377	THR	CA-CB-CG2	5.44	120.02	112.40
2	B	1069	PHE	CD1-CG-CD2	-5.44	111.22	118.30
2	B	1181	GLU	CA-CB-CG	5.44	125.37	113.40
6	H	12	VAL	N-CA-C	5.44	125.69	111.00
8	J	32	GLU	OE1-CD-OE2	-5.44	116.77	123.30
1	A	196	GLU	CA-CB-CG	5.44	125.36	113.40
1	A	789	LYS	N-CA-CB	-5.44	100.81	110.60
1	A	876	ALA	N-CA-C	5.44	125.68	111.00
1	A	1032	LEU	CB-CG-CD2	5.44	120.25	111.00
1	A	1224	LEU	CB-CA-C	-5.44	99.87	110.20
2	B	106	ASP	N-CA-C	5.44	125.68	111.00
3	C	253	LYS	N-CA-C	5.44	125.68	111.00
3	C	19	ASP	N-CA-CB	-5.44	100.81	110.60
10	L	60	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	A	721	PHE	CB-CG-CD2	5.43	124.61	120.80
2	B	597	MET	CG-SD-CE	-5.43	91.50	100.20
3	C	132	PRO	CA-C-O	-5.43	107.16	120.20
2	B	173	MET	CG-SD-CE	5.43	108.89	100.20
2	B	246	LYS	N-CA-C	5.43	125.67	111.00
1	A	408	ASP	CB-CG-OD1	-5.43	113.41	118.30
2	B	25	ILE	CB-CG1-CD1	-5.43	98.69	113.90
1	A	247	ARG	NE-CZ-NH1	-5.43	117.59	120.30
2	B	340	ALA	N-CA-CB	-5.43	102.50	110.10
1	A	494	SER	N-CA-CB	-5.43	102.36	110.50
1	A	547	LEU	CB-CG-CD1	5.43	120.23	111.00
3	C	90	ASP	CB-CG-OD2	-5.43	113.42	118.30
2	B	687	GLU	OE1-CD-OE2	-5.42	116.79	123.30
2	B	899	ILE	CG1-CB-CG2	-5.42	99.47	111.40
1	A	485	ASP	CB-CG-OD2	5.42	123.18	118.30
2	B	325	GLN	CB-CA-C	-5.42	99.56	110.40
2	B	1150	ARG	O-C-N	-5.42	114.03	122.70
3	C	62	PHE	CG-CD1-CE1	-5.42	114.84	120.80
3	C	227	THR	CA-CB-OG1	5.42	120.38	109.00
2	B	878	GLN	N-CA-C	5.42	125.62	111.00
2	B	1064	TYR	CD1-CE1-CZ	5.42	124.67	119.80
1	A	430	TRP	CD1-NE1-CE2	-5.42	104.13	109.00
4	E	204	THR	N-CA-CB	-5.42	100.01	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	HIS	CB-CA-C	5.41	121.23	110.40
1	A	630	ILE	N-CA-C	-5.41	96.38	111.00
1	A	708	MET	CB-CA-C	5.41	121.23	110.40
10	L	26	THR	CA-CB-CG2	5.41	119.98	112.40
1	A	498	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	A	1034	GLU	CG-CD-OE2	5.41	129.12	118.30
4	E	147	HIS	CB-CG-ND1	-5.41	109.67	123.20
4	E	156	LEU	O-C-N	5.41	131.36	122.70
9	K	70	ARG	NE-CZ-NH2	5.41	123.01	120.30
1	A	421	ALA	N-CA-CB	-5.41	102.53	110.10
3	C	61	GLU	OE1-CD-OE2	5.41	129.79	123.30
7	I	70	ARG	N-CA-CB	-5.41	100.86	110.60
1	A	271	LYS	CD-CE-NZ	5.41	124.14	111.70
2	B	738	PHE	CG-CD1-CE1	-5.41	114.85	120.80
9	K	74	ARG	NE-CZ-NH2	5.41	123.00	120.30
2	B	974	PRO	CB-CG-CD	-5.41	85.41	106.50
2	B	1219	ASP	CB-CG-OD1	5.41	123.17	118.30
7	I	93	LYS	N-CA-CB	5.41	120.33	110.60
1	A	793	SER	N-CA-C	5.40	125.59	111.00
2	B	697	GLU	CG-CD-OE1	-5.40	107.49	118.30
1	A	919	ILE	N-CA-CB	5.40	123.22	110.80
2	B	851	PHE	CB-CG-CD2	5.40	124.58	120.80
2	B	1079	LYS	CB-CA-C	-5.40	99.60	110.40
4	E	190	LEU	CB-CA-C	-5.40	99.94	110.20
1	A	69	THR	C-N-CA	5.40	135.20	121.70
2	B	763	GLN	CB-CA-C	-5.40	99.60	110.40
1	A	919	ILE	CG1-CB-CG2	-5.40	99.53	111.40
1	A	1055	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	1212	VAL	CG1-CB-CG2	-5.40	102.27	110.90
6	H	89	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	1022	LEU	CB-CG-CD2	-5.40	101.83	111.00
2	B	789	MET	CA-CB-CG	5.40	122.47	113.30
1	A	968	GLN	N-CA-CB	5.39	120.31	110.60
1	A	1269	GLU	CB-CA-C	-5.39	99.61	110.40
1	A	4	GLN	N-CA-CB	-5.39	100.89	110.60
1	A	465	TYR	CA-C-N	5.39	129.06	117.20
1	A	1305	VAL	CA-CB-CG1	-5.39	102.81	110.90
1	A	1447	GLU	N-CA-CB	5.39	120.31	110.60
3	C	123	ASN	C-N-CA	-5.39	108.22	121.70
2	B	836	GLU	CA-C-O	-5.39	108.78	120.10
1	A	437	MET	CB-CA-C	-5.39	99.62	110.40
1	A	629	LEU	CD1-CG-CD2	-5.39	94.33	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	802	PRO	O-C-N	5.39	131.32	122.70
6	H	121	LEU	N-CA-CB	-5.39	99.62	110.40
9	K	35	PHE	CG-CD1-CE1	5.39	126.73	120.80
1	A	412	ARG	CG-CD-NE	-5.39	100.48	111.80
1	A	261	ASP	CB-CG-OD2	5.38	123.15	118.30
2	B	595	ARG	N-CA-CB	5.38	120.29	110.60
3	C	63	ILE	CA-CB-CG2	-5.38	100.13	110.90
2	B	644	GLU	OE1-CD-OE2	5.38	129.76	123.30
1	A	1024	SER	CA-CB-OG	5.38	125.73	111.20
1	A	380	VAL	CG1-CB-CG2	-5.38	102.30	110.90
1	A	1209	MET	C-N-CA	-5.38	111.01	122.30
2	B	118	ARG	CD-NE-CZ	5.38	131.13	123.60
2	B	166	PHE	CZ-CE2-CD2	-5.38	113.65	120.10
2	B	1156	ASP	CB-CA-C	5.38	121.15	110.40
10	L	31	CYS	CA-CB-SG	5.37	123.67	114.00
1	A	387	ARG	NE-CZ-NH2	-5.37	117.61	120.30
2	B	651	LEU	CB-CG-CD2	-5.37	101.87	111.00
2	B	904	ARG	CG-CD-NE	-5.37	100.52	111.80
8	J	49	MET	CB-CA-C	5.37	121.14	110.40
1	A	595	THR	CA-CB-CG2	-5.37	104.88	112.40
1	A	731	ARG	O-C-N	-5.37	114.11	122.70
1	A	1119	TYR	CB-CG-CD2	5.37	124.22	121.00
6	H	9	ILE	CG1-CB-CG2	-5.37	99.59	111.40
2	B	711	GLU	N-CA-C	5.37	125.49	111.00
3	C	239	PRO	CA-C-O	5.37	133.08	120.20
2	B	24	PRO	CA-N-CD	-5.36	103.99	111.50
5	F	112	GLU	N-CA-CB	5.36	120.26	110.60
8	J	14	VAL	CA-C-O	5.36	131.36	120.10
8	J	56	LEU	CD1-CG-CD2	-5.36	94.41	110.50
1	A	1291	VAL	N-CA-CB	-5.36	99.70	111.50
1	A	152	VAL	CA-CB-CG1	5.36	118.94	110.90
2	B	1151	LEU	O-C-N	-5.36	114.12	122.70
4	E	100	ILE	CB-CA-C	-5.36	100.88	111.60
1	A	1102	LYS	N-CA-CB	-5.36	100.96	110.60
2	B	1106	ARG	CG-CD-NE	5.36	123.05	111.80
4	E	61	GLN	N-CA-C	-5.36	96.54	111.00
1	A	462	VAL	O-C-N	5.35	131.27	122.70
1	A	951	GLU	CA-C-N	-5.35	105.43	117.20
1	A	418	SER	CA-CB-OG	-5.35	96.75	111.20
1	A	923	LEU	O-C-N	5.35	131.26	122.70
1	A	518	LYS	CD-CE-NZ	-5.35	99.39	111.70
1	A	1062	GLU	CB-CG-CD	5.35	128.64	114.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	183	GLY	CA-C-O	-5.35	110.97	120.60
1	A	1267	MET	CB-CA-C	5.35	121.09	110.40
1	A	1382	THR	N-CA-CB	-5.35	100.14	110.30
4	E	102	GLU	OE1-CD-OE2	-5.35	116.88	123.30
7	I	67	THR	N-CA-CB	5.35	120.46	110.30
2	B	258	LEU	CD1-CG-CD2	-5.35	94.46	110.50
4	E	167	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	A	614	PHE	CB-CG-CD2	-5.34	117.06	120.80
3	C	180	TYR	CD1-CE1-CZ	5.34	124.61	119.80
7	I	27	PHE	CD1-CG-CD2	-5.34	111.36	118.30
2	B	348	ARG	NE-CZ-NH1	-5.34	117.63	120.30
2	B	1091	TYR	OH-CZ-CE2	5.34	134.52	120.10
5	F	140	ASP	N-CA-C	5.34	125.42	111.00
7	I	101	PHE	CD1-CE1-CZ	5.34	126.51	120.10
2	B	262	GLU	CA-CB-CG	5.34	125.14	113.40
2	B	329	THR	N-CA-CB	-5.34	100.16	110.30
4	E	169	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	A	1015	VAL	CG1-CB-CG2	-5.34	102.36	110.90
8	J	63	TYR	CA-C-N	5.34	128.94	117.20
10	L	42	ARG	N-CA-CB	5.34	120.21	110.60
2	B	213	ILE	CG1-CB-CG2	-5.33	99.66	111.40
5	F	81	THR	CA-CB-CG2	5.33	119.87	112.40
1	A	1046	LEU	O-C-N	-5.33	114.17	122.70
2	B	267	ARG	N-CA-C	5.33	125.40	111.00
1	A	674	PRO	N-CD-CG	5.33	111.20	103.20
3	C	11	ARG	NE-CZ-NH1	5.33	122.97	120.30
4	E	106	GLN	CB-CA-C	5.33	121.06	110.40
6	H	27	GLU	CB-CA-C	5.33	121.06	110.40
1	A	751	SER	CA-C-O	-5.33	108.91	120.10
8	J	61	LEU	O-C-N	-5.33	114.17	122.70
1	A	559	VAL	CA-CB-CG1	5.33	118.89	110.90
2	B	566	LEU	CD1-CG-CD2	-5.33	94.52	110.50
1	A	788	SER	CA-CB-OG	-5.33	96.82	111.20
3	C	94	LYS	CB-CG-CD	5.33	125.45	111.60
4	E	85	GLU	CA-CB-CG	5.33	125.11	113.40
1	A	427	GLN	N-CA-CB	-5.32	101.02	110.60
2	B	542	MET	CA-CB-CG	5.32	122.35	113.30
3	C	49	VAL	CA-C-O	-5.32	108.92	120.10
6	H	55	LEU	N-CA-C	5.32	125.37	111.00
9	K	64	GLU	OE1-CD-OE2	-5.32	116.91	123.30
1	A	464	PRO	CA-C-N	5.32	128.90	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1046	LEU	CB-CA-C	-5.32	100.09	110.20
1	A	1113	THR	N-CA-C	5.32	125.37	111.00
2	B	31	TRP	CD1-NE1-CE2	-5.32	104.21	109.00
2	B	982	SER	C-N-CA	-5.32	108.40	121.70
4	E	46	TYR	CD1-CE1-CZ	5.32	124.59	119.80
1	A	113	LEU	CA-CB-CG	5.32	127.53	115.30
1	A	267	ALA	N-CA-CB	-5.32	102.66	110.10
3	C	104	PHE	N-CA-C	-5.32	96.64	111.00
3	C	116	LYS	CD-CE-NZ	-5.32	99.47	111.70
7	I	45	ARG	NH1-CZ-NH2	5.32	125.25	119.40
2	B	1101	ASP	CB-CG-OD1	5.32	123.08	118.30
2	B	104	GLU	N-CA-C	5.31	125.35	111.00
2	B	492	LEU	CB-CG-CD2	-5.31	101.97	111.00
1	A	1116	LEU	N-CA-C	-5.31	96.66	111.00
1	A	1167	GLU	CB-CA-C	5.31	121.03	110.40
2	B	895	ASP	OD1-CG-OD2	-5.31	113.21	123.30
2	B	120	ARG	NH1-CZ-NH2	5.31	125.24	119.40
2	B	994	TYR	CB-CG-CD2	5.31	124.19	121.00
4	E	161	LYS	CA-CB-CG	5.31	125.08	113.40
9	K	34	THR	CA-C-O	5.31	131.25	120.10
2	B	531	GLN	N-CA-C	-5.31	96.67	111.00
2	B	531	GLN	CB-CG-CD	5.31	125.39	111.60
1	A	779	PHE	CB-CG-CD2	5.30	124.51	120.80
4	E	53	PRO	N-CD-CG	-5.30	95.24	103.20
4	E	162	ARG	NE-CZ-NH1	5.30	122.95	120.30
4	E	200	ARG	NE-CZ-NH2	-5.30	117.65	120.30
7	I	110	PHE	CZ-CE2-CD2	5.30	126.46	120.10
1	A	133	LYS	N-CA-CB	-5.30	101.06	110.60
1	A	377	PRO	CB-CA-C	-5.30	98.75	112.00
1	A	653	VAL	CG1-CB-CG2	-5.30	102.42	110.90
1	A	482	PHE	O-C-N	-5.30	114.22	122.70
1	A	932	GLU	CA-CB-CG	5.30	125.06	113.40
3	C	97	VAL	CA-CB-CG1	-5.30	102.95	110.90
1	A	486	GLU	CG-CD-OE1	5.30	128.89	118.30
1	A	1232	ASN	CB-CG-OD1	5.30	132.19	121.60
2	B	257	LYS	CD-CE-NZ	-5.30	99.52	111.70
2	B	1198	TYR	CB-CG-CD2	-5.30	117.82	121.00
3	C	36	VAL	CA-CB-CG2	5.30	118.84	110.90
9	K	95	ILE	O-C-N	5.29	131.17	122.70
4	E	90	VAL	N-CA-CB	-5.29	99.86	111.50
1	A	218	ASP	CA-C-N	5.29	128.84	117.20
7	I	72	ASP	OD1-CG-OD2	-5.29	113.25	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	441	PRO	N-CA-CB	-5.29	96.78	102.60
10	L	40	LEU	CB-CG-CD1	5.29	119.99	111.00
1	A	186	LYS	CG-CD-CE	5.29	127.77	111.90
4	E	81	GLU	CG-CD-OE2	-5.29	107.72	118.30
1	A	710	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	1192	LEU	CA-CB-CG	5.29	127.45	115.30
3	C	75	MET	CB-CG-SD	5.28	128.25	112.40
4	E	11	ARG	NE-CZ-NH2	-5.28	117.66	120.30
3	C	10	ILE	CG1-CB-CG2	-5.28	99.78	111.40
1	A	801	GLU	CG-CD-OE2	-5.28	107.74	118.30
2	B	215	GLN	O-C-N	-5.28	114.25	122.70
3	C	51	VAL	O-C-N	-5.28	114.25	122.70
8	J	64	ASN	CB-CA-C	5.28	120.96	110.40
1	A	621	THR	OG1-CB-CG2	-5.28	97.86	110.00
2	B	944	THR	CA-CB-CG2	-5.28	105.01	112.40
1	A	991	LYS	CA-CB-CG	5.28	125.01	113.40
2	B	206	ASN	N-CA-C	-5.28	96.75	111.00
3	C	228	PHE	N-CA-CB	-5.28	101.10	110.60
1	A	412	ARG	CB-CG-CD	5.27	125.31	111.60
3	C	178	PHE	CG-CD1-CE1	-5.27	115.00	120.80
1	A	399	HIS	C-N-CA	5.27	144.14	122.00
1	A	1021	LEU	CD1-CG-CD2	-5.27	94.68	110.50
7	I	71	SER	CB-CA-C	-5.27	100.08	110.10
1	A	1172	LEU	CB-CG-CD1	-5.27	102.04	111.00
2	B	259	TYR	CB-CG-CD2	5.27	124.16	121.00
2	B	1003	ALA	N-CA-CB	-5.27	102.72	110.10
1	A	685	GLU	CB-CA-C	5.27	120.94	110.40
1	A	1238	ILE	CA-C-N	5.27	128.79	117.20
2	B	114	PRO	N-CD-CG	5.27	111.10	103.20
2	B	272	THR	O-C-N	5.27	131.13	122.70
2	B	633	VAL	CB-CA-C	-5.27	101.39	111.40
2	B	1023	VAL	CA-C-N	5.27	128.79	117.20
3	C	62	PHE	CD1-CE1-CZ	5.27	126.42	120.10
1	A	63	ARG	NE-CZ-NH1	5.27	122.93	120.30
2	B	259	TYR	N-CA-CB	5.27	120.08	110.60
3	C	183	TRP	N-CA-CB	5.27	120.08	110.60
4	E	122	LYS	CB-CA-C	5.27	120.93	110.40
2	B	570	VAL	CG1-CB-CG2	-5.26	102.48	110.90
2	B	828	ALA	N-CA-C	5.26	125.21	111.00
3	C	11	ARG	C-N-CA	-5.26	108.54	121.70
2	B	251	ILE	CA-CB-CG1	-5.26	101.00	111.00
3	C	255	VAL	CA-CB-CG2	-5.26	103.01	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	50	ASP	CB-CA-C	5.26	120.92	110.40
1	A	598	LEU	CB-CA-C	-5.26	100.21	110.20
1	A	525	GLN	CG-CD-NE2	-5.26	104.08	116.70
2	B	1110	PRO	CA-C-O	5.26	132.82	120.20
1	A	978	PRO	CA-C-O	5.25	132.81	120.20
4	E	21	GLU	CG-CD-OE1	5.25	128.81	118.30
4	E	83	CYS	CA-CB-SG	5.25	123.46	114.00
1	A	761	MET	CB-CA-C	-5.25	99.89	110.40
1	A	1121	GLU	OE1-CD-OE2	-5.25	117.00	123.30
2	B	968	VAL	CG1-CB-CG2	-5.25	102.49	110.90
7	I	19	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	368	LYS	CA-CB-CG	5.25	124.95	113.40
1	A	668	ASP	N-CA-CB	-5.25	101.15	110.60
1	A	1309	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	1368	MET	O-C-N	-5.25	114.30	122.70
1	A	143	LYS	CD-CE-NZ	5.25	123.78	111.70
1	A	411	ASP	N-CA-CB	5.25	120.05	110.60
1	A	672	ASP	OD1-CG-OD2	-5.25	113.32	123.30
2	B	60	GLN	CA-C-N	5.25	128.74	117.20
2	B	728	ARG	NH1-CZ-NH2	5.25	125.17	119.40
1	A	1281	ARG	NH1-CZ-NH2	-5.25	113.63	119.40
2	B	267	ARG	O-C-N	-5.25	114.31	122.70
1	A	844	ALA	CB-CA-C	-5.24	102.23	110.10
1	A	1228	TRP	CD1-NE1-CE2	5.24	113.72	109.00
2	B	102	VAL	CB-CA-C	-5.24	101.44	111.40
2	B	685	LEU	CD1-CG-CD2	-5.24	94.77	110.50
1	A	351	THR	N-CA-CB	5.24	120.26	110.30
1	A	691	LEU	CB-CG-CD2	-5.24	102.09	111.00
1	A	1155	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	864	ILE	O-C-N	5.24	131.08	122.70
2	B	662	MET	O-C-N	-5.24	114.32	122.70
7	I	91	ARG	N-CA-C	-5.24	96.86	111.00
1	A	278	THR	OG1-CB-CG2	-5.23	97.96	110.00
4	E	148	GLU	OE1-CD-OE2	-5.23	117.02	123.30
1	A	1001	ARG	NH1-CZ-NH2	5.23	125.16	119.40
4	E	175	LEU	CB-CG-CD1	5.23	119.89	111.00
6	H	35	GLN	CA-CB-CG	5.23	124.91	113.40
8	J	48	ARG	CA-CB-CG	5.23	124.91	113.40
9	K	8	GLU	CG-CD-OE1	-5.23	107.83	118.30
1	A	920	LEU	C-N-CA	-5.23	111.32	122.30
4	E	147	HIS	CB-CA-C	-5.23	99.94	110.40
3	C	92	CYS	O-C-N	-5.23	114.33	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	82	TYR	OH-CZ-CE2	5.23	134.21	120.10
1	A	738	LYS	CA-C-O	-5.22	109.13	120.10
1	A	806	ARG	CD-NE-CZ	-5.22	116.28	123.60
8	J	63	TYR	CA-C-O	-5.22	109.13	120.10
2	B	893	LEU	CB-CA-C	-5.22	100.28	110.20
1	A	1233	ASP	N-CA-CB	5.22	120.00	110.60
1	A	1356	ILE	CB-CG1-CD1	-5.22	99.28	113.90
1	A	433	GLU	CG-CD-OE2	-5.22	107.86	118.30
1	A	832	ALA	N-CA-C	5.22	125.09	111.00
1	A	1445	ILE	CA-CB-CG2	-5.22	100.46	110.90
2	B	724	ASP	N-CA-C	5.22	125.09	111.00
2	B	912	ILE	CB-CA-C	-5.22	101.16	111.60
4	E	31	THR	N-CA-C	-5.22	96.91	111.00
4	E	203	GLU	CB-CA-C	-5.22	99.96	110.40
1	A	1057	VAL	CG1-CB-CG2	-5.21	102.56	110.90
2	B	21	GLU	CB-CA-C	5.21	120.83	110.40
2	B	540	SER	N-CA-CB	-5.21	102.68	110.50
2	B	1176	ASN	CA-C-O	-5.21	109.15	120.10
8	J	30	LEU	CA-CB-CG	5.21	127.29	115.30
10	L	56	LEU	CB-CG-CD2	-5.21	102.14	111.00
2	B	285	ILE	CA-C-O	5.21	131.05	120.10
1	A	159	THR	N-CA-CB	5.21	120.20	110.30
1	A	584	ASN	C-N-CA	-5.21	111.36	122.30
5	F	103	MET	CG-SD-CE	5.21	108.53	100.20
1	A	1418	LEU	CB-CG-CD2	-5.21	102.15	111.00
1	A	93	VAL	CG1-CB-CG2	5.21	119.23	110.90
1	A	849	MET	CG-SD-CE	-5.21	91.87	100.20
9	K	85	ASP	N-CA-C	-5.21	96.95	111.00
1	A	789	LYS	N-CA-C	5.20	125.05	111.00
2	B	168	GLY	O-C-N	5.20	131.03	122.70
9	K	84	LYS	CA-CB-CG	5.20	124.85	113.40
3	C	7	GLN	CB-CA-C	-5.20	100.00	110.40
9	K	31	VAL	CA-CB-CG1	5.20	118.70	110.90
2	B	723	VAL	CG1-CB-CG2	5.20	119.22	110.90
7	I	43	VAL	CG1-CB-CG2	-5.20	102.58	110.90
9	K	54	ARG	CD-NE-CZ	5.20	130.88	123.60
1	A	974	ASP	O-C-N	5.20	131.02	122.70
1	A	982	THR	N-CA-C	5.20	125.04	111.00
1	A	1135	ARG	CA-CB-CG	5.20	124.84	113.40
2	B	420	LEU	CB-CG-CD2	5.20	119.84	111.00
2	B	521	LEU	CA-CB-CG	-5.20	103.34	115.30
2	B	1064	TYR	C-N-CA	-5.20	108.70	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	98	ILE	CA-CB-CG2	5.20	121.30	110.90
2	B	362	PRO	CA-C-O	-5.20	107.73	120.20
1	A	671	ALA	N-CA-CB	-5.20	102.83	110.10
2	B	983	ARG	CG-CD-NE	-5.20	100.89	111.80
3	C	172	PRO	N-CD-CG	5.20	110.99	103.20
1	A	444	PHE	N-CA-C	-5.19	96.98	111.00
1	A	1442	ASP	O-C-N	5.19	131.01	122.70
2	B	711	GLU	CG-CD-OE2	5.19	128.69	118.30
8	J	17	LYS	CB-CG-CD	5.19	125.10	111.60
1	A	1031	VAL	CG1-CB-CG2	5.19	119.21	110.90
2	B	401	PHE	CG-CD2-CE2	5.19	126.51	120.80
4	E	200	ARG	N-CA-CB	5.19	119.94	110.60
7	I	30	ARG	CB-CA-C	-5.19	100.02	110.40
1	A	790	ASP	CA-C-O	-5.19	109.20	120.10
2	B	853	SER	CA-CB-OG	5.19	125.21	111.20
2	B	879	ARG	N-CA-CB	5.19	119.94	110.60
4	E	22	MET	CA-CB-CG	5.19	122.12	113.30
4	E	162	ARG	CB-CA-C	5.19	120.78	110.40
9	K	51	LEU	N-CA-CB	-5.19	100.02	110.40
2	B	773	MET	CG-SD-CE	5.19	108.50	100.20
1	A	175	ARG	N-CA-CB	-5.18	101.27	110.60
1	A	1018	PHE	CD1-CG-CD2	-5.18	111.56	118.30
3	C	48	SER	CB-CA-C	-5.18	100.25	110.10
6	H	91	ASP	CA-C-O	5.18	130.99	120.10
2	B	175	ARG	NE-CZ-NH2	5.18	122.89	120.30
2	B	969	ARG	NE-CZ-NH1	-5.18	117.71	120.30
3	C	229	TYR	CG-CD1-CE1	5.18	125.45	121.30
9	K	51	LEU	CB-CG-CD2	-5.18	102.19	111.00
6	H	111	LEU	CB-CA-C	-5.18	100.36	110.20
2	B	130	VAL	CA-CB-CG1	5.18	118.67	110.90
2	B	833	TYR	CE1-CZ-OH	5.18	134.09	120.10
2	B	1040	ASN	CB-CG-OD1	-5.18	111.24	121.60
4	E	110	PHE	CB-CG-CD2	5.18	124.42	120.80
9	K	95	ILE	CA-C-N	-5.18	105.81	117.20
2	B	724	ASP	CA-C-O	5.18	130.97	120.10
1	A	138	ILE	CA-CB-CG2	5.17	121.25	110.90
1	A	895	LYS	CB-CG-CD	5.17	125.05	111.60
1	A	1099	PRO	CA-N-CD	5.17	118.94	111.70
2	B	864	LYS	CD-CE-NZ	5.17	123.60	111.70
1	A	922	ASP	CB-CA-C	-5.17	100.05	110.40
1	A	1154	TYR	OH-CZ-CE2	5.17	134.07	120.10
1	A	981	LEU	CB-CG-CD1	5.17	119.79	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1230	GLU	N-CA-CB	5.17	119.91	110.60
2	B	38	PHE	CB-CG-CD2	5.17	124.42	120.80
2	B	1082	MET	CB-CA-C	5.17	120.74	110.40
1	A	179	LEU	O-C-N	5.17	130.97	122.70
1	A	591	PHE	CB-CA-C	5.17	120.74	110.40
1	A	734	GLU	CA-CB-CG	5.17	124.77	113.40
2	B	206	ASN	N-CA-CB	5.17	119.90	110.60
2	B	608	ASP	N-CA-CB	5.17	119.91	110.60
2	B	644	GLU	CG-CD-OE2	-5.17	107.97	118.30
2	B	746	SER	O-C-N	5.17	130.97	122.70
2	B	843	GLN	C-N-CA	-5.17	108.78	121.70
5	F	108	PHE	CD1-CE1-CZ	-5.17	113.90	120.10
1	A	1384	VAL	CA-C-O	-5.17	109.25	120.10
1	A	468	PHE	CG-CD1-CE1	-5.16	115.12	120.80
2	B	122	LEU	CA-CB-CG	-5.16	103.42	115.30
1	A	40	THR	N-CA-C	-5.16	97.06	111.00
6	H	91	ASP	CA-C-N	-5.16	105.84	117.20
1	A	1345	ARG	CB-CA-C	-5.16	100.08	110.40
6	H	125	LEU	CB-CG-CD1	5.16	119.77	111.00
1	A	452	LYS	CB-CG-CD	-5.16	98.19	111.60
1	A	1093	LYS	CB-CG-CD	5.16	125.01	111.60
1	A	46	THR	CA-CB-CG2	5.16	119.62	112.40
2	B	1073	TYR	CB-CG-CD2	5.15	124.09	121.00
8	J	52	THR	OG1-CB-CG2	-5.15	98.15	110.00
1	A	227	VAL	CA-C-N	-5.15	105.87	117.20
2	B	242	SER	CA-CB-OG	5.15	125.10	111.20
2	B	1183	LYS	CB-CG-CD	5.15	124.99	111.60
9	K	12	LEU	N-CA-CB	5.15	120.70	110.40
10	L	61	THR	N-CA-CB	5.15	120.09	110.30
2	B	685	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	393	ARG	CD-NE-CZ	5.15	130.81	123.60
2	B	227	LYS	CG-CD-CE	-5.15	96.46	111.90
3	C	199	LYS	CA-CB-CG	-5.15	102.08	113.40
1	A	1234	GLU	CG-CD-OE1	5.14	128.59	118.30
2	B	452	THR	CA-CB-CG2	5.14	119.60	112.40
2	B	463	THR	CB-CA-C	-5.14	97.71	111.60
2	B	1064	TYR	CE1-CZ-CE2	-5.14	111.57	119.80
1	A	41	MET	CB-CG-SD	5.14	127.83	112.40
1	A	685	GLU	CA-CB-CG	5.14	124.72	113.40
2	B	895	ASP	N-CA-CB	5.14	119.86	110.60
4	E	19	VAL	CA-CB-CG1	-5.14	103.19	110.90
10	L	59	ALA	CB-CA-C	-5.14	102.39	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	678	GLU	CA-CB-CG	5.14	124.71	113.40
10	L	42	ARG	CD-NE-CZ	5.14	130.80	123.60
1	A	1430	LEU	C-N-CA	-5.14	111.51	122.30
4	E	47	CYS	CB-CA-C	5.14	120.68	110.40
1	A	49	LYS	CB-CG-CD	5.14	124.96	111.60
1	A	161	LEU	O-C-N	5.14	130.92	122.70
1	A	1143	LEU	CB-CG-CD2	-5.14	102.27	111.00
2	B	995	ARG	NH1-CZ-NH2	5.14	125.05	119.40
1	A	852	TYR	CD1-CE1-CZ	-5.13	115.18	119.80
1	A	1287	TYR	OH-CZ-CE2	-5.13	106.24	120.10
2	B	57	TYR	CD1-CG-CD2	-5.13	112.25	117.90
2	B	288	ALA	O-C-N	5.13	130.91	122.70
3	C	92	CYS	CA-CB-SG	5.13	123.24	114.00
3	C	144	ILE	CB-CA-C	-5.13	101.33	111.60
3	C	189	THR	N-CA-C	-5.13	97.14	111.00
4	E	207	ARG	CB-CG-CD	5.13	124.95	111.60
6	H	142	LEU	CB-CG-CD1	-5.13	102.27	111.00
9	K	42	LEU	CA-CB-CG	5.13	127.11	115.30
2	B	591	ARG	NE-CZ-NH1	5.13	122.87	120.30
2	B	606	LYS	CB-CG-CD	5.13	124.94	111.60
2	B	915	THR	CA-CB-OG1	5.13	119.78	109.00
4	E	192	ARG	NE-CZ-NH1	5.13	122.86	120.30
5	F	84	TYR	CE1-CZ-CE2	-5.13	111.59	119.80
1	A	1422	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	626	ASN	N-CA-C	-5.12	97.17	111.00
1	A	794	PRO	CA-N-CD	-5.12	104.33	111.50
1	A	1003	LYS	CB-CG-CD	5.12	124.92	111.60
1	A	1261	LYS	CG-CD-CE	5.12	127.27	111.90
4	E	165	LEU	CB-CG-CD2	-5.12	102.29	111.00
5	F	94	LEU	CA-CB-CG	-5.12	103.52	115.30
5	F	136	ARG	CA-C-O	-5.12	109.34	120.10
7	I	70	ARG	NE-CZ-NH1	5.12	122.86	120.30
9	K	1	MET	CB-CG-SD	-5.12	97.03	112.40
9	K	35	PHE	CA-C-N	5.12	128.47	117.20
8	J	30	LEU	CD1-CG-CD2	-5.12	95.14	110.50
8	J	47	ARG	N-CA-CB	5.12	119.82	110.60
1	A	507	VAL	CG1-CB-CG2	-5.12	102.71	110.90
1	A	696	GLU	CG-CD-OE1	-5.12	108.06	118.30
3	C	78	GLU	OE1-CD-OE2	5.12	129.44	123.30
1	A	560	ILE	C-N-CD	5.12	139.15	128.40
1	A	1167	GLU	CG-CD-OE1	5.12	128.53	118.30
2	B	57	TYR	CA-CB-CG	5.12	123.12	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	727	ASP	OD1-CG-OD2	-5.11	113.58	123.30
2	B	1128	LEU	CA-CB-CG	-5.11	103.54	115.30
7	I	30	ARG	CG-CD-NE	-5.11	101.06	111.80
1	A	156	ASP	N-CA-C	5.11	124.80	111.00
3	C	186	LEU	N-CA-CB	-5.11	100.18	110.40
8	J	28	ASP	O-C-N	5.11	130.88	122.70
9	K	30	ALA	CB-CA-C	-5.11	102.44	110.10
2	B	910	VAL	CA-CB-CG1	5.11	118.56	110.90
6	H	21	ASN	N-CA-C	5.11	124.79	111.00
6	H	38	LEU	CD1-CG-CD2	-5.11	95.17	110.50
1	A	633	VAL	C-N-CA	-5.11	108.93	121.70
2	B	164	LYS	CA-C-O	-5.11	109.38	120.10
2	B	1154	ALA	CB-CA-C	5.11	117.76	110.10
2	B	760	ASP	OD1-CG-OD2	-5.11	113.60	123.30
2	B	896	ASP	N-CA-CB	5.11	119.79	110.60
4	E	107	THR	N-CA-C	5.11	124.79	111.00
7	I	92	ARG	NH1-CZ-NH2	5.11	125.02	119.40
1	A	1381	LEU	CB-CA-C	-5.10	100.50	110.20
2	B	870	ILE	CG1-CB-CG2	5.10	122.63	111.40
2	B	1165	ILE	N-CA-C	-5.10	97.22	111.00
1	A	462	VAL	CA-CB-CG2	-5.10	103.25	110.90
2	B	804	GLY	N-CA-C	5.10	125.86	113.10
3	C	111	THR	CA-CB-OG1	5.10	119.72	109.00
1	A	893	PHE	CA-C-N	5.10	128.42	117.20
1	A	974	ASP	CB-CG-OD1	5.10	122.89	118.30
6	H	104	PHE	N-CA-C	5.10	124.77	111.00
2	B	181	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	A	1105	LEU	CB-CG-CD2	5.10	119.67	111.00
2	B	19	GLU	O-C-N	-5.10	114.55	122.70
3	C	56	THR	OG1-CB-CG2	-5.10	98.28	110.00
3	C	219	PHE	CB-CG-CD1	5.10	124.37	120.80
2	B	699	GLU	CB-CA-C	-5.09	100.21	110.40
4	E	103	LYS	CA-CB-CG	5.09	124.61	113.40
1	A	779	PHE	O-C-N	-5.09	114.55	122.70
2	B	185	THR	OG1-CB-CG2	-5.09	98.29	110.00
2	B	217	ARG	CA-CB-CG	5.09	124.60	113.40
2	B	908	GLU	CG-CD-OE2	5.09	128.49	118.30
3	C	158	VAL	CG1-CB-CG2	-5.09	102.75	110.90
5	F	73	ALA	N-CA-C	5.09	124.75	111.00
1	A	594	GLY	CA-C-O	5.09	129.76	120.60
2	B	289	LEU	CB-CG-CD1	-5.09	102.35	111.00
7	I	97	MET	C-N-CA	-5.09	108.97	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	218	SER	O-C-N	-5.09	114.56	122.70
7	I	72	ASP	CB-CA-C	5.09	120.58	110.40
1	A	212	LYS	CA-CB-CG	5.09	124.59	113.40
1	A	243	PRO	CB-CA-C	-5.09	99.28	112.00
2	B	228	LYS	CA-C-O	-5.09	109.42	120.10
7	I	17	ARG	CB-CA-C	-5.09	100.23	110.40
9	K	35	PHE	CA-C-O	-5.09	109.42	120.10
4	E	74	ASP	CA-C-O	5.08	130.78	120.10
5	F	75	PRO	N-CA-C	5.08	125.32	112.10
1	A	93	VAL	CA-C-O	5.08	130.78	120.10
1	A	247	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	A	585	GLY	O-C-N	5.08	130.83	122.70
4	E	21	GLU	CG-CD-OE2	-5.08	108.13	118.30
10	L	45	ALA	O-C-N	5.08	130.83	122.70
1	A	1064	VAL	CA-CB-CG1	5.08	118.52	110.90
2	B	788	ARG	N-CA-CB	-5.08	101.45	110.60
9	K	4	PRO	N-CA-C	-5.08	98.89	112.10
1	A	1062	GLU	N-CA-CB	5.08	119.74	110.60
7	I	22	ASN	CB-CA-C	-5.08	100.24	110.40
1	A	95	PHE	CB-CG-CD1	5.08	124.36	120.80
1	A	1207	LEU	CB-CA-C	5.08	119.85	110.20
2	B	788	ARG	C-N-CA	-5.08	109.01	121.70
1	A	1118	VAL	CA-CB-CG1	5.08	118.52	110.90
2	B	490	SER	O-C-N	5.08	130.82	122.70
2	B	167	ILE	CB-CA-C	-5.08	101.45	111.60
2	B	556	THR	CA-CB-CG2	-5.08	105.29	112.40
2	B	288	ALA	CA-C-N	-5.07	106.04	117.20
3	C	207	CYS	CB-CA-C	-5.07	100.25	110.40
2	B	41	LYS	CB-CG-CD	5.07	124.79	111.60
2	B	710	LEU	CA-C-N	5.07	128.35	117.20
4	E	156	LEU	CD1-CG-CD2	5.07	125.71	110.50
1	A	931	GLU	O-C-N	5.07	130.81	122.70
2	B	356	LEU	CB-CG-CD2	-5.07	102.39	111.00
2	B	1148	LYS	CA-C-O	-5.07	109.46	120.10
6	H	16	ASP	CB-CA-C	-5.07	100.26	110.40
6	H	102	TYR	CA-CB-CG	5.07	123.03	113.40
1	A	182	VAL	CG1-CB-CG2	-5.07	102.79	110.90
1	A	1256	GLU	CA-CB-CG	5.07	124.54	113.40
6	H	57	VAL	N-CA-C	5.07	124.68	111.00
7	I	76	PRO	CA-CB-CG	-5.07	94.37	104.00
4	E	12	LEU	CB-CG-CD2	5.06	119.61	111.00
1	A	188	ASP	CA-C-N	5.06	128.33	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	621	THR	N-CA-CB	-5.06	100.69	110.30
1	A	1243	VAL	CA-CB-CG2	5.06	118.49	110.90
2	B	355	ILE	CA-CB-CG2	-5.06	100.78	110.90
2	B	406	LEU	O-C-N	-5.06	114.61	122.70
1	A	264	PHE	CB-CA-C	5.06	120.51	110.40
1	A	626	ASN	CB-CA-C	5.06	120.51	110.40
4	E	32	GLN	C-N-CA	-5.06	109.06	121.70
2	B	1158	PHE	N-CA-C	5.05	124.64	111.00
6	H	10	PHE	CB-CG-CD2	-5.05	117.26	120.80
1	A	527	THR	CA-CB-OG1	5.05	119.61	109.00
1	A	1109	LYS	CB-CG-CD	5.05	124.73	111.60
1	A	1219	THR	CA-CB-OG1	5.05	119.61	109.00
1	A	1238	ILE	CA-CB-CG1	5.05	120.60	111.00
2	B	803	LEU	CB-CG-CD1	-5.05	102.41	111.00
1	A	982	THR	OG1-CB-CG2	-5.05	98.39	110.00
1	A	1006	ILE	CA-CB-CG1	5.05	120.59	111.00
1	A	1064	VAL	CA-CB-CG2	5.05	118.47	110.90
10	L	29	TYR	O-C-N	-5.05	114.62	122.70
2	B	311	LEU	O-C-N	-5.05	114.62	122.70
2	B	595	ARG	CG-CD-NE	5.05	122.40	111.80
6	H	10	PHE	CA-C-N	-5.05	106.10	117.20
3	C	75	MET	CB-CA-C	5.04	120.49	110.40
2	B	1168	LEU	C-N-CA	-5.04	109.09	121.70
9	K	99	GLY	CA-C-N	-5.04	106.10	117.20
1	A	433	GLU	N-CA-CB	-5.04	101.53	110.60
1	A	607	ILE	CA-C-N	5.04	128.29	117.20
2	B	345	LYS	O-C-N	-5.04	114.63	122.70
2	B	979	LYS	CB-CG-CD	5.04	124.71	111.60
1	A	1223	ASP	OD1-CG-OD2	-5.04	113.72	123.30
2	B	164	LYS	CD-CE-NZ	5.04	123.29	111.70
2	B	600	LEU	CA-CB-CG	-5.04	103.71	115.30
2	B	792	MET	CA-CB-CG	-5.04	104.73	113.30
4	E	33	GLU	CA-CB-CG	5.04	124.49	113.40
4	E	130	ALA	CB-CA-C	5.04	117.66	110.10
1	A	706	HIS	N-CA-C	-5.04	97.39	111.00
1	A	1026	LEU	O-C-N	-5.04	114.64	122.70
2	B	312	GLU	N-CA-CB	-5.04	101.53	110.60
4	E	63	ASN	N-CA-C	5.04	124.61	111.00
1	A	1304	TRP	CB-CA-C	-5.04	100.33	110.40
2	B	569	TYR	CG-CD1-CE1	5.04	125.33	121.30
3	C	251	LEU	CA-CB-CG	5.04	126.88	115.30
1	A	595	THR	CB-CA-C	-5.04	98.00	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	656	GLY	O-C-N	5.04	130.76	122.70
7	I	85	PHE	O-C-N	-5.04	114.64	122.70
10	L	40	LEU	CA-C-O	-5.04	109.53	120.10
4	E	187	TYR	CE1-CZ-CE2	-5.03	111.75	119.80
6	H	39	THR	CA-CB-CG2	-5.03	105.35	112.40
2	B	1210	MET	CB-CA-C	-5.03	100.34	110.40
2	B	705	MET	CA-C-N	5.03	128.27	117.20
2	B	802	PRO	N-CD-CG	5.03	110.75	103.20
2	B	890	TYR	CB-CG-CD2	-5.03	117.98	121.00
3	C	15	LYS	CD-CE-NZ	-5.03	100.13	111.70
5	F	132	LEU	CB-CG-CD2	5.03	119.55	111.00
8	J	24	LEU	O-C-N	-5.03	114.65	122.70
1	A	162	VAL	CG1-CB-CG2	5.03	118.95	110.90
1	A	1365	TYR	CD1-CE1-CZ	5.03	124.33	119.80
4	E	100	ILE	CA-C-N	-5.03	106.14	117.20
1	A	840	ARG	NE-CZ-NH1	5.03	122.81	120.30
6	H	38	LEU	CB-CG-CD2	5.03	119.55	111.00
1	A	443	LEU	CB-CG-CD1	-5.03	102.45	111.00
3	C	69	LEU	O-C-N	-5.03	114.66	122.70
8	J	18	TRP	CD1-NE1-CE2	-5.03	104.48	109.00
1	A	1191	TRP	CD1-CG-CD2	-5.02	102.28	106.30
2	B	768	THR	CA-C-N	5.02	128.25	117.20
4	E	137	GLU	CG-CD-OE2	-5.02	108.25	118.30
2	B	302	CYS	N-CA-C	-5.02	97.44	111.00
4	E	158	SER	CB-CA-C	5.02	119.64	110.10
1	A	1310	GLY	O-C-N	5.02	130.73	122.70
4	E	175	LEU	N-CA-C	-5.02	97.44	111.00
1	A	670	ILE	CA-CB-CG1	5.02	120.54	111.00
2	B	1085	ILE	O-C-N	-5.02	114.67	122.70
2	B	1220	ARG	CG-CD-NE	5.02	122.34	111.80
4	E	72	PHE	CG-CD2-CE2	-5.02	115.28	120.80
10	L	42	ARG	CG-CD-NE	5.02	122.34	111.80
2	B	620	ARG	N-CA-CB	-5.02	101.57	110.60
1	A	1137	ALA	C-N-CA	-5.02	109.16	121.70
2	B	54	PHE	CB-CG-CD2	-5.02	117.29	120.80
1	A	806	ARG	CB-CA-C	-5.01	100.37	110.40
1	A	906	HIS	N-CA-CB	-5.01	101.58	110.60
3	C	8	VAL	CG1-CB-CG2	5.01	118.92	110.90
2	B	722	ASP	OD1-CG-OD2	-5.01	113.78	123.30
2	B	1155	SER	CB-CA-C	5.01	119.62	110.10
6	H	53	ASP	C-N-CA	-5.01	109.17	121.70
1	A	1316	VAL	CA-CB-CG2	-5.01	103.38	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	65	GLU	N-CA-C	-5.01	97.47	111.00
5	F	120	ILE	CG1-CB-CG2	-5.01	100.37	111.40
9	K	27	ALA	CB-CA-C	5.01	117.62	110.10
10	L	48	CYS	CB-CA-C	5.01	120.42	110.40
1	A	857	ARG	NH1-CZ-NH2	-5.01	113.89	119.40
3	C	5	GLY	N-CA-C	5.01	125.62	113.10
3	C	148	ARG	CB-CG-CD	5.01	124.63	111.60
5	F	129	LYS	CD-CE-NZ	5.01	123.22	111.70
6	H	92	ASP	OD1-CG-OD2	-5.01	113.78	123.30
9	K	72	LYS	N-CA-C	-5.01	97.47	111.00
1	A	228	PHE	CG-CD2-CE2	-5.01	115.29	120.80
2	B	1097	HIS	O-C-N	-5.01	114.69	122.70
2	B	852	ARG	CB-CA-C	5.00	120.41	110.40
6	H	19	ARG	N-CA-CB	5.00	119.61	110.60
1	A	1151	GLU	CG-CD-OE1	5.00	128.31	118.30
2	B	429	PHE	CB-CA-C	5.00	120.41	110.40
2	B	535	LEU	CD1-CG-CD2	-5.00	95.49	110.50
7	I	72	ASP	O-C-N	-5.00	114.69	122.70
9	K	79	GLU	CB-CA-C	5.00	120.41	110.40
1	A	87	ALA	N-CA-CB	-5.00	103.10	110.10
1	A	954	TRP	CD1-NE1-CE2	-5.00	104.50	109.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	204	THR	CB

All (159) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1027	ALA	Mainchain
1	A	1035	TYR	Sidechain
1	A	1064	VAL	Mainchain,Peptide
1	A	1093	LYS	Peptide
1	A	1111	MET	Mainchain
1	A	1119	TYR	Sidechain
1	A	1155	ASP	Mainchain,Peptide
1	A	120	GLU	Peptide
1	A	1232	ASN	Peptide
1	A	1254	ALA	Peptide
1	A	1267	MET	Peptide
1	A	1298	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	1301	GLU	Mainchain
1	A	1361	SER	Mainchain
1	A	1375	MET	Mainchain
1	A	1384	VAL	Peptide
1	A	154	SER	Peptide
1	A	158	PRO	Peptide
1	A	165	GLY	Peptide
1	A	187	LYS	Peptide
1	A	191	THR	Peptide
1	A	31	SER	Peptide
1	A	325	ILE	Peptide
1	A	399	HIS	Peptide
1	A	417	TYR	Mainchain
1	A	434	ARG	Sidechain
1	A	44	THR	Peptide
1	A	444	PHE	Sidechain
1	A	464	PRO	Mainchain,Peptide
1	A	469	ARG	Sidechain,Mainchain
1	A	484	GLY	Mainchain
1	A	52	GLY	Peptide
1	A	538	ASP	Mainchain
1	A	555	ASP	Peptide
1	A	591	PHE	Sidechain
1	A	60	SER	Peptide
1	A	631	HIS	Sidechain,Mainchain
1	A	659	HIS	Sidechain
1	A	705	LYS	Peptide
1	A	706	HIS	Peptide
1	A	707	GLY	Peptide
1	A	74	MET	Peptide
1	A	751	SER	Mainchain
1	A	759	ALA	Mainchain
1	A	787	PHE	Sidechain
1	A	790	ASP	Mainchain
1	A	852	TYR	Sidechain
1	A	877	HIS	Sidechain
1	A	893	PHE	Sidechain
1	A	936	LEU	Mainchain
1	A	938	LYS	Mainchain
1	A	941	LYS	Mainchain
2	B	1025	HIS	Sidechain
2	B	104	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	B	107	GLY	Peptide
2	B	1092	TYR	Sidechain
2	B	1097	HIS	Sidechain
2	B	1101	ASP	Peptide
2	B	1102	LYS	Peptide
2	B	1103	ILE	Peptide
2	B	1109	GLY	Peptide
2	B	1141	HIS	Sidechain
2	B	1152	MET	Peptide
2	B	1155	SER	Peptide
2	B	1157	ALA	Peptide
2	B	1159	ARG	Peptide
2	B	1166	CYS	Mainchain
2	B	1175	LEU	Peptide
2	B	1177	HIS	Sidechain
2	B	1181	GLU	Peptide
2	B	1183	LYS	Peptide
2	B	1221	SER	Peptide
2	B	1222	ARG	Peptide
2	B	123	THR	Peptide
2	B	248	SER	Peptide
2	B	262	GLU	Peptide
2	B	276	ILE	Peptide
2	B	277	LYS	Mainchain
2	B	369	GLY	Peptide
2	B	434	ARG	Peptide
2	B	479	VAL	Mainchain
2	B	501	PRO	Peptide
2	B	51	PHE	Sidechain
2	B	515	HIS	Sidechain
2	B	517	THR	Mainchain
2	B	518	HIS	Sidechain
2	B	535	LEU	Mainchain
2	B	543	SER	Mainchain
2	B	586	TRP	Mainchain
2	B	589	VAL	Mainchain
2	B	627	PHE	Sidechain
2	B	641	GLU	Mainchain
2	B	642	ASP	Peptide
2	B	643	ASP	Peptide
2	B	644	GLU	Peptide
2	B	646	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	B	732	SER	Peptide
2	B	742	GLU	Mainchain
2	B	745	PRO	Mainchain
2	B	832	GLY	Mainchain
2	B	868	MET	Peptide
2	B	870	ILE	Peptide
2	B	878	GLN	Peptide
2	B	882	THR	Peptide
2	B	915	THR	Peptide
2	B	984	HIS	Sidechain
2	B	995	ARG	Sidechain
3	C	103	ALA	Mainchain
3	C	124	LEU	Mainchain
3	C	126	GLY	Peptide
3	C	155	LEU	Mainchain
3	C	156	THR	Mainchain
3	C	157	CYS	Mainchain
3	C	171	GLY	Mainchain
3	C	184	ASN	Mainchain,Peptide
3	C	190	ASP	Peptide
3	C	240	VAL	Mainchain
3	C	261	ALA	Peptide
3	C	267	GLN	Peptide
3	C	4	GLU	Peptide
3	C	92	CYS	Mainchain
4	E	128	PRO	Peptide
4	E	147	HIS	Sidechain
4	E	153	HIS	Sidechain
4	E	170	LEU	Peptide
4	E	195	VAL	Mainchain
4	E	211	TYR	Sidechain
4	E	212	ARG	Sidechain
4	E	48	ASP	Peptide
4	E	56	LYS	Peptide
5	F	135	ARG	Mainchain
6	H	102	TYR	Peptide
6	H	103	LYS	Peptide
6	H	110	ASP	Peptide
6	H	131	ASN	Peptide
6	H	135	LEU	Peptide
6	H	136	LYS	Peptide
6	H	26	ILE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
6	H	31	THR	Peptide
6	H	61	SER	Peptide
6	H	62	SER	Peptide
6	H	86	ASP	Peptide
6	H	87	ARG	Peptide
7	I	26	LEU	Peptide
7	I	27	PHE	Sidechain
7	I	3	THR	Peptide
7	I	42	LEU	Mainchain
7	I	43	VAL	Mainchain
7	I	79	HIS	Sidechain
9	K	11	LEU	Peptide
9	K	70	ARG	Mainchain
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	10606	0	10662	1053	0
2	B	8690	0	8707	916	0
3	C	2095	0	2054	224	0
4	E	1760	0	1788	222	0
5	F	670	0	689	58	0
6	H	1068	0	1040	220	0
7	I	990	0	948	100	0
8	J	525	0	537	58	0
9	K	919	0	928	108	0
10	L	364	0	387	91	0
11	A	2	0	0	0	0
12	A	2	0	0	1	0
12	B	1	0	0	0	0
12	C	1	0	0	3	0
12	I	2	0	0	0	0
12	J	1	0	0	2	0
12	L	1	0	0	1	0
13	A	30	0	9	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	B	1	0	0	0	0
All	All	27728	0	27749	2904	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 53.

All (2904) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:TYR:CG	2:B:137:TYR:CB	1.77	1.66
9:K:26:LYS:CE	9:K:26:LYS:CD	1.74	1.66
1:A:1225:PHE:CG	1:A:1225:PHE:CB	1.78	1.65
2:B:884:ARG:CG	2:B:884:ARG:CD	1.75	1.64
1:A:977:LYS:CD	1:A:977:LYS:CG	1.74	1.64
7:I:20:LYS:CD	7:I:20:LYS:CG	1.74	1.64
2:B:846:ILE:CB	2:B:846:ILE:CA	1.75	1.63
2:B:908:GLU:CB	2:B:908:GLU:CG	1.76	1.63
1:A:860:LEU:CG	1:A:860:LEU:CD2	1.76	1.63
1:A:1176:LEU:CD2	1:A:1176:LEU:CG	1.74	1.63
2:B:418:LYS:CG	2:B:418:LYS:CD	1.76	1.63
5:F:135:ARG:CD	5:F:135:ARG:CG	1.74	1.63
2:B:228:LYS:CG	2:B:228:LYS:CB	1.75	1.62
2:B:368:GLU:CA	2:B:368:GLU:CB	1.75	1.62
1:A:191:THR:CG2	1:A:191:THR:CB	1.76	1.62
2:B:423:LYS:CD	2:B:423:LYS:CE	1.76	1.62
1:A:720:ARG:CG	1:A:720:ARG:CD	1.77	1.62
2:B:423:LYS:CG	2:B:423:LYS:CD	1.77	1.62
4:E:1:MET:CG	4:E:1:MET:CB	1.75	1.62
2:B:1172:ILE:CG2	2:B:1172:ILE:CB	1.76	1.62
2:B:266:ALA:CB	2:B:266:ALA:CA	1.76	1.62
4:E:45:LYS:CG	4:E:45:LYS:CD	1.75	1.62
1:A:132:LYS:CG	1:A:132:LYS:CD	1.77	1.62
1:A:1238:ILE:CB	1:A:1238:ILE:CG2	1.78	1.62
1:A:895:LYS:CD	1:A:895:LYS:CG	1.77	1.62
2:B:426:LYS:CD	2:B:426:LYS:CE	1.78	1.61
6:H:11:GLN:CG	6:H:11:GLN:CB	1.78	1.61
9:K:56:VAL:CB	9:K:56:VAL:CA	1.74	1.61
2:B:227:LYS:CE	2:B:227:LYS:CD	1.77	1.61
1:A:1080:THR:CB	1:A:1080:THR:CA	1.76	1.61
2:B:1163:CYS:CB	2:B:1163:CYS:CA	1.74	1.61
2:B:646:LEU:CB	2:B:646:LEU:CG	1.74	1.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1162:VAL:CG1	1:A:1162:VAL:CB	1.77	1.61
3:C:94:LYS:CG	3:C:94:LYS:CB	1.74	1.61
2:B:1058:LEU:CG	2:B:1058:LEU:CD1	1.76	1.61
1:A:1159:ARG:CB	1:A:1159:ARG:CG	1.74	1.61
10:L:43:THR:CA	10:L:43:THR:CB	1.76	1.61
5:F:80:ALA:CA	5:F:80:ALA:CB	1.77	1.61
4:E:118:PRO:CD	4:E:118:PRO:CG	1.78	1.61
2:B:328:GLU:CG	2:B:328:GLU:CB	1.79	1.61
1:A:860:LEU:CG	1:A:860:LEU:CD1	1.79	1.61
2:B:875:GLU:CB	2:B:875:GLU:CG	1.75	1.61
3:C:199:LYS:CE	3:C:199:LYS:CD	1.77	1.61
3:C:137:LYS:CD	3:C:137:LYS:CE	1.78	1.61
10:L:65:VAL:CB	10:L:65:VAL:CG2	1.74	1.61
1:A:393:ARG:CG	1:A:393:ARG:CD	1.76	1.61
2:B:1183:LYS:CG	2:B:1183:LYS:CD	1.79	1.60
1:A:412:ARG:CG	1:A:412:ARG:CD	1.76	1.60
1:A:1450:LEU:CD1	1:A:1450:LEU:CG	1.76	1.60
4:E:213:ILE:CG1	4:E:213:ILE:CD1	1.80	1.60
3:C:263:THR:CG2	3:C:263:THR:CB	1.79	1.60
2:B:393:LYS:CG	2:B:393:LYS:CD	1.79	1.60
2:B:1156:ASP:CA	2:B:1156:ASP:CB	1.76	1.60
2:B:358:LYS:CB	2:B:358:LYS:CG	1.78	1.60
2:B:367:LEU:CD1	2:B:367:LEU:CG	1.75	1.60
1:A:1148:ILE:CG1	1:A:1148:ILE:CD1	1.76	1.60
2:B:191:LYS:CD	2:B:191:LYS:CG	1.77	1.60
7:I:109:ILE:CD1	7:I:109:ILE:CG1	1.76	1.60
7:I:117:LYS:CE	7:I:117:LYS:CD	1.75	1.60
4:E:44:ALA:CB	4:E:44:ALA:CA	1.77	1.60
7:I:8:ARG:CB	7:I:8:ARG:CG	1.76	1.60
2:B:620:ARG:CG	2:B:620:ARG:CB	1.77	1.60
1:A:66:LYS:CG	1:A:66:LYS:CB	1.75	1.60
2:B:458:LYS:CE	2:B:458:LYS:CD	1.76	1.60
1:A:4:GLN:CG	1:A:4:GLN:CB	1.80	1.60
1:A:61:ILE:CB	1:A:61:ILE:CG2	1.77	1.60
1:A:1144:LYS:CE	1:A:1144:LYS:CD	1.79	1.59
1:A:44:THR:CB	1:A:44:THR:CG2	1.79	1.59
3:C:205:LYS:CG	3:C:205:LYS:CD	1.78	1.59
2:B:345:LYS:CD	2:B:345:LYS:CE	1.79	1.59
1:A:271:LYS:CG	1:A:271:LYS:CD	1.79	1.59
3:C:156:THR:CB	3:C:156:THR:CG2	1.76	1.59
4:E:57:MET:CB	4:E:57:MET:CG	1.76	1.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:LEU:CD2	2:B:192:LEU:CG	1.80	1.59
2:B:446:LEU:CG	2:B:446:LEU:CD2	1.75	1.59
4:E:91:LYS:CA	4:E:91:LYS:CB	1.74	1.59
4:E:98:ILE:CD1	4:E:98:ILE:CG1	1.76	1.59
4:E:66:GLU:CB	4:E:66:GLU:CA	1.75	1.59
9:K:88:LYS:CE	9:K:88:LYS:CD	1.79	1.59
1:A:427:GLN:CB	1:A:427:GLN:CG	1.76	1.59
2:B:1148:LYS:CE	2:B:1148:LYS:CD	1.77	1.59
1:A:1003:LYS:CD	1:A:1003:LYS:CG	1.78	1.59
4:E:98:ILE:CA	4:E:98:ILE:CB	1.74	1.59
9:K:11:LEU:CG	9:K:11:LEU:CD1	1.81	1.59
9:K:26:LYS:CB	9:K:26:LYS:CG	1.75	1.58
1:A:705:LYS:CB	1:A:705:LYS:CA	1.76	1.58
3:C:154:LYS:CG	3:C:154:LYS:CB	1.77	1.58
10:L:30:ILE:CD1	10:L:30:ILE:CG1	1.81	1.58
1:A:176:LYS:CG	1:A:176:LYS:CD	1.80	1.58
5:F:129:LYS:CG	5:F:129:LYS:CD	1.75	1.58
2:B:193:LYS:CD	2:B:193:LYS:CE	1.77	1.58
1:A:1112:LYS:CG	1:A:1112:LYS:CD	1.79	1.58
1:A:1144:LYS:CG	1:A:1144:LYS:CD	1.81	1.58
4:E:7:ARG:CD	4:E:7:ARG:CG	1.74	1.58
1:A:326:ARG:CD	1:A:326:ARG:CG	1.80	1.58
1:A:1109:LYS:CB	1:A:1109:LYS:CG	1.81	1.58
2:B:1183:LYS:CD	2:B:1183:LYS:CE	1.76	1.58
1:A:705:LYS:CG	1:A:705:LYS:CD	1.76	1.58
4:E:7:ARG:CB	4:E:7:ARG:CG	1.81	1.58
1:A:1164:PRO:CB	1:A:1164:PRO:CG	1.75	1.58
1:A:596:THR:CB	1:A:596:THR:CG2	1.77	1.58
7:I:118:ARG:CG	7:I:118:ARG:CD	1.74	1.58
2:B:1097:HIS:CB	2:B:1097:HIS:CA	1.77	1.58
2:B:94:LYS:CB	2:B:94:LYS:CG	1.74	1.58
2:B:18:PHE:CB	2:B:18:PHE:CA	1.74	1.58
6:H:51:ALA:CA	6:H:51:ALA:CB	1.75	1.58
1:A:1112:LYS:CB	1:A:1112:LYS:CG	1.75	1.58
2:B:1155:SER:CB	2:B:1155:SER:CA	1.81	1.58
1:A:1221:LYS:CG	1:A:1221:LYS:CD	1.82	1.58
6:H:32:THR:CA	6:H:32:THR:CB	1.77	1.58
4:E:94:LYS:CG	4:E:94:LYS:CD	1.81	1.58
1:A:934:LYS:CG	1:A:934:LYS:CD	1.76	1.58
1:A:469:ARG:CG	1:A:469:ARG:CD	1.82	1.58
6:H:87:ARG:CD	6:H:87:ARG:CG	1.79	1.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:LYS:CD	2:B:99:LYS:CE	1.75	1.58
2:B:249:ARG:CD	2:B:249:ARG:CG	1.79	1.58
9:K:88:LYS:CG	9:K:88:LYS:CD	1.82	1.58
1:A:601:LYS:CG	1:A:601:LYS:CD	1.76	1.58
2:B:231:PRO:CG	2:B:231:PRO:CB	1.79	1.58
2:B:25:ILE:CB	2:B:25:ILE:CG2	1.82	1.57
7:I:3:THR:CG2	7:I:3:THR:CB	1.77	1.57
1:A:838:GLN:CB	1:A:838:GLN:CG	1.76	1.57
2:B:1189:ILE:CB	2:B:1189:ILE:CG2	1.79	1.57
1:A:1187:GLN:CG	1:A:1187:GLN:CB	1.80	1.57
9:K:26:LYS:CG	9:K:26:LYS:CD	1.79	1.57
2:B:227:LYS:CD	2:B:227:LYS:CG	1.82	1.57
1:A:1262:LYS:CB	1:A:1262:LYS:CG	1.76	1.57
6:H:131:ASN:CB	6:H:131:ASN:CA	1.79	1.57
10:L:26:THR:CG2	10:L:26:THR:CB	1.80	1.57
1:A:53:LEU:CD1	1:A:53:LEU:CG	1.78	1.57
1:A:1092:LYS:CG	1:A:1092:LYS:CD	1.76	1.57
1:A:143:LYS:CG	1:A:143:LYS:CD	1.75	1.57
2:B:807:ARG:CB	2:B:807:ARG:CG	1.77	1.57
4:E:20:LYS:CD	4:E:20:LYS:CE	1.76	1.57
2:B:1057:LYS:CD	2:B:1057:LYS:CG	1.77	1.57
1:A:274:ILE:CG1	1:A:274:ILE:CD1	1.80	1.57
2:B:723:VAL:CB	2:B:723:VAL:CG2	1.82	1.57
1:A:46:THR:CA	1:A:46:THR:CB	1.77	1.57
6:H:135:LEU:CG	6:H:135:LEU:CD2	1.76	1.57
4:E:207:ARG:CD	4:E:207:ARG:CG	1.74	1.57
1:A:180:LYS:CB	1:A:180:LYS:CG	1.77	1.57
1:A:1092:LYS:CB	1:A:1092:LYS:CG	1.78	1.57
1:A:827:THR:CG2	1:A:827:THR:CB	1.76	1.57
7:I:30:ARG:CD	7:I:30:ARG:CG	1.76	1.57
8:J:43:ARG:CG	8:J:43:ARG:CD	1.79	1.57
1:A:1012:ARG:CD	1:A:1012:ARG:CG	1.83	1.57
3:C:120:ILE:CG1	3:C:120:ILE:CD1	1.79	1.56
1:A:1272:THR:CB	1:A:1272:THR:CG2	1.75	1.56
10:L:25:ALA:CA	10:L:25:ALA:CB	1.75	1.56
1:A:1081:LEU:CG	1:A:1081:LEU:CD2	1.77	1.56
2:B:801:LYS:CG	2:B:801:LYS:CD	1.76	1.56
1:A:633:VAL:CB	1:A:633:VAL:CG2	1.78	1.56
1:A:1445:ILE:CD1	1:A:1445:ILE:CG1	1.83	1.56
2:B:228:LYS:CD	2:B:228:LYS:CE	1.77	1.56
2:B:344:LYS:CG	2:B:344:LYS:CD	1.78	1.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:40:LEU:CD2	10:L:40:LEU:CG	1.78	1.56
2:B:1102:LYS:CG	2:B:1102:LYS:CB	1.78	1.56
2:B:164:LYS:CD	2:B:164:LYS:CG	1.77	1.56
2:B:958:GLN:CB	2:B:958:GLN:CG	1.83	1.56
1:A:1093:LYS:CD	1:A:1093:LYS:CG	1.82	1.56
3:C:84:ARG:CB	3:C:84:ARG:CG	1.82	1.56
10:L:40:LEU:CB	10:L:40:LEU:CG	1.77	1.56
4:E:71:LYS:CB	4:E:71:LYS:CG	1.74	1.56
2:B:871:THR:CA	2:B:871:THR:CB	1.77	1.56
1:A:567:LYS:CD	1:A:567:LYS:CE	1.75	1.56
2:B:935:ARG:CG	2:B:935:ARG:CD	1.81	1.56
7:I:1:MET:CG	7:I:1:MET:CB	1.84	1.56
2:B:880:THR:CB	2:B:880:THR:CG2	1.77	1.56
1:A:217:LYS:CE	1:A:217:LYS:CD	1.83	1.56
3:C:260:LEU:CD2	3:C:260:LEU:CG	1.81	1.56
1:A:34:LYS:CD	1:A:34:LYS:CG	1.80	1.56
4:E:113:GLN:CG	4:E:113:GLN:CB	1.75	1.56
1:A:544:ASP:CG	1:A:544:ASP:CB	1.74	1.56
1:A:1385:THR:CB	1:A:1385:THR:CG2	1.79	1.56
1:A:212:LYS:CD	1:A:212:LYS:CG	1.83	1.56
1:A:368:LYS:CE	1:A:368:LYS:CD	1.78	1.56
3:C:199:LYS:CD	3:C:199:LYS:CG	1.84	1.56
1:A:1112:LYS:CE	1:A:1112:LYS:CD	1.84	1.55
3:C:116:LYS:CE	3:C:116:LYS:CD	1.82	1.55
1:A:186:LYS:CB	1:A:186:LYS:CG	1.81	1.55
2:B:191:LYS:CG	2:B:191:LYS:CB	1.83	1.55
1:A:1221:LYS:CG	1:A:1221:LYS:CB	1.79	1.55
10:L:54:ARG:CG	10:L:54:ARG:CD	1.80	1.55
1:A:991:LYS:CE	1:A:991:LYS:NZ	1.69	1.55
2:B:70:ILE:CD1	2:B:70:ILE:CG1	1.78	1.55
2:B:245:GLU:CA	2:B:245:GLU:C	1.75	1.55
2:B:435:THR:CA	2:B:435:THR:C	1.74	1.55
4:E:116:ILE:CG1	4:E:116:ILE:CD1	1.77	1.55
2:B:191:LYS:CD	2:B:191:LYS:CE	1.81	1.55
2:B:1101:ASP:C	2:B:1101:ASP:CA	1.75	1.55
2:B:723:VAL:CB	2:B:723:VAL:CG1	1.81	1.55
2:B:622:LYS:CG	2:B:622:LYS:CB	1.77	1.55
6:H:139:ASN:CA	6:H:139:ASN:CB	1.79	1.55
2:B:706:GLN:CG	2:B:706:GLN:CB	1.83	1.55
2:B:1106:ARG:CD	2:B:1106:ARG:CG	1.83	1.55
1:A:1055:ARG:CD	1:A:1055:ARG:CG	1.80	1.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:VAL:CB	1:A:829:VAL:CG2	1.77	1.55
1:A:40:THR:CB	1:A:40:THR:CA	1.80	1.55
7:I:1:MET:CA	7:I:1:MET:CB	1.78	1.55
5:F:87:LYS:CE	5:F:87:LYS:CD	1.84	1.55
1:A:302:THR:CG2	1:A:302:THR:CB	1.82	1.55
1:A:28:ARG:CG	1:A:28:ARG:CD	1.83	1.55
10:L:38:LEU:CD1	10:L:38:LEU:CG	1.81	1.55
2:B:961:LEU:CG	2:B:961:LEU:CD1	1.80	1.55
2:B:916:THR:CG2	2:B:916:THR:CB	1.79	1.55
2:B:870:ILE:CB	2:B:870:ILE:CG2	1.77	1.55
2:B:986:GLN:CB	2:B:986:GLN:CG	1.85	1.55
2:B:110:HIS:CA	2:B:110:HIS:C	1.75	1.55
1:A:830:LYS:NZ	1:A:830:LYS:CE	1.68	1.55
2:B:620:ARG:CG	2:B:620:ARG:CD	1.81	1.54
1:A:271:LYS:CE	1:A:271:LYS:CD	1.78	1.54
2:B:958:GLN:CD	2:B:958:GLN:CG	1.74	1.54
2:B:965:LYS:CE	2:B:965:LYS:CD	1.76	1.54
1:A:186:LYS:CD	1:A:186:LYS:CG	1.80	1.54
1:A:199:LEU:CG	1:A:199:LEU:CD1	1.82	1.54
2:B:477:ALA:CA	2:B:477:ALA:CB	1.79	1.54
1:A:688:LYS:CD	1:A:688:LYS:CE	1.79	1.54
1:A:962:ARG:CD	1:A:962:ARG:CG	1.76	1.54
9:K:110:ASN:CG	9:K:110:ASN:CB	1.75	1.54
1:A:840:ARG:CD	1:A:840:ARG:CG	1.80	1.54
3:C:199:LYS:CB	3:C:199:LYS:CG	1.82	1.54
1:A:264:PHE:CG	1:A:264:PHE:CB	1.84	1.54
9:K:20:LYS:CE	9:K:20:LYS:CD	1.84	1.54
1:A:1318:THR:CB	1:A:1318:THR:CG2	1.82	1.54
1:A:1204:ASP:CB	1:A:1204:ASP:CG	1.75	1.54
1:A:61:ILE:CB	1:A:61:ILE:CA	1.79	1.54
1:A:1003:LYS:CD	1:A:1003:LYS:CE	1.83	1.54
1:A:1385:THR:CA	1:A:1385:THR:C	1.75	1.54
2:B:436:VAL:CB	2:B:436:VAL:CA	1.84	1.54
2:B:1154:ALA:CA	2:B:1154:ALA:CB	1.85	1.54
3:C:137:LYS:CG	3:C:137:LYS:CD	1.84	1.54
9:K:20:LYS:CD	9:K:20:LYS:CG	1.86	1.54
6:H:41:ASP:CG	6:H:41:ASP:CB	1.76	1.54
1:A:133:LYS:CE	1:A:133:LYS:NZ	1.71	1.54
4:E:31:THR:CB	4:E:31:THR:CG2	1.83	1.54
4:E:103:LYS:CE	4:E:103:LYS:CD	1.80	1.54
2:B:1183:LYS:CG	2:B:1183:LYS:CB	1.76	1.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:154:LYS:CE	3:C:154:LYS:NZ	1.68	1.54
1:A:1217:LYS:CE	1:A:1217:LYS:NZ	1.70	1.54
9:K:102:LYS:CG	9:K:102:LYS:CD	1.80	1.54
1:A:637:LYS:CE	1:A:637:LYS:NZ	1.68	1.54
1:A:620:LYS:CB	1:A:620:LYS:CG	1.86	1.54
2:B:39:ARG:CB	2:B:39:ARG:CG	1.81	1.54
4:E:98:ILE:CG2	4:E:98:ILE:CB	1.81	1.53
6:H:107:VAL:CB	6:H:107:VAL:CG1	1.80	1.53
1:A:744:LYS:CE	1:A:744:LYS:CD	1.86	1.53
5:F:76:LYS:CD	5:F:76:LYS:CG	1.78	1.53
1:A:1405:THR:CA	1:A:1405:THR:CB	1.85	1.53
4:E:43:LYS:CB	4:E:43:LYS:CG	1.83	1.53
4:E:129:PRO:CG	4:E:129:PRO:CB	1.82	1.53
1:A:291:GLU:CD	1:A:291:GLU:CG	1.76	1.53
1:A:931:GLU:CG	1:A:931:GLU:CD	1.75	1.53
4:E:115:ASN:CB	4:E:115:ASN:CG	1.75	1.53
3:C:253:LYS:CE	3:C:253:LYS:CD	1.80	1.53
10:L:50:ASP:C	10:L:50:ASP:CA	1.74	1.53
6:H:131:ASN:C	6:H:131:ASN:CA	1.74	1.53
2:B:870:ILE:CA	2:B:870:ILE:CB	1.84	1.53
4:E:54:GLN:CG	4:E:54:GLN:CB	1.86	1.53
2:B:134:LYS:CB	2:B:134:LYS:CG	1.78	1.53
1:A:518:LYS:CD	1:A:518:LYS:CE	1.86	1.53
10:L:61:THR:CG2	10:L:61:THR:CB	1.80	1.53
1:A:121:LEU:CG	1:A:121:LEU:CD1	1.84	1.53
6:H:76:THR:CG2	6:H:76:THR:CB	1.80	1.53
1:A:49:LYS:NZ	1:A:49:LYS:CE	1.71	1.53
1:A:689:LYS:CE	1:A:689:LYS:CD	1.82	1.53
6:H:111:LEU:CD1	6:H:111:LEU:CG	1.86	1.53
1:A:1222:ASN:CB	1:A:1222:ASN:CA	1.77	1.53
2:B:1150:ARG:NH2	2:B:1150:ARG:CZ	1.69	1.53
1:A:977:LYS:CB	1:A:977:LYS:CG	1.86	1.53
2:B:358:LYS:NZ	2:B:358:LYS:CE	1.68	1.53
4:E:66:GLU:CD	4:E:66:GLU:CG	1.77	1.53
4:E:47:CYS:C	4:E:47:CYS:CA	1.75	1.53
1:A:1261:LYS:CD	1:A:1261:LYS:CE	1.78	1.53
2:B:944:THR:CB	2:B:944:THR:CG2	1.82	1.53
7:I:20:LYS:CD	7:I:20:LYS:CE	1.84	1.53
1:A:191:THR:CB	1:A:191:THR:CA	1.80	1.53
1:A:934:LYS:CE	1:A:934:LYS:NZ	1.72	1.53
1:A:274:ILE:CG2	1:A:274:ILE:CB	1.82	1.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:595:ARG:CG	2:B:595:ARG:CD	1.81	1.53
4:E:90:VAL:CG1	4:E:90:VAL:CB	1.82	1.53
1:A:274:ILE:CA	1:A:274:ILE:CB	1.80	1.52
3:C:102:GLN:CG	3:C:102:GLN:CB	1.84	1.52
1:A:566:ILE:CB	1:A:566:ILE:CG2	1.85	1.52
1:A:569:LYS:CE	1:A:569:LYS:NZ	1.72	1.52
2:B:343:ILE:CD1	2:B:343:ILE:CG1	1.85	1.52
3:C:9:LYS:CD	3:C:9:LYS:CE	1.85	1.52
1:A:1262:LYS:CD	1:A:1262:LYS:CE	1.78	1.52
2:B:733:HIS:CA	2:B:733:HIS:C	1.77	1.52
1:A:1120:LEU:CD1	1:A:1120:LEU:CG	1.82	1.52
1:A:1350:LYS:CD	1:A:1350:LYS:CG	1.88	1.52
4:E:91:LYS:CG	4:E:91:LYS:CB	1.82	1.52
1:A:705:LYS:CE	1:A:705:LYS:NZ	1.69	1.52
2:B:965:LYS:NZ	2:B:965:LYS:CE	1.72	1.52
1:A:49:LYS:CD	1:A:49:LYS:CG	1.87	1.52
3:C:9:LYS:CD	3:C:9:LYS:CG	1.78	1.52
1:A:423:ASP:CB	1:A:423:ASP:CG	1.77	1.52
2:B:531:GLN:CG	2:B:531:GLN:CB	1.87	1.52
1:A:71:GLN:CG	1:A:71:GLN:CD	1.75	1.52
1:A:728:LYS:CE	1:A:728:LYS:NZ	1.69	1.52
6:H:77:ARG:CB	6:H:77:ARG:CG	1.85	1.52
2:B:775:LYS:CB	2:B:775:LYS:CG	1.84	1.52
1:A:880:LYS:CG	1:A:880:LYS:CD	1.84	1.52
2:B:418:LYS:CE	2:B:418:LYS:CD	1.84	1.52
2:B:120:ARG:CB	2:B:120:ARG:CG	1.82	1.52
2:B:1150:ARG:NH1	2:B:1150:ARG:CZ	1.67	1.52
3:C:127:ARG:CA	3:C:127:ARG:N	1.68	1.52
1:A:1132:LYS:CE	1:A:1132:LYS:CD	1.88	1.52
1:A:1359:ASP:CG	1:A:1359:ASP:CB	1.76	1.52
1:A:187:LYS:CA	1:A:187:LYS:C	1.76	1.52
2:B:270:LYS:NZ	2:B:270:LYS:CE	1.72	1.52
10:L:43:THR:CG2	10:L:43:THR:CB	1.82	1.51
10:L:47:ARG:CG	10:L:47:ARG:CD	1.84	1.51
4:E:43:LYS:CE	4:E:43:LYS:NZ	1.70	1.51
7:I:36:GLU:CD	7:I:36:GLU:CG	1.77	1.51
1:A:1194:ARG:CB	1:A:1194:ARG:CG	1.83	1.51
2:B:915:THR:CA	2:B:915:THR:CB	1.83	1.51
1:A:1206:ASP:CG	1:A:1206:ASP:CB	1.77	1.51
2:B:652:LYS:CE	2:B:652:LYS:NZ	1.69	1.51
4:E:56:LYS:CD	4:E:56:LYS:CG	1.84	1.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:LEU:CD2	1:A:571:LEU:CG	1.88	1.51
1:A:282:ASN:CG	1:A:282:ASN:CB	1.79	1.51
2:B:279:ASP:CB	2:B:279:ASP:CG	1.76	1.51
1:A:5:GLN:CG	1:A:5:GLN:CB	1.87	1.51
4:E:37:LEU:CD1	4:E:37:LEU:CG	1.86	1.51
3:C:50:GLU:CD	3:C:50:GLU:CG	1.76	1.51
8:J:26:GLN:CG	8:J:26:GLN:CD	1.77	1.51
2:B:1219:ASP:CB	2:B:1219:ASP:CG	1.79	1.51
6:H:137:GLN:CD	6:H:137:GLN:CG	1.75	1.51
2:B:959:ASP:CG	2:B:959:ASP:CB	1.77	1.51
1:A:1080:THR:C	1:A:1080:THR:CA	1.74	1.51
2:B:625:LYS:NZ	2:B:625:LYS:CE	1.74	1.51
2:B:106:ASP:CG	2:B:106:ASP:CB	1.77	1.51
4:E:161:LYS:CD	4:E:161:LYS:CE	1.89	1.51
1:A:188:ASP:CG	1:A:188:ASP:CB	1.78	1.51
2:B:1188:LYS:CE	2:B:1188:LYS:CD	1.88	1.51
6:H:27:GLU:CA	6:H:27:GLU:C	1.76	1.51
2:B:552:MET:CG	2:B:552:MET:CB	1.86	1.51
3:C:205:LYS:CD	3:C:205:LYS:CE	1.84	1.50
1:A:268:ASP:CG	1:A:268:ASP:CB	1.79	1.50
1:A:217:LYS:CD	1:A:217:LYS:CG	1.88	1.50
1:A:1419:ASP:CG	1:A:1419:ASP:CB	1.77	1.50
2:B:183:GLU:CD	2:B:183:GLU:CG	1.77	1.50
1:A:601:LYS:CD	1:A:601:LYS:CE	1.85	1.50
1:A:1130:GLN:CG	1:A:1130:GLN:CD	1.79	1.50
2:B:1188:LYS:NZ	2:B:1188:LYS:CE	1.67	1.50
1:A:1129:GLU:CG	1:A:1129:GLU:CD	1.77	1.50
2:B:668:ASP:CB	2:B:668:ASP:CG	1.75	1.50
1:A:1277:GLU:CD	1:A:1277:GLU:CG	1.78	1.50
1:A:695:LYS:NZ	1:A:695:LYS:CE	1.67	1.50
1:A:177:ASP:CG	1:A:177:ASP:CB	1.77	1.50
2:B:353:LYS:CD	2:B:353:LYS:CG	1.85	1.50
2:B:641:GLU:CD	2:B:641:GLU:CG	1.78	1.50
2:B:892:LYS:CE	2:B:892:LYS:CD	1.84	1.50
2:B:1101:ASP:CB	2:B:1101:ASP:CG	1.77	1.50
6:H:136:LYS:C	6:H:136:LYS:CA	1.74	1.50
3:C:220:ASP:CB	3:C:220:ASP:CG	1.79	1.50
1:A:193:ASP:CB	1:A:193:ASP:CG	1.78	1.50
1:A:941:LYS:CG	1:A:941:LYS:CD	1.84	1.50
1:A:1235:LYS:CD	1:A:1235:LYS:CE	1.86	1.50
10:L:62:LYS:CD	10:L:62:LYS:CE	1.86	1.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1221:LYS:NZ	1:A:1221:LYS:CE	1.69	1.50
3:C:187:LYS:NZ	3:C:187:LYS:CE	1.74	1.50
2:B:239:GLU:CG	2:B:239:GLU:CD	1.78	1.50
2:B:1176:ASN:CB	2:B:1176:ASN:CG	1.75	1.50
2:B:646:LEU:CD1	2:B:646:LEU:CG	1.90	1.50
5:F:129:LYS:CE	5:F:129:LYS:CD	1.89	1.50
2:B:1155:SER:N	2:B:1155:SER:CA	1.68	1.50
8:J:42:LYS:CG	8:J:42:LYS:CD	1.90	1.50
4:E:52:ARG:CB	4:E:52:ARG:CG	1.84	1.50
8:J:26:GLN:CB	8:J:26:GLN:CG	1.84	1.50
1:A:705:LYS:CG	1:A:705:LYS:CB	1.86	1.49
1:A:143:LYS:NZ	1:A:143:LYS:CE	1.74	1.49
2:B:347:LYS:CD	2:B:347:LYS:CG	1.87	1.49
4:E:191:LYS:CE	4:E:191:LYS:CD	1.89	1.49
4:E:41:ASP:CB	4:E:41:ASP:CG	1.77	1.49
10:L:64:LEU:CD1	10:L:64:LEU:CG	1.88	1.49
6:H:2:SER:CA	6:H:2:SER:C	1.75	1.49
7:I:82:GLU:CD	7:I:82:GLU:CG	1.74	1.49
1:A:1239:ARG:CD	1:A:1239:ARG:CG	1.87	1.49
2:B:962:LYS:CD	2:B:962:LYS:CG	1.83	1.49
1:A:186:LYS:CD	1:A:186:LYS:CE	1.86	1.49
3:C:267:GLN:C	3:C:267:GLN:CA	1.81	1.49
2:B:736:THR:CB	2:B:736:THR:CG2	1.89	1.49
1:A:101:LYS:CE	1:A:101:LYS:NZ	1.71	1.49
1:A:795:GLU:CD	1:A:795:GLU:CG	1.80	1.49
1:A:644:LYS:NZ	1:A:644:LYS:CE	1.76	1.49
1:A:1109:LYS:CD	1:A:1109:LYS:CE	1.87	1.49
7:I:45:ARG:CD	7:I:45:ARG:CG	1.87	1.49
1:A:295:LEU:CD2	1:A:295:LEU:CG	1.89	1.49
3:C:196:ASP:CB	3:C:196:ASP:CG	1.79	1.49
1:A:934:LYS:CE	1:A:934:LYS:CD	1.87	1.49
2:B:451:LYS:CD	2:B:451:LYS:CG	1.88	1.49
2:B:305:VAL:CG1	2:B:305:VAL:CB	1.88	1.49
7:I:93:LYS:CG	7:I:93:LYS:CD	1.87	1.49
1:A:895:LYS:NZ	1:A:895:LYS:CE	1.72	1.48
1:A:45:GLN:C	1:A:45:GLN:CA	1.79	1.48
6:H:19:ARG:CG	6:H:19:ARG:CB	1.90	1.48
2:B:1186:ASP:CB	2:B:1186:ASP:CG	1.79	1.48
2:B:962:LYS:CE	2:B:962:LYS:CD	1.88	1.48
3:C:116:LYS:CE	3:C:116:LYS:NZ	1.68	1.48
6:H:63:LEU:C	6:H:63:LEU:CA	1.79	1.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:1:MET:CE	8:J:1:MET:SD	2.02	1.48
2:B:251:ILE:CG2	2:B:251:ILE:CB	1.89	1.48
2:B:426:LYS:NZ	2:B:426:LYS:CE	1.73	1.48
2:B:986:GLN:CG	2:B:986:GLN:CD	1.80	1.48
2:B:1132:GLU:CD	2:B:1132:GLU:CG	1.80	1.48
4:E:73:PRO:CB	4:E:73:PRO:CG	1.77	1.48
2:B:962:LYS:CE	2:B:962:LYS:NZ	1.74	1.48
2:B:706:GLN:CG	2:B:706:GLN:CD	1.81	1.48
1:A:687:LYS:NZ	1:A:687:LYS:CE	1.77	1.48
4:E:93:MET:SD	4:E:93:MET:CG	2.02	1.48
1:A:69:THR:CA	1:A:69:THR:C	1.79	1.48
5:F:129:LYS:CE	5:F:129:LYS:NZ	1.75	1.48
5:F:87:LYS:CE	5:F:87:LYS:NZ	1.73	1.48
1:A:157:ASP:CB	1:A:157:ASP:CG	1.79	1.48
2:B:563:MET:CG	2:B:563:MET:SD	2.02	1.48
3:C:15:LYS:CE	3:C:15:LYS:NZ	1.72	1.47
2:B:415:GLN:CB	2:B:415:GLN:CG	1.89	1.47
1:A:977:LYS:NZ	1:A:977:LYS:CE	1.76	1.47
1:A:601:LYS:NZ	1:A:601:LYS:CE	1.73	1.47
3:C:15:LYS:CB	3:C:15:LYS:CG	1.89	1.47
4:E:201:LYS:CG	4:E:201:LYS:CD	1.91	1.47
6:H:9:ILE:CD1	6:H:9:ILE:CG1	1.91	1.47
10:L:26:THR:CB	10:L:26:THR:CA	1.91	1.47
2:B:434:ARG:CG	2:B:434:ARG:CB	1.90	1.47
1:A:1408:ILE:CG1	1:A:1408:ILE:CD1	1.93	1.47
9:K:88:LYS:CE	9:K:88:LYS:NZ	1.77	1.46
1:A:1112:LYS:CE	1:A:1112:LYS:NZ	1.75	1.46
2:B:428:ILE:CG1	2:B:428:ILE:CD1	1.91	1.46
2:B:1188:LYS:CG	2:B:1188:LYS:CD	1.89	1.46
10:L:62:LYS:NZ	10:L:62:LYS:CE	1.77	1.46
1:A:843:LYS:CE	1:A:843:LYS:CD	1.90	1.46
1:A:895:LYS:CD	1:A:895:LYS:CE	1.87	1.46
7:I:93:LYS:CE	7:I:93:LYS:CD	1.90	1.46
3:C:15:LYS:CG	3:C:15:LYS:CD	1.91	1.46
2:B:895:ASP:CB	2:B:895:ASP:CG	1.80	1.46
1:A:368:LYS:CD	1:A:368:LYS:CG	1.90	1.46
6:H:19:ARG:CD	6:H:19:ARG:CG	1.92	1.46
1:A:1171:GLN:CG	1:A:1171:GLN:CD	1.85	1.46
8:J:38:ARG:CG	8:J:38:ARG:CB	1.92	1.46
2:B:509:ALA:CA	2:B:509:ALA:CB	1.92	1.46
10:L:45:ALA:CA	10:L:45:ALA:CB	1.94	1.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASP:C	1:A:188:ASP:CA	1.84	1.45
2:B:712:PRO:CB	2:B:712:PRO:CG	1.78	1.45
2:B:502:ILE:CB	2:B:502:ILE:CA	1.94	1.45
9:K:26:LYS:CE	9:K:26:LYS:NZ	1.76	1.45
2:B:346:GLU:CG	2:B:346:GLU:CD	1.84	1.45
1:A:1262:LYS:CD	1:A:1262:LYS:CG	1.94	1.45
2:B:622:LYS:NZ	2:B:622:LYS:CE	1.76	1.45
1:A:1290:LYS:CD	1:A:1290:LYS:CE	1.94	1.45
2:B:933:SER:C	2:B:933:SER:CA	1.83	1.45
10:L:48:CYS:CA	10:L:48:CYS:C	1.80	1.45
2:B:705:MET:CG	2:B:705:MET:SD	2.04	1.45
3:C:230:MET:SD	3:C:230:MET:CG	2.05	1.45
9:K:111:LEU:CD1	9:K:111:LEU:CG	1.93	1.45
2:B:347:LYS:CD	2:B:347:LYS:CE	1.95	1.44
1:A:1425:SER:CB	1:A:1425:SER:OG	1.64	1.44
1:A:41:MET:SD	1:A:41:MET:CE	2.05	1.44
1:A:1080:THR:CG2	1:A:1080:THR:CB	1.93	1.44
1:A:144:THR:CB	1:A:144:THR:CG2	1.91	1.44
1:A:941:LYS:CE	1:A:941:LYS:NZ	1.81	1.44
4:E:191:LYS:CE	4:E:191:LYS:NZ	1.77	1.44
1:A:1290:LYS:NZ	1:A:1290:LYS:CE	1.81	1.44
5:F:123:LYS:CE	5:F:123:LYS:NZ	1.77	1.44
2:B:246:LYS:C	2:B:246:LYS:CA	1.85	1.44
8:J:42:LYS:CD	8:J:42:LYS:CE	1.93	1.43
1:A:1450:LEU:CG	1:A:1450:LEU:CD2	1.93	1.43
1:A:738:LYS:CE	1:A:738:LYS:NZ	1.81	1.43
1:A:123:ARG:CB	1:A:123:ARG:CG	1.95	1.43
1:A:1111:MET:CG	1:A:1111:MET:SD	2.06	1.43
1:A:1235:LYS:NZ	1:A:1235:LYS:CE	1.79	1.43
7:I:93:LYS:CE	7:I:93:LYS:NZ	1.77	1.43
3:C:197:SER:OG	3:C:197:SER:CB	1.65	1.43
1:A:1232:ASN:CG	1:A:1232:ASN:CB	1.87	1.43
2:B:711:GLU:CG	2:B:711:GLU:CD	1.87	1.43
4:E:118:PRO:CB	4:E:118:PRO:CG	1.97	1.42
1:A:751:SER:CB	1:A:751:SER:OG	1.64	1.42
2:B:172:ILE:CD1	2:B:172:ILE:CG1	1.98	1.42
1:A:843:LYS:CG	1:A:843:LYS:CD	1.94	1.42
2:B:768:THR:CA	2:B:768:THR:C	1.86	1.42
2:B:344:LYS:CD	2:B:344:LYS:CE	1.93	1.42
2:B:434:ARG:CG	2:B:434:ARG:CD	1.95	1.42
2:B:233:PRO:CB	2:B:233:PRO:CG	1.94	1.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:789:MET:SD	2:B:789:MET:CE	2.06	1.42
1:A:1064:VAL:O	1:A:1064:VAL:CA	1.66	1.42
2:B:951:GLN:CD	2:B:951:GLN:CG	1.87	1.42
2:B:315:LYS:CE	2:B:315:LYS:NZ	1.80	1.42
1:A:1223:ASP:CG	1:A:1223:ASP:CB	1.89	1.42
3:C:125:MET:SD	3:C:125:MET:CG	2.07	1.42
3:C:94:LYS:NZ	3:C:94:LYS:CE	1.82	1.41
1:A:49:LYS:CD	1:A:49:LYS:CE	1.98	1.41
1:A:1263:ILE:CG1	1:A:1263:ILE:CD1	1.97	1.41
4:E:45:LYS:CE	4:E:45:LYS:CD	1.95	1.41
1:A:830:LYS:CD	1:A:830:LYS:CG	1.97	1.41
1:A:346:ASP:CB	1:A:346:ASP:CG	1.89	1.41
1:A:427:GLN:CD	1:A:427:GLN:CG	1.87	1.41
6:H:131:ASN:CG	6:H:131:ASN:CB	1.88	1.41
10:L:28:LYS:NZ	10:L:28:LYS:CE	1.82	1.41
3:C:195:GLN:CD	3:C:195:GLN:CG	1.89	1.41
1:A:248:PRO:CG	1:A:248:PRO:CB	1.89	1.41
1:A:555:ASP:CG	1:A:555:ASP:CB	1.88	1.40
9:K:12:LEU:CG	9:K:12:LEU:CD1	1.98	1.40
10:L:50:ASP:CB	10:L:50:ASP:CG	1.87	1.40
1:A:728:LYS:CD	1:A:728:LYS:CG	1.99	1.40
2:B:344:LYS:CB	2:B:344:LYS:CG	1.99	1.40
1:A:597:LEU:CG	1:A:597:LEU:CD1	1.99	1.40
1:A:703:THR:CG2	1:A:703:THR:CB	1.99	1.40
2:B:103:ASN:CB	2:B:103:ASN:CG	1.89	1.40
1:A:984:LYS:CE	1:A:984:LYS:NZ	1.82	1.40
1:A:1132:LYS:CE	1:A:1132:LYS:NZ	1.83	1.39
2:B:1156:ASP:CG	2:B:1156:ASP:CB	1.91	1.39
1:A:1109:LYS:CD	1:A:1109:LYS:CG	1.99	1.39
1:A:1285:MET:CG	1:A:1285:MET:SD	2.10	1.39
4:E:57:MET:CG	4:E:57:MET:SD	2.11	1.39
3:C:154:LYS:CG	3:C:154:LYS:CD	1.99	1.39
1:A:695:LYS:CD	1:A:695:LYS:CE	1.99	1.39
5:F:106:PRO:CB	5:F:106:PRO:CG	1.79	1.39
1:A:1110:ASN:CB	1:A:1110:ASN:CG	1.91	1.38
1:A:304:MET:CG	1:A:304:MET:SD	2.09	1.38
4:E:162:ARG:CB	4:E:162:ARG:CG	1.98	1.38
3:C:29:MET:SD	3:C:29:MET:CE	2.09	1.38
7:I:1:MET:CE	7:I:1:MET:SD	2.11	1.38
1:A:676:MET:CG	1:A:676:MET:SD	2.12	1.38
6:H:52:GLN:CD	6:H:52:GLN:CG	1.91	1.38

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:LYS:CE	2:B:164:LYS:CD	2.00	1.38
6:H:104:PHE:C	6:H:104:PHE:CA	1.93	1.38
2:B:598:GLU:CD	2:B:598:GLU:CG	1.93	1.37
7:I:72:ASP:CG	7:I:72:ASP:CB	1.92	1.37
7:I:120:GLN:CG	7:I:120:GLN:CB	2.00	1.37
4:E:53:PRO:CB	4:E:53:PRO:CG	1.90	1.37
1:A:941:LYS:CD	1:A:941:LYS:CE	2.02	1.37
4:E:162:ARG:CG	4:E:162:ARG:CD	2.03	1.36
2:B:745:PRO:CD	2:B:745:PRO:CG	1.79	1.36
1:A:1102:LYS:CG	1:A:1102:LYS:CD	2.02	1.36
6:H:139:ASN:CB	6:H:139:ASN:CG	1.95	1.36
1:A:600:PRO:CB	1:A:600:PRO:CG	1.76	1.35
1:A:1350:LYS:NZ	1:A:1350:LYS:CE	1.90	1.35
4:E:152:LYS:CE	4:E:152:LYS:CD	2.05	1.35
3:C:154:LYS:CD	3:C:154:LYS:CE	2.03	1.34
2:B:1189:ILE:CG1	2:B:1189:ILE:CD1	2.02	1.34
1:A:1190:PRO:CG	1:A:1190:PRO:CB	1.91	1.34
1:A:1444:MET:CE	1:A:1444:MET:SD	2.15	1.34
4:E:215:MET:CE	4:E:215:MET:SD	2.15	1.34
7:I:117:LYS:CE	7:I:117:LYS:NZ	1.89	1.33
2:B:870:ILE:CG1	2:B:870:ILE:CD1	2.04	1.33
7:I:17:ARG:CG	7:I:17:ARG:CD	2.06	1.33
3:C:165:LYS:NZ	3:C:165:LYS:CE	1.91	1.33
1:A:1222:ASN:CB	1:A:1222:ASN:CG	1.97	1.32
4:E:131:THR:CG2	4:E:131:THR:CB	2.05	1.32
4:E:1:MET:CG	4:E:1:MET:SD	2.18	1.32
1:A:620:LYS:CE	1:A:620:LYS:CD	2.06	1.32
1:A:44:THR:CB	1:A:44:THR:CA	2.07	1.32
2:B:531:GLN:CG	2:B:531:GLN:CD	1.97	1.32
9:K:23:PRO:CB	9:K:23:PRO:CG	1.90	1.32
2:B:987:LYS:NZ	2:B:987:LYS:CE	1.93	1.32
1:A:752:LYS:CD	1:A:752:LYS:CE	2.08	1.31
1:A:1135:ARG:CD	1:A:1135:ARG:CG	2.08	1.30
1:A:978:PRO:CG	1:A:978:PRO:CB	2.06	1.30
4:E:93:MET:CE	4:E:93:MET:SD	2.20	1.30
1:A:938:LYS:CE	1:A:938:LYS:CD	2.09	1.30
2:B:999:MET:CE	2:B:999:MET:SD	1.20	1.30
10:L:68:GLU:CG	10:L:68:GLU:CD	2.00	1.30
2:B:646:LEU:CD2	2:B:646:LEU:CG	2.10	1.29
1:A:728:LYS:CE	1:A:728:LYS:CD	2.11	1.28
1:A:1064:VAL:O	1:A:1064:VAL:HA	1.10	1.28

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1259:MET:CE	1:A:1259:MET:SD	2.21	1.28
2:B:662:MET:CE	2:B:662:MET:SD	2.21	1.28
7:I:55:THR:CG2	7:I:55:THR:CB	2.10	1.28
2:B:381:MET:CE	2:B:381:MET:SD	1.19	1.28
2:B:955:THR:HG22	10:L:54:ARG:O	1.24	1.26
4:E:20:LYS:NZ	4:E:20:LYS:CE	1.98	1.26
1:A:1259:MET:CG	1:A:1259:MET:SD	2.23	1.26
7:I:1:MET:CG	7:I:1:MET:SD	2.24	1.26
1:A:42:ASP:OD2	1:A:47:ARG:N	1.70	1.24
1:A:1064:VAL:C	1:A:1066:VAL:N	1.90	1.24
2:B:100:PRO:HD2	2:B:180:TYR:CE1	1.74	1.22
2:B:999:MET:CG	2:B:999:MET:CE	2.17	1.22
1:A:549:MET:SD	1:A:549:MET:CE	1.10	1.20
1:A:620:LYS:CE	1:A:620:LYS:NZ	2.06	1.19
4:E:1:MET:CE	4:E:1:MET:SD	2.30	1.19
1:A:74:MET:SD	1:A:74:MET:CE	2.31	1.18
4:E:12:LEU:HD21	4:E:58:MET:SD	1.84	1.18
2:B:1097:HIS:HA	2:B:1097:HIS:ND1	1.58	1.18
6:H:138:GLU:O	6:H:139:ASN:C	1.78	1.17
2:B:999:MET:HE1	2:B:999:MET:SD	1.78	1.17
2:B:792:MET:CE	2:B:792:MET:SD	2.33	1.17
1:A:567:LYS:HD3	6:H:95:TYR:CG	1.78	1.16
1:A:752:LYS:NZ	1:A:752:LYS:CE	2.08	1.16
8:J:1:MET:CE	8:J:1:MET:CG	2.22	1.15
1:A:73:GLY:O	1:A:75:ASN:N	1.78	1.15
1:A:567:LYS:HD3	6:H:95:TYR:CA	1.78	1.14
2:B:381:MET:HE3	2:B:381:MET:SD	1.77	1.13
6:H:130:ARG:C	6:H:130:ARG:HD2	1.68	1.13
2:B:999:MET:HE3	2:B:999:MET:SD	1.78	1.13
3:C:54:ASN:OD1	3:C:56:THR:HB	1.49	1.12
2:B:381:MET:CE	2:B:381:MET:CG	2.26	1.12
1:A:1064:VAL:O	1:A:1064:VAL:C	1.87	1.12
2:B:1097:HIS:ND1	2:B:1097:HIS:CA	2.11	1.11
2:B:104:GLU:OE1	10:L:54:ARG:NE	1.80	1.11
1:A:567:LYS:CD	6:H:95:TYR:HA	1.81	1.11
1:A:708:MET:SD	1:A:708:MET:CE	2.39	1.10
2:B:381:MET:HE1	2:B:381:MET:SD	1.77	1.10
2:B:381:MET:HE2	2:B:381:MET:SD	1.77	1.10
9:K:110:ASN:O	9:K:112:GLN:N	1.84	1.10
1:A:1064:VAL:CA	1:A:1065:GLY:N	2.14	1.10
6:H:138:GLU:O	6:H:140:ALA:N	1.84	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:91:ASP:OD1	6:H:91:ASP:O	1.70	1.09
1:A:549:MET:SD	1:A:549:MET:HE1	1.69	1.09
1:A:567:LYS:HB3	6:H:96:VAL:N	1.65	1.09
1:A:567:LYS:HG3	1:A:568:PRO:CD	1.83	1.09
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.14	1.08
2:B:705:MET:CE	2:B:705:MET:CG	2.30	1.08
6:H:5:LEU:O	6:H:133:ASN:ND2	1.86	1.07
2:B:885:MET:CE	2:B:885:MET:SD	2.42	1.07
2:B:134:LYS:O	2:B:135:ARG:HG3	1.54	1.07
1:A:535:THR:HG21	1:A:617:VAL:N	1.69	1.07
1:A:567:LYS:HB3	6:H:96:VAL:H	1.12	1.07
2:B:999:MET:SD	2:B:999:MET:HE2	1.78	1.07
1:A:549:MET:HE2	1:A:549:MET:SD	1.69	1.07
1:A:549:MET:SD	1:A:549:MET:HE3	1.69	1.06
2:B:646:LEU:CB	2:B:646:LEU:HG	1.81	1.06
4:E:100:ILE:HG22	4:E:101:GLN:N	1.67	1.06
5:F:103:MET:SD	5:F:103:MET:CE	2.44	1.06
6:H:130:ARG:O	6:H:130:ARG:HD2	1.54	1.05
2:B:114:PRO:HD3	2:B:124:TYR:CE1	1.91	1.05
1:A:1285:MET:SD	1:A:1285:MET:CE	2.45	1.05
1:A:304:MET:CE	1:A:304:MET:SD	2.45	1.05
6:H:128:ASN:O	6:H:131:ASN:ND2	1.91	1.04
1:A:752:LYS:HE2	2:B:1019:SER:OG	1.57	1.04
9:K:1:MET:SD	9:K:1:MET:CE	2.46	1.04
7:I:58:VAL:O	7:I:58:VAL:HG12	1.55	1.03
2:B:1128:LEU:HD12	2:B:1128:LEU:C	1.76	1.03
2:B:643:ASP:O	2:B:644:GLU:CB	2.02	1.03
4:E:98:ILE:HA	4:E:98:ILE:CB	1.83	1.03
6:H:59:ILE:HG22	6:H:60:ALA:N	1.71	1.03
2:B:643:ASP:O	2:B:644:GLU:HB2	1.24	1.02
2:B:294:ASP:H	7:I:12:ASN:ND2	1.56	1.02
10:L:40:LEU:HG	10:L:40:LEU:CB	1.86	1.02
1:A:369:SER:OG	9:K:2:ASN:ND2	1.93	1.01
1:A:31:SER:CB	1:A:83:HIS:HD2	1.74	1.00
1:A:567:LYS:CB	6:H:96:VAL:H	1.75	1.00
7:I:109:ILE:CD1	7:I:109:ILE:CB	2.40	1.00
1:A:535:THR:HG21	1:A:617:VAL:H	0.85	1.00
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.01	0.99
1:A:1064:VAL:O	1:A:1065:GLY:N	1.93	0.99
6:H:103:LYS:NZ	6:H:105:GLU:OE2	1.95	0.99
2:B:58:THR:O	2:B:62:ILE:HG12	1.61	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:4:PHE:CE1	7:I:13:MET:HE2	1.98	0.98
6:H:135:LEU:HG	6:H:135:LEU:CD2	1.88	0.98
1:A:32:VAL:HG23	1:A:33:ALA:H	1.27	0.98
2:B:1220:ARG:O	2:B:1222:ARG:HD3	1.63	0.97
1:A:1079:MET:SD	1:A:1359:ASP:OD2	2.23	0.97
2:B:1084:GLN:HE22	3:C:192:TRP:H	1.03	0.97
4:E:98:ILE:CG2	4:E:98:ILE:CG1	2.41	0.97
1:A:711:ARG:HE	7:I:95:THR:HG22	1.27	0.96
1:A:1064:VAL:CA	1:A:1064:VAL:C	2.34	0.96
1:A:535:THR:CG2	1:A:617:VAL:H	1.76	0.96
2:B:101:MET:HA	2:B:110:HIS:O	1.63	0.96
7:I:4:PHE:HE1	7:I:13:MET:HE2	1.30	0.96
1:A:567:LYS:CG	1:A:568:PRO:HD3	1.95	0.96
1:A:549:MET:CG	1:A:549:MET:CE	2.42	0.96
8:J:10:CYS:HG	8:J:45:CYS:HG	1.05	0.95
2:B:1198:TYR:OH	2:B:1201:LYS:NZ	2.00	0.95
6:H:4:THR:C	6:H:5:LEU:HD23	1.87	0.95
2:B:1097:HIS:CA	2:B:1097:HIS:CG	2.50	0.95
2:B:101:MET:SD	2:B:101:MET:CE	2.54	0.95
6:H:63:LEU:C	6:H:90:ALA:HB3	1.86	0.95
1:A:752:LYS:HZ3	2:B:1019:SER:H	1.14	0.95
2:B:1156:ASP:HA	2:B:1156:ASP:CB	1.97	0.94
3:C:125:MET:SD	3:C:125:MET:CE	2.56	0.94
1:A:567:LYS:HD3	6:H:95:TYR:HA	1.37	0.94
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.47	0.94
1:A:55:ASP:N	1:A:56:PRO:CD	2.30	0.94
2:B:1051:THR:HG22	2:B:1053:GLU:N	1.82	0.94
2:B:552:MET:CG	2:B:552:MET:SD	2.55	0.94
2:B:999:MET:CG	2:B:999:MET:HE3	1.85	0.94
1:A:982:THR:HB	1:A:985:ASP:OD2	1.67	0.94
2:B:1150:ARG:HD2	2:B:1150:ARG:HH11	1.33	0.93
2:B:846:ILE:HD12	2:B:974:PRO:HB2	1.50	0.93
1:A:588:LEU:HD23	1:A:588:LEU:C	1.89	0.93
2:B:789:MET:HE3	2:B:965:LYS:HB3	1.51	0.93
6:H:103:LYS:HB3	6:H:105:GLU:OE1	1.66	0.93
1:A:567:LYS:CD	6:H:95:TYR:CG	2.51	0.93
2:B:566:LEU:HD13	2:B:588:GLY:HA2	1.51	0.93
3:C:156:THR:CA	3:C:156:THR:CG2	2.46	0.93
1:A:64:ASN:OD1	1:A:64:ASN:O	1.87	0.92
4:E:66:GLU:HA	4:E:66:GLU:CB	1.99	0.92
4:E:47:CYS:C	4:E:47:CYS:HA	1.85	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1025:HIS:HE1	2:B:1090:THR:HG21	1.35	0.92
2:B:1172:ILE:CG2	2:B:1172:ILE:CG1	2.48	0.92
2:B:90:ILE:N	2:B:90:ILE:HD12	1.85	0.92
5:F:111:LEU:O	5:F:113:GLY:N	2.02	0.92
1:A:901:LEU:H	1:A:926:GLN:NE2	1.68	0.91
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.35	0.91
7:I:4:PHE:CE1	7:I:13:MET:CE	2.52	0.91
2:B:417:PHE:CD2	2:B:417:PHE:O	2.23	0.91
9:K:35:PHE:HE1	9:K:73:LEU:HD12	1.36	0.91
1:A:909:ASP:OD1	1:A:911:SER:N	2.01	0.91
2:B:381:MET:HE2	2:B:381:MET:CG	1.92	0.91
2:B:99:LYS:HB3	2:B:100:PRO:HD3	1.52	0.91
1:A:469:ARG:CG	1:A:469:ARG:NE	2.33	0.91
1:A:1079:MET:HG2	1:A:1359:ASP:OD2	1.71	0.91
2:B:18:PHE:HA	2:B:18:PHE:CB	2.00	0.90
5:F:75:PRO:O	5:F:77:ASP:O	1.89	0.90
1:A:1233:ASP:O	1:A:1234:GLU:HB3	1.68	0.90
2:B:515:HIS:H	2:B:518:HIS:HD2	1.16	0.90
1:A:503:GLN:NE2	5:F:90:ARG:NH2	2.19	0.90
1:A:55:ASP:O	1:A:57:ARG:N	2.04	0.90
6:H:77:ARG:O	6:H:78:SER:O	1.89	0.90
7:I:45:ARG:HG2	7:I:45:ARG:HH11	1.34	0.89
1:A:203:SER:OG	1:A:206:GLU:HG2	1.72	0.89
2:B:294:ASP:H	7:I:12:ASN:HD22	1.17	0.89
4:E:117:THR:O	4:E:119:SER:N	2.05	0.89
3:C:120:ILE:CB	3:C:120:ILE:CD1	2.51	0.89
7:I:120:GLN:O	7:I:121:PHE:HB2	1.73	0.89
2:B:916:THR:N	2:B:935:ARG:O	2.06	0.88
3:C:8:VAL:HG12	3:C:9:LYS:H	1.37	0.88
6:H:6:PHE:CD2	6:H:7:ASP:N	2.42	0.88
3:C:263:THR:CG2	3:C:263:THR:HB	2.03	0.88
1:A:903:ASN:ND2	1:A:905:ASP:H	1.71	0.88
1:A:596:THR:CG2	1:A:596:THR:CA	2.52	0.88
2:B:955:THR:CG2	10:L:54:ARG:O	2.17	0.88
1:A:567:LYS:CG	1:A:568:PRO:CD	2.49	0.88
1:A:567:LYS:HD3	6:H:95:TYR:CB	2.03	0.88
1:A:752:LYS:HG3	1:A:753:GLY:N	1.88	0.88
2:B:705:MET:SD	2:B:705:MET:CB	2.62	0.87
3:C:8:VAL:HG12	3:C:9:LYS:N	1.88	0.87
1:A:517:ASN:ND2	1:A:1364:ASN:OD1	2.08	0.87
10:L:34:CYS:HG	12:L:3005:ZN:ZN	0.57	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:167:HIS:HD2	3:C:169:LYS:H	1.19	0.87
10:L:58:LYS:O	10:L:59:ALA:HB3	1.74	0.87
8:J:43:ARG:NE	8:J:43:ARG:CG	2.38	0.87
1:A:633:VAL:CG1	1:A:633:VAL:CG2	2.53	0.87
10:L:38:LEU:O	10:L:39:SER:HB2	1.72	0.87
1:A:596:THR:HG22	1:A:597:LEU:H	1.39	0.87
2:B:1084:GLN:NE2	3:C:192:TRP:H	1.71	0.87
3:C:88:CYS:HG	12:C:3002:ZN:ZN	0.81	0.87
1:A:901:LEU:H	1:A:926:GLN:HE22	1.20	0.86
4:E:79:TRP:HB2	4:E:105:PHE:CE1	2.10	0.86
1:A:1385:THR:HG22	1:A:1385:THR:O	1.76	0.86
1:A:187:LYS:HB2	1:A:194:ALA:HB3	1.55	0.86
1:A:503:GLN:NE2	5:F:90:ARG:HH21	1.73	0.86
6:H:2:SER:HA	6:H:2:SER:C	1.96	0.86
10:L:47:ARG:HG2	10:L:48:CYS:H	1.40	0.86
6:H:59:ILE:CG2	6:H:60:ALA:N	2.37	0.86
1:A:42:ASP:OD2	1:A:46:THR:C	2.13	0.86
2:B:770:GLN:HG2	2:B:983:ARG:O	1.76	0.86
2:B:999:MET:HE3	2:B:999:MET:HG2	1.57	0.86
1:A:324:SER:O	1:A:327:ALA:HB3	1.75	0.86
3:C:50:GLU:HB3	10:L:64:LEU:HD13	1.57	0.86
4:E:98:ILE:CA	4:E:98:ILE:HB	2.04	0.86
2:B:102:VAL:O	2:B:109:THR:HA	1.76	0.85
1:A:1366:ARG:NH1	1:A:1366:ARG:HB3	1.91	0.85
1:A:567:LYS:CG	6:H:96:VAL:H	1.89	0.85
2:B:955:THR:HG23	10:L:55:ILE:HA	1.57	0.85
8:J:1:MET:HG3	8:J:1:MET:HE2	1.57	0.85
2:B:129:PHE:CD2	2:B:166:PHE:HA	2.12	0.85
1:A:1081:LEU:HG	1:A:1081:LEU:CD2	2.05	0.85
1:A:1079:MET:CG	1:A:1359:ASP:OD2	2.24	0.85
8:J:1:MET:CE	8:J:1:MET:HG3	2.06	0.85
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.75	0.85
3:C:99:LEU:HD12	3:C:99:LEU:N	1.92	0.85
8:J:1:MET:CE	8:J:1:MET:CB	2.55	0.84
9:K:101:LEU:O	9:K:101:LEU:HD13	1.77	0.84
2:B:1189:ILE:HG22	2:B:1190:ASP:N	1.92	0.84
6:H:89:LEU:HB3	6:H:91:ASP:OD1	1.78	0.84
2:B:129:PHE:CE2	2:B:166:PHE:CA	2.60	0.84
6:H:4:THR:O	6:H:5:LEU:HD23	1.76	0.84
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	1.91	0.84
3:C:75:MET:SD	3:C:75:MET:CE	2.65	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:620:ARG:NE	2:B:620:ARG:CG	2.41	0.84
7:I:16:PRO:O	7:I:17:ARG:HD3	1.78	0.84
4:E:91:LYS:CB	4:E:91:LYS:HA	2.08	0.84
2:B:428:ILE:HG12	2:B:448:ILE:HD11	1.60	0.84
1:A:535:THR:O	1:A:575:LYS:HE2	1.78	0.83
2:B:1190:ASP:O	2:B:1191:ILE:HG13	1.77	0.83
2:B:1065:GLN:HE22	2:B:1067:ARG:HB2	1.42	0.83
1:A:709:THR:HG22	1:A:712:GLU:H	1.43	0.83
2:B:1150:ARG:NH1	2:B:1150:ARG:HD2	1.92	0.83
1:A:156:ASP:O	1:A:158:PRO:HD3	1.79	0.83
10:L:34:CYS:CB	10:L:51:CYS:HB3	2.09	0.83
2:B:477:ALA:CB	2:B:477:ALA:HA	2.08	0.83
6:H:103:LYS:O	6:H:115:TYR:HD1	1.62	0.82
2:B:251:ILE:HB	2:B:251:ILE:CG2	2.07	0.82
2:B:1051:THR:CG2	2:B:1053:GLU:H	1.92	0.82
9:K:65:HIS:HD2	9:K:67:PHE:H	1.24	0.82
2:B:393:LYS:NZ	2:B:621:GLU:OE2	2.12	0.82
2:B:192:LEU:CD2	2:B:192:LEU:CD1	2.57	0.82
2:B:516:ASN:H	2:B:516:ASN:HD22	1.25	0.82
1:A:982:THR:HG22	1:A:985:ASP:H	1.44	0.82
2:B:99:LYS:HB3	2:B:100:PRO:CD	2.10	0.82
1:A:324:SER:O	1:A:327:ALA:CB	2.28	0.82
2:B:956:THR:HA	2:B:961:LEU:O	1.80	0.82
1:A:829:VAL:CG1	1:A:829:VAL:CG2	2.58	0.82
7:I:120:GLN:O	7:I:121:PHE:CB	2.27	0.81
1:A:1151:GLU:CG	7:I:45:ARG:HD2	2.10	0.81
1:A:567:LYS:CD	1:A:568:PRO:HD3	2.09	0.81
2:B:487:THR:HG22	2:B:490:SER:H	1.44	0.81
1:A:1162:VAL:CG1	1:A:1162:VAL:CA	2.58	0.81
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.78	0.81
1:A:351:THR:CG2	2:B:1103:ILE:HG12	2.11	0.81
2:B:625:LYS:CD	2:B:625:LYS:NZ	2.44	0.81
6:H:130:ARG:O	6:H:130:ARG:CD	2.29	0.81
1:A:46:THR:HB	1:A:46:THR:CA	2.10	0.81
1:A:567:LYS:CD	6:H:95:TYR:CD1	2.64	0.81
2:B:1084:GLN:HE22	3:C:192:TRP:N	1.78	0.81
2:B:552:MET:SD	2:B:552:MET:CE	2.68	0.81
1:A:61:ILE:CB	1:A:61:ILE:HA	2.10	0.80
10:L:64:LEU:CD1	10:L:64:LEU:HG	2.09	0.80
7:I:3:THR:CG2	7:I:3:THR:CA	2.60	0.80
6:H:25:ARG:NH2	6:H:41:ASP:OD2	2.13	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1058:LEU:CD2	2:B:1058:LEU:CD1	2.58	0.80
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.63	0.80
8:J:1:MET:CG	8:J:1:MET:HE2	2.12	0.80
7:I:4:PHE:CZ	7:I:13:MET:HE1	2.17	0.80
1:A:962:ARG:CG	1:A:962:ARG:NE	2.43	0.80
3:C:73:GLN:HE21	3:C:75:MET:H	1.30	0.80
9:K:24:ASP:OD1	9:K:74:ARG:NH1	2.15	0.80
1:A:41:MET:O	1:A:50:ILE:HD11	1.82	0.80
10:L:34:CYS:HB3	10:L:51:CYS:HB3	1.63	0.79
1:A:1111:MET:CG	1:A:1111:MET:CE	2.60	0.79
2:B:1198:TYR:CE1	2:B:1201:LYS:HD2	2.17	0.79
7:I:45:ARG:HH11	7:I:45:ARG:CG	1.96	0.79
6:H:139:ASN:HA	6:H:139:ASN:CB	2.09	0.79
1:A:69:THR:C	1:A:69:THR:HA	2.01	0.79
5:F:123:LYS:NZ	5:F:123:LYS:CD	2.45	0.79
1:A:73:GLY:C	1:A:75:ASN:N	2.29	0.79
7:I:4:PHE:HE1	7:I:13:MET:CE	1.89	0.79
2:B:424:LEU:HD21	2:B:428:ILE:HD11	1.64	0.79
6:H:103:LYS:CB	6:H:105:GLU:OE1	2.29	0.79
2:B:1222:ARG:HH11	2:B:1222:ARG:HB2	1.47	0.79
4:E:55:ARG:O	4:E:56:LYS:C	2.19	0.79
2:B:381:MET:HE2	2:B:381:MET:HG3	1.64	0.79
2:B:1220:ARG:O	2:B:1222:ARG:CD	2.31	0.79
6:H:104:PHE:C	6:H:104:PHE:HA	2.02	0.79
2:B:680:THR:HG22	2:B:682:SER:H	1.48	0.79
1:A:1385:THR:CB	1:A:1385:THR:C	2.50	0.78
2:B:502:ILE:HD13	2:B:502:ILE:HA	1.63	0.78
4:E:207:ARG:NE	4:E:207:ARG:CG	2.46	0.78
2:B:915:THR:CA	2:B:915:THR:HB	2.10	0.78
7:I:16:PRO:HG3	7:I:27:PHE:CE2	2.17	0.78
2:B:185:THR:HG23	2:B:188:ASP:OD2	1.83	0.78
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.19	0.78
2:B:246:LYS:C	2:B:246:LYS:HA	2.01	0.78
4:E:47:CYS:SG	4:E:52:ARG:O	2.40	0.78
1:A:518:LYS:NZ	1:A:518:LYS:CD	2.46	0.78
6:H:103:LYS:CG	6:H:105:GLU:OE1	2.32	0.78
2:B:134:LYS:HB2	2:B:134:LYS:HE3	1.66	0.78
1:A:752:LYS:CE	2:B:1019:SER:OG	2.30	0.78
1:A:503:GLN:HE22	5:F:90:ARG:NH2	1.81	0.78
9:K:101:LEU:C	9:K:101:LEU:HD13	2.04	0.78
4:E:117:THR:O	4:E:118:PRO:C	2.18	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:199:LYS:CA	3:C:199:LYS:CG	2.62	0.78
6:H:91:ASP:OD1	6:H:91:ASP:C	2.22	0.78
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.64	0.78
7:I:35:VAL:O	7:I:35:VAL:HG23	1.81	0.78
1:A:1012:ARG:NE	1:A:1012:ARG:CG	2.45	0.78
2:B:129:PHE:CE2	2:B:166:PHE:HA	2.19	0.78
1:A:920:LEU:HD22	1:A:921:GLY:N	1.99	0.78
10:L:34:CYS:HB3	10:L:51:CYS:CB	2.14	0.78
2:B:1222:ARG:NH1	2:B:1222:ARG:HG2	1.98	0.78
1:A:282:ASN:C	1:A:283:GLY:O	2.23	0.78
2:B:561:TRP:O	2:B:590:HIS:HE1	1.66	0.78
3:C:8:VAL:CG1	3:C:9:LYS:H	1.96	0.77
2:B:1025:HIS:CE1	2:B:1090:THR:HG21	2.19	0.77
5:F:135:ARG:CG	5:F:135:ARG:NE	2.47	0.77
4:E:116:ILE:CD1	4:E:116:ILE:CB	2.61	0.77
1:A:567:LYS:HD2	1:A:568:PRO:HD3	1.63	0.77
7:I:5:ARG:HD3	7:I:36:GLU:OE2	1.84	0.77
3:C:25:VAL:HG11	3:C:29:MET:HG2	1.67	0.77
1:A:1238:ILE:CG2	1:A:1238:ILE:CA	2.62	0.77
1:A:1385:THR:CA	1:A:1385:THR:CG2	2.60	0.77
2:B:270:LYS:CD	2:B:270:LYS:NZ	2.48	0.77
2:B:744:HIS:HD2	2:B:746:SER:H	1.32	0.77
6:H:27:GLU:HA	6:H:27:GLU:C	1.98	0.77
1:A:896:ARG:HD3	1:A:897:TYR:CZ	2.19	0.77
2:B:724:ASP:O	2:B:726:ALA:N	2.17	0.77
1:A:595:THR:HG22	1:A:596:THR:N	1.96	0.77
3:C:267:GLN:C	3:C:267:GLN:HA	1.99	0.77
4:E:116:ILE:H	4:E:116:ILE:HD12	1.50	0.77
2:B:871:THR:HA	2:B:871:THR:CB	2.09	0.77
1:A:412:ARG:CG	1:A:412:ARG:NE	2.48	0.77
2:B:484:ASN:OD1	2:B:486:TYR:CE1	2.38	0.77
2:B:986:GLN:CG	2:B:986:GLN:CA	2.62	0.77
2:B:237:VAL:HG12	2:B:238:ALA:N	1.98	0.77
2:B:1166:CYS:O	2:B:1168:LEU:HG	1.85	0.77
2:B:944:THR:CG2	2:B:944:THR:CA	2.63	0.77
9:K:35:PHE:CE1	9:K:73:LEU:HD12	2.19	0.77
1:A:1055:ARG:CG	1:A:1055:ARG:NE	2.48	0.76
1:A:752:LYS:HZ3	2:B:1019:SER:N	1.82	0.76
2:B:952:VAL:HG22	2:B:966:VAL:HG22	1.66	0.76
2:B:367:LEU:CB	2:B:367:LEU:CD1	2.63	0.76
1:A:1080:THR:C	1:A:1080:THR:HA	2.00	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:116:ILE:N	4:E:116:ILE:HD12	2.01	0.76
9:K:11:LEU:HG	9:K:11:LEU:CD1	2.10	0.76
2:B:510:LYS:N	2:B:511:PRO:CD	2.48	0.76
10:L:65:VAL:CG2	10:L:65:VAL:CA	2.59	0.76
1:A:1063:MET:O	1:A:1064:VAL:C	2.23	0.76
6:H:93:TYR:HB3	6:H:144:ILE:O	1.85	0.76
1:A:121:LEU:HG	1:A:121:LEU:CD1	2.14	0.76
6:H:13:SER:N	6:H:27:GLU:O	2.19	0.76
1:A:547:LEU:HB3	9:K:58:PHE:CE1	2.21	0.76
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.18	0.76
6:H:32:THR:HA	6:H:32:THR:CB	2.12	0.76
1:A:1385:THR:C	1:A:1385:THR:CG2	2.55	0.76
1:A:858:ASN:HD22	1:A:858:ASN:C	1.87	0.75
1:A:413:ILE:HD13	1:A:413:ILE:N	1.99	0.75
2:B:1166:CYS:O	2:B:1167:GLY:C	2.24	0.75
1:A:148:CYS:HG	12:A:3006:ZN:ZN	0.43	0.75
2:B:358:LYS:CA	2:B:358:LYS:CG	2.64	0.75
2:B:129:PHE:HE2	2:B:166:PHE:HB2	1.50	0.75
2:B:1198:TYR:CZ	2:B:1201:LYS:NZ	2.54	0.75
2:B:228:LYS:CA	2:B:228:LYS:CG	2.65	0.75
10:L:34:CYS:SG	10:L:36:SER:OG	2.43	0.75
2:B:100:PRO:HD2	2:B:180:TYR:CZ	2.21	0.75
2:B:999:MET:HB3	2:B:1000:PRO:HD2	1.68	0.75
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.68	0.75
6:H:89:LEU:C	6:H:91:ASP:H	1.89	0.75
1:A:40:THR:HB	1:A:40:THR:CA	2.11	0.74
2:B:1154:ALA:HA	2:B:1154:ALA:CB	2.13	0.74
2:B:654:ARG:H	2:B:657:HIS:HD2	1.35	0.74
1:A:61:ILE:HB	1:A:61:ILE:CG2	2.14	0.74
9:K:102:LYS:O	9:K:106:GLU:HB2	1.87	0.74
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.85	0.74
1:A:886:ILE:HD12	1:A:943:LEU:HB3	1.68	0.74
1:A:1161:THR:CG2	1:A:1163:ILE:H	1.98	0.74
4:E:116:ILE:HG22	4:E:120:ALA:HB3	1.69	0.74
1:A:535:THR:CG2	1:A:616:VAL:HA	2.16	0.74
1:A:351:THR:CG2	2:B:1103:ILE:CG1	2.65	0.74
2:B:846:ILE:CD1	2:B:974:PRO:HB2	2.18	0.74
1:A:166:GLY:O	1:A:167:CYS:HB3	1.86	0.74
2:B:955:THR:CG2	10:L:55:ILE:HA	2.18	0.74
8:J:10:CYS:HG	12:J:3001:ZN:ZN	0.43	0.74
5:F:133:VAL:HG22	5:F:147:SER:HA	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1152:MET:CE	2:B:1152:MET:HA	2.18	0.74
6:H:103:LYS:NZ	6:H:105:GLU:CD	2.39	0.74
3:C:242:GLN:HE21	3:C:246:ARG:HH21	1.36	0.74
4:E:79:TRP:HB2	4:E:105:PHE:CD1	2.22	0.74
1:A:1318:THR:HG23	4:E:11:ARG:HH12	1.52	0.74
2:B:424:LEU:HG	2:B:424:LEU:O	1.85	0.74
2:B:787:VAL:O	2:B:787:VAL:CG1	2.36	0.74
9:K:56:VAL:CB	9:K:56:VAL:HA	2.11	0.73
6:H:4:THR:O	6:H:5:LEU:CD2	2.35	0.73
1:A:711:ARG:NE	7:I:95:THR:HG22	2.01	0.73
1:A:567:LYS:CB	6:H:95:TYR:HA	2.18	0.73
2:B:1222:ARG:CG	2:B:1222:ARG:NH1	2.48	0.73
1:A:108:MET:H	1:A:171:GLN:HE22	1.36	0.73
4:E:117:THR:OG1	4:E:120:ALA:HB2	1.88	0.73
4:E:12:LEU:CD2	4:E:58:MET:SD	2.73	0.73
2:B:323:VAL:C	2:B:324:ILE:HD12	2.08	0.73
3:C:196:ASP:HB3	3:C:199:LYS:HG3	1.70	0.73
4:E:52:ARG:HG3	4:E:53:PRO:HD3	1.71	0.73
2:B:129:PHE:CD2	2:B:166:PHE:CA	2.71	0.73
2:B:164:LYS:CD	2:B:164:LYS:CB	2.66	0.73
7:I:16:PRO:HG3	7:I:27:PHE:HE2	1.54	0.73
2:B:206:ASN:OD1	2:B:458:LYS:CE	2.36	0.73
2:B:1155:SER:CB	2:B:1155:SER:HA	2.11	0.73
2:B:789:MET:CE	2:B:965:LYS:HB3	2.17	0.73
1:A:567:LYS:HE2	6:H:95:TYR:CE2	2.22	0.73
3:C:8:VAL:CG1	3:C:9:LYS:N	2.51	0.73
4:E:50:MET:SD	4:E:50:MET:CE	2.77	0.73
8:J:7:CYS:HG	8:J:10:CYS:HG	1.35	0.73
4:E:90:VAL:CG1	4:E:90:VAL:HB	2.15	0.72
2:B:261:ARG:O	2:B:264:SER:N	2.22	0.72
10:L:51:CYS:SG	10:L:53:HIS:HB2	2.28	0.72
1:A:302:THR:CG2	1:A:302:THR:OG1	2.36	0.72
1:A:351:THR:HG23	2:B:1103:ILE:CG1	2.18	0.72
1:A:31:SER:CB	1:A:83:HIS:CD2	2.67	0.72
2:B:705:MET:CG	2:B:705:MET:HE2	2.19	0.72
1:A:752:LYS:NZ	2:B:1019:SER:H	1.85	0.72
2:B:313:MET:CE	2:B:386:LEU:HD22	2.18	0.72
4:E:63:ASN:O	4:E:64:PRO:O	2.08	0.72
1:A:1080:THR:HB	1:A:1080:THR:CG2	2.13	0.72
2:B:1166:CYS:O	2:B:1168:LEU:N	2.22	0.72
1:A:369:SER:H	9:K:2:ASN:HD21	1.38	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:N	1:A:56:PRO:HD3	2.04	0.72
2:B:227:LYS:CE	2:B:227:LYS:CG	2.68	0.72
2:B:25:ILE:CG1	2:B:25:ILE:CG2	2.67	0.72
6:H:59:ILE:HG22	6:H:60:ALA:H	1.54	0.72
5:F:77:ASP:O	5:F:78:GLN:HB2	1.89	0.72
1:A:1148:ILE:CB	1:A:1148:ILE:CD1	2.67	0.72
1:A:571:LEU:HG	1:A:571:LEU:CD2	2.16	0.72
1:A:1226:VAL:HG12	1:A:1227:ILE:N	2.01	0.72
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.72	0.71
8:J:45:CYS:HG	12:J:3001:ZN:ZN	1.02	0.71
2:B:365:THR:HG22	2:B:367:LEU:H	1.54	0.71
1:A:909:ASP:OD1	1:A:911:SER:OG	2.05	0.71
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.26	0.71
1:A:1233:ASP:O	1:A:1234:GLU:CB	2.38	0.71
2:B:95:ILE:HG22	2:B:96:TYR:N	2.04	0.71
2:B:644:GLU:OE1	2:B:646:LEU:HB2	1.90	0.71
2:B:1222:ARG:HH11	2:B:1222:ARG:CG	2.03	0.71
1:A:711:ARG:HE	7:I:95:THR:CG2	2.02	0.71
1:A:351:THR:HG23	2:B:1103:ILE:HG12	1.70	0.71
7:I:30:ARG:NE	7:I:30:ARG:CG	2.54	0.71
1:A:1064:VAL:CA	1:A:1065:GLY:H	2.01	0.71
2:B:984:HIS:CD2	2:B:1025:HIS:HA	2.26	0.71
2:B:1152:MET:HA	2:B:1152:MET:HE2	1.73	0.71
7:I:71:SER:O	7:I:83:ASN:ND2	2.24	0.71
9:K:56:VAL:CG1	9:K:56:VAL:CA	2.67	0.71
1:A:120:GLU:HG2	1:A:123:ARG:HH22	1.56	0.71
1:A:35:ILE:HD12	1:A:35:ILE:H	1.54	0.71
3:C:196:ASP:CB	3:C:199:LYS:HG3	2.21	0.71
1:A:11:LEU:HD11	2:B:1195:HIS:CD2	2.26	0.71
3:C:50:GLU:HB3	10:L:64:LEU:CD1	2.20	0.71
2:B:1128:LEU:O	2:B:1128:LEU:HG	1.89	0.71
2:B:1150:ARG:CD	2:B:1150:ARG:NH1	2.54	0.70
2:B:169:ARG:O	2:B:457:LEU:HD12	1.89	0.70
2:B:846:ILE:HB	2:B:846:ILE:CA	2.11	0.70
2:B:436:VAL:HB	2:B:436:VAL:CA	2.15	0.70
2:B:914:LYS:H	2:B:938:SER:HB2	1.56	0.70
1:A:1162:VAL:HG12	1:A:1162:VAL:O	1.92	0.70
1:A:101:LYS:NZ	1:A:101:LYS:CD	2.53	0.70
3:C:86:CYS:HG	12:C:3002:ZN:ZN	1.06	0.70
1:A:903:ASN:HD22	1:A:905:ASP:H	1.40	0.70
2:B:542:MET:HG3	2:B:747:MET:HE3	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:32:THR:CG2	6:H:33:GLN:OE1	2.40	0.70
1:A:1081:LEU:CD1	1:A:1081:LEU:CD2	2.69	0.70
2:B:129:PHE:CE2	2:B:166:PHE:HB2	2.25	0.70
1:A:212:LYS:CB	1:A:212:LYS:CD	2.70	0.70
2:B:1222:ARG:HH11	2:B:1222:ARG:CB	2.03	0.70
2:B:498:THR:HG21	2:B:537:LYS:HB2	1.73	0.70
6:H:27:GLU:CA	6:H:28:ALA:N	2.55	0.70
2:B:662:MET:CG	2:B:662:MET:CE	2.70	0.70
1:A:89:PRO:HB2	1:A:204:THR:HG21	1.74	0.70
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.32	0.70
10:L:40:LEU:CD1	10:L:40:LEU:CD2	2.69	0.70
4:E:28:TYR:CE1	4:E:75:MET:CE	2.75	0.70
1:A:1364:ASN:ND2	1:A:1366:ARG:CD	2.54	0.70
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.21	0.70
1:A:243:PRO:O	1:A:243:PRO:HG2	1.91	0.70
3:C:252:GLN:HE22	9:K:99:GLY:HA2	1.56	0.70
2:B:446:LEU:CD1	2:B:446:LEU:CD2	2.70	0.70
1:A:187:LYS:CB	1:A:194:ALA:HB3	2.22	0.69
1:A:535:THR:HG23	1:A:616:VAL:HA	1.72	0.69
1:A:206:GLU:O	1:A:210:ILE:HD13	1.92	0.69
2:B:723:VAL:HB	2:B:723:VAL:CG2	2.16	0.69
9:K:111:LEU:N	9:K:111:LEU:HD23	2.07	0.69
2:B:515:HIS:H	2:B:518:HIS:CD2	2.03	0.69
1:A:636:GLU:OE2	1:A:962:ARG:HD2	1.92	0.69
4:E:36:GLU:O	4:E:37:LEU:C	2.29	0.69
2:B:323:VAL:HG12	2:B:323:VAL:O	1.92	0.69
1:A:353:ILE:HD13	1:A:487:MET:SD	2.31	0.69
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.27	0.69
6:H:63:LEU:C	6:H:90:ALA:CB	2.60	0.69
1:A:1385:THR:HA	1:A:1385:THR:C	2.06	0.69
6:H:59:ILE:HD12	6:H:59:ILE:H	1.56	0.69
1:A:176:LYS:NZ	1:A:178:GLY:O	2.17	0.69
6:H:59:ILE:CG2	6:H:60:ALA:H	2.03	0.69
6:H:105:GLU:HB3	6:H:107:VAL:HG23	1.75	0.69
6:H:115:TYR:O	6:H:123:MET:O	2.10	0.69
2:B:792:MET:SD	2:B:857:ARG:NH2	2.66	0.69
3:C:172:PRO:O	3:C:235:VAL:HG12	1.92	0.69
6:H:131:ASN:CB	6:H:131:ASN:HA	2.11	0.69
2:B:736:THR:CA	2:B:736:THR:CG2	2.67	0.69
1:A:1213:GLY:HA3	1:A:1228:TRP:CZ3	2.28	0.69
6:H:26:ILE:HD12	6:H:42:ILE:HD12	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ASP:OD2	1:A:47:ARG:CA	2.41	0.69
6:H:18:GLY:O	6:H:19:ARG:HB2	1.93	0.69
2:B:324:ILE:N	2:B:324:ILE:HD12	2.08	0.69
6:H:123:MET:HE3	6:H:142:LEU:HD22	1.75	0.68
2:B:94:LYS:CA	2:B:94:LYS:CG	2.69	0.68
1:A:31:SER:HB3	1:A:83:HIS:HD2	1.58	0.68
4:E:127:ILE:N	4:E:128:PRO:CD	2.56	0.68
2:B:165:VAL:HG12	2:B:167:ILE:HD13	1.74	0.68
5:F:80:ALA:N	5:F:80:ALA:CB	2.51	0.68
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.28	0.68
6:H:113:ALA:HA	6:H:125:LEU:O	1.94	0.68
2:B:345:LYS:CG	2:B:345:LYS:CE	2.72	0.68
2:B:578:THR:OG1	2:B:593:PRO:HG3	1.93	0.68
2:B:217:ARG:HD3	2:B:407:ASP:OD2	1.93	0.68
2:B:542:MET:HG3	2:B:747:MET:CE	2.23	0.68
1:A:1146:VAL:O	1:A:1146:VAL:CG1	2.38	0.68
2:B:227:LYS:CB	2:B:227:LYS:CD	2.68	0.68
1:A:827:THR:CG2	1:A:827:THR:CA	2.69	0.68
2:B:916:THR:HB	2:B:935:ARG:HB2	1.76	0.68
2:B:431:TYR:O	2:B:431:TYR:HD2	1.76	0.68
1:A:751:SER:OG	2:B:1015:HIS:HE1	1.76	0.68
5:F:73:ALA:HB2	5:F:143:PHE:CZ	2.28	0.68
2:B:1163:CYS:HB3	2:B:1166:CYS:SG	2.35	0.67
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.09	0.67
2:B:282:ILE:H	2:B:282:ILE:HD13	1.59	0.67
2:B:172:ILE:CB	2:B:172:ILE:CD1	2.71	0.67
10:L:65:VAL:HB	10:L:65:VAL:CG2	2.15	0.67
1:A:55:ASP:H	1:A:56:PRO:HD3	1.59	0.67
4:E:156:LEU:HB3	4:E:160:GLU:HB3	1.75	0.67
2:B:772:ALA:O	2:B:775:LYS:HB2	1.94	0.67
2:B:624:LEU:C	2:B:624:LEU:HD12	2.14	0.67
5:F:105:ALA:HB1	5:F:106:PRO:HD2	1.76	0.67
1:A:1146:VAL:O	1:A:1146:VAL:HG13	1.93	0.67
10:L:38:LEU:O	10:L:39:SER:CB	2.42	0.67
3:C:167:HIS:HE1	10:L:70:ARG:O	1.77	0.67
1:A:32:VAL:CG2	1:A:33:ALA:H	2.02	0.67
1:A:132:LYS:CE	1:A:132:LYS:CG	2.70	0.67
2:B:98:THR:OG1	2:B:127:GLY:O	2.12	0.67
2:B:1189:ILE:CA	2:B:1189:ILE:CG2	2.72	0.67
1:A:423:ASP:O	1:A:423:ASP:CG	2.33	0.67
1:A:658:LEU:HD12	1:A:658:LEU:O	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:HG22	1:A:52:GLY:N	2.10	0.67
1:A:903:ASN:ND2	1:A:905:ASP:N	2.42	0.67
2:B:680:THR:HG22	2:B:682:SER:N	2.08	0.67
1:A:912:LEU:N	1:A:912:LEU:HD23	2.10	0.67
2:B:864:LYS:HB3	2:B:872:GLU:H	1.60	0.67
5:F:76:LYS:CB	5:F:76:LYS:CD	2.72	0.67
2:B:424:LEU:O	2:B:424:LEU:CG	2.43	0.67
3:C:86:CYS:HG	3:C:95:CYS:HG	0.68	0.67
1:A:199:LEU:CD2	1:A:199:LEU:CD1	2.72	0.67
1:A:840:ARG:NE	1:A:840:ARG:CG	2.57	0.67
2:B:884:ARG:CG	2:B:884:ARG:NE	2.57	0.67
1:A:1109:LYS:CG	1:A:1109:LYS:CA	2.71	0.67
1:A:566:ILE:CA	1:A:566:ILE:CG2	2.71	0.67
2:B:424:LEU:HD23	2:B:424:LEU:C	2.15	0.67
1:A:150:THR:HA	1:A:166:GLY:HA2	1.75	0.67
4:E:116:ILE:HG22	4:E:120:ALA:CB	2.25	0.66
1:A:199:LEU:HG	1:A:199:LEU:CD1	2.15	0.66
2:B:736:THR:OG1	2:B:736:THR:CG2	2.42	0.66
6:H:63:LEU:HA	6:H:63:LEU:C	2.09	0.66
1:A:351:THR:HG21	2:B:1103:ILE:HG12	1.77	0.66
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.76	0.66
1:A:55:ASP:OD1	1:A:55:ASP:O	2.12	0.66
3:C:18:VAL:HG23	3:C:240:VAL:HG11	1.77	0.66
2:B:431:TYR:O	2:B:431:TYR:CD2	2.48	0.66
1:A:216:VAL:HG22	1:A:219:PHE:CZ	2.30	0.66
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.31	0.66
4:E:127:ILE:N	4:E:128:PRO:HD3	2.10	0.66
1:A:1350:LYS:CD	1:A:1350:LYS:CB	2.72	0.66
6:H:6:PHE:CG	6:H:7:ASP:N	2.60	0.66
2:B:393:LYS:CD	2:B:393:LYS:CB	2.72	0.66
6:H:89:LEU:O	6:H:91:ASP:N	2.28	0.66
2:B:90:ILE:N	2:B:90:ILE:CD1	2.59	0.66
7:I:45:ARG:NH1	7:I:45:ARG:HG2	2.08	0.66
1:A:55:ASP:N	1:A:56:PRO:HD2	2.10	0.66
3:C:88:CYS:HG	3:C:95:CYS:HG	1.36	0.66
2:B:228:LYS:O	2:B:261:ARG:NH2	2.21	0.66
2:B:106:ASP:OD1	2:B:106:ASP:CB	2.41	0.66
1:A:72:GLU:OE2	2:B:1175:LEU:HD11	1.96	0.66
6:H:63:LEU:HB2	6:H:90:ALA:HB2	1.76	0.66
1:A:155:GLU:HB2	1:A:156:ASP:OD2	1.96	0.66
3:C:181:ASP:N	3:C:182:PRO:CD	2.58	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:TYR:CG	2:B:137:TYR:HB2	2.21	0.66
1:A:601:LYS:CD	1:A:601:LYS:NZ	2.59	0.66
1:A:32:VAL:HG23	1:A:33:ALA:N	2.06	0.66
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.75	0.66
2:B:733:HIS:CA	2:B:734:HIS:N	2.59	0.66
3:C:240:VAL:C	3:C:242:GLN:N	2.46	0.66
2:B:1182:CYS:O	2:B:1183:LYS:C	2.34	0.66
2:B:305:VAL:CG1	2:B:305:VAL:CA	2.71	0.66
2:B:768:THR:C	2:B:768:THR:HG22	2.16	0.66
2:B:890:TYR:OH	2:B:936:ASP:OD1	2.11	0.65
2:B:1195:HIS:C	2:B:1196:ILE:HG23	2.16	0.65
1:A:64:ASN:O	1:A:66:LYS:N	2.29	0.65
1:A:1166:ASP:O	1:A:1170:ILE:HD13	1.96	0.65
7:I:45:ARG:CD	7:I:45:ARG:CB	2.71	0.65
3:C:239:PRO:O	3:C:242:GLN:HB2	1.97	0.65
1:A:531:ILE:O	1:A:535:THR:HB	1.95	0.65
2:B:1002:THR:HG21	2:B:1006:ILE:HB	1.79	0.65
8:J:53:HIS:ND1	8:J:54:VAL:N	2.43	0.65
1:A:903:ASN:HD22	1:A:905:ASP:N	1.94	0.65
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.78	0.65
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.77	0.65
1:A:555:ASP:OD1	9:K:26:LYS:NZ	2.30	0.65
4:E:117:THR:OG1	4:E:120:ALA:CB	2.45	0.65
4:E:94:LYS:CG	4:E:94:LYS:CE	2.75	0.65
1:A:53:LEU:CD1	1:A:53:LEU:HG	2.15	0.65
4:E:213:ILE:CB	4:E:213:ILE:CD1	2.71	0.65
4:E:76:GLY:HA3	4:E:106:GLN:HB3	1.77	0.65
1:A:551:TYR:CD2	9:K:62:LYS:HD3	2.32	0.65
4:E:98:ILE:O	4:E:101:GLN:HB3	1.96	0.65
1:A:53:LEU:CD1	1:A:53:LEU:CD2	2.73	0.65
1:A:567:LYS:CG	6:H:95:TYR:HA	2.25	0.65
7:I:4:PHE:CE1	7:I:13:MET:HE1	2.30	0.65
2:B:724:ASP:O	2:B:725:PRO:C	2.31	0.65
1:A:89:PRO:HB2	1:A:204:THR:CG2	2.26	0.65
2:B:213:ILE:N	2:B:213:ILE:HD12	2.10	0.65
2:B:1097:HIS:CB	2:B:1097:HIS:N	2.57	0.65
2:B:916:THR:HB	2:B:935:ARG:CB	2.25	0.65
6:H:103:LYS:HZ2	6:H:105:GLU:CD	2.00	0.65
2:B:294:ASP:N	7:I:12:ASN:HD22	1.92	0.65
1:A:208:LEU:HB2	1:A:235:ILE:HG21	1.79	0.65
4:E:71:LYS:CA	4:E:71:LYS:CG	2.72	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:VAL:C	1:A:1066:VAL:H	1.96	0.65
2:B:431:TYR:O	2:B:432:MET:HG3	1.97	0.65
1:A:894:GLU:HB2	1:A:933:TYR:OH	1.96	0.65
2:B:995:ARG:HD2	2:B:997:GLU:OE2	1.97	0.65
1:A:1293:SER:HB2	1:A:1294:PRO:HD2	1.78	0.65
2:B:1022:THR:HG23	2:B:1022:THR:O	1.97	0.65
1:A:896:ARG:HG2	1:A:897:TYR:CD1	2.32	0.64
2:B:510:LYS:N	2:B:511:PRO:HD3	2.11	0.64
2:B:360:PHE:O	2:B:361:LEU:C	2.33	0.64
1:A:741:ASN:C	1:A:741:ASN:HD22	2.00	0.64
10:L:65:VAL:N	10:L:65:VAL:CG2	2.61	0.64
1:A:838:GLN:CB	1:A:838:GLN:CD	2.65	0.64
2:B:789:MET:CG	2:B:789:MET:CE	2.75	0.64
1:A:752:LYS:CG	1:A:752:LYS:CE	2.74	0.64
7:I:65:ASP:C	7:I:65:ASP:OD1	2.32	0.64
6:H:51:ALA:CB	6:H:51:ALA:HA	2.16	0.64
1:A:46:THR:HB	1:A:46:THR:O	1.96	0.64
4:E:52:ARG:CG	4:E:53:PRO:HD3	2.27	0.64
1:A:1064:VAL:O	1:A:1065:GLY:CA	2.44	0.64
1:A:1004:ASN:CG	4:E:167:ARG:HG3	2.17	0.64
2:B:328:GLU:CG	2:B:328:GLU:CA	2.73	0.64
1:A:1194:ARG:CD	1:A:1194:ARG:CB	2.74	0.64
2:B:516:ASN:ND2	2:B:516:ASN:H	1.85	0.64
1:A:23:SER:O	1:A:27:VAL:HG23	1.96	0.64
2:B:1077:THR:HG22	2:B:1079:LYS:H	1.62	0.64
1:A:187:LYS:HG3	1:A:194:ALA:CB	2.27	0.64
2:B:323:VAL:CG1	2:B:323:VAL:O	2.46	0.64
1:A:551:TYR:CE2	9:K:62:LYS:HD3	2.33	0.64
2:B:645:SER:OG	2:B:646:LEU:N	2.27	0.64
1:A:66:LYS:CB	1:A:66:LYS:CD	2.74	0.64
2:B:1148:LYS:NZ	2:B:1148:LYS:CD	2.60	0.64
2:B:864:LYS:HG3	2:B:865:LYS:N	2.12	0.64
10:L:32:ALA:HB2	10:L:55:ILE:HG22	1.79	0.64
2:B:1058:LEU:CD1	2:B:1058:LEU:CB	2.72	0.64
10:L:38:LEU:HD23	10:L:39:SER:H	1.62	0.64
1:A:356:ASP:OD2	1:A:469:ARG:HD3	1.98	0.64
4:E:157:SER:O	4:E:160:GLU:HB2	1.97	0.64
2:B:933:SER:C	2:B:933:SER:HA	2.09	0.64
1:A:703:THR:CA	1:A:703:THR:CG2	2.77	0.64
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.61	0.64
2:B:167:ILE:HG22	2:B:167:ILE:O	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:VAL:HG12	2:B:226:PHE:N	2.13	0.63
2:B:821:GLN:OE1	2:B:850:LEU:HD12	1.98	0.63
1:A:1290:LYS:HA	1:A:1299:VAL:O	1.98	0.63
1:A:107:CYS:HB2	1:A:148:CYS:HB2	1.79	0.63
1:A:1176:LEU:CD2	1:A:1176:LEU:HG	2.14	0.63
2:B:368:GLU:C	2:B:368:GLU:CB	2.63	0.63
9:K:56:VAL:HB	9:K:56:VAL:CA	2.13	0.63
8:J:1:MET:C	8:J:2:ILE:HD12	2.19	0.63
1:A:26:GLU:HA	1:A:29:ALA:HB3	1.79	0.63
3:C:40:GLU:OE1	3:C:254:LYS:NZ	2.31	0.63
1:A:46:THR:C	1:A:46:THR:CB	2.63	0.63
3:C:253:LYS:CE	3:C:253:LYS:CG	2.71	0.63
3:C:100:THR:HG22	3:C:101:LEU:N	2.14	0.63
2:B:653:VAL:O	2:B:654:ARG:HD3	1.98	0.63
1:A:720:ARG:O	1:A:724:GLU:HB3	1.98	0.63
4:E:7:ARG:O	4:E:8:ASN:C	2.36	0.63
1:A:601:LYS:CD	1:A:601:LYS:CB	2.69	0.63
1:A:1151:GLU:HG3	7:I:45:ARG:HD2	1.80	0.63
4:E:156:LEU:HD23	4:E:156:LEU:N	2.13	0.63
6:H:142:LEU:HG	6:H:143:LEU:N	2.12	0.63
2:B:775:LYS:CA	2:B:775:LYS:CG	2.74	0.63
3:C:167:HIS:CD2	3:C:169:LYS:H	2.10	0.63
2:B:1172:ILE:CG2	2:B:1172:ILE:HG12	2.29	0.63
10:L:26:THR:CG2	10:L:27:LEU:H	2.12	0.63
10:L:25:ALA:HA	10:L:25:ALA:CB	2.14	0.63
2:B:104:GLU:HB2	2:B:108:VAL:HA	1.80	0.63
2:B:595:ARG:CB	2:B:595:ARG:CD	2.77	0.63
2:B:97:VAL:HG12	2:B:178:ASN:HD21	1.62	0.63
1:A:860:LEU:CB	1:A:860:LEU:CD2	2.76	0.62
10:L:38:LEU:HD21	10:L:40:LEU:HB2	1.80	0.62
2:B:417:PHE:CD2	2:B:417:PHE:C	2.71	0.62
2:B:863:GLU:OE1	2:B:962:LYS:HD3	1.99	0.62
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.14	0.62
2:B:291:ILE:O	2:B:297:ILE:HD11	1.99	0.62
1:A:274:ILE:CA	1:A:274:ILE:HB	2.16	0.62
2:B:987:LYS:CD	2:B:987:LYS:NZ	2.62	0.62
1:A:1080:THR:CB	1:A:1080:THR:N	2.61	0.62
3:C:19:ASP:C	3:C:19:ASP:OD1	2.33	0.62
1:A:203:SER:OG	1:A:206:GLU:CG	2.46	0.62
2:B:498:THR:CG2	2:B:537:LYS:HB2	2.28	0.62
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1039:LYS:HG3	1:A:1039:LYS:O	1.99	0.62
2:B:307:ASP:O	2:B:308:TRP:C	2.30	0.62
2:B:1163:CYS:CB	2:B:1163:CYS:HA	2.13	0.62
3:C:84:ARG:HD2	9:K:11:LEU:HD21	1.81	0.62
2:B:662:MET:HG3	2:B:662:MET:CE	2.30	0.62
2:B:958:GLN:HG2	2:B:958:GLN:H	1.65	0.62
2:B:775:LYS:CD	2:B:775:LYS:CB	2.75	0.62
1:A:571:LEU:CD2	1:A:571:LEU:CD1	2.72	0.62
1:A:1366:ARG:HH11	1:A:1366:ARG:HB3	1.63	0.62
1:A:1004:ASN:OD1	4:E:167:ARG:HG3	1.98	0.62
2:B:1101:ASP:HA	2:B:1101:ASP:C	2.08	0.62
10:L:25:ALA:CB	10:L:25:ALA:C	2.65	0.62
7:I:64:SER:O	7:I:66:PRO:HD3	1.99	0.62
6:H:83:GLN:C	6:H:85:GLY:N	2.48	0.62
9:K:93:SER:O	9:K:97:LYS:HG3	2.00	0.62
2:B:165:VAL:HG12	2:B:167:ILE:CD1	2.30	0.62
1:A:133:LYS:O	1:A:136:ALA:HB3	1.99	0.62
1:A:1222:ASN:HA	1:A:1222:ASN:CB	2.13	0.62
9:K:101:LEU:C	9:K:101:LEU:CD1	2.68	0.62
4:E:66:GLU:O	4:E:67:GLU:C	2.35	0.61
1:A:858:ASN:ND2	1:A:858:ASN:C	2.53	0.61
1:A:719:VAL:O	1:A:719:VAL:HG12	1.95	0.61
1:A:1055:ARG:CB	1:A:1055:ARG:CD	2.76	0.61
1:A:203:SER:HG	1:A:206:GLU:HG2	1.65	0.61
2:B:341:LEU:HD12	2:B:342:GLY:H	1.65	0.61
4:E:44:ALA:CB	4:E:45:LYS:N	2.63	0.61
2:B:25:ILE:HD11	2:B:651:LEU:HD12	1.80	0.61
2:B:1189:ILE:CG2	2:B:1189:ILE:C	2.67	0.61
1:A:966:ASN:O	1:A:967:ALA:C	2.39	0.61
1:A:752:LYS:NZ	2:B:1019:SER:N	2.47	0.61
2:B:1166:CYS:CB	2:B:1185:CYS:SG	2.87	0.61
1:A:1348:LEU:HG	1:A:1372:VAL:CG2	2.30	0.61
4:E:91:LYS:CD	4:E:91:LYS:CB	2.74	0.61
1:A:596:THR:HG22	1:A:597:LEU:N	2.11	0.61
1:A:903:ASN:HD22	1:A:904:THR:N	1.98	0.61
9:K:103:THR:C	9:K:105:PHE:N	2.52	0.61
1:A:172:PRO:HG2	1:A:174:ILE:HD11	1.82	0.61
1:A:472:LEU:O	1:A:475:THR:HB	2.00	0.61
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	2.00	0.61
2:B:127:GLY:HA2	2:B:168:GLY:O	2.00	0.61
3:C:120:ILE:HB	3:C:120:ILE:CD1	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:HIS:HD2	1:A:966:ASN:OD1	1.82	0.61
1:A:880:LYS:CG	1:A:880:LYS:CE	2.78	0.61
1:A:1259:MET:CB	1:A:1259:MET:SD	2.89	0.61
1:A:1077:THR:HG22	1:A:1078:GLN:NE2	2.16	0.61
1:A:1445:ILE:CD1	1:A:1445:ILE:CB	2.77	0.61
1:A:567:LYS:CD	1:A:567:LYS:HE3	2.18	0.61
7:I:1:MET:HA	7:I:1:MET:CB	2.18	0.61
4:E:191:LYS:O	4:E:192:ARG:C	2.36	0.61
1:A:1100:ARG:O	1:A:1103:GLU:HB3	2.01	0.61
2:B:129:PHE:CE2	2:B:166:PHE:CB	2.83	0.61
1:A:587:HIS:CE1	1:A:609:ASP:H	2.19	0.61
1:A:120:GLU:HG2	1:A:123:ARG:NH2	2.15	0.61
3:C:133:ILE:C	3:C:134:ILE:HG12	2.19	0.61
6:H:84:ALA:O	6:H:88:SER:OG	2.09	0.61
2:B:1012:ILE:HD12	2:B:1012:ILE:C	2.21	0.61
2:B:129:PHE:HD2	2:B:165:VAL:C	2.04	0.61
1:A:217:LYS:CD	1:A:217:LYS:NZ	2.63	0.61
2:B:424:LEU:O	2:B:428:ILE:HG13	2.01	0.61
6:H:59:ILE:HD12	6:H:59:ILE:N	2.16	0.61
6:H:7:ASP:OD1	6:H:8:ASP:N	2.34	0.61
2:B:1002:THR:CG2	2:B:1006:ILE:HB	2.31	0.61
1:A:901:LEU:HD22	1:A:919:ILE:HD13	1.83	0.61
6:H:81:PRO:CB	6:H:82:PRO:CD	2.78	0.61
6:H:81:PRO:CB	6:H:82:PRO:HD3	2.31	0.61
2:B:1221:SER:OG	5:F:72:LYS:HD2	2.00	0.61
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.03	0.61
2:B:282:ILE:H	2:B:282:ILE:CD1	2.14	0.60
1:A:1383:SER:OG	1:A:1384:VAL:N	2.32	0.60
6:H:32:THR:CA	6:H:32:THR:CG2	2.72	0.60
6:H:136:LYS:CA	6:H:137:GLN:N	2.61	0.60
1:A:535:THR:HG22	1:A:616:VAL:HG13	1.83	0.60
1:A:1325:THR:O	4:E:147:HIS:CD2	2.53	0.60
1:A:595:THR:CG2	1:A:596:THR:N	2.64	0.60
2:B:39:ARG:CB	2:B:39:ARG:CD	2.75	0.60
6:H:105:GLU:H	6:H:105:GLU:CD	2.05	0.60
2:B:428:ILE:HG12	2:B:448:ILE:CD1	2.30	0.60
1:A:1098:VAL:N	1:A:1099:PRO:CD	2.64	0.60
4:E:153:HIS:CE1	4:E:184:VAL:HG11	2.36	0.60
1:A:1450:LEU:HG	1:A:1450:LEU:CD2	2.22	0.60
2:B:193:LYS:CG	2:B:193:LYS:CE	2.77	0.60
2:B:120:ARG:NH2	2:B:956:THR:O	2.29	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:111:LEU:CD1	6:H:111:LEU:HG	2.17	0.60
2:B:624:LEU:HD12	2:B:625:LYS:N	2.16	0.60
1:A:1236:LEU:C	1:A:1237:ILE:HD12	2.20	0.60
4:E:127:ILE:H	4:E:128:PRO:HD3	1.65	0.60
4:E:6:GLU:OE2	4:E:43:LYS:NZ	2.34	0.60
1:A:1425:SER:CB	1:A:1425:SER:HG	2.08	0.60
1:A:1242:VAL:C	1:A:1243:VAL:HG12	2.20	0.60
2:B:1097:HIS:CE1	2:B:1102:LYS:HG3	2.35	0.60
2:B:1153:GLU:HB3	2:B:1155:SER:HB3	1.84	0.60
1:A:567:LYS:HD3	6:H:95:TYR:CD2	2.34	0.60
9:K:110:ASN:ND2	9:K:110:ASN:CB	2.60	0.60
6:H:89:LEU:C	6:H:91:ASP:N	2.54	0.60
1:A:1283:VAL:HG12	1:A:1284:MET:O	2.01	0.60
8:J:1:MET:CE	8:J:1:MET:HB2	2.30	0.60
6:H:130:ARG:C	6:H:130:ARG:CD	2.59	0.60
1:A:903:ASN:C	1:A:903:ASN:HD22	2.05	0.60
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.00	0.60
2:B:903:VAL:HG12	2:B:904:ARG:N	2.16	0.60
6:H:56:THR:HG21	6:H:145:ARG:NE	2.16	0.60
1:A:1166:ASP:OD2	1:A:1239:ARG:NH2	2.31	0.60
2:B:961:LEU:CD2	2:B:961:LEU:CD1	2.76	0.60
2:B:1177:HIS:HB2	2:B:1179:GLN:NE2	2.17	0.60
1:A:1239:ARG:NE	1:A:1239:ARG:CG	2.64	0.60
1:A:1272:THR:CA	1:A:1272:THR:CG2	2.76	0.60
2:B:654:ARG:N	2:B:657:HIS:HD2	2.00	0.60
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.36	0.60
1:A:605:MET:CE	1:A:607:ILE:HG13	2.32	0.60
1:A:673:GLY:N	1:A:674:PRO:HD2	2.17	0.60
7:I:98:VAL:HG22	7:I:99:LEU:N	2.15	0.60
1:A:215:SER:OG	1:A:218:ASP:HB2	2.02	0.60
6:H:93:TYR:CD1	6:H:93:TYR:N	2.70	0.59
6:H:17:PRO:HB3	6:H:24:CYS:SG	2.42	0.59
9:K:46:ILE:O	9:K:47:ARG:C	2.32	0.59
2:B:906:SER:O	2:B:907:GLY:C	2.40	0.59
3:C:11:ARG:NE	3:C:209:TYR:CE2	2.70	0.59
2:B:55:VAL:HG12	2:B:56:ASP:N	2.17	0.59
2:B:846:ILE:N	2:B:846:ILE:CB	2.58	0.59
1:A:1385:THR:HG22	1:A:1385:THR:C	2.18	0.59
6:H:107:VAL:CG2	6:H:107:VAL:CG1	2.76	0.59
1:A:1366:ARG:CZ	1:A:1366:ARG:HB3	2.30	0.59
10:L:58:LYS:O	10:L:59:ALA:CB	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:PRO:O	2:B:111:ALA:HA	2.02	0.59
1:A:31:SER:HB2	1:A:83:HIS:HD2	1.63	0.59
2:B:986:GLN:NE2	2:B:987:LYS:O	2.31	0.59
1:A:1293:SER:CB	1:A:1294:PRO:HD2	2.33	0.59
1:A:947:PHE:CE2	1:A:954:TRP:CE2	2.90	0.59
2:B:1189:ILE:HG22	2:B:1190:ASP:H	1.66	0.59
10:L:26:THR:HB	10:L:26:THR:CA	2.20	0.59
2:B:807:ARG:CB	2:B:807:ARG:CD	2.74	0.59
1:A:567:LYS:CB	6:H:96:VAL:N	2.46	0.59
2:B:705:MET:HE3	2:B:705:MET:CG	2.32	0.59
3:C:15:LYS:NZ	3:C:15:LYS:CD	2.64	0.59
5:F:109:VAL:HG22	5:F:127:GLU:OE1	2.02	0.59
4:E:123:LEU:O	4:E:126:SER:HB2	2.02	0.59
1:A:567:LYS:HG2	6:H:96:VAL:H	1.66	0.59
7:I:49:ILE:O	7:I:49:ILE:HG22	2.01	0.59
2:B:1189:ILE:CG2	2:B:1190:ASP:N	2.64	0.59
1:A:533:LYS:NZ	1:A:745:GLN:HE22	2.00	0.59
1:A:1208:THR:O	1:A:1209:MET:C	2.36	0.59
1:A:804:TYR:O	2:B:761:HIS:ND1	2.33	0.59
2:B:1101:ASP:CA	2:B:1102:LYS:N	2.62	0.59
1:A:1151:GLU:OE2	7:I:45:ARG:HD3	2.03	0.59
1:A:274:ILE:CG2	1:A:274:ILE:CG1	2.76	0.59
2:B:871:THR:CA	2:B:871:THR:HB	2.16	0.59
2:B:39:ARG:CA	2:B:39:ARG:CG	2.78	0.59
6:H:103:LYS:O	6:H:115:TYR:CD1	2.50	0.59
9:K:111:LEU:CB	9:K:111:LEU:CD1	2.77	0.59
10:L:68:GLU:O	10:L:69:ALA:HB3	2.03	0.59
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.85	0.59
9:K:78:THR:HG22	9:K:79:GLU:H	1.66	0.59
3:C:10:ILE:HD13	3:C:10:ILE:H	1.68	0.59
1:A:751:SER:OG	2:B:1015:HIS:CE1	2.55	0.59
9:K:65:HIS:CD2	9:K:67:PHE:H	2.13	0.59
3:C:218:PRO:O	3:C:218:PRO:HG2	2.02	0.59
1:A:909:ASP:CG	1:A:910:PRO:HD2	2.22	0.59
2:B:100:PRO:CD	2:B:180:TYR:CE1	2.69	0.59
1:A:50:ILE:HG22	1:A:52:GLY:H	1.65	0.59
3:C:92:CYS:SG	3:C:95:CYS:SG	3.00	0.59
2:B:428:ILE:CG1	2:B:448:ILE:HD11	2.33	0.59
1:A:676:MET:CB	1:A:676:MET:SD	2.90	0.59
1:A:1155:ASP:O	1:A:1241:ARG:NH2	2.33	0.58
4:E:7:ARG:O	4:E:9:ILE:N	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1134:ILE:HG22	1:A:1306:LEU:HD11	1.84	0.58
1:A:369:SER:CB	9:K:2:ASN:ND2	2.66	0.58
9:K:65:HIS:HD2	9:K:67:PHE:N	1.97	0.58
2:B:744:HIS:CD2	2:B:746:SER:H	2.17	0.58
1:A:446:ARG:CG	1:A:446:ARG:HH11	2.14	0.58
2:B:754:SER:O	2:B:806:THR:HG21	2.03	0.58
1:A:852:TYR:CE2	5:F:136:ARG:HD3	2.37	0.58
2:B:68:THR:HG23	2:B:91:SER:HB3	1.84	0.58
4:E:43:LYS:CB	4:E:43:LYS:CD	2.78	0.58
1:A:325:ILE:HG22	1:A:325:ILE:O	2.03	0.58
2:B:787:VAL:O	2:B:787:VAL:HG12	2.02	0.58
1:A:1027:ALA:O	1:A:1030:ARG:HB2	2.03	0.58
2:B:357:GLN:NE2	2:B:368:GLU:HG2	2.18	0.58
1:A:1148:ILE:HD13	1:A:1148:ILE:HG21	1.85	0.58
2:B:121:ASN:HD22	2:B:121:ASN:N	2.01	0.58
1:A:200:ARG:NH2	1:A:206:GLU:OE2	2.36	0.58
3:C:97:VAL:HG12	3:C:98:VAL:N	2.14	0.58
1:A:596:THR:HG22	1:A:597:LEU:HD12	1.86	0.58
2:B:1097:HIS:C	2:B:1097:HIS:ND1	2.57	0.58
6:H:47:PHE:O	6:H:47:PHE:CD2	2.56	0.58
2:B:353:LYS:CD	2:B:353:LYS:CB	2.78	0.58
1:A:751:SER:HG	1:A:751:SER:CB	2.07	0.58
1:A:938:LYS:CE	1:A:938:LYS:CG	2.81	0.58
3:C:234:SER:OG	3:C:235:VAL:N	2.35	0.58
1:A:378:GLU:OE1	1:A:434:ARG:HD3	2.03	0.58
4:E:44:ALA:CB	4:E:44:ALA:C	2.68	0.58
6:H:131:ASN:CA	6:H:132:LEU:N	2.64	0.58
2:B:70:ILE:CB	2:B:70:ILE:CD1	2.80	0.58
2:B:870:ILE:HA	2:B:870:ILE:CB	2.20	0.58
5:F:77:ASP:O	5:F:78:GLN:CB	2.48	0.58
1:A:243:PRO:CB	1:A:245:PRO:HD2	2.33	0.58
2:B:549:THR:HG22	2:B:628:THR:HB	1.85	0.58
4:E:44:ALA:CB	4:E:44:ALA:N	2.64	0.58
1:A:599:SER:O	1:A:600:PRO:C	2.37	0.58
1:A:164:ARG:O	1:A:166:GLY:N	2.36	0.58
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.03	0.58
1:A:931:GLU:CB	1:A:931:GLU:CD	2.67	0.58
2:B:531:GLN:H	2:B:531:GLN:CD	2.07	0.58
2:B:915:THR:C	2:B:915:THR:CB	2.67	0.58
1:A:1111:MET:HE2	1:A:1111:MET:CG	2.33	0.58
3:C:197:SER:HG	3:C:197:SER:CB	2.08	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:ASP:N	7:I:12:ASN:ND2	2.39	0.58
3:C:73:GLN:HE21	3:C:75:MET:N	2.00	0.58
4:E:117:THR:C	4:E:119:SER:N	2.54	0.58
3:C:102:GLN:CA	3:C:102:GLN:CG	2.75	0.58
2:B:1098:MET:O	2:B:1100:ASP:N	2.36	0.58
6:H:7:ASP:HB2	6:H:58:THR:OG1	2.04	0.58
3:C:95:CYS:HG	12:C:3002:ZN:ZN	1.13	0.58
2:B:1162:ILE:HD11	2:B:1169:MET:HG2	1.85	0.58
9:K:26:LYS:CB	9:K:26:LYS:CD	2.81	0.58
1:A:1162:VAL:CG1	1:A:1162:VAL:O	2.51	0.58
1:A:61:ILE:CG1	1:A:61:ILE:CA	2.78	0.58
2:B:879:ARG:NH2	2:B:885:MET:CE	2.67	0.58
7:I:4:PHE:HZ	7:I:13:MET:HE1	1.68	0.58
1:A:243:PRO:CG	1:A:245:PRO:HD2	2.34	0.58
9:K:82:ASP:OD1	9:K:83:PRO:HG2	2.04	0.58
2:B:859:TYR:CD1	2:B:859:TYR:N	2.71	0.58
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.38	0.57
7:I:45:ARG:NH1	7:I:45:ARG:CG	2.67	0.57
6:H:103:LYS:HG2	6:H:105:GLU:OE2	2.03	0.57
2:B:768:THR:CG2	2:B:768:THR:C	2.72	0.57
1:A:541:ILE:N	1:A:541:ILE:HD12	2.19	0.57
10:L:47:ARG:HG2	10:L:48:CYS:N	2.16	0.57
1:A:1165:GLU:C	1:A:1167:GLU:H	2.05	0.57
3:C:214:ASN:O	3:C:216:GLY:N	2.37	0.57
6:H:32:THR:HB	6:H:32:THR:CA	2.17	0.57
2:B:552:MET:O	2:B:553:PRO:C	2.34	0.57
1:A:982:THR:HB	1:A:985:ASP:CG	2.24	0.57
1:A:1282:VAL:HG12	1:A:1283:VAL:N	2.14	0.57
4:E:112:TYR:CE2	4:E:116:ILE:HD11	2.39	0.57
6:H:32:THR:HG22	6:H:33:GLN:CD	2.24	0.57
6:H:136:LYS:C	6:H:136:LYS:HA	2.08	0.57
1:A:565:ILE:HD12	6:H:97:MET:HG2	1.87	0.57
2:B:446:LEU:CB	2:B:446:LEU:CD2	2.78	0.57
1:A:53:LEU:HD23	1:A:54:ASN:N	2.20	0.57
1:A:1127:ASP:HB3	1:A:1130:GLN:H	1.70	0.57
7:I:32:CYS:HB2	7:I:34:TYR:H	1.69	0.57
1:A:347:PHE:H	2:B:1107:ALA:HA	1.69	0.57
2:B:324:ILE:N	2:B:324:ILE:CD1	2.67	0.57
1:A:834:THR:HG21	1:A:1077:THR:HA	1.86	0.57
1:A:98:LYS:C	1:A:100:LYS:N	2.54	0.57
2:B:249:ARG:CZ	2:B:415:GLN:HG3	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:LYS:CD	1:A:895:LYS:NZ	2.68	0.57
2:B:1182:CYS:O	2:B:1184:GLY:N	2.37	0.57
4:E:58:MET:O	4:E:59:SER:C	2.43	0.57
2:B:113:TYR:CD2	2:B:192:LEU:CD2	2.87	0.57
2:B:724:ASP:HB3	2:B:727:LYS:HG3	1.86	0.57
2:B:282:ILE:HD13	2:B:282:ILE:N	2.19	0.57
2:B:369:GLY:N	2:B:370:PHE:HD1	2.02	0.57
2:B:418:LYS:CD	2:B:418:LYS:CB	2.79	0.57
1:A:567:LYS:HB2	6:H:95:TYR:HA	1.86	0.57
2:B:609:ILE:HG22	2:B:610:ASN:N	2.20	0.57
1:A:1176:LEU:CD2	1:A:1176:LEU:CD1	2.81	0.57
1:A:35:ILE:HG22	1:A:270:LEU:HD21	1.86	0.57
1:A:598:LEU:HD21	6:H:124:ARG:HB2	1.87	0.57
5:F:76:LYS:CE	5:F:76:LYS:CG	2.79	0.57
5:F:76:LYS:O	5:F:79:ARG:HD2	2.04	0.57
10:L:61:THR:CG2	10:L:61:THR:OG1	2.46	0.57
6:H:102:TYR:O	6:H:104:PHE:N	2.37	0.57
1:A:1151:GLU:CG	7:I:45:ARG:CD	2.82	0.57
1:A:1151:GLU:HG2	7:I:45:ARG:HD2	1.85	0.57
2:B:826:ALA:HB3	2:B:1011:ILE:HD12	1.86	0.57
1:A:571:LEU:HD22	6:H:46:LEU:HD11	1.87	0.57
2:B:367:LEU:CD1	2:B:367:LEU:CD2	2.79	0.57
1:A:920:LEU:CD2	1:A:921:GLY:N	2.67	0.57
4:E:28:TYR:CZ	4:E:75:MET:CE	2.88	0.57
1:A:243:PRO:HB2	1:A:245:PRO:CD	2.34	0.57
3:C:156:THR:HG22	3:C:157:CYS:N	2.20	0.56
2:B:121:ASN:H	2:B:121:ASN:HD22	1.53	0.56
6:H:138:GLU:C	6:H:140:ALA:N	2.51	0.56
3:C:56:THR:HG22	3:C:58:LEU:H	1.70	0.56
1:A:869:GLY:O	4:E:204:THR:HG21	2.05	0.56
2:B:192:LEU:CD2	2:B:192:LEU:HG	2.19	0.56
1:A:567:LYS:CE	6:H:95:TYR:CE2	2.85	0.56
4:E:83:CYS:O	4:E:113:GLN:NE2	2.37	0.56
1:A:830:LYS:NZ	1:A:830:LYS:CD	2.66	0.56
2:B:134:LYS:CE	2:B:134:LYS:HB2	2.34	0.56
3:C:66:ARG:CG	3:C:66:ARG:NH1	2.58	0.56
7:I:55:THR:CG2	7:I:55:THR:HB	2.24	0.56
2:B:1128:LEU:CD1	2:B:1128:LEU:C	2.53	0.56
2:B:914:LYS:CD	2:B:937:ALA:HB3	2.36	0.56
1:A:1146:VAL:HG12	1:A:1197:LEU:HD22	1.87	0.56
2:B:369:GLY:N	2:B:370:PHE:CD1	2.73	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:914:GLU:C	1:A:916:GLY:H	2.08	0.56
1:A:1238:ILE:CG1	1:A:1238:ILE:CG2	2.81	0.56
6:H:6:PHE:C	6:H:6:PHE:CD2	2.73	0.56
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.41	0.56
10:L:47:ARG:CG	10:L:48:CYS:H	2.17	0.56
2:B:663:ALA:O	2:B:667:GLN:HG3	2.05	0.56
1:A:244:PRO:HA	1:A:247:ARG:HG3	1.86	0.56
3:C:56:THR:CG2	3:C:57:VAL:N	2.67	0.56
2:B:114:PRO:HD3	2:B:124:TYR:HE1	1.60	0.56
3:C:40:GLU:O	3:C:163:ILE:HD11	2.06	0.56
2:B:900:ALA:O	2:B:901:PRO:C	2.40	0.56
3:C:11:ARG:NH2	3:C:206:ASN:OD1	2.30	0.56
1:A:1449:SER:HB2	5:F:149:GLU:OE2	2.05	0.56
2:B:467:GLY:H	2:B:477:ALA:CB	2.18	0.56
10:L:61:THR:HB	10:L:63:ARG:H	1.70	0.56
1:A:689:LYS:O	1:A:693:VAL:HG23	2.05	0.56
2:B:424:LEU:HD23	2:B:424:LEU:O	2.06	0.56
2:B:1065:GLN:NE2	2:B:1067:ARG:HB2	2.16	0.56
6:H:26:ILE:CD1	6:H:42:ILE:HD12	2.34	0.56
2:B:431:TYR:CE1	2:B:447:ALA:HB1	2.40	0.56
1:A:507:VAL:HB	1:A:508:PRO:HD3	1.88	0.56
3:C:25:VAL:CG1	3:C:29:MET:HG2	2.34	0.56
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.41	0.56
8:J:14:VAL:HG13	8:J:50:ILE:HD11	1.88	0.56
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.20	0.56
2:B:1150:ARG:NH1	2:B:1150:ARG:NE	2.44	0.56
3:C:242:GLN:O	3:C:246:ARG:HB2	2.06	0.56
1:A:50:ILE:HG22	1:A:51:GLY:N	2.21	0.56
2:B:90:ILE:HA	2:B:133:LYS:O	2.05	0.56
3:C:11:ARG:O	3:C:12:GLU:CB	2.45	0.56
1:A:545:GLN:O	1:A:546:VAL:C	2.36	0.56
2:B:544:CYS:HB2	2:B:634:TYR:CE1	2.40	0.56
6:H:10:PHE:HD1	6:H:57:VAL:HG23	1.71	0.56
2:B:227:LYS:HG3	2:B:395:GLN:NE2	2.20	0.56
10:L:38:LEU:CG	10:L:39:SER:H	2.19	0.56
3:C:116:LYS:NZ	3:C:116:LYS:CD	2.67	0.56
6:H:76:THR:HG22	6:H:76:THR:O	2.06	0.56
1:A:1208:THR:OG1	1:A:1211:GLN:CD	2.44	0.56
1:A:557:ASP:O	1:A:559:VAL:N	2.39	0.56
2:B:1163:CYS:HB2	2:B:1182:CYS:SG	2.46	0.56
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:594:ALA:HB2	2:B:617:ARG:HH12	1.71	0.56
2:B:453:ILE:HG22	2:B:454:THR:N	2.20	0.56
2:B:879:ARG:NH2	2:B:885:MET:HE2	2.21	0.56
2:B:1128:LEU:O	2:B:1128:LEU:CG	2.54	0.56
1:A:351:THR:CG2	2:B:1103:ILE:HG13	2.36	0.56
1:A:606:LEU:HD23	1:A:613:ILE:HG21	1.87	0.56
2:B:870:ILE:HB	2:B:870:ILE:CG2	2.17	0.56
2:B:110:HIS:C	2:B:110:HIS:HA	2.11	0.56
1:A:503:GLN:HE21	5:F:90:ARG:HH21	1.53	0.56
2:B:291:ILE:HG22	2:B:297:ILE:HD13	1.88	0.56
3:C:80:LEU:HD12	3:C:94:LYS:O	2.06	0.56
10:L:38:LEU:CD2	10:L:39:SER:H	2.18	0.56
2:B:347:LYS:CB	2:B:347:LYS:CD	2.83	0.56
1:A:752:LYS:HG3	1:A:753:GLY:H	1.68	0.56
2:B:114:PRO:HD3	2:B:124:TYR:CZ	2.35	0.56
6:H:81:PRO:C	6:H:82:PRO:O	2.44	0.56
1:A:216:VAL:HA	1:A:219:PHE:CZ	2.40	0.56
1:A:189:ARG:HG2	1:A:189:ARG:O	2.06	0.56
10:L:43:THR:CB	10:L:43:THR:C	2.72	0.55
10:L:31:CYS:SG	10:L:34:CYS:SG	3.04	0.55
4:E:161:LYS:NZ	4:E:193:GLY:O	2.39	0.55
2:B:117:ALA:CB	2:B:122:LEU:HB2	2.37	0.55
4:E:61:GLN:HB2	4:E:79:TRP:HE3	1.70	0.55
1:A:324:SER:O	1:A:327:ALA:HB2	2.05	0.55
2:B:296:GLU:O	2:B:300:HIS:CD2	2.59	0.55
2:B:755:ILE:HG22	2:B:755:ILE:O	2.05	0.55
1:A:1265:ASN:O	1:A:1266:THR:C	2.44	0.55
3:C:260:LEU:O	3:C:260:LEU:HD12	2.06	0.55
8:J:53:HIS:HD1	8:J:54:VAL:N	2.04	0.55
1:A:903:ASN:HD21	1:A:905:ASP:HB2	1.69	0.55
6:H:81:PRO:HB2	6:H:82:PRO:HD3	1.87	0.55
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.41	0.55
2:B:296:GLU:O	2:B:300:HIS:HD2	1.89	0.55
1:A:555:ASP:OD1	9:K:26:LYS:HE3	2.05	0.55
4:E:96:PHE:CE2	4:E:100:ILE:HD11	2.40	0.55
10:L:38:LEU:HG	10:L:39:SER:H	1.70	0.55
10:L:48:CYS:C	10:L:48:CYS:HA	2.09	0.55
1:A:1232:ASN:ND2	1:A:1232:ASN:CB	2.65	0.55
4:E:116:ILE:CD1	4:E:116:ILE:N	2.68	0.55
1:A:4:GLN:CG	1:A:4:GLN:N	2.68	0.55
4:E:65:THR:OG1	4:E:68:SER:OG	2.23	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:50:ASP:CA	10:L:51:CYS:N	2.62	0.55
6:H:103:LYS:HG2	6:H:105:GLU:CD	2.26	0.55
3:C:267:GLN:CA	3:C:268:ASP:N	2.63	0.55
2:B:658:ILE:O	2:B:658:ILE:HG22	2.04	0.55
1:A:1341:ILE:HD13	1:A:1379:GLY:O	2.06	0.55
2:B:1098:MET:O	2:B:1099:VAL:C	2.40	0.55
8:J:6:ARG:HD2	8:J:11:GLY:O	2.06	0.55
9:K:49:GLU:HG2	9:K:94:ILE:HD11	1.88	0.55
1:A:1264:GLU:OE1	7:I:44:TYR:HE2	1.89	0.55
1:A:1150:SER:OG	7:I:46:HIS:HB3	2.07	0.55
2:B:1025:HIS:HE1	2:B:1090:THR:CG2	2.16	0.55
5:F:138:LEU:HB3	5:F:139:PRO:HD2	1.89	0.55
6:H:27:GLU:HA	6:H:28:ALA:N	2.22	0.55
8:J:1:MET:HB2	8:J:1:MET:HE3	1.88	0.55
2:B:424:LEU:CD2	2:B:424:LEU:O	2.54	0.55
1:A:446:ARG:HH11	1:A:446:ARG:HG2	1.72	0.55
4:E:118:PRO:HA	4:E:121:MET:SD	2.47	0.55
10:L:32:ALA:HB2	10:L:55:ILE:CG2	2.36	0.55
2:B:846:ILE:C	2:B:846:ILE:CB	2.71	0.55
2:B:423:LYS:CD	2:B:423:LYS:CB	2.80	0.55
5:F:129:LYS:CB	5:F:129:LYS:CD	2.78	0.55
1:A:274:ILE:CG1	1:A:274:ILE:CA	2.81	0.55
2:B:451:LYS:HA	2:B:454:THR:HB	1.88	0.55
7:I:120:GLN:O	7:I:121:PHE:CD1	2.60	0.55
4:E:28:TYR:CE1	4:E:75:MET:HE2	2.42	0.55
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.88	0.55
6:H:10:PHE:CD1	6:H:57:VAL:HG23	2.41	0.55
2:B:458:LYS:CE	2:B:458:LYS:CG	2.83	0.55
2:B:28:GLU:CD	2:B:807:ARG:HH22	2.10	0.55
2:B:768:THR:N	2:B:768:THR:C	2.57	0.55
6:H:7:ASP:C	6:H:7:ASP:OD1	2.45	0.55
1:A:34:LYS:HG2	1:A:83:HIS:HE1	1.72	0.55
3:C:102:GLN:N	3:C:102:GLN:CG	2.70	0.55
1:A:203:SER:H	1:A:206:GLU:HG3	1.72	0.55
2:B:561:TRP:O	2:B:590:HIS:CE1	2.55	0.55
2:B:269:ILE:HB	2:B:282:ILE:HD12	1.88	0.55
9:K:55:LYS:HB3	9:K:81:TYR:HD1	1.72	0.55
1:A:1172:LEU:O	1:A:1173:HIS:CD2	2.60	0.55
2:B:830:TYR:O	2:B:831:SER:CB	2.52	0.55
2:B:120:ARG:CG	2:B:120:ARG:CA	2.79	0.54
6:H:77:ARG:C	6:H:78:SER:O	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1159:ARG:HG2	2:B:1160:VAL:H	1.72	0.54
3:C:55:THR:O	3:C:55:THR:HG22	2.07	0.54
4:E:213:ILE:HG21	4:E:213:ILE:CD1	2.37	0.54
2:B:127:GLY:CA	2:B:168:GLY:O	2.55	0.54
2:B:417:PHE:O	2:B:417:PHE:HD2	1.83	0.54
1:A:562:THR:HG22	6:H:98:TYR:CD2	2.42	0.54
1:A:976:THR:O	1:A:977:LYS:HG3	2.06	0.54
2:B:531:GLN:CG	2:B:531:GLN:CA	2.78	0.54
1:A:325:ILE:C	1:A:327:ALA:H	2.11	0.54
2:B:100:PRO:HD2	2:B:180:TYR:HE1	1.61	0.54
1:A:752:LYS:HE2	2:B:1019:SER:HG	1.67	0.54
1:A:497:THR:HG21	2:B:1149:GLU:OE1	2.08	0.54
2:B:191:LYS:CG	2:B:191:LYS:CA	2.79	0.54
2:B:458:LYS:CD	2:B:458:LYS:NZ	2.67	0.54
6:H:138:GLU:HG2	6:H:139:ASN:N	2.22	0.54
2:B:169:ARG:HG3	2:B:454:THR:OG1	2.07	0.54
1:A:119:ASN:O	1:A:120:GLU:HB2	2.07	0.54
3:C:11:ARG:HE	3:C:209:TYR:HE2	1.48	0.54
1:A:464:PRO:O	1:A:465:TYR:O	2.24	0.54
2:B:705:MET:CE	2:B:705:MET:HG3	2.33	0.54
4:E:41:ASP:O	4:E:42:PHE:C	2.45	0.54
6:H:130:ARG:HB2	6:H:133:ASN:HB3	1.89	0.54
6:H:59:ILE:H	6:H:59:ILE:CD1	2.20	0.54
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.89	0.54
2:B:820:GLY:HA3	2:B:1091:TYR:CZ	2.43	0.54
1:A:1349:TYR:CD2	1:A:1349:TYR:C	2.80	0.54
10:L:48:CYS:CA	10:L:49:LYS:N	2.64	0.54
1:A:274:ILE:CD1	1:A:274:ILE:HA	2.37	0.54
2:B:864:LYS:HG3	2:B:865:LYS:H	1.72	0.54
5:F:87:LYS:CD	5:F:87:LYS:NZ	2.70	0.54
7:I:40:SER:CB	7:I:41:PRO:CD	2.85	0.54
1:A:1267:MET:O	1:A:1268:LEU:C	2.41	0.54
2:B:414:ALA:O	2:B:418:LYS:N	2.41	0.54
2:B:25:ILE:HD12	2:B:25:ILE:CG2	2.38	0.54
4:E:71:LYS:NZ	4:E:160:GLU:OE2	2.24	0.54
6:H:2:SER:CA	6:H:3:ASN:N	2.65	0.54
2:B:914:LYS:HD3	2:B:937:ALA:HB3	1.89	0.54
9:K:49:GLU:CG	9:K:94:ILE:HD11	2.38	0.54
2:B:520:GLY:O	2:B:521:LEU:HD23	2.07	0.54
6:H:48:PRO:C	6:H:49:VAL:HG23	2.28	0.54
1:A:1313:LEU:O	1:A:1314:SER:C	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:THR:O	1:A:278:THR:HG22	2.07	0.54
9:K:26:LYS:CA	9:K:26:LYS:CG	2.80	0.54
1:A:407:ARG:HG2	1:A:430:TRP:CZ3	2.43	0.54
1:A:1359:ASP:CG	1:A:1359:ASP:CA	2.72	0.54
1:A:1203:ASN:C	1:A:1205:LYS:N	2.62	0.54
1:A:120:GLU:CG	1:A:123:ARG:HH22	2.19	0.54
2:B:369:GLY:CA	2:B:370:PHE:CD1	2.91	0.54
2:B:991:GLY:O	2:B:992:ILE:HB	2.08	0.54
1:A:274:ILE:CD1	1:A:274:ILE:CB	2.80	0.54
2:B:129:PHE:CD2	2:B:166:PHE:N	2.75	0.54
2:B:172:ILE:HG21	2:B:172:ILE:HD13	1.90	0.54
1:A:366:VAL:CG2	1:A:460:VAL:HG13	2.38	0.54
1:A:366:VAL:HG21	1:A:460:VAL:HG13	1.89	0.54
1:A:182:VAL:HG22	1:A:201:VAL:HG22	1.90	0.54
3:C:63:ILE:O	3:C:66:ARG:HB2	2.08	0.53
1:A:884:ASP:O	1:A:886:ILE:N	2.41	0.53
1:A:216:VAL:HA	1:A:219:PHE:CE2	2.43	0.53
1:A:1172:LEU:O	1:A:1173:HIS:CG	2.60	0.53
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.72	0.53
1:A:191:THR:HB	1:A:192:GLY:N	2.22	0.53
4:E:213:ILE:CD1	4:E:213:ILE:CG2	2.86	0.53
4:E:47:CYS:HA	4:E:48:ASP:N	2.23	0.53
1:A:741:ASN:ND2	1:A:741:ASN:C	2.60	0.53
9:K:103:THR:C	9:K:105:PHE:H	2.11	0.53
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.90	0.53
3:C:148:ARG:HH12	8:J:64:ASN:CG	2.12	0.53
1:A:534:LEU:O	1:A:574:GLY:HA3	2.08	0.53
2:B:205:ILE:HG22	2:B:205:ILE:O	2.06	0.53
4:E:47:CYS:CA	4:E:48:ASP:N	2.61	0.53
2:B:103:ASN:HB2	2:B:169:ARG:HH22	1.73	0.53
8:J:53:HIS:HE1	8:J:55:ASP:CA	2.21	0.53
1:A:537:ARG:NH2	1:A:600:PRO:O	2.41	0.53
2:B:237:VAL:CG1	2:B:238:ALA:N	2.71	0.53
3:C:40:GLU:HA	3:C:163:ILE:HG12	1.91	0.53
2:B:886:LYS:C	2:B:888:GLY:H	2.11	0.53
2:B:958:GLN:CG	2:B:958:GLN:CA	2.83	0.53
1:A:1203:ASN:O	1:A:1205:LYS:N	2.41	0.53
3:C:66:ARG:O	3:C:67:LEU:C	2.45	0.53
1:A:92:HIS:HD2	1:A:94:GLY:H	1.56	0.53
3:C:99:LEU:CD1	3:C:99:LEU:N	2.68	0.53
1:A:420:ARG:O	1:A:421:ALA:C	2.37	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:HIS:O	1:A:287:HIS:C	2.46	0.53
3:C:233:GLU:OE1	8:J:12:LYS:HE2	2.08	0.53
7:I:20:LYS:CD	7:I:20:LYS:CB	2.80	0.53
4:E:65:THR:O	4:E:69:ILE:HG13	2.07	0.53
2:B:864:LYS:N	2:B:872:GLU:HB2	2.24	0.53
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.90	0.53
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.44	0.53
3:C:10:ILE:HD13	3:C:10:ILE:N	2.20	0.53
1:A:274:ILE:HA	1:A:274:ILE:CB	2.20	0.53
1:A:633:VAL:O	1:A:634:THR:C	2.41	0.53
6:H:93:TYR:HD1	6:H:93:TYR:N	2.07	0.53
1:A:588:LEU:C	1:A:588:LEU:CD2	2.70	0.53
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.89	0.53
3:C:252:GLN:HE22	9:K:99:GLY:CA	2.22	0.53
2:B:282:ILE:HD11	2:B:317:CYS:SG	2.48	0.53
1:A:1287:TYR:O	1:A:1302:PRO:HA	2.08	0.53
2:B:807:ARG:CA	2:B:807:ARG:CG	2.80	0.53
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.74	0.53
8:J:42:LYS:HG3	8:J:43:ARG:N	2.23	0.53
4:E:80:VAL:HG22	4:E:109:ILE:HD12	1.91	0.53
1:A:1039:LYS:HE3	1:A:1043:ASP:OD2	2.08	0.53
1:A:587:HIS:CE1	1:A:969:GLN:HG2	2.44	0.53
1:A:644:LYS:NZ	1:A:644:LYS:CD	2.70	0.53
1:A:295:LEU:CB	1:A:295:LEU:CD2	2.82	0.53
2:B:1152:MET:HE3	2:B:1152:MET:HA	1.88	0.53
2:B:60:GLN:O	2:B:60:GLN:HG3	1.98	0.53
2:B:137:TYR:CG	2:B:137:TYR:HB3	2.21	0.53
10:L:65:VAL:CG1	10:L:65:VAL:CG2	2.78	0.53
1:A:1450:LEU:CD1	1:A:1450:LEU:CB	2.83	0.53
8:J:43:ARG:O	8:J:47:ARG:HG3	2.09	0.53
1:A:28:ARG:CG	1:A:28:ARG:NE	2.67	0.53
2:B:806:THR:HG23	2:B:808:ALA:H	1.73	0.53
1:A:476:SER:N	1:A:477:PRO:HD2	2.24	0.53
6:H:10:PHE:O	6:H:55:LEU:N	2.39	0.53
3:C:196:ASP:CG	3:C:199:LYS:HG3	2.29	0.53
1:A:596:THR:CG2	1:A:597:LEU:N	2.72	0.53
1:A:567:LYS:CE	1:A:567:LYS:CG	2.82	0.53
2:B:705:MET:CE	2:B:745:PRO:HG3	2.39	0.53
9:K:40:HIS:O	9:K:41:THR:C	2.43	0.53
1:A:4:GLN:CG	1:A:4:GLN:H	2.22	0.52
1:A:271:LYS:CB	1:A:271:LYS:CD	2.80	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:864:LYS:CB	2:B:872:GLU:H	2.22	0.52
3:C:253:LYS:NZ	3:C:253:LYS:CD	2.67	0.52
1:A:518:LYS:CG	1:A:518:LYS:CE	2.83	0.52
8:J:2:ILE:HD11	8:J:57:ILE:HD12	1.91	0.52
3:C:56:THR:HG23	3:C:57:VAL:N	2.22	0.52
1:A:547:LEU:HB3	9:K:58:PHE:HE1	1.71	0.52
1:A:353:ILE:HG21	1:A:487:MET:SD	2.49	0.52
2:B:1182:CYS:HB3	2:B:1185:CYS:HB2	1.91	0.52
2:B:705:MET:HE3	2:B:745:PRO:HG3	1.92	0.52
8:J:3:VAL:HA	8:J:53:HIS:CD2	2.44	0.52
9:K:1:MET:HB3	9:K:3:ALA:H	1.73	0.52
1:A:418:SER:C	1:A:420:ARG:N	2.60	0.52
1:A:1226:VAL:CG1	1:A:1227:ILE:N	2.65	0.52
2:B:25:ILE:HD13	2:B:25:ILE:N	2.24	0.52
3:C:66:ARG:CG	3:C:66:ARG:HH11	2.00	0.52
3:C:35:ARG:HH11	9:K:41:THR:H	1.58	0.52
2:B:95:ILE:CG2	2:B:96:TYR:N	2.70	0.52
2:B:603:LEU:HD22	2:B:608:ASP:HB2	1.91	0.52
2:B:962:LYS:CD	2:B:962:LYS:CB	2.80	0.52
1:A:567:LYS:HB3	6:H:96:VAL:HG23	1.92	0.52
2:B:625:LYS:NZ	2:B:625:LYS:HD2	2.22	0.52
1:A:1408:ILE:HG22	1:A:1408:ILE:O	2.09	0.52
2:B:502:ILE:HA	2:B:502:ILE:CD1	2.37	0.52
2:B:914:LYS:N	2:B:938:SER:HB2	2.22	0.52
4:E:85:GLU:OE2	4:E:92:THR:OG1	2.22	0.52
2:B:414:ALA:O	2:B:415:GLN:C	2.47	0.52
10:L:51:CYS:SG	10:L:51:CYS:O	2.68	0.52
1:A:11:LEU:CD1	2:B:1195:HIS:CD2	2.92	0.52
1:A:7:SER:O	1:A:9:ALA:N	2.42	0.52
3:C:205:LYS:O	3:C:207:CYS:N	2.42	0.52
9:K:111:LEU:CD1	9:K:111:LEU:HG	2.25	0.52
8:J:7:CYS:SG	8:J:46:CYS:N	2.82	0.52
1:A:103:CYS:SG	1:A:207:ILE:HD12	2.50	0.52
1:A:555:ASP:OD1	9:K:26:LYS:CE	2.58	0.52
2:B:1172:ILE:CG2	2:B:1172:ILE:CA	2.75	0.52
8:J:42:LYS:CD	8:J:42:LYS:CB	2.80	0.52
2:B:117:ALA:O	2:B:207:GLY:HA2	2.10	0.52
1:A:744:LYS:HD3	1:A:748:MET:SD	2.49	0.52
1:A:45:GLN:C	1:A:45:GLN:HA	2.13	0.52
1:A:768:GLN:NE2	1:A:816:HIS:HA	2.25	0.52
2:B:1172:ILE:O	2:B:1180:PHE:HA	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1008:PRO:HG2	2:B:1011:ILE:HD11	1.91	0.52
2:B:958:GLN:H	2:B:958:GLN:CG	2.23	0.52
2:B:245:GLU:CA	2:B:246:LYS:N	2.67	0.52
4:E:90:VAL:CG1	4:E:90:VAL:CA	2.80	0.52
2:B:1222:ARG:N	2:B:1222:ARG:HD3	2.25	0.52
1:A:606:LEU:HD23	1:A:613:ILE:CG2	2.40	0.52
1:A:4:GLN:HG2	1:A:4:GLN:N	2.24	0.52
1:A:1264:GLU:OE2	7:I:46:HIS:HD2	1.92	0.52
1:A:180:LYS:CA	1:A:180:LYS:CG	2.80	0.52
2:B:1006:ILE:HD12	2:B:1006:ILE:N	2.25	0.52
2:B:965:LYS:NZ	2:B:965:LYS:CD	2.72	0.52
1:A:786:HIS:CD2	1:A:786:HIS:H	2.25	0.52
5:F:80:ALA:C	5:F:80:ALA:CB	2.71	0.52
1:A:934:LYS:NZ	1:A:934:LYS:CD	2.73	0.52
8:J:53:HIS:C	8:J:53:HIS:ND1	2.63	0.52
3:C:112:ASN:HB2	3:C:114:TYR:CE1	2.45	0.52
2:B:733:HIS:C	2:B:733:HIS:CB	2.76	0.51
2:B:563:MET:CB	2:B:563:MET:SD	2.91	0.51
1:A:50:ILE:CG2	1:A:51:GLY:N	2.71	0.51
1:A:1146:VAL:CG1	1:A:1197:LEU:HD22	2.40	0.51
1:A:134:ARG:HD2	1:A:221:SER:O	2.10	0.51
1:A:39:GLU:HB3	1:A:50:ILE:CD1	2.40	0.51
1:A:1259:MET:O	1:A:1260:LEU:C	2.47	0.51
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.45	0.51
2:B:249:ARG:CD	2:B:249:ARG:CB	2.86	0.51
2:B:25:ILE:HD12	2:B:25:ILE:HG23	1.92	0.51
6:H:95:TYR:HB3	6:H:144:ILE:HB	1.92	0.51
2:B:594:ALA:HB2	2:B:617:ARG:NH1	2.25	0.51
1:A:1315:GLU:O	1:A:1318:THR:HG22	2.09	0.51
1:A:1127:ASP:O	1:A:1128:GLN:C	2.49	0.51
1:A:346:ASP:O	1:A:347:PHE:HB2	2.11	0.51
1:A:709:THR:HB	1:A:712:GLU:HG3	1.92	0.51
9:K:77:THR:OG1	9:K:83:PRO:HD3	2.10	0.51
2:B:830:TYR:O	2:B:831:SER:OG	2.21	0.51
2:B:884:ARG:O	2:B:936:ASP:HB3	2.09	0.51
1:A:976:THR:O	1:A:977:LYS:CG	2.58	0.51
4:E:7:ARG:CA	4:E:7:ARG:CG	2.82	0.51
1:A:55:ASP:C	1:A:57:ARG:H	1.93	0.51
2:B:130:VAL:CG2	2:B:167:ILE:HD11	2.41	0.51
4:E:156:LEU:HB3	4:E:160:GLU:CB	2.40	0.51
3:C:56:THR:CG2	3:C:58:LEU:H	2.23	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:CYS:SG	1:A:167:CYS:CB	2.96	0.51
1:A:369:SER:CB	9:K:2:ASN:HD21	2.23	0.51
1:A:901:LEU:N	1:A:926:GLN:NE2	2.50	0.51
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.11	0.51
3:C:26:ASP:O	3:C:27:LEU:C	2.47	0.51
4:E:117:THR:C	4:E:119:SER:H	2.12	0.51
10:L:38:LEU:HG	10:L:39:SER:N	2.25	0.51
2:B:25:ILE:H	2:B:25:ILE:HD13	1.75	0.51
1:A:143:LYS:CG	1:A:143:LYS:CE	2.81	0.51
7:I:30:ARG:CD	7:I:30:ARG:CB	2.80	0.51
3:C:166:GLU:O	3:C:167:HIS:HB2	2.10	0.51
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.74	0.51
9:K:103:THR:O	9:K:105:PHE:N	2.42	0.51
1:A:844:ALA:HB2	1:A:1384:VAL:HG12	1.92	0.51
3:C:69:LEU:HB2	8:J:5:VAL:HG11	1.93	0.51
1:A:780:VAL:O	1:A:781:ASP:HB2	2.10	0.51
1:A:789:LYS:HG3	7:I:67:THR:HB	1.92	0.51
2:B:1163:CYS:CB	2:B:1166:CYS:SG	2.98	0.51
6:H:103:LYS:HG2	6:H:105:GLU:OE1	2.08	0.51
6:H:4:THR:C	6:H:5:LEU:CD2	2.70	0.51
1:A:1364:ASN:HD22	1:A:1365:TYR:N	2.08	0.51
3:C:43:THR:CG2	3:C:44:LEU:N	2.74	0.51
2:B:458:LYS:O	2:B:459:TYR:C	2.49	0.51
1:A:53:LEU:O	1:A:56:PRO:HD3	2.11	0.51
2:B:165:VAL:O	2:B:165:VAL:HG12	2.11	0.51
9:K:28:PRO:O	9:K:29:ASN:HB2	2.09	0.51
7:I:40:SER:HB2	7:I:41:PRO:CD	2.41	0.51
2:B:692:TYR:O	2:B:693:ILE:HD13	2.10	0.51
2:B:35:SER:HA	2:B:811:TYR:CE2	2.46	0.51
2:B:1002:THR:HG22	2:B:1006:ILE:N	2.25	0.51
3:C:120:ILE:C	3:C:121:VAL:HG23	2.31	0.51
1:A:187:LYS:CA	1:A:188:ASP:N	2.68	0.51
2:B:1065:GLN:NE2	2:B:1067:ARG:N	2.58	0.51
1:A:154:SER:C	1:A:155:GLU:O	2.49	0.51
1:A:351:THR:HG21	2:B:1103:ILE:CG1	2.36	0.51
9:K:83:PRO:C	9:K:85:ASP:N	2.62	0.51
1:A:902:LEU:N	1:A:902:LEU:HD23	2.25	0.51
4:E:154:ILE:HD12	4:E:154:ILE:N	2.26	0.51
6:H:32:THR:HG22	6:H:33:GLN:OE1	2.10	0.51
2:B:98:THR:O	2:B:126:SER:OG	2.23	0.51
7:I:120:GLN:O	7:I:121:PHE:CG	2.63	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:HIS:CD2	1:A:786:HIS:N	2.78	0.51
1:A:979:SER:OG	1:A:981:LEU:HB2	2.10	0.51
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.45	0.51
2:B:206:ASN:OD1	2:B:458:LYS:HE3	2.10	0.51
1:A:176:LYS:CG	1:A:176:LYS:CE	2.82	0.51
6:H:40:LEU:HD12	6:H:41:ASP:H	1.76	0.51
3:C:230:MET:SD	3:C:230:MET:CB	2.98	0.51
3:C:167:HIS:CE1	10:L:70:ARG:O	2.62	0.51
2:B:89:GLU:C	2:B:90:ILE:HD12	2.31	0.51
1:A:834:THR:HG21	1:A:1077:THR:CA	2.41	0.51
3:C:44:LEU:HG	3:C:45:ALA:N	2.26	0.51
2:B:26:THR:O	2:B:27:ALA:C	2.49	0.51
2:B:129:PHE:CE2	2:B:166:PHE:N	2.79	0.50
10:L:60:ARG:O	10:L:61:THR:C	2.42	0.50
3:C:124:LEU:O	3:C:127:ARG:HG3	2.11	0.50
2:B:654:ARG:H	2:B:657:HIS:CD2	2.22	0.50
2:B:225:VAL:CG1	2:B:226:PHE:N	2.74	0.50
6:H:83:GLN:O	6:H:84:ALA:C	2.49	0.50
8:J:24:LEU:HD22	8:J:30:LEU:HD12	1.93	0.50
2:B:1020:ARG:O	2:B:1021:MET:HB2	2.10	0.50
2:B:419:THR:HG22	2:B:419:THR:O	2.09	0.50
6:H:11:GLN:HB3	6:H:29:ALA:HB3	1.94	0.50
4:E:57:MET:SD	4:E:57:MET:CE	2.99	0.50
2:B:121:ASN:HD21	2:B:965:LYS:NZ	2.09	0.50
2:B:592:ASN:O	2:B:593:PRO:C	2.47	0.50
1:A:941:LYS:CB	1:A:941:LYS:CD	2.78	0.50
4:E:93:MET:CE	4:E:93:MET:CG	2.89	0.50
1:A:369:SER:N	9:K:2:ASN:HD21	2.08	0.50
1:A:741:ASN:ND2	1:A:743:VAL:H	2.09	0.50
9:K:82:ASP:OD1	9:K:83:PRO:N	2.43	0.50
3:C:33:LEU:HD13	3:C:248:ILE:HD13	1.93	0.50
6:H:10:PHE:HB3	6:H:29:ALA:O	2.12	0.50
2:B:643:ASP:CG	2:B:644:GLU:O	2.50	0.50
4:E:97:VAL:HG13	4:E:127:ILE:HD13	1.93	0.50
3:C:19:ASP:OD1	3:C:20:PHE:N	2.44	0.50
1:A:950:GLY:CA	1:A:1298:TYR:CZ	2.95	0.50
1:A:1259:MET:HB2	1:A:1259:MET:SD	2.51	0.50
2:B:341:LEU:HD12	2:B:342:GLY:N	2.27	0.50
7:I:41:PRO:HD2	7:I:42:LEU:H	1.76	0.50
9:K:88:LYS:CB	9:K:88:LYS:CD	2.85	0.50
1:A:35:ILE:HD12	1:A:35:ILE:N	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:181:ASP:N	3:C:182:PRO:HD2	2.26	0.50
3:C:209:TYR:CD1	3:C:209:TYR:N	2.80	0.50
3:C:218:PRO:O	3:C:218:PRO:CG	2.59	0.50
1:A:722:LEU:HD22	1:A:799:PHE:CD1	2.47	0.50
1:A:365:GLY:HA2	1:A:461:LYS:O	2.11	0.50
1:A:560:ILE:O	1:A:561:PRO:C	2.49	0.50
1:A:191:THR:CA	1:A:191:THR:HB	2.20	0.50
4:E:213:ILE:HG21	4:E:213:ILE:HD13	1.92	0.50
4:E:56:LYS:CG	4:E:56:LYS:CE	2.85	0.50
4:E:96:PHE:CE2	4:E:100:ILE:CD1	2.95	0.50
4:E:39:LEU:O	4:E:43:LYS:N	2.45	0.50
3:C:127:ARG:C	3:C:127:ARG:N	2.57	0.50
8:J:1:MET:HG3	8:J:60:PHE:HE2	1.77	0.50
1:A:844:ALA:CB	1:A:1384:VAL:HG12	2.40	0.50
9:K:83:PRO:O	9:K:84:LYS:C	2.46	0.50
6:H:118:PHE:C	6:H:120:GLY:N	2.63	0.50
2:B:373:ARG:HD2	2:B:567:GLU:OE1	2.12	0.50
6:H:63:LEU:H	6:H:63:LEU:HD12	1.77	0.50
2:B:235:SER:OG	2:B:236:HIS:HD2	1.94	0.50
4:E:14:ARG:O	4:E:15:ALA:C	2.43	0.50
1:A:1203:ASN:C	1:A:1205:LYS:H	2.14	0.50
1:A:1135:ARG:CG	1:A:1135:ARG:NE	2.70	0.50
6:H:48:PRO:O	6:H:49:VAL:CG2	2.59	0.50
2:B:1184:GLY:H	2:B:1186:ASP:H	1.58	0.50
4:E:65:THR:O	4:E:66:GLU:C	2.48	0.50
3:C:121:VAL:HG12	3:C:121:VAL:O	2.11	0.50
1:A:1271:ILE:HG22	1:A:1272:THR:N	2.26	0.50
7:I:7:CYS:SG	7:I:29:CYS:SG	3.10	0.50
1:A:982:THR:O	1:A:985:ASP:HB2	2.12	0.50
3:C:181:ASP:OD2	3:C:186:LEU:HB2	2.11	0.50
1:A:853:ASP:OD2	1:A:857:ARG:NH2	2.42	0.50
4:E:1:MET:CG	4:E:1:MET:CA	2.82	0.50
2:B:130:VAL:HG23	2:B:167:ILE:HD11	1.94	0.50
3:C:29:MET:HB2	3:C:29:MET:CE	2.42	0.50
2:B:68:THR:CG2	2:B:91:SER:HB3	2.41	0.50
1:A:7:SER:O	1:A:8:SER:C	2.48	0.50
2:B:64:CYS:C	2:B:65:GLU:O	2.49	0.50
1:A:1132:LYS:O	1:A:1133:LEU:C	2.46	0.49
1:A:295:LEU:CD1	1:A:295:LEU:CD2	2.88	0.49
8:J:1:MET:CB	8:J:1:MET:HE3	2.37	0.49
2:B:657:HIS:O	2:B:658:ILE:C	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:28:TYR:CZ	4:E:75:MET:HE2	2.47	0.49
4:E:28:TYR:CZ	4:E:75:MET:HE3	2.47	0.49
1:A:914:GLU:C	1:A:916:GLY:N	2.66	0.49
4:E:44:ALA:HB3	4:E:45:LYS:H	1.77	0.49
2:B:99:LYS:CB	2:B:100:PRO:CD	2.85	0.49
8:J:53:HIS:CE1	8:J:54:VAL:C	2.85	0.49
2:B:502:ILE:CA	2:B:502:ILE:CG1	2.85	0.49
3:C:195:GLN:CD	3:C:195:GLN:CB	2.77	0.49
3:C:180:TYR:OH	3:C:188:HIS:ND1	2.30	0.49
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.94	0.49
7:I:40:SER:HB2	7:I:41:PRO:HD3	1.94	0.49
1:A:1318:THR:HB	1:A:1318:THR:CG2	2.20	0.49
3:C:102:GLN:N	3:C:102:GLN:HG2	2.27	0.49
8:J:2:ILE:O	8:J:3:VAL:C	2.50	0.49
1:A:950:GLY:HA2	1:A:1298:TYR:CZ	2.46	0.49
2:B:417:PHE:C	2:B:417:PHE:HD2	2.15	0.49
1:A:920:LEU:HD22	1:A:921:GLY:H	1.74	0.49
3:C:100:THR:CG2	3:C:101:LEU:N	2.71	0.49
2:B:904:ARG:C	2:B:905:VAL:HG13	2.32	0.49
1:A:826:ASP:O	1:A:827:THR:C	2.44	0.49
1:A:1012:ARG:CB	1:A:1012:ARG:CD	2.85	0.49
1:A:982:THR:HG22	1:A:984:LYS:N	2.27	0.49
9:K:23:PRO:O	9:K:23:PRO:HD2	2.12	0.49
1:A:1198:ASP:OD1	1:A:1200:ALA:HB3	2.13	0.49
4:E:118:PRO:CA	4:E:118:PRO:CG	2.88	0.49
3:C:260:LEU:CD1	3:C:260:LEU:CD2	2.87	0.49
1:A:535:THR:CG2	1:A:617:VAL:N	2.55	0.49
2:B:516:ASN:N	2:B:516:ASN:ND2	2.59	0.49
2:B:658:ILE:CG2	2:B:658:ILE:O	2.59	0.49
3:C:47:ASP:CG	3:C:47:ASP:O	2.51	0.49
2:B:345:LYS:O	2:B:346:GLU:C	2.46	0.49
1:A:1217:LYS:CD	1:A:1217:LYS:NZ	2.67	0.49
7:I:83:ASN:HA	7:I:102:VAL:O	2.13	0.49
2:B:118:ARG:HH22	2:B:194:GLU:CG	2.24	0.49
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.12	0.49
9:K:49:GLU:HG3	9:K:94:ILE:CD1	2.42	0.49
1:A:1411:GLU:O	1:A:1412:ALA:C	2.48	0.49
3:C:266:ASP:OD1	3:C:266:ASP:N	2.45	0.49
4:E:118:PRO:O	4:E:121:MET:SD	2.70	0.49
7:I:109:ILE:HD12	7:I:109:ILE:N	2.28	0.49
4:E:58:MET:O	4:E:59:SER:O	2.31	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:57:ILE:O	8:J:60:PHE:N	2.46	0.49
5:F:123:LYS:HD2	5:F:123:LYS:NZ	2.27	0.49
1:A:67:CYS:SG	1:A:77:CYS:SG	3.08	0.49
2:B:266:ALA:CB	2:B:266:ALA:C	2.73	0.49
1:A:132:LYS:CB	1:A:132:LYS:CD	2.83	0.49
2:B:365:THR:HG22	2:B:366:GLN:N	2.27	0.49
1:A:1151:GLU:HG2	7:I:45:ARG:CD	2.43	0.49
2:B:1006:ILE:CD1	8:J:43:ARG:HD2	2.42	0.49
2:B:960:GLY:O	2:B:961:LEU:C	2.47	0.49
2:B:1176:ASN:ND2	2:B:1176:ASN:CB	2.69	0.49
1:A:1258:HIS:O	1:A:1259:MET:C	2.51	0.49
1:A:1122:PRO:O	1:A:1123:GLY:C	2.49	0.49
2:B:739:THR:O	2:B:740:HIS:CG	2.66	0.49
10:L:30:ILE:CD1	10:L:30:ILE:CB	2.78	0.49
6:H:4:THR:O	6:H:5:LEU:CB	2.60	0.49
1:A:672:ASP:HB2	1:A:736:ASN:ND2	2.28	0.49
3:C:77:ILE:HG13	3:C:77:ILE:O	2.11	0.49
4:E:112:TYR:CZ	4:E:116:ILE:HD11	2.47	0.49
3:C:208:GLU:O	3:C:210:GLU:N	2.45	0.49
4:E:97:VAL:HG12	4:E:97:VAL:O	2.13	0.49
1:A:636:GLU:OE2	1:A:962:ARG:CD	2.60	0.49
1:A:325:ILE:C	1:A:327:ALA:N	2.67	0.49
2:B:421:PHE:O	2:B:425:THR:HB	2.13	0.48
1:A:1264:GLU:OE1	7:I:44:TYR:CE2	2.66	0.48
1:A:35:ILE:HG23	1:A:53:LEU:HB2	1.95	0.48
8:J:2:ILE:N	8:J:2:ILE:HD12	2.25	0.48
1:A:926:GLN:HG3	1:A:926:GLN:O	2.13	0.48
1:A:325:ILE:CG2	1:A:325:ILE:O	2.61	0.48
1:A:265:LYS:HE2	1:A:299:HIS:O	2.13	0.48
1:A:387:ARG:O	1:A:388:LEU:C	2.52	0.48
1:A:1148:ILE:CD1	1:A:1148:ILE:HG21	2.43	0.48
2:B:705:MET:HB2	2:B:705:MET:SD	2.50	0.48
2:B:134:LYS:CB	2:B:134:LYS:HE3	2.39	0.48
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.78	0.48
2:B:515:HIS:N	2:B:518:HIS:HD2	1.98	0.48
8:J:14:VAL:HG13	8:J:14:VAL:O	2.13	0.48
2:B:276:ILE:HD11	2:B:355:ILE:HG13	1.94	0.48
1:A:373:THR:O	1:A:373:THR:HG22	2.10	0.48
2:B:864:LYS:HD2	2:B:871:THR:OG1	2.13	0.48
1:A:567:LYS:CE	6:H:95:TYR:CG	2.89	0.48
1:A:156:ASP:O	1:A:158:PRO:CD	2.57	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1162:ILE:HD13	2:B:1162:ILE:HA	1.54	0.48
1:A:125:ALA:HA	1:A:128:ILE:HG12	1.95	0.48
2:B:206:ASN:OD1	2:B:458:LYS:HE2	2.12	0.48
1:A:44:THR:OG1	1:A:44:THR:CG2	2.57	0.48
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.95	0.48
6:H:17:PRO:O	6:H:18:GLY:C	2.50	0.48
4:E:61:GLN:HB2	4:E:79:TRP:CE3	2.47	0.48
4:E:98:ILE:HA	4:E:98:ILE:CG1	2.42	0.48
1:A:567:LYS:CG	6:H:96:VAL:N	2.67	0.48
1:A:1171:GLN:CG	1:A:1171:GLN:NE2	2.67	0.48
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.96	0.48
3:C:131:HIS:O	3:C:132:PRO:C	2.47	0.48
2:B:910:VAL:C	2:B:911:ILE:HD12	2.33	0.48
7:I:50:THR:HG23	7:I:50:THR:O	2.12	0.48
2:B:25:ILE:CD1	2:B:25:ILE:CG2	2.91	0.48
2:B:110:HIS:C	2:B:110:HIS:CB	2.73	0.48
8:J:53:HIS:C	8:J:53:HIS:HD1	2.16	0.48
2:B:313:MET:HE3	2:B:386:LEU:CD2	2.32	0.48
5:F:138:LEU:HB3	5:F:139:PRO:CD	2.44	0.48
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.49	0.48
2:B:710:LEU:N	2:B:710:LEU:HD23	2.29	0.48
1:A:982:THR:HG22	1:A:984:LYS:H	1.78	0.48
2:B:307:ASP:C	2:B:309:GLN:N	2.64	0.48
7:I:50:THR:CG2	7:I:50:THR:O	2.61	0.48
1:A:1224:LEU:HG	1:A:1225:PHE:N	2.26	0.48
1:A:1262:LYS:O	1:A:1265:ASN:N	2.46	0.48
4:E:159:ASP:O	4:E:162:ARG:N	2.46	0.48
6:H:105:GLU:N	6:H:105:GLU:CD	2.66	0.48
3:C:126:GLY:C	3:C:127:ARG:CA	2.70	0.48
5:F:111:LEU:C	5:F:113:GLY:N	2.67	0.48
1:A:896:ARG:CD	1:A:897:TYR:CE1	2.97	0.48
1:A:870:GLU:HG2	4:E:208:TYR:CD1	2.48	0.48
10:L:30:ILE:HG22	10:L:31:CYS:N	2.27	0.48
10:L:34:CYS:SG	10:L:51:CYS:HB3	2.54	0.48
6:H:123:MET:HG2	6:H:124:ARG:N	2.28	0.48
2:B:933:SER:CA	2:B:934:LYS:N	2.67	0.48
7:I:98:VAL:CG1	7:I:98:VAL:O	2.61	0.48
1:A:98:LYS:O	1:A:99:ILE:C	2.52	0.48
2:B:755:ILE:HD13	2:B:755:ILE:N	2.26	0.48
1:A:445:ASN:HA	1:A:454:SER:O	2.13	0.48
1:A:650:GLN:O	1:A:654:ASN:HB2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:135:ARG:CB	5:F:135:ARG:CD	2.82	0.48
2:B:357:GLN:HE21	2:B:368:GLU:HG2	1.77	0.48
1:A:1112:LYS:CA	1:A:1112:LYS:CG	2.78	0.48
1:A:1239:ARG:HG3	1:A:1239:ARG:O	2.13	0.48
2:B:127:GLY:C	2:B:128:LEU:HD13	2.34	0.48
1:A:1272:THR:OG1	1:A:1272:THR:CG2	2.55	0.48
6:H:101:ALA:HB2	6:H:116:TYR:CD2	2.49	0.48
4:E:43:LYS:CA	4:E:43:LYS:CG	2.83	0.48
8:J:26:GLN:CA	8:J:26:GLN:CG	2.84	0.48
2:B:515:HIS:CD2	2:B:517:THR:H	2.32	0.48
6:H:81:PRO:HB2	6:H:82:PRO:HD2	1.93	0.48
1:A:852:TYR:CD2	5:F:136:ARG:HD3	2.49	0.48
1:A:1287:TYR:O	1:A:1303:GLU:N	2.37	0.48
2:B:794:ASN:O	2:B:795:ILE:HD13	2.13	0.48
2:B:600:LEU:O	2:B:601:ARG:C	2.50	0.48
2:B:845:SER:O	2:B:846:ILE:C	2.49	0.47
6:H:32:THR:CB	6:H:33:GLN:OE1	2.62	0.47
1:A:566:ILE:HD12	1:A:566:ILE:CG2	2.43	0.47
9:K:39:ASP:HB2	9:K:40:HIS:H	1.36	0.47
3:C:209:TYR:N	3:C:209:TYR:HD1	2.10	0.47
1:A:296:LEU:HA	1:A:296:LEU:HD12	1.42	0.47
1:A:44:THR:CA	1:A:44:THR:HB	2.30	0.47
1:A:1213:GLY:HA3	1:A:1228:TRP:CH2	2.48	0.47
1:A:1449:SER:CB	5:F:149:GLU:OE2	2.61	0.47
9:K:49:GLU:C	9:K:51:LEU:N	2.67	0.47
2:B:287:ARG:O	2:B:327:ARG:HG3	2.13	0.47
4:E:140:LEU:O	4:E:141:VAL:C	2.49	0.47
9:K:11:LEU:CD1	9:K:11:LEU:CB	2.81	0.47
1:A:217:LYS:O	1:A:221:SER:HB2	2.14	0.47
6:H:130:ARG:HB2	6:H:133:ASN:CB	2.44	0.47
2:B:984:HIS:CD2	2:B:1025:HIS:CA	2.96	0.47
1:A:503:GLN:HE21	5:F:90:ARG:NH2	2.07	0.47
1:A:1282:VAL:CG1	1:A:1283:VAL:N	2.72	0.47
2:B:942:ARG:HB2	2:B:945:GLU:HB2	1.95	0.47
6:H:10:PHE:CD1	6:H:57:VAL:CG2	2.97	0.47
6:H:8:ASP:OD2	6:H:9:ILE:N	2.37	0.47
2:B:642:ASP:HA	2:B:643:ASP:HA	1.28	0.47
4:E:57:MET:CA	4:E:57:MET:CG	2.84	0.47
10:L:26:THR:CG2	10:L:26:THR:OG1	2.58	0.47
6:H:138:GLU:O	6:H:139:ASN:O	2.27	0.47
1:A:858:ASN:ND2	1:A:862:ASN:H	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:ARG:NH2	5:F:139:PRO:HG2	2.29	0.47
1:A:1153:TYR:CZ	7:I:42:LEU:HD13	2.50	0.47
6:H:48:PRO:O	6:H:49:VAL:HG23	2.14	0.47
1:A:7:SER:C	1:A:9:ALA:H	2.18	0.47
1:A:970:THR:HG22	1:A:970:THR:O	2.14	0.47
6:H:15:VAL:HG12	6:H:15:VAL:O	2.14	0.47
2:B:1058:LEU:O	2:B:1062:HIS:HD2	1.96	0.47
1:A:35:ILE:H	1:A:35:ILE:CD1	2.20	0.47
1:A:633:VAL:CG2	1:A:633:VAL:CA	2.83	0.47
2:B:101:MET:CA	2:B:110:HIS:O	2.51	0.47
3:C:239:PRO:O	3:C:240:VAL:C	2.51	0.47
2:B:224:GLN:HB3	2:B:226:PHE:CZ	2.49	0.47
9:K:105:PHE:C	9:K:107:THR:N	2.67	0.47
3:C:214:ASN:O	3:C:217:ASP:N	2.47	0.47
1:A:567:LYS:CD	1:A:567:LYS:HE2	2.18	0.47
2:B:487:THR:HG23	2:B:488:TYR:N	2.30	0.47
1:A:1004:ASN:ND2	4:E:167:ARG:HG3	2.30	0.47
2:B:827:ILE:HG21	2:B:827:ILE:HD13	1.23	0.47
1:A:384:ASN:C	1:A:384:ASN:OD1	2.53	0.47
1:A:913:LEU:HD12	1:A:913:LEU:C	2.31	0.47
2:B:1173:ALA:HA	2:B:1180:PHE:HD2	1.80	0.47
2:B:875:GLU:O	2:B:876:LYS:C	2.52	0.47
1:A:1217:LYS:O	1:A:1221:LYS:N	2.47	0.47
2:B:801:LYS:CG	2:B:801:LYS:CE	2.83	0.47
1:A:187:LYS:CG	1:A:194:ALA:CB	2.91	0.47
2:B:172:ILE:HG21	2:B:172:ILE:CD1	2.44	0.47
1:A:1220:PHE:CE2	1:A:1263:ILE:HD12	2.50	0.47
2:B:89:GLU:C	2:B:90:ILE:CD1	2.83	0.47
1:A:470:LEU:HD11	1:A:487:MET:SD	2.54	0.47
2:B:1079:LYS:HE3	3:C:188:HIS:CE1	2.50	0.47
3:C:11:ARG:O	3:C:12:GLU:HB2	2.13	0.47
2:B:65:GLU:HG2	2:B:66:ASP:H	1.80	0.47
2:B:1082:MET:HA	3:C:189:THR:HA	1.95	0.47
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.94	0.47
1:A:78:PRO:HB2	1:A:79:GLY:O	2.14	0.47
1:A:1148:ILE:CG2	1:A:1148:ILE:CD1	2.92	0.47
1:A:1109:LYS:HA	1:A:1109:LYS:CG	2.43	0.47
2:B:789:MET:CE	2:B:965:LYS:CB	2.88	0.47
1:A:71:GLN:CG	1:A:71:GLN:NE2	2.69	0.47
1:A:571:LEU:HA	1:A:571:LEU:HD12	1.68	0.47
1:A:843:LYS:NZ	1:A:843:LYS:CD	2.69	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:502:ILE:CA	2:B:502:ILE:CD1	2.93	0.47
2:B:768:THR:O	2:B:769:TYR:C	2.50	0.47
7:I:16:PRO:O	7:I:17:ARG:CD	2.57	0.47
1:A:216:VAL:HG22	1:A:219:PHE:HZ	1.80	0.47
2:B:661:LEU:HD23	2:B:679:TYR:CD2	2.50	0.47
7:I:118:ARG:CD	7:I:118:ARG:CB	2.85	0.47
1:A:829:VAL:HB	1:A:829:VAL:CG2	2.20	0.47
1:A:620:LYS:CE	1:A:620:LYS:CG	2.91	0.47
2:B:882:THR:HG1	2:B:933:SER:N	2.13	0.47
1:A:557:ASP:OD1	1:A:557:ASP:C	2.51	0.47
2:B:240:ILE:HG13	2:B:241:ARG:N	2.30	0.47
1:A:1161:THR:CG2	1:A:1162:VAL:N	2.77	0.47
1:A:567:LYS:CD	1:A:568:PRO:CD	2.88	0.47
2:B:916:THR:HB	2:B:935:ARG:HB3	1.96	0.47
1:A:31:SER:HB2	1:A:83:HIS:CD2	2.46	0.47
3:C:9:LYS:CD	3:C:9:LYS:CB	2.77	0.47
1:A:92:HIS:HD2	1:A:94:GLY:N	2.12	0.47
1:A:1106:ASN:O	1:A:1107:VAL:C	2.49	0.47
2:B:1182:CYS:HB3	2:B:1185:CYS:CB	2.43	0.46
4:E:74:ASP:N	4:E:74:ASP:OD1	2.48	0.46
6:H:131:ASN:HD22	6:H:131:ASN:H	1.63	0.46
6:H:100:THR:HG22	6:H:101:ALA:N	2.29	0.46
9:K:110:ASN:CA	9:K:110:ASN:CG	2.71	0.46
4:E:48:ASP:HB3	4:E:54:GLN:HG2	1.97	0.46
1:A:868:TYR:HE1	1:A:1064:VAL:HG13	1.81	0.46
1:A:58:LEU:HB3	1:A:80:HIS:O	2.14	0.46
1:A:533:LYS:HZ3	1:A:745:GLN:HE22	1.62	0.46
2:B:225:VAL:O	2:B:226:PHE:CD2	2.68	0.46
1:A:507:VAL:N	1:A:508:PRO:CD	2.77	0.46
1:A:775:ILE:HG22	1:A:776:ALA:N	2.28	0.46
2:B:189:LEU:HA	2:B:189:LEU:HD23	1.46	0.46
3:C:199:LYS:N	3:C:199:LYS:CG	2.78	0.46
4:E:12:LEU:HD13	4:E:55:ARG:NE	2.30	0.46
4:E:55:ARG:O	4:E:57:MET:N	2.48	0.46
3:C:120:ILE:H	3:C:120:ILE:HD12	1.80	0.46
1:A:984:LYS:HG2	1:A:988:LEU:HD11	1.97	0.46
2:B:355:ILE:HD12	2:B:355:ILE:HG23	1.45	0.46
2:B:893:LEU:HD13	2:B:897:GLY:C	2.34	0.46
2:B:281:PRO:HB2	2:B:284:ILE:HD13	1.97	0.46
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.96	0.46
7:I:51:ASN:HB2	7:I:118:ARG:CZ	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:CB	6:H:95:TYR:CA	2.90	0.46
4:E:13:TRP:CE3	4:E:39:LEU:HD13	2.50	0.46
5:F:147:SER:O	5:F:148:VAL:C	2.50	0.46
1:A:523:ILE:CB	1:A:622:VAL:HG13	2.43	0.46
2:B:286:PHE:HB3	2:B:297:ILE:HD12	1.96	0.46
1:A:1172:LEU:C	1:A:1173:HIS:CD2	2.88	0.46
2:B:599:THR:O	2:B:600:LEU:C	2.51	0.46
8:J:62:ARG:HB3	8:J:62:ARG:HE	1.24	0.46
2:B:880:THR:CG2	2:B:880:THR:CA	2.82	0.46
1:A:31:SER:HB3	1:A:83:HIS:CD2	2.45	0.46
2:B:1045:SER:HB3	2:B:1046:PRO:HD2	1.98	0.46
2:B:416:LEU:HB3	2:B:420:LEU:HD12	1.97	0.46
1:A:860:LEU:CB	1:A:860:LEU:CD1	2.86	0.46
6:H:32:THR:HB	6:H:33:GLN:OE1	2.16	0.46
2:B:863:GLU:C	2:B:864:LYS:O	2.54	0.46
1:A:599:SER:HA	1:A:600:PRO:HD2	1.58	0.46
1:A:1364:ASN:HB3	1:A:1366:ARG:HG2	1.97	0.46
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.97	0.46
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.15	0.46
1:A:1023:ARG:HH21	1:A:1023:ARG:HD3	1.60	0.46
1:A:567:LYS:CB	1:A:568:PRO:CD	2.90	0.46
6:H:101:ALA:HA	6:H:116:TYR:HA	1.97	0.46
1:A:920:LEU:CD2	1:A:921:GLY:H	2.28	0.46
6:H:56:THR:HG21	6:H:145:ARG:HE	1.79	0.46
1:A:706:HIS:O	1:A:707:GLY:C	2.53	0.46
1:A:1112:LYS:CB	1:A:1112:LYS:CD	2.90	0.46
1:A:46:THR:C	1:A:46:THR:HB	2.35	0.46
1:A:34:LYS:HG2	1:A:83:HIS:CE1	2.50	0.46
1:A:1205:LYS:O	1:A:1206:ASP:C	2.50	0.46
1:A:144:THR:O	1:A:146:MET:HG2	2.16	0.46
3:C:95:CYS:O	3:C:96:SER:HB3	2.16	0.46
2:B:400:HIS:CE1	2:B:517:THR:HG21	2.51	0.46
4:E:78:LEU:HD21	4:E:80:VAL:CG2	2.45	0.46
3:C:252:GLN:HB2	9:K:98:LEU:HD12	1.98	0.46
6:H:98:TYR:C	6:H:118:PHE:HD2	2.19	0.46
1:A:971:PHE:O	1:A:972:HIS:C	2.49	0.46
2:B:408:LEU:O	2:B:409:ALA:C	2.52	0.46
2:B:547:VAL:O	2:B:547:VAL:HG13	2.16	0.46
1:A:46:THR:O	1:A:48:ALA:N	2.49	0.46
2:B:864:LYS:NZ	2:B:865:LYS:H	2.13	0.46
1:A:566:ILE:CG2	1:A:566:ILE:CD1	2.94	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LYS:O	1:A:188:ASP:CG	2.54	0.46
2:B:736:THR:HA	2:B:736:THR:CG2	2.45	0.46
4:E:28:TYR:CE1	4:E:75:MET:HE3	2.51	0.46
5:F:109:VAL:CG1	5:F:110:ASP:N	2.76	0.46
1:A:767:GLN:HA	1:A:799:PHE:HA	1.98	0.46
2:B:639:ILE:HG22	2:B:640:VAL:N	2.30	0.46
8:J:48:ARG:CD	8:J:48:ARG:C	2.83	0.46
1:A:635:ARG:HD3	1:A:635:ARG:HH11	1.59	0.46
1:A:1225:PHE:CA	1:A:1225:PHE:CG	2.90	0.46
9:K:88:LYS:O	9:K:89:ASN:C	2.51	0.46
1:A:356:ASP:OD2	1:A:469:ARG:CD	2.62	0.46
1:A:42:ASP:OD2	1:A:47:ARG:HA	2.16	0.46
2:B:1006:ILE:HG22	2:B:1007:VAL:N	2.29	0.46
2:B:864:LYS:HZ3	2:B:865:LYS:H	1.62	0.46
1:A:567:LYS:CE	6:H:95:TYR:CD2	2.99	0.46
1:A:1204:ASP:CG	1:A:1204:ASP:O	2.54	0.46
6:H:18:GLY:O	6:H:19:ARG:CB	2.54	0.46
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.80	0.46
2:B:1081:LEU:O	2:B:1082:MET:C	2.50	0.46
3:C:145:CYS:SG	3:C:146:LYS:N	2.89	0.46
1:A:999:VAL:HG12	1:A:1000:LEU:HG	1.98	0.46
5:F:125:LEU:HA	5:F:130:ILE:HD12	1.97	0.46
1:A:135:PHE:CD1	1:A:222:LEU:HD22	2.51	0.46
2:B:418:LYS:CE	2:B:418:LYS:CG	2.92	0.46
2:B:1182:CYS:CB	2:B:1185:CYS:HB2	2.39	0.46
2:B:643:ASP:HB3	2:B:644:GLU:C	2.36	0.46
1:A:4:GLN:CG	1:A:4:GLN:CA	2.85	0.46
1:A:1150:SER:O	1:A:1151:GLU:HG3	2.16	0.46
2:B:269:ILE:O	2:B:282:ILE:HD12	2.15	0.46
2:B:235:SER:C	2:B:236:HIS:CD2	2.89	0.46
2:B:758:PHE:N	2:B:759:PRO:CD	2.79	0.46
1:A:860:LEU:HG	1:A:860:LEU:CD1	2.21	0.45
4:E:98:ILE:CG2	4:E:98:ILE:HG12	2.39	0.45
2:B:130:VAL:O	2:B:164:LYS:O	2.33	0.45
9:K:110:ASN:C	9:K:112:GLN:N	2.60	0.45
2:B:879:ARG:NH2	2:B:885:MET:HE1	2.31	0.45
3:C:181:ASP:CG	3:C:181:ASP:O	2.49	0.45
2:B:242:SER:OG	2:B:363:HIS:ND1	2.49	0.45
4:E:44:ALA:HB3	4:E:45:LYS:N	2.31	0.45
4:E:161:LYS:CG	4:E:161:LYS:CE	2.77	0.45
1:A:1120:LEU:HD21	1:A:1131:ALA:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:773:MET:O	2:B:774:GLY:C	2.51	0.45
3:C:195:GLN:NE2	3:C:195:GLN:CG	2.73	0.45
1:A:588:LEU:HD23	1:A:589:GLN:N	2.29	0.45
1:A:466:SER:HB3	2:B:1103:ILE:HD11	1.98	0.45
2:B:521:LEU:CD2	2:B:635:ARG:HD3	2.45	0.45
3:C:80:LEU:HD12	3:C:80:LEU:HA	1.55	0.45
1:A:1003:LYS:CG	1:A:1003:LYS:CE	2.91	0.45
6:H:32:THR:CG2	6:H:33:GLN:CD	2.83	0.45
1:A:1066:VAL:O	1:A:1067:LEU:C	2.51	0.45
4:E:63:ASN:C	4:E:64:PRO:O	2.54	0.45
1:A:974:ASP:N	1:A:974:ASP:OD1	2.49	0.45
3:C:241:ASP:CG	3:C:242:GLN:N	2.69	0.45
4:E:78:LEU:HG	4:E:79:TRP:N	2.32	0.45
3:C:180:TYR:CD1	3:C:180:TYR:C	2.89	0.45
2:B:900:ALA:O	2:B:903:VAL:HG23	2.17	0.45
2:B:609:ILE:O	2:B:610:ASN:C	2.52	0.45
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.52	0.45
2:B:259:TYR:HB2	2:B:268:THR:HG22	1.98	0.45
1:A:878:ILE:HG23	1:A:878:ILE:HD12	1.60	0.45
2:B:435:THR:HA	2:B:435:THR:C	2.11	0.45
4:E:2:ASP:HB3	4:E:6:GLU:HB2	1.98	0.45
1:A:1134:ILE:HG22	1:A:1306:LEU:CD1	2.46	0.45
2:B:552:MET:N	2:B:553:PRO:HD2	2.31	0.45
3:C:230:MET:CE	3:C:230:MET:CG	2.82	0.45
2:B:711:GLU:CB	2:B:711:GLU:CD	2.76	0.45
2:B:232:SER:OG	2:B:233:PRO:HD2	2.16	0.45
2:B:999:MET:HB3	2:B:1000:PRO:CD	2.40	0.45
1:A:589:GLN:HB2	1:A:961:ARG:HH22	1.80	0.45
2:B:724:ASP:C	2:B:726:ALA:H	2.19	0.45
3:C:179:GLU:CG	3:C:180:TYR:N	2.79	0.45
2:B:372:SER:O	2:B:373:ARG:C	2.53	0.45
4:E:137:GLU:O	4:E:138:ALA:C	2.53	0.45
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.46	0.45
2:B:423:LYS:NZ	2:B:423:LYS:CD	2.69	0.45
3:C:205:LYS:HG3	3:C:205:LYS:H	1.64	0.45
2:B:69:LEU:O	2:B:70:ILE:HD13	2.17	0.45
3:C:169:LYS:NZ	10:L:69:ALA:O	2.44	0.45
1:A:219:PHE:CD1	1:A:219:PHE:C	2.88	0.45
1:A:567:LYS:CD	6:H:95:TYR:CA	2.53	0.45
1:A:931:GLU:OE1	1:A:991:LYS:NZ	2.28	0.45
6:H:138:GLU:CG	6:H:139:ASN:N	2.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:37:LEU:HA	4:E:38:PRO:HD2	1.61	0.45
1:A:1364:ASN:ND2	1:A:1365:TYR:N	2.65	0.45
1:A:1348:LEU:CG	1:A:1372:VAL:HG22	2.40	0.45
2:B:254:LEU:HD23	2:B:361:LEU:HD21	1.98	0.45
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	2.51	0.45
2:B:1002:THR:O	2:B:1003:ALA:C	2.51	0.45
6:H:47:PHE:O	6:H:47:PHE:HD2	2.00	0.45
2:B:343:ILE:CD1	2:B:343:ILE:CB	2.83	0.45
9:K:35:PHE:CD1	9:K:71:PHE:CE1	3.04	0.45
1:A:903:ASN:HD21	1:A:905:ASP:H	1.57	0.45
2:B:827:ILE:HG12	2:B:1012:ILE:HD11	1.99	0.45
2:B:1162:ILE:HG23	2:B:1162:ILE:HD12	1.54	0.45
1:A:95:PHE:O	1:A:99:ILE:HD12	2.15	0.45
1:A:562:THR:HA	1:A:563:PRO:HD3	1.79	0.45
1:A:418:SER:C	1:A:420:ARG:H	2.19	0.45
1:A:116:ASP:C	1:A:116:ASP:OD2	2.55	0.45
6:H:10:PHE:O	6:H:54:SER:HB2	2.16	0.45
4:E:65:THR:OG1	4:E:68:SER:CB	2.65	0.45
4:E:69:ILE:HG22	4:E:73:PRO:HA	1.98	0.45
2:B:25:ILE:CA	2:B:25:ILE:CG2	2.86	0.45
2:B:958:GLN:HG2	2:B:958:GLN:N	2.30	0.45
4:E:161:LYS:O	4:E:162:ARG:C	2.55	0.45
1:A:1405:THR:CA	1:A:1405:THR:HB	2.23	0.45
2:B:134:LYS:CB	2:B:134:LYS:CE	2.94	0.45
2:B:498:THR:HG22	2:B:537:LYS:H	1.81	0.45
1:A:446:ARG:CG	1:A:446:ARG:NH1	2.76	0.45
1:A:741:ASN:O	1:A:745:GLN:HG3	2.16	0.45
2:B:520:GLY:C	2:B:521:LEU:HD23	2.37	0.45
2:B:416:LEU:HD11	2:B:466:TRP:CZ2	2.52	0.45
1:A:849:MET:HE2	1:A:1061:GLY:HA2	1.99	0.45
1:A:1322:ILE:O	1:A:1324:PRO:HD3	2.16	0.45
1:A:899:VAL:CG1	1:A:929:LEU:HD13	2.47	0.45
3:C:262:LEU:HA	3:C:262:LEU:HD23	1.62	0.45
1:A:913:LEU:HD12	1:A:914:GLU:N	2.32	0.45
6:H:105:GLU:C	6:H:107:VAL:N	2.70	0.45
3:C:127:ARG:CG	3:C:127:ARG:N	2.80	0.45
1:A:1194:ARG:C	1:A:1194:ARG:CG	2.85	0.45
1:A:848:ILE:HA	1:A:857:ARG:O	2.17	0.45
6:H:114:VAL:HG11	6:H:134:ASN:ND2	2.32	0.45
2:B:644:GLU:HA	2:B:645:SER:HB3	1.99	0.44
4:E:115:ASN:ND2	4:E:115:ASN:CB	2.67	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:531:GLN:H	2:B:531:GLN:CG	2.30	0.44
1:A:880:LYS:CB	1:A:880:LYS:CD	2.88	0.44
2:B:92:PHE:N	2:B:92:PHE:CD1	2.85	0.44
1:A:920:LEU:HA	1:A:920:LEU:HD23	1.45	0.44
1:A:80:HIS:O	1:A:243:PRO:HB3	2.17	0.44
1:A:70:CYS:O	1:A:72:GLU:OE1	2.34	0.44
4:E:123:LEU:O	4:E:126:SER:CB	2.64	0.44
1:A:878:ILE:HD13	1:A:878:ILE:HA	1.35	0.44
2:B:249:ARG:HB2	2:B:418:LYS:NZ	2.32	0.44
1:A:1112:LYS:CE	1:A:1112:LYS:CG	2.92	0.44
2:B:381:MET:CE	2:B:381:MET:HG3	2.22	0.44
1:A:516:SER:O	1:A:517:ASN:C	2.51	0.44
1:A:541:ILE:HG22	1:A:542:GLU:N	2.32	0.44
2:B:886:LYS:O	2:B:888:GLY:N	2.49	0.44
2:B:911:ILE:N	2:B:911:ILE:CD1	2.80	0.44
1:A:138:ILE:HD12	1:A:142:CYS:SG	2.57	0.44
1:A:964:ILE:HD13	1:A:964:ILE:HA	1.70	0.44
10:L:30:ILE:HG21	10:L:30:ILE:CD1	2.47	0.44
2:B:129:PHE:HE2	2:B:166:PHE:CB	2.18	0.44
2:B:916:THR:CA	2:B:916:THR:CG2	2.86	0.44
1:A:184:SER:HB2	1:A:199:LEU:HD23	2.00	0.44
1:A:1425:SER:O	1:A:1428:VAL:HB	2.17	0.44
1:A:93:VAL:H	1:A:304:MET:HE3	1.82	0.44
1:A:752:LYS:HZ3	2:B:1018:PRO:HD2	1.82	0.44
2:B:361:LEU:N	2:B:362:PRO:CD	2.79	0.44
1:A:125:ALA:O	1:A:126:LEU:C	2.47	0.44
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	1.99	0.44
1:A:980:ASP:OD1	1:A:980:ASP:N	2.32	0.44
1:A:1116:LEU:HD22	1:A:1311:VAL:HA	1.99	0.44
2:B:1163:CYS:SG	2:B:1165:ILE:HG12	2.58	0.44
1:A:268:ASP:HA	1:A:271:LYS:HB2	1.99	0.44
6:H:33:GLN:O	6:H:34:ASP:C	2.54	0.44
2:B:958:GLN:CG	2:B:958:GLN:N	2.80	0.44
2:B:578:THR:HG23	2:B:622:LYS:C	2.37	0.44
6:H:123:MET:HG2	6:H:124:ARG:H	1.83	0.44
1:A:1405:THR:CB	1:A:1405:THR:C	2.82	0.44
6:H:118:PHE:O	6:H:119:GLY:C	2.52	0.44
2:B:893:LEU:HD23	2:B:893:LEU:N	2.33	0.44
1:A:138:ILE:HG12	1:A:222:LEU:HD23	1.99	0.44
1:A:1415:SER:O	1:A:1416:ALA:HB3	2.17	0.44
2:B:1050:ILE:H	2:B:1050:ILE:HD12	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:94:LYS:HB2	3:C:94:LYS:CG	2.20	0.44
4:E:65:THR:O	4:E:69:ILE:CG1	2.66	0.44
1:A:633:VAL:HG21	1:A:645:LEU:HD22	1.98	0.44
2:B:529:GLU:O	2:B:531:GLN:NE2	2.50	0.44
6:H:16:ASP:O	6:H:24:CYS:HB3	2.17	0.44
1:A:1208:THR:OG1	1:A:1211:GLN:NE2	2.50	0.44
3:C:147:LEU:HD13	3:C:151:GLN:O	2.17	0.44
5:F:94:LEU:HD23	5:F:94:LEU:HA	1.66	0.44
2:B:1206:GLU:O	2:B:1209:ALA:HB3	2.17	0.44
4:E:132:ILE:HD13	4:E:132:ILE:HA	1.75	0.44
2:B:137:TYR:CD2	2:B:137:TYR:CB	2.83	0.44
1:A:274:ILE:C	1:A:274:ILE:CB	2.74	0.44
6:H:76:THR:CG2	6:H:76:THR:O	2.66	0.44
4:E:37:LEU:CD1	4:E:37:LEU:CB	2.85	0.44
3:C:73:GLN:NE2	3:C:74:SER:H	2.16	0.44
9:K:65:HIS:CD2	9:K:67:PHE:HB2	2.53	0.44
2:B:214:ALA:HB3	2:B:498:THR:HA	2.00	0.44
2:B:498:THR:HG22	2:B:498:THR:O	2.18	0.44
2:B:355:ILE:O	2:B:355:ILE:HG22	2.15	0.44
2:B:816:GLU:C	2:B:818:PRO:HD3	2.38	0.44
2:B:1172:ILE:HD12	2:B:1181:GLU:O	2.18	0.44
4:E:37:LEU:C	4:E:38:PRO:O	2.54	0.44
2:B:1188:LYS:CB	2:B:1188:LYS:CD	2.87	0.44
9:K:65:HIS:CD2	9:K:66:PRO:HD2	2.53	0.44
1:A:108:MET:N	1:A:171:GLN:HE22	2.09	0.44
2:B:269:ILE:HG13	2:B:317:CYS:SG	2.57	0.44
9:K:47:ARG:O	9:K:48:ALA:C	2.50	0.44
4:E:32:GLN:O	4:E:35:VAL:HB	2.18	0.44
1:A:1138:ILE:HD13	1:A:1138:ILE:HG21	1.30	0.44
1:A:1339:LEU:HA	1:A:1339:LEU:HD23	1.75	0.44
3:C:144:ILE:HG21	3:C:144:ILE:HD12	1.68	0.44
2:B:423:LYS:O	2:B:425:THR:N	2.51	0.44
10:L:47:ARG:CG	10:L:48:CYS:N	2.78	0.44
1:A:1262:LYS:C	1:A:1264:GLU:N	2.70	0.44
2:B:772:ALA:O	2:B:775:LYS:N	2.40	0.44
1:A:1298:TYR:O	1:A:1299:VAL:HG23	2.18	0.44
2:B:769:TYR:O	2:B:770:GLN:C	2.55	0.44
1:A:1260:LEU:HA	1:A:1260:LEU:HD12	1.69	0.44
1:A:606:LEU:HD11	1:A:608:ILE:HD11	1.99	0.44
1:A:463:ILE:HD13	1:A:463:ILE:HG21	1.64	0.44
8:J:4:PRO:HD3	8:J:53:HIS:HD2	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLU:HB3	1:A:50:ILE:HD12	2.00	0.44
2:B:1051:THR:HG22	2:B:1054:GLY:H	1.82	0.44
1:A:446:ARG:HB2	1:A:487:MET:CE	2.48	0.44
1:A:607:ILE:HD13	1:A:607:ILE:HG21	1.65	0.44
2:B:609:ILE:CG2	2:B:610:ASN:N	2.77	0.44
1:A:509:LEU:H	1:A:509:LEU:HG	1.54	0.44
2:B:319:GLU:HG3	2:B:319:GLU:H	1.66	0.44
1:A:915:SER:O	1:A:916:GLY:C	2.50	0.43
7:I:3:THR:CG2	7:I:3:THR:C	2.86	0.43
2:B:773:MET:C	2:B:775:LYS:N	2.69	0.43
3:C:73:GLN:HB3	3:C:131:HIS:H	1.82	0.43
3:C:235:VAL:HG13	3:C:236:GLY:N	2.32	0.43
2:B:755:ILE:CG2	2:B:755:ILE:O	2.66	0.43
1:A:672:ASP:HB2	1:A:675:THR:OG1	2.18	0.43
1:A:793:SER:O	1:A:794:PRO:C	2.56	0.43
2:B:737:THR:O	2:B:738:PHE:C	2.55	0.43
4:E:82:PHE:N	4:E:82:PHE:CD1	2.86	0.43
2:B:890:TYR:C	2:B:892:LYS:H	2.22	0.43
1:A:1164:PRO:O	1:A:1167:GLU:N	2.51	0.43
2:B:958:GLN:CG	2:B:958:GLN:NE2	2.69	0.43
2:B:119:LEU:HD23	2:B:119:LEU:HA	1.63	0.43
9:K:20:LYS:CE	9:K:20:LYS:CG	2.95	0.43
9:K:49:GLU:HG3	9:K:94:ILE:HD13	1.99	0.43
2:B:1010:LEU:HD12	2:B:1010:LEU:HA	1.34	0.43
4:E:124:VAL:HB	4:E:125:PRO:HD3	2.01	0.43
3:C:251:LEU:HA	3:C:251:LEU:HD12	1.72	0.43
1:A:911:SER:O	1:A:978:PRO:HB3	2.19	0.43
6:H:100:THR:OG1	6:H:138:GLU:HG3	2.18	0.43
1:A:587:HIS:NE2	1:A:969:GLN:HG2	2.33	0.43
1:A:264:PHE:O	1:A:267:ALA:HB3	2.18	0.43
4:E:11:ARG:HD2	4:E:11:ARG:HH11	1.32	0.43
4:E:43:LYS:CE	4:E:43:LYS:CB	2.96	0.43
8:J:53:HIS:HE1	8:J:55:ASP:HA	1.82	0.43
1:A:247:ARG:HH11	1:A:247:ARG:HD2	1.61	0.43
2:B:566:LEU:HA	2:B:566:LEU:HD12	1.71	0.43
1:A:861:GLY:O	1:A:862:ASN:C	2.50	0.43
1:A:613:ILE:HD12	1:A:613:ILE:HG23	1.75	0.43
2:B:1031:LEU:O	2:B:1031:LEU:HG	2.17	0.43
10:L:32:ALA:CB	10:L:55:ILE:CG2	2.96	0.43
1:A:587:HIS:CD2	1:A:966:ASN:OD1	2.68	0.43
2:B:913:GLY:HA2	2:B:938:SER:HB2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:PRO:HG2	1:A:174:ILE:CD1	2.47	0.43
2:B:898:LEU:C	2:B:899:ILE:O	2.53	0.43
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.17	0.43
1:A:890:ASP:O	1:A:891:ALA:C	2.56	0.43
3:C:255:VAL:O	3:C:255:VAL:HG12	2.18	0.43
1:A:188:ASP:HA	1:A:188:ASP:C	2.15	0.43
1:A:101:LYS:HD3	1:A:139:TRP:CE2	2.53	0.43
6:H:23:VAL:HG12	6:H:24:CYS:N	2.32	0.43
3:C:66:ARG:NH2	8:J:3:VAL:O	2.51	0.43
2:B:878:GLN:H	2:B:934:LYS:HD2	1.83	0.43
2:B:172:ILE:CD1	2:B:172:ILE:CG2	2.96	0.43
1:A:809:THR:HB	1:A:810:PRO:CD	2.48	0.43
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.78	0.43
2:B:59:LEU:HD12	2:B:59:LEU:HA	1.73	0.43
1:A:1142:THR:C	1:A:1144:LYS:N	2.68	0.43
4:E:100:ILE:CG2	4:E:101:GLN:N	2.39	0.43
2:B:1161:HIS:HA	2:B:1192:TYR:O	2.19	0.43
2:B:129:PHE:HD2	2:B:166:PHE:N	2.15	0.43
1:A:567:LYS:HB3	6:H:95:TYR:C	2.32	0.43
1:A:31:SER:OG	1:A:83:HIS:CD2	2.72	0.43
1:A:518:LYS:HE3	1:A:624:SER:O	2.18	0.43
4:E:37:LEU:HD23	4:E:42:PHE:HB2	1.99	0.43
3:C:19:ASP:HA	3:C:231:ASN:HA	2.00	0.43
9:K:49:GLU:CG	9:K:94:ILE:CD1	2.96	0.43
6:H:99:GLY:HA3	6:H:118:PHE:CD2	2.53	0.43
2:B:817:LEU:N	2:B:818:PRO:HD3	2.33	0.43
1:A:1052:GLN:O	1:A:1053:PHE:C	2.52	0.43
1:A:550:LEU:HD13	1:A:556:TRP:CZ2	2.53	0.43
1:A:269:ILE:HG21	1:A:269:ILE:HD13	1.82	0.43
2:B:249:ARG:NH2	2:B:415:GLN:HG3	2.33	0.43
2:B:1006:ILE:HD11	8:J:43:ARG:HD2	2.00	0.43
1:A:535:THR:CG2	1:A:616:VAL:CA	2.92	0.43
3:C:73:GLN:HA	3:C:133:ILE:HD11	1.99	0.43
1:A:11:LEU:O	1:A:12:ARG:HG2	2.18	0.43
7:I:59:VAL:O	7:I:60:GLN:C	2.55	0.43
1:A:1328:TYR:CG	1:A:1329:THR:N	2.87	0.43
1:A:1059:HIS:CD2	1:A:1059:HIS:N	2.85	0.43
1:A:289:ILE:HA	1:A:289:ILE:HD13	1.80	0.43
1:A:977:LYS:HA	1:A:978:PRO:HD2	1.79	0.43
2:B:228:LYS:HA	2:B:228:LYS:CG	2.47	0.43
2:B:122:LEU:HA	2:B:122:LEU:HD23	1.56	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:987:LYS:NZ	2:B:987:LYS:HD2	2.34	0.43
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.72	0.43
1:A:1213:GLY:HA3	1:A:1228:TRP:CE3	2.53	0.43
7:I:41:PRO:CD	7:I:42:LEU:H	2.31	0.43
2:B:311:LEU:O	2:B:312:GLU:C	2.53	0.43
3:C:211:ASP:O	3:C:212:PRO:C	2.57	0.43
2:B:106:ASP:O	10:L:47:ARG:NH2	2.52	0.43
1:A:469:ARG:CD	1:A:469:ARG:CB	2.88	0.43
2:B:100:PRO:CD	2:B:180:TYR:CZ	2.99	0.43
6:H:142:LEU:HD12	6:H:142:LEU:HA	1.74	0.43
2:B:353:LYS:CE	2:B:353:LYS:CG	2.88	0.43
1:A:203:SER:N	1:A:206:GLU:HG3	2.33	0.43
4:E:78:LEU:HD21	4:E:80:VAL:HG23	2.01	0.43
9:K:65:HIS:CD2	9:K:66:PRO:N	2.86	0.43
1:A:243:PRO:O	1:A:243:PRO:CG	2.61	0.43
2:B:409:ALA:O	2:B:410:GLY:C	2.54	0.43
1:A:882:SER:OG	1:A:882:SER:O	2.35	0.43
5:F:97:ARG:NH2	5:F:124:GLU:OE2	2.46	0.43
3:C:84:ARG:CA	3:C:84:ARG:CG	2.82	0.43
1:A:827:THR:CG2	1:A:827:THR:C	2.87	0.43
4:E:160:GLU:O	4:E:161:LYS:C	2.57	0.43
2:B:120:ARG:HB2	2:B:122:LEU:HG	2.01	0.43
2:B:770:GLN:OE1	2:B:770:GLN:HA	2.18	0.43
1:A:247:ARG:HA	1:A:248:PRO:HD3	1.70	0.43
10:L:58:LYS:O	10:L:59:ALA:O	2.36	0.43
2:B:557:PHE:CZ	2:B:561:TRP:CD1	3.06	0.43
4:E:63:ASN:OD1	4:E:77:SER:HB3	2.19	0.43
3:C:55:THR:O	3:C:151:GLN:HG2	2.19	0.43
2:B:373:ARG:HG3	2:B:373:ARG:H	1.66	0.43
2:B:613:VAL:HG12	2:B:614:SER:N	2.34	0.43
2:B:756:ILE:HD13	2:B:756:ILE:HG21	1.76	0.43
5:F:120:ILE:HD12	5:F:120:ILE:HG23	1.66	0.43
1:A:1166:ASP:O	1:A:1170:ILE:CD1	2.64	0.42
2:B:98:THR:HB	2:B:99:LYS:O	2.19	0.42
1:A:274:ILE:CD1	1:A:274:ILE:CA	2.97	0.42
2:B:121:ASN:HA	2:B:207:GLY:HA3	2.01	0.42
6:H:100:THR:O	6:H:116:TYR:HA	2.19	0.42
6:H:111:LEU:HB3	6:H:127:GLY:O	2.19	0.42
2:B:879:ARG:HH21	2:B:885:MET:HE1	1.84	0.42
1:A:771:GLU:CD	2:B:510:LYS:HZ3	2.23	0.42
3:C:34:ARG:O	3:C:35:ARG:C	2.57	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:185:LYS:HB2	3:C:185:LYS:HE2	1.90	0.42
1:A:1446:ASP:OD1	1:A:1448:GLU:HG3	2.19	0.42
1:A:670:ILE:HD12	1:A:670:ILE:HG21	1.77	0.42
2:B:1191:ILE:HD13	2:B:1191:ILE:HG21	1.74	0.42
2:B:789:MET:HG3	2:B:789:MET:HE2	2.01	0.42
10:L:55:ILE:HG21	10:L:55:ILE:HD12	1.82	0.42
4:E:103:LYS:CE	4:E:103:LYS:CG	2.83	0.42
4:E:43:LYS:O	4:E:47:CYS:HB3	2.19	0.42
3:C:241:ASP:OD1	3:C:241:ASP:N	2.51	0.42
9:K:58:PHE:HB3	9:K:76:GLN:CB	2.50	0.42
2:B:34:ILE:O	2:B:35:SER:C	2.56	0.42
1:A:973:ILE:HD11	1:A:1038:THR:HG23	2.01	0.42
4:E:176:PRO:O	4:E:212:ARG:HA	2.19	0.42
2:B:202:TYR:N	2:B:202:TYR:CD2	2.84	0.42
2:B:764:SER:HB3	2:B:765:PRO:HD3	2.01	0.42
2:B:648:HIS:ND1	2:B:648:HIS:N	2.67	0.42
2:B:1003:ALA:C	2:B:1005:GLY:H	2.22	0.42
2:B:1008:PRO:CG	2:B:1011:ILE:HD11	2.49	0.42
1:A:842:VAL:O	1:A:846:GLU:HB2	2.20	0.42
3:C:148:ARG:O	3:C:149:LYS:C	2.57	0.42
2:B:1205:GLN:O	2:B:1206:GLU:C	2.55	0.42
1:A:882:SER:CB	1:A:953:ASN:OD1	2.68	0.42
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.55	0.42
8:J:49:MET:HE3	8:J:49:MET:HB2	1.69	0.42
2:B:215:GLN:HE21	2:B:215:GLN:HB3	1.62	0.42
6:H:44:VAL:HG13	6:H:44:VAL:O	2.18	0.42
5:F:128:LYS:HD3	5:F:128:LYS:HA	1.83	0.42
4:E:23:VAL:HG11	4:E:30:ILE:HD11	2.01	0.42
1:A:1157:ASP:O	1:A:1159:ARG:N	2.52	0.42
2:B:130:VAL:HB	2:B:131:ASP:H	1.80	0.42
2:B:789:MET:HG3	2:B:789:MET:CE	2.50	0.42
2:B:864:LYS:O	2:B:961:LEU:CD2	2.67	0.42
2:B:705:MET:CE	2:B:745:PRO:CG	2.97	0.42
2:B:92:PHE:HZ	2:B:428:ILE:HD12	1.84	0.42
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.29	0.42
1:A:816:HIS:HE2	2:B:763:GLN:HA	1.84	0.42
4:E:125:PRO:CD	4:E:125:PRO:O	2.67	0.42
9:K:18:LYS:HE3	9:K:38:GLU:HG2	2.00	0.42
1:A:885:THR:O	1:A:940:ARG:HG3	2.20	0.42
3:C:183:TRP:NE1	3:C:207:CYS:HB3	2.34	0.42
4:E:100:ILE:HG22	4:E:101:GLN:CA	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:29:TYR:O	10:L:30:ILE:HG13	2.19	0.42
1:A:53:LEU:HD23	1:A:54:ASN:H	1.84	0.42
6:H:47:PHE:C	6:H:47:PHE:CD2	2.91	0.42
1:A:829:VAL:CA	1:A:829:VAL:CG2	2.80	0.42
10:L:61:THR:HG21	10:L:63:ARG:HD3	2.02	0.42
4:E:109:ILE:HG22	4:E:110:PHE:N	2.33	0.42
3:C:181:ASP:OD2	3:C:185:LYS:N	2.49	0.42
9:K:94:ILE:HG23	9:K:94:ILE:HD12	1.88	0.42
1:A:827:THR:O	1:A:828:ALA:C	2.56	0.42
1:A:636:GLU:OE1	1:A:966:ASN:ND2	2.52	0.42
3:C:186:LEU:HA	3:C:186:LEU:HD12	1.57	0.42
1:A:853:ASP:O	1:A:854:ASN:HB2	2.20	0.42
3:C:43:THR:HG23	3:C:44:LEU:N	2.33	0.42
2:B:839:MET:CE	2:B:1010:LEU:HD11	2.50	0.42
2:B:978:ASP:O	2:B:989:THR:HA	2.20	0.42
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.20	0.42
2:B:646:LEU:CA	2:B:646:LEU:HG	2.48	0.42
4:E:73:PRO:HD2	4:E:74:ASP:H	1.84	0.42
2:B:772:ALA:O	2:B:773:MET:C	2.57	0.42
1:A:842:VAL:O	1:A:843:LYS:C	2.58	0.42
1:A:1430:LEU:O	1:A:1432:GLN:HG3	2.19	0.42
9:K:55:LYS:HB2	9:K:81:TYR:CE1	2.54	0.42
2:B:521:LEU:HD21	2:B:635:ARG:HD3	2.01	0.42
1:A:870:GLU:HG2	4:E:208:TYR:CG	2.54	0.42
9:K:21:ILE:HG21	9:K:21:ILE:HD13	1.78	0.42
2:B:949:VAL:HG12	2:B:950:ASP:N	2.31	0.42
2:B:846:ILE:CD1	2:B:974:PRO:CB	2.94	0.42
4:E:72:PHE:HA	4:E:73:PRO:HD3	1.74	0.42
3:C:63:ILE:HG23	3:C:63:ILE:HD12	1.43	0.42
2:B:791:THR:O	2:B:857:ARG:HA	2.20	0.42
2:B:307:ASP:C	2:B:307:ASP:OD1	2.57	0.42
9:K:29:ASN:HB3	9:K:77:THR:O	2.20	0.42
1:A:562:THR:CG2	6:H:98:TYR:CD2	3.02	0.42
1:A:418:SER:O	1:A:419:LYS:C	2.56	0.42
1:A:388:LEU:O	1:A:392:VAL:HG23	2.20	0.42
1:A:1053:PHE:O	1:A:1054:LEU:C	2.58	0.42
5:F:117:PRO:O	5:F:118:LEU:C	2.57	0.42
3:C:207:CYS:O	3:C:208:GLU:C	2.59	0.42
2:B:1191:ILE:HG22	2:B:1192:TYR:N	2.34	0.42
1:A:1305:VAL:HG12	1:A:1306:LEU:N	2.34	0.42
3:C:29:MET:HB2	3:C:29:MET:HE2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:88:CYS:SG	3:C:92:CYS:SG	3.17	0.42
2:B:1051:THR:O	2:B:1055:ILE:HG12	2.20	0.42
2:B:984:HIS:HD2	2:B:1025:HIS:HA	1.81	0.42
1:A:926:GLN:HE21	1:A:926:GLN:HB2	1.38	0.42
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.54	0.42
1:A:613:ILE:HA	1:A:613:ILE:HD13	1.81	0.42
2:B:639:ILE:CG2	2:B:640:VAL:N	2.81	0.42
5:F:140:ASP:OD1	5:F:140:ASP:C	2.56	0.42
2:B:846:ILE:CG1	2:B:846:ILE:CA	2.81	0.42
1:A:705:LYS:CE	1:A:705:LYS:CG	2.87	0.42
2:B:956:THR:CA	2:B:961:LEU:O	2.61	0.42
4:E:191:LYS:CE	4:E:191:LYS:CG	2.88	0.42
8:J:45:CYS:SG	8:J:46:CYS:SG	3.17	0.42
9:K:91:CYS:O	9:K:94:ILE:HB	2.20	0.42
1:A:1116:LEU:HD12	1:A:1116:LEU:HA	1.71	0.42
1:A:241:VAL:HA	1:A:242:PRO:HD2	1.96	0.42
1:A:867:ILE:HD13	1:A:867:ILE:HG21	1.73	0.42
2:B:492:LEU:HA	2:B:492:LEU:HD23	1.81	0.42
1:A:1433:MET:HB2	1:A:1433:MET:HE2	1.80	0.42
2:B:582:VAL:O	2:B:583:ASN:C	2.55	0.42
2:B:620:ARG:N	2:B:620:ARG:CG	2.83	0.41
1:A:1143:LEU:O	1:A:1144:LYS:C	2.57	0.41
1:A:596:THR:CG2	1:A:596:THR:C	2.88	0.41
2:B:98:THR:OG1	2:B:127:GLY:N	2.52	0.41
2:B:956:THR:CG2	2:B:961:LEU:O	2.68	0.41
6:H:123:MET:CE	6:H:142:LEU:HD22	2.45	0.41
1:A:644:LYS:HB3	1:A:644:LYS:HE3	1.73	0.41
3:C:15:LYS:CA	3:C:15:LYS:CG	2.89	0.41
1:A:119:ASN:O	1:A:120:GLU:CB	2.68	0.41
2:B:661:LEU:HD23	2:B:679:TYR:HD2	1.85	0.41
2:B:571:PRO:O	2:B:573:GLN:N	2.53	0.41
1:A:924:LYS:HB2	1:A:924:LYS:HE2	1.60	0.41
1:A:1044:TRP:CZ2	1:A:1048:ASN:ND2	2.88	0.41
6:H:9:ILE:HA	6:H:55:LEU:O	2.19	0.41
1:A:1217:LYS:O	1:A:1221:LYS:HA	2.20	0.41
1:A:270:LEU:HA	1:A:270:LEU:HD13	1.86	0.41
2:B:166:PHE:HE2	2:B:450:ALA:HB1	1.85	0.41
2:B:622:LYS:CB	2:B:622:LYS:CD	2.87	0.41
4:E:43:LYS:HE2	4:E:43:LYS:CB	2.50	0.41
9:K:23:PRO:CD	9:K:23:PRO:O	2.68	0.41
1:A:752:LYS:HG2	1:A:752:LYS:CE	2.48	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:PRO:HA	1:A:160:GLN:H	1.85	0.41
5:F:147:SER:OG	5:F:150:GLU:HB2	2.19	0.41
2:B:914:LYS:HD2	2:B:937:ALA:O	2.20	0.41
2:B:1159:ARG:CG	2:B:1160:VAL:N	2.82	0.41
6:H:48:PRO:C	6:H:49:VAL:CG2	2.88	0.41
1:A:1358:SER:C	1:A:1360:GLY:H	2.23	0.41
1:A:399:HIS:HE1	1:A:436:ILE:O	2.04	0.41
1:A:393:ARG:NE	1:A:393:ARG:CG	2.75	0.41
4:E:96:PHE:O	4:E:97:VAL:C	2.52	0.41
10:L:30:ILE:CG2	10:L:31:CYS:N	2.83	0.41
2:B:1153:GLU:CB	2:B:1155:SER:HB3	2.50	0.41
2:B:1191:ILE:CG2	2:B:1192:TYR:N	2.80	0.41
6:H:47:PHE:CB	6:H:95:TYR:HD1	2.32	0.41
6:H:62:SER:O	6:H:63:LEU:C	2.58	0.41
1:A:353:ILE:HG21	1:A:353:ILE:HD13	1.12	0.41
3:C:114:TYR:HB3	3:C:140:ASN:O	2.20	0.41
2:B:1144:ALA:O	2:B:1145:SER:C	2.56	0.41
2:B:1035:ALA:HB1	2:B:1040:ASN:O	2.21	0.41
1:A:910:PRO:HA	1:A:916:GLY:HA3	2.03	0.41
10:L:48:CYS:HB3	10:L:51:CYS:O	2.21	0.41
2:B:134:LYS:CB	2:B:134:LYS:CD	2.86	0.41
8:J:56:LEU:O	8:J:57:ILE:C	2.56	0.41
2:B:424:LEU:CD2	2:B:428:ILE:HD11	2.41	0.41
1:A:1424:VAL:O	1:A:1428:VAL:HG23	2.20	0.41
1:A:709:THR:CG2	1:A:712:GLU:HG3	2.50	0.41
9:K:103:THR:O	9:K:104:ASN:C	2.58	0.41
1:A:1154:TYR:CZ	1:A:1156:PRO:HB3	2.55	0.41
2:B:170:LEU:HA	2:B:171:PRO:HD3	1.76	0.41
2:B:123:THR:O	2:B:123:THR:HG22	2.09	0.41
2:B:646:LEU:CD2	2:B:646:LEU:HG	2.32	0.41
1:A:54:ASN:C	1:A:56:PRO:HD2	2.40	0.41
1:A:567:LYS:HD3	6:H:95:TYR:C	2.36	0.41
6:H:47:PHE:CZ	6:H:146:ARG:HD2	2.55	0.41
2:B:667:GLN:O	2:B:668:ASP:OD1	2.38	0.41
3:C:15:LYS:O	3:C:240:VAL:HG23	2.20	0.41
1:A:150:THR:HG22	1:A:151:ASP:OD2	2.21	0.41
2:B:515:HIS:HD2	2:B:517:THR:H	1.67	0.41
3:C:26:ASP:N	3:C:26:ASP:OD1	2.50	0.41
2:B:416:LEU:HD23	2:B:416:LEU:HA	1.51	0.41
1:A:275:SER:O	1:A:279:LEU:HG	2.21	0.41
2:B:387:LEU:HD12	2:B:387:LEU:HA	1.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:LYS:NZ	2:B:621:GLU:CD	2.72	0.41
2:B:28:GLU:OE1	2:B:807:ARG:NH2	2.54	0.41
2:B:1007:VAL:HA	2:B:1008:PRO:HD3	1.97	0.41
2:B:705:MET:HB3	2:B:706:GLN:HE21	1.85	0.41
4:E:36:GLU:O	4:E:38:PRO:N	2.53	0.41
3:C:15:LYS:NZ	3:C:15:LYS:HD2	2.36	0.41
1:A:300:VAL:HG12	1:A:304:MET:HE1	2.03	0.41
1:A:92:HIS:O	1:A:93:VAL:C	2.58	0.41
1:A:875:ALA:HB2	1:A:1366:ARG:HG3	2.02	0.41
1:A:1236:LEU:O	1:A:1237:ILE:HD12	2.20	0.41
1:A:542:GLU:O	1:A:546:VAL:HG23	2.20	0.41
1:A:557:ASP:O	1:A:558:GLY:C	2.41	0.41
8:J:5:VAL:HG12	8:J:6:ARG:HG2	2.03	0.41
2:B:820:GLY:HA3	2:B:1091:TYR:CE2	2.56	0.41
9:K:33:ILE:CD1	9:K:87:LEU:HD22	2.51	0.41
1:A:820:GLY:O	1:A:821:ARG:C	2.54	0.41
2:B:292:ILE:N	2:B:293:PRO:CD	2.83	0.41
1:A:922:ASP:OD1	1:A:922:ASP:C	2.58	0.41
3:C:53:THR:HB	3:C:154:LYS:HG3	2.02	0.41
10:L:30:ILE:HG21	10:L:30:ILE:HD13	2.02	0.41
1:A:186:LYS:CA	1:A:186:LYS:CG	2.88	0.41
1:A:1132:LYS:C	1:A:1134:ILE:N	2.68	0.41
1:A:1111:MET:CE	1:A:1111:MET:CB	2.99	0.41
7:I:14:LEU:HB3	7:I:27:PHE:HB3	2.03	0.41
2:B:565:PRO:O	2:B:566:LEU:C	2.58	0.41
1:A:1372:VAL:HG12	1:A:1373:ASP:N	2.34	0.41
2:B:555:ILE:HD12	2:B:587:HIS:CE1	2.56	0.41
4:E:88:VAL:HG12	4:E:116:ILE:HG23	2.02	0.41
1:A:1166:ASP:O	1:A:1167:GLU:C	2.58	0.41
3:C:124:LEU:HD23	3:C:124:LEU:N	2.36	0.41
6:H:22:LYS:C	6:H:23:VAL:HG23	2.38	0.41
2:B:877:PRO:O	2:B:878:GLN:HG2	2.21	0.41
1:A:243:PRO:C	1:A:245:PRO:HD2	2.40	0.41
4:E:167:ARG:HD3	4:E:167:ARG:HA	1.92	0.41
9:K:105:PHE:C	9:K:107:THR:H	2.23	0.41
1:A:1107:VAL:O	1:A:1107:VAL:HG12	2.20	0.41
2:B:170:LEU:HD12	2:B:170:LEU:HA	1.83	0.41
1:A:553:VAL:O	1:A:554:PRO:C	2.56	0.41
5:F:74:ILE:HG23	5:F:74:ILE:HD12	1.80	0.41
3:C:22:LEU:HD23	3:C:22:LEU:HA	1.82	0.41
10:L:38:LEU:HD13	10:L:48:CYS:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:51:ALA:CB	6:H:51:ALA:N	2.67	0.41
2:B:1006:ILE:CG2	2:B:1007:VAL:N	2.83	0.41
6:H:138:GLU:CG	6:H:139:ASN:H	2.33	0.41
1:A:40:THR:CB	1:A:40:THR:HA	2.21	0.41
1:A:1318:THR:HG23	4:E:11:ARG:NH1	2.28	0.41
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.56	0.41
4:E:79:TRP:HE1	4:E:81:GLU:HB2	1.86	0.41
2:B:199:MET:HE1	2:B:488:TYR:CE1	2.56	0.41
1:A:456:MET:HB2	1:A:478:TYR:OH	2.21	0.41
1:A:1209:MET:O	1:A:1210:GLY:C	2.59	0.41
6:H:118:PHE:O	6:H:120:GLY:N	2.54	0.41
1:A:489:LEU:C	1:A:489:LEU:HD23	2.40	0.41
7:I:111:THR:HG21	7:I:113:ASP:HB2	2.02	0.41
7:I:111:THR:HB	7:I:113:ASP:H	1.86	0.41
1:A:1225:PHE:C	1:A:1226:VAL:HG23	2.41	0.41
6:H:11:GLN:NE2	6:H:52:GLN:HG2	2.35	0.41
2:B:344:LYS:O	2:B:345:LYS:C	2.59	0.41
4:E:55:ARG:C	4:E:57:MET:N	2.73	0.41
1:A:84:ILE:HD13	1:A:270:LEU:HD11	2.02	0.41
8:J:36:LEU:HD13	8:J:47:ARG:HB3	2.03	0.41
1:A:567:LYS:O	1:A:568:PRO:C	2.57	0.41
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.21	0.41
2:B:92:PHE:CZ	2:B:428:ILE:HD12	2.55	0.41
4:E:78:LEU:CD2	4:E:80:VAL:HG23	2.51	0.41
9:K:58:PHE:HB3	9:K:76:GLN:HB3	2.03	0.41
1:A:11:LEU:HD11	2:B:1195:HIS:HD2	1.82	0.41
1:A:478:TYR:CD1	1:A:487:MET:HE1	2.56	0.41
9:K:83:PRO:C	9:K:85:ASP:H	2.25	0.41
9:K:21:ILE:HG12	9:K:33:ILE:HG12	2.03	0.41
2:B:539:LEU:H	2:B:539:LEU:HG	1.69	0.41
2:B:423:LYS:O	2:B:426:LYS:N	2.47	0.40
4:E:44:ALA:O	4:E:46:TYR:N	2.54	0.40
10:L:38:LEU:CD2	10:L:40:LEU:HB2	2.49	0.40
1:A:1318:THR:CG2	4:E:11:ARG:HH12	2.27	0.40
1:A:1130:GLN:NE2	1:A:1134:ILE:CD1	2.84	0.40
3:C:15:LYS:O	3:C:240:VAL:CG2	2.70	0.40
1:A:370:ILE:HD11	2:B:1103:ILE:HG23	2.02	0.40
2:B:787:VAL:O	2:B:787:VAL:HG13	2.20	0.40
1:A:606:LEU:HB3	1:A:614:PHE:CD2	2.56	0.40
2:B:764:SER:HB3	2:B:765:PRO:CD	2.51	0.40
1:A:577:ILE:HG23	1:A:577:ILE:HD12	1.83	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1207:LEU:HD23	1:A:1207:LEU:HA	2.00	0.40
7:I:45:ARG:HG3	7:I:46:HIS:N	2.35	0.40
2:B:723:VAL:CA	2:B:723:VAL:CG1	2.92	0.40
2:B:119:LEU:O	2:B:965:LYS:NZ	2.49	0.40
2:B:117:ALA:HB1	2:B:122:LEU:HB2	2.03	0.40
2:B:121:ASN:ND2	2:B:965:LYS:NZ	2.69	0.40
6:H:95:TYR:HB3	6:H:144:ILE:CG2	2.52	0.40
2:B:435:THR:CA	2:B:436:VAL:N	2.69	0.40
5:F:89:GLU:O	5:F:90:ARG:C	2.56	0.40
3:C:73:GLN:HG3	3:C:74:SER:N	2.36	0.40
2:B:56:ASP:N	2:B:56:ASP:OD1	2.53	0.40
1:A:970:THR:O	1:A:970:THR:CG2	2.68	0.40
2:B:404:LYS:C	2:B:405:ARG:HG2	2.41	0.40
1:A:993:LEU:O	1:A:994:GLN:C	2.56	0.40
1:A:1327:ILE:HD13	1:A:1327:ILE:HG21	1.90	0.40
2:B:328:GLU:CG	2:B:328:GLU:HA	2.50	0.40
1:A:44:THR:CB	1:A:44:THR:HA	2.33	0.40
1:A:187:LYS:O	1:A:188:ASP:OD1	2.40	0.40
1:A:941:LYS:CD	1:A:941:LYS:NZ	2.84	0.40
9:K:74:ARG:HD2	9:K:74:ARG:HH11	1.50	0.40
1:A:1293:SER:OG	1:A:1294:PRO:N	2.45	0.40
2:B:899:ILE:HD13	2:B:899:ILE:HG21	1.72	0.40
2:B:899:ILE:HG22	2:B:900:ALA:H	1.86	0.40
2:B:911:ILE:O	2:B:912:ILE:HG13	2.21	0.40
2:B:405:ARG:HA	2:B:631:GLY:O	2.20	0.40
7:I:104:LEU:HD23	7:I:104:LEU:HA	1.90	0.40
7:I:15:TYR:CD1	7:I:30:ARG:HG3	2.57	0.40
6:H:2:SER:HA	6:H:3:ASN:N	2.32	0.40
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.86	0.40
1:A:300:VAL:O	1:A:303:TYR:HB3	2.20	0.40
3:C:167:HIS:CD2	3:C:169:LYS:HG2	2.56	0.40
2:B:1131:GLY:C	2:B:1133:MET:N	2.74	0.40
2:B:422:LYS:HD3	2:B:422:LYS:HA	1.95	0.40
2:B:191:LYS:CG	2:B:191:LYS:CE	2.94	0.40
9:K:7:PHE:CD1	9:K:7:PHE:C	2.93	0.40
1:A:567:LYS:HB2	1:A:568:PRO:HD3	2.03	0.40
2:B:101:MET:CG	2:B:101:MET:O	2.69	0.40
1:A:187:LYS:CG	1:A:194:ALA:HB3	2.51	0.40
1:A:616:VAL:HG12	1:A:617:VAL:N	2.35	0.40
2:B:739:THR:C	2:B:740:HIS:CG	2.95	0.40
2:B:1204:PHE:O	2:B:1205:GLN:C	2.58	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:16:ASP:OD1	8:J:17:LYS:HE2	2.22	0.40
2:B:973:ILE:HD13	2:B:973:ILE:HG21	1.91	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	1332/1733 (77%)	1173 (88%)	93 (7%)	66 (5%)	3	24
2	B	1071/1224 (88%)	914 (85%)	110 (10%)	47 (4%)	3	28
3	C	264/318 (83%)	230 (87%)	22 (8%)	12 (4%)	3	27
4	E	213/215 (99%)	182 (85%)	20 (9%)	11 (5%)	2	23
5	F	81/155 (52%)	72 (89%)	7 (9%)	2 (2%)	7	43
6	H	129/146 (88%)	82 (64%)	21 (16%)	26 (20%)	0	1
7	I	119/122 (98%)	107 (90%)	11 (9%)	1 (1%)	24	67
8	J	62/70 (89%)	58 (94%)	3 (5%)	1 (2%)	12	53
9	K	112/120 (93%)	99 (88%)	9 (8%)	4 (4%)	4	34
10	L	44/70 (63%)	24 (54%)	9 (20%)	11 (25%)	0	0
All	All	3427/4173 (82%)	2941 (86%)	305 (9%)	181 (5%)	2	22

All (181) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	38	PRO
1	A	45	GLN
1	A	47	ARG
1	A	59	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	60	SER
1	A	62	ASP
1	A	65	LEU
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	190	ALA
1	A	193	ASP
1	A	286	HIS
1	A	326	ARG
1	A	465	TYR
1	A	567	LYS
1	A	672	ASP
1	A	707	GLY
1	A	1064	VAL
1	A	1065	GLY
1	A	1080	THR
1	A	1221	LYS
1	A	1263	ILE
1	A	1448	GLU
2	B	66	ASP
2	B	105	SER
2	B	109	THR
2	B	230	ALA
2	B	646	LEU
2	B	733	HIS
2	B	864	LYS
2	B	879	ARG
2	B	887	HIS
2	B	957	ASN
2	B	1108	ARG
2	B	1128	LEU
2	B	1167	GLY
3	C	4	GLU
3	C	206	ASN
4	E	48	ASP
4	E	59	SER
5	F	73	ALA
6	H	32	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	H	52	GLN
6	H	53	ASP
6	H	78	SER
6	H	104	PHE
6	H	105	GLU
6	H	107	VAL
6	H	116	TYR
6	H	132	LEU
6	H	136	LYS
6	H	139	ASN
7	I	4	PHE
9	K	111	LEU
10	L	28	LYS
10	L	39	SER
10	L	45	ALA
10	L	46	VAL
10	L	50	ASP
10	L	58	LYS
1	A	57	ARG
1	A	64	ASN
1	A	226	GLU
1	A	418	SER
1	A	464	PRO
1	A	885	THR
1	A	1128	GLN
1	A	1234	GLU
2	B	106	ASP
2	B	108	VAL
2	B	165	VAL
2	B	307	ASP
2	B	424	LEU
2	B	432	MET
2	B	451	LYS
2	B	643	ASP
2	B	1078	GLY
2	B	1099	VAL
2	B	1155	SER
2	B	1190	ASP
3	C	9	LYS
3	C	56	THR
3	C	231	ASN
4	E	126	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	H	18	GLY
6	H	19	ARG
6	H	34	ASP
6	H	81	PRO
6	H	82	PRO
6	H	86	ASP
6	H	90	ALA
6	H	128	ASN
9	K	99	GLY
1	A	29	ALA
1	A	56	PRO
1	A	75	ASN
1	A	136	ALA
1	A	188	ASP
1	A	196	GLU
1	A	1204	ASP
1	A	1366	ARG
2	B	263	GLY
2	B	266	ALA
2	B	865	LYS
2	B	868	MET
2	B	940	PRO
2	B	1097	HIS
2	B	1140	ALA
2	B	1221	SER
3	C	10	ILE
3	C	215	GLU
3	C	266	ASP
4	E	41	ASP
4	E	118	PRO
6	H	5	LEU
9	K	50	LEU
9	K	104	ASN
1	A	167	CYS
1	A	400	PRO
1	A	408	ASP
1	A	599	SER
1	A	706	HIS
1	A	1232	ASN
1	A	1255	GLU
1	A	1280	GLU
1	A	1359	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	56	ASP
2	B	90	ILE
2	B	645	SER
2	B	1105	ALA
4	E	56	LYS
4	E	64	PRO
6	H	77	ARG
6	H	88	SER
6	H	89	LEU
10	L	35	SER
10	L	41	SER
10	L	49	LYS
10	L	54	ARG
1	A	63	ARG
1	A	78	PRO
1	A	279	LEU
1	A	287	HIS
1	A	915	SER
2	B	115	GLN
2	B	436	VAL
3	C	208	GLU
4	E	127	ILE
5	F	112	GLU
6	H	7	ASP
6	H	8	ASP
10	L	59	ALA
1	A	128	ILE
1	A	191	THR
1	A	958	VAL
1	A	1189	SER
1	A	1223	ASP
2	B	644	GLU
2	B	943	SER
2	B	1176	ASN
2	B	1214	PRO
3	C	137	LYS
4	E	50	MET
4	E	73	PRO
6	H	83	GLN
2	B	1103	ILE
1	A	32	VAL
3	C	18	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	99	LYS
2	B	1189	ILE
3	C	217	ASP
8	J	14	VAL
1	A	55	ASP
2	B	364	ILE
4	E	37	LEU
1	A	1002	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	1181/1520 (78%)	971 (82%)	210 (18%)	2	12
2	B	947/1061 (89%)	788 (83%)	159 (17%)	2	14
3	C	234/274 (85%)	194 (83%)	40 (17%)	2	14
4	E	197/197 (100%)	145 (74%)	52 (26%)	0	3
5	F	73/137 (53%)	62 (85%)	11 (15%)	3	19
6	H	117/128 (91%)	71 (61%)	46 (39%)	0	1
7	I	115/116 (99%)	82 (71%)	33 (29%)	0	2
8	J	59/65 (91%)	45 (76%)	14 (24%)	1	4
9	K	99/102 (97%)	81 (82%)	18 (18%)	2	11
10	L	40/57 (70%)	21 (52%)	19 (48%)	0	0
All	All	3062/3657 (84%)	2460 (80%)	602 (20%)	1	8

All (602) 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	28	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	34	LYS
1	A	36	ARG
1	A	39	GLU
1	A	46	THR
1	A	49	LYS
1	A	54	ASN
1	A	57	ARG
1	A	58	LEU
1	A	60	SER
1	A	62	ASP
1	A	65	LEU
1	A	68	GLN
1	A	70	CYS
1	A	72	GLU
1	A	77	CYS
1	A	84	ILE
1	A	85	ASP
1	A	90	VAL
1	A	93	VAL
1	A	98	LYS
1	A	106	VAL
1	A	107	CYS
1	A	110	CYS
1	A	112	LYS
1	A	114	LEU
1	A	120	GLU
1	A	123	ARG
1	A	129	LYS
1	A	133	LYS
1	A	138	ILE
1	A	141	LEU
1	A	143	LYS
1	A	144	THR
1	A	145	LYS
1	A	147	VAL
1	A	156	ASP
1	A	159	THR
1	A	160	GLN
1	A	162	VAL
1	A	163	SER
1	A	167	CYS
1	A	174	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	176	LYS
1	A	184	SER
1	A	186	LYS
1	A	191	THR
1	A	198	GLU
1	A	205	GLU
1	A	206	GLU
1	A	210	ILE
1	A	225	ASN
1	A	226	GLU
1	A	239	LEU
1	A	247	ARG
1	A	261	ASP
1	A	265	LYS
1	A	268	ASP
1	A	270	LEU
1	A	274	ILE
1	A	275	SER
1	A	286	HIS
1	A	289	ILE
1	A	294	SER
1	A	297	GLN
1	A	299	HIS
1	A	324	SER
1	A	326	ARG
1	A	346	ASP
1	A	351	THR
1	A	354	SER
1	A	368	LYS
1	A	383	TYR
1	A	413	ILE
1	A	416	ARG
1	A	419	LYS
1	A	423	ASP
1	A	434	ARG
1	A	446	ARG
1	A	451	HIS
1	A	455	MET
1	A	461	LYS
1	A	466	SER
1	A	472	LEU
1	A	474	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	475	THR
1	A	493	GLN
1	A	495	GLU
1	A	497	THR
1	A	498	ARG
1	A	504	LEU
1	A	508	PRO
1	A	513	SER
1	A	518	LYS
1	A	535	THR
1	A	537	ARG
1	A	543	LEU
1	A	565	ILE
1	A	566	ILE
1	A	571	LEU
1	A	586	ILE
1	A	588	LEU
1	A	597	LEU
1	A	599	SER
1	A	618	GLU
1	A	620	LYS
1	A	622	VAL
1	A	630	ILE
1	A	644	LYS
1	A	666	ILE
1	A	681	GLU
1	A	688	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	728	LYS
1	A	741	ASN
1	A	744	LYS
1	A	752	LYS
1	A	794	PRO
1	A	810	PRO
1	A	821	ARG
1	A	830	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	840	ARG
1	A	858	ASN
1	A	880	LYS
1	A	882	SER
1	A	885	THR
1	A	893	PHE
1	A	894	GLU
1	A	895	LYS
1	A	903	ASN
1	A	907	THR
1	A	909	ASP
1	A	919	ILE
1	A	920	LEU
1	A	973	ILE
1	A	974	ASP
1	A	978	PRO
1	A	979	SER
1	A	1001	ARG
1	A	1006	ILE
1	A	1015	VAL
1	A	1030	ARG
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	1120	LEU
1	A	1127	ASP
1	A	1129	GLU
1	A	1133	LEU
1	A	1134	ILE
1	A	1146	VAL
1	A	1161	THR
1	A	1165	GLU
1	A	1168	GLU
1	A	1171	GLN
1	A	1176	LEU
1	A	1187	GLN
1	A	1217	LYS
1	A	1222	ASN
1	A	1225	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1230	GLU
1	A	1235	LYS
1	A	1237	ILE
1	A	1239	ARG
1	A	1243	VAL
1	A	1255	GLU
1	A	1257	ASP
1	A	1258	HIS
1	A	1259	MET
1	A	1260	LEU
1	A	1267	MET
1	A	1269	GLU
1	A	1277	GLU
1	A	1280	GLU
1	A	1281	ARG
1	A	1291	VAL
1	A	1293	SER
1	A	1299	VAL
1	A	1309	ASP
1	A	1314	SER
1	A	1318	THR
1	A	1325	THR
1	A	1359	ASP
1	A	1364	ASN
1	A	1366	ARG
1	A	1372	VAL
1	A	1376	THR
1	A	1377	THR
1	A	1384	VAL
1	A	1405	THR
1	A	1411	GLU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	65	GLU
2	B	68	THR
2	B	69	LEU
2	B	89	GLU
2	B	90	ILE
2	B	92	PHE
2	B	98	THR
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	167	ILE
2	B	169	ARG
2	B	179	CYS
2	B	183	GLU
2	B	187	SER
2	B	199	MET
2	B	205	ILE
2	B	217	ARG
2	B	228	LYS
2	B	239	GLU
2	B	242	SER
2	B	248	SER
2	B	249	ARG
2	B	252	SER
2	B	261	ARG
2	B	264	SER
2	B	276	ILE
2	B	277	LYS
2	B	282	ILE
2	B	283	VAL
2	B	305	VAL
2	B	306	ASN
2	B	315	LYS
2	B	357	GLN
2	B	358	LYS
2	B	367	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	373	ARG
2	B	383	ASN
2	B	384	ARG
2	B	387	LEU
2	B	394	ASP
2	B	417	PHE
2	B	423	LYS
2	B	425	THR
2	B	429	PHE
2	B	434	ARG
2	B	435	THR
2	B	446	LEU
2	B	448	ILE
2	B	452	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	513	GLN
2	B	516	ASN
2	B	524	PRO
2	B	531	GLN
2	B	547	VAL
2	B	549	THR
2	B	552	MET
2	B	566	LEU
2	B	589	VAL
2	B	591	ARG
2	B	595	ARG
2	B	598	GLU
2	B	612	GLU
2	B	614	SER
2	B	641	GLU
2	B	648	HIS
2	B	653	VAL
2	B	666	TYR
2	B	680	THR
2	B	691	GLU
2	B	693	ILE
2	B	706	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	710	LEU
2	B	723	VAL
2	B	733	HIS
2	B	736	THR
2	B	775	LYS
2	B	788	ARG
2	B	802	PRO
2	B	806	THR
2	B	838	SER
2	B	857	ARG
2	B	864	LYS
2	B	868	MET
2	B	871	THR
2	B	878	GLN
2	B	879	ARG
2	B	880	THR
2	B	881	ASN
2	B	882	THR
2	B	883	LEU
2	B	884	ARG
2	B	889	THR
2	B	891	ASP
2	B	895	ASP
2	B	896	ASP
2	B	908	GLU
2	B	933	SER
2	B	938	SER
2	B	944	THR
2	B	955	THR
2	B	956	THR
2	B	958	GLN
2	B	964	VAL
2	B	973	ILE
2	B	974	PRO
2	B	975	GLN
2	B	983	ARG
2	B	987	LYS
2	B	996	ARG
2	B	997	GLU
2	B	1007	VAL
2	B	1045	SER
2	B	1056	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1060	ARG
2	B	1065	GLN
2	B	1077	THR
2	B	1085	ILE
2	B	1097	HIS
2	B	1099	VAL
2	B	1101	ASP
2	B	1106	ARG
2	B	1150	ARG
2	B	1152	MET
2	B	1155	SER
2	B	1156	ASP
2	B	1159	ARG
2	B	1165	ILE
2	B	1174	LYS
2	B	1175	LEU
2	B	1177	HIS
2	B	1178	ASN
2	B	1179	GLN
2	B	1183	LYS
2	B	1185	CYS
2	B	1187	ASN
2	B	1190	ASP
2	B	1211	ASN
2	B	1218	THR
2	B	1220	ARG
2	B	1222	ARG
2	B	1224	PHE
3	C	3	GLU
3	C	4	GLU
3	C	14	SER
3	C	23	SER
3	C	25	VAL
3	C	26	ASP
3	C	29	MET
3	C	33	LEU
3	C	43	THR
3	C	56	THR
3	C	57	VAL
3	C	62	PHE
3	C	83	SER
3	C	86	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	93	ASP
3	C	102	GLN
3	C	119	VAL
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	137	LYS
3	C	154	LYS
3	C	156	THR
3	C	163	ILE
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	218	PRO
3	C	235	VAL
3	C	238	ILE
3	C	241	ASP
3	C	242	GLN
3	C	245	VAL
3	C	246	ARG
3	C	252	GLN
3	C	266	ASP
4	E	3	GLN
4	E	6	GLU
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	47	CYS
4	E	49	SER
4	E	50	MET
4	E	52	ARG
4	E	56	LYS
4	E	57	MET
4	E	61	GLN
4	E	69	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	E	70	SER
4	E	74	ASP
4	E	78	LEU
4	E	81	GLU
4	E	82	PHE
4	E	84	ASP
4	E	85	GLU
4	E	91	LYS
4	E	92	THR
4	E	93	MET
4	E	100	ILE
4	E	102	GLU
4	E	103	LYS
4	E	107	THR
4	E	115	ASN
4	E	116	ILE
4	E	117	THR
4	E	118	PRO
4	E	121	MET
4	E	123	LEU
4	E	129	PRO
4	E	137	GLU
4	E	148	GLU
4	E	149	LEU
4	E	158	SER
4	E	159	ASP
4	E	161	LYS
4	E	167	ARG
4	E	169	ARG
4	E	179	GLN
4	E	183	PRO
4	E	192	ARG
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	81	THR
5	F	82	THR
5	F	92	ARG
5	F	97	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	F	110	ASP
5	F	111	LEU
5	F	117	PRO
5	F	119	ARG
5	F	128	LYS
6	H	4	THR
6	H	5	LEU
6	H	6	PHE
6	H	7	ASP
6	H	13	SER
6	H	17	PRO
6	H	19	ARG
6	H	22	LYS
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	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	91	ASP
6	H	92	ASP
6	H	93	TYR
6	H	105	GLU
6	H	106	GLU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	H	131	ASN
6	H	135	LEU
6	H	136	LYS
6	H	137	GLN
6	H	138	GLU
6	H	143	LEU
6	H	144	ILE
6	H	145	ARG
6	H	146	ARG
7	I	1	MET
7	I	2	THR
7	I	4	PHE
7	I	7	CYS
7	I	8	ARG
7	I	10	CYS
7	I	18	GLU
7	I	21	GLU
7	I	31	THR
7	I	41	PRO
7	I	45	ARG
7	I	46	HIS
7	I	55	THR
7	I	58	VAL
7	I	59	VAL
7	I	61	ASP
7	I	74	GLU
7	I	75	CYS
7	I	76	PRO
7	I	77	LYS
7	I	78	CYS
7	I	81	ARG
7	I	83	ASN
7	I	84	VAL
7	I	93	LYS
7	I	95	THR
7	I	105	SER
7	I	111	THR
7	I	116	ASN
7	I	117	LYS
7	I	118	ARG
7	I	119	THR
7	I	120	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	J	2	ILE
8	J	3	VAL
8	J	7	CYS
8	J	9	SER
8	J	14	VAL
8	J	20	SER
8	J	25	LEU
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	14	GLU
9	K	20	LYS
9	K	31	VAL
9	K	42	LEU
9	K	47	ARG
9	K	54	ARG
9	K	63	VAL
9	K	73	LEU
9	K	78	THR
9	K	93	SER
9	K	94	ILE
9	K	101	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	42	ARG
10	L	43	THR
10	L	44	ASP
10	L	46	VAL
10	L	47	ARG
10	L	49	LYS
10	L	51	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	L	53	HIS
10	L	54	ARG
10	L	58	LYS
10	L	60	ARG
10	L	61	THR
10	L	62	LYS
10	L	64	LEU
10	L	65	VAL
10	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	92	HIS
1	A	171	GLN
1	A	299	HIS
1	A	390	GLN
1	A	399	HIS
1	A	451	HIS
1	A	479	ASN
1	A	503	GLN
1	A	515	GLN
1	A	517	ASN
1	A	587	HIS
1	A	736	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	877	HIS
1	A	903	ASN
1	A	926	GLN
1	A	1078	GLN
1	A	1130	GLN
1	A	1140	HIS
1	A	1173	HIS
1	A	1364	ASN
1	A	1432	GLN
2	B	121	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS
2	B	300	HIS
2	B	325	GLN
2	B	357	GLN
2	B	366	GLN
2	B	395	GLN
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	531	GLN
2	B	538	ASN
2	B	590	HIS
2	B	657	HIS
2	B	706	GLN
2	B	744	HIS
2	B	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	1161	HIS
2	B	1177	HIS
2	B	1179	GLN
2	B	1193	GLN
3	C	73	GLN
3	C	112	ASN
3	C	167	HIS
3	C	242	GLN
3	C	252	GLN
4	E	3	GLN
4	E	101	GLN
4	E	104	ASN
4	E	113	GLN
4	E	147	HIS
6	H	11	GLN
6	H	131	ASN
6	H	134	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	I	12	ASN
7	I	46	HIS
7	I	83	ASN
7	I	116	ASN
9	K	2	ASN
9	K	65	HIS
9	K	110	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	ATP	A	3011	11	24,32,33	1.05	2 (8%)	32,50,52	2.63	8 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	ATP	A	3011	11	1/1/6/7	0/18/34/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	3011	ATP	C8-N7	-2.37	1.30	1.34
13	A	3011	ATP	C4-N3	3.39	1.40	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	3011	ATP	PA-O3A-PB	-4.31	120.63	132.73
13	A	3011	ATP	PB-O3B-PG	-3.46	121.06	132.67
13	A	3011	ATP	C2'-C3'-C4'	2.18	107.29	102.77
13	A	3011	ATP	C2'-C1'-N9	2.58	120.42	114.16
13	A	3011	ATP	C4-C5-N7	2.85	112.10	109.48
13	A	3011	ATP	O4'-C1'-C2'	3.42	113.08	106.27
13	A	3011	ATP	C1'-N9-C4	6.46	138.10	127.16
13	A	3011	ATP	O4'-C1'-N9	10.09	125.18	107.72

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	3011	ATP	C1'

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	1349/1733 (77%)	-0.32	29 (2%) 67 61	1, 22, 99, 165	0
2	B	1091/1224 (89%)	-0.29	51 (4%) 35 32	1, 22, 107, 155	0
3	C	266/318 (83%)	-0.52	1 (0%) 93 91	1, 22, 72, 145	0
4	E	215/215 (100%)	-0.28	4 (1%) 70 64	1, 40, 102, 138	0
5	F	83/155 (53%)	-0.30	1 (1%) 81 75	1, 21, 63, 89	0
6	H	133/146 (91%)	0.22	7 (5%) 30 27	14, 65, 120, 167	0
7	I	121/122 (99%)	-0.14	4 (3%) 50 45	1, 30, 79, 120	0
8	J	64/70 (91%)	-0.50	0 100 100	3, 18, 64, 91	0
9	K	114/120 (95%)	-0.31	0 100 100	1, 32, 72, 103	0
10	L	46/70 (65%)	0.12	2 (4%) 39 34	16, 72, 123, 140	0
All	All	3482/4173 (83%)	-0.29	99 (2%) 56 52	1, 25, 103, 167	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	THR	8.1
2	B	1109	GLY	7.2
2	B	882	THR	7.1
1	A	1450	LEU	6.4
1	A	1449	SER	6.4
2	B	1110	PRO	6.3
6	H	85	GLY	5.8
2	B	869	SER	5.5
2	B	1223	ASP	5.4
2	B	1104	HIS	5.4
2	B	137	TYR	5.2
4	E	1	MET	5.2
1	A	188	ASP	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	248	PRO	5.2
1	A	65	LEU	4.7
2	B	433	GLN	4.6
1	A	44	THR	4.5
2	B	871	THR	4.3
2	B	870	ILE	4.2
2	B	1176	ASN	4.1
1	A	45	GLN	4.0
2	B	959	ASP	3.9
2	B	1105	ALA	3.9
2	B	90	ILE	3.8
2	B	246	LYS	3.8
1	A	43	GLU	3.7
2	B	432	MET	3.7
2	B	866	TYR	3.6
2	B	89	GLU	3.6
10	L	45	ALA	3.6
2	B	136	THR	3.6
7	I	79	HIS	3.5
2	B	1106	ARG	3.5
2	B	130	VAL	3.4
2	B	883	LEU	3.4
2	B	935	ARG	3.4
2	B	868	MET	3.4
2	B	887	HIS	3.4
1	A	191	THR	3.3
2	B	1103	ILE	3.3
3	C	268	ASP	3.2
1	A	190	ALA	3.2
1	A	193	ASP	3.2
2	B	429	PHE	3.0
2	B	68	THR	3.0
6	H	146	ARG	3.0
2	B	1224	PHE	3.0
2	B	69	LEU	3.0
1	A	1448	GLU	3.0
1	A	157	ASP	2.9
2	B	1102	LYS	2.9
1	A	41	MET	2.9
1	A	192	GLY	2.9
2	B	428	ILE	2.9
2	B	938	SER	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	3	GLY	2.8
1	A	62	ASP	2.8
1	A	6	TYR	2.7
6	H	131	ASN	2.6
2	B	1179	GLN	2.6
2	B	135	ARG	2.5
6	H	86	ASP	2.5
4	E	50	MET	2.5
7	I	114	GLN	2.4
2	B	250	PHE	2.4
2	B	131	ASP	2.4
2	B	881	ASN	2.4
2	B	132	VAL	2.4
2	B	1178	ASN	2.4
7	I	74	GLU	2.3
1	A	33	ALA	2.3
6	H	132	LEU	2.3
6	H	127	GLY	2.3
1	A	49	LYS	2.3
6	H	84	ALA	2.3
2	B	936	ASP	2.3
2	B	70	ILE	2.3
2	B	451	LYS	2.3
4	E	51	GLY	2.2
7	I	112	SER	2.2
1	A	7	SER	2.2
1	A	71	GLN	2.2
2	B	92	PHE	2.2
2	B	886	LYS	2.2
5	F	110	ASP	2.1
10	L	25	ALA	2.1
2	B	436	VAL	2.1
1	A	40	THR	2.1
1	A	1079	MET	2.1
2	B	247	GLY	2.1
4	E	52	ARG	2.1
1	A	153	PRO	2.1
2	B	430	ARG	2.1
1	A	66	LYS	2.1
2	B	733	HIS	2.1
2	B	91	SER	2.0
1	A	46	THR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	35	ILE	2.0
2	B	434	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
13	ATP	A	3011	30/31	0.80	0.30	2.28	5,46,82,85	0
12	ZN	C	3002	1/1	0.98	0.07	-1.23	42,42,42,42	0
12	ZN	I	3004	1/1	0.94	0.07	-1.23	66,66,66,66	0
12	ZN	L	3005	1/1	0.96	0.11	-1.43	90,90,90,90	0
12	ZN	A	3008	1/1	0.95	0.05	-1.44	91,91,91,91	0
12	ZN	A	3006	1/1	0.95	0.05	-1.76	47,47,47,47	0
12	ZN	B	3007	1/1	0.98	0.06	-2.00	57,57,57,57	0
12	ZN	I	3003	1/1	0.98	0.03	-2.67	46,46,46,46	0
12	ZN	J	3001	1/1	0.95	0.06	-3.87	34,34,34,34	0
11	MN	A	3009	1/1	0.94	0.09	-	4,4,4,4	0
11	MN	A	3010	1/1	0.97	0.05	-	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.