Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2026 – 04:25 AM UTC

PDB ID	:	1TWH / pdb_00001twh
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

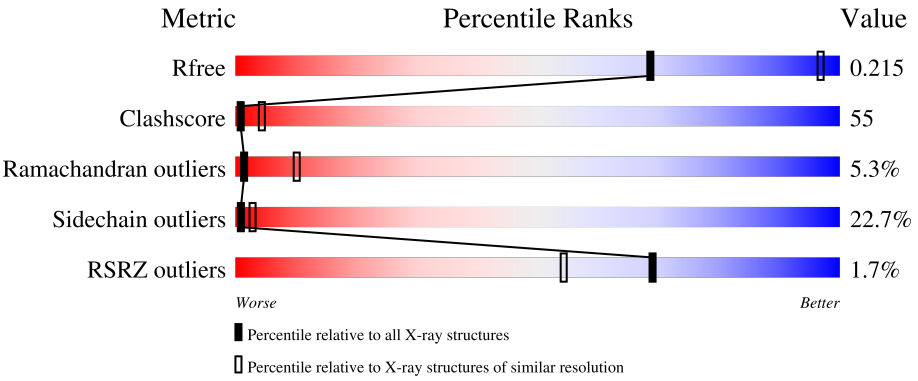
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	32% 31% 13% 22%
2	B	1224	35% 37% 15% 11%
3	C	318	31% 37% 15% 16%
4	E	215	32% 43% 24%
5	F	155	22% 24% 7% 46%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	H	146	8% 14% 37% 40% 9%
7	I	122	% 40% 43% 16%
8	J	70	36% 40% 16% 9%
9	K	120	% 32% 48% 15% 5%
10	L	70	% 9% 26% 30% 34%

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	-	-	-

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 (CCD ID: MN) (formula: Mn).

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

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

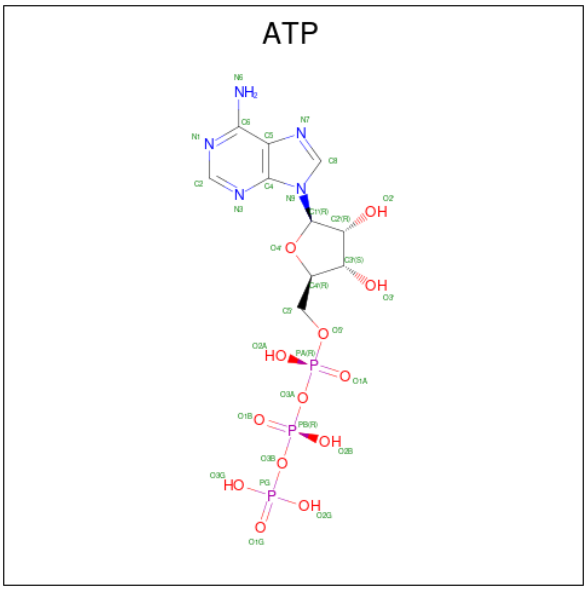
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	2	Total	Zn	0	0
			2	2		
12	B	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C N O P 30 10 5 12 3	0	0

- Molecule 14 is water.

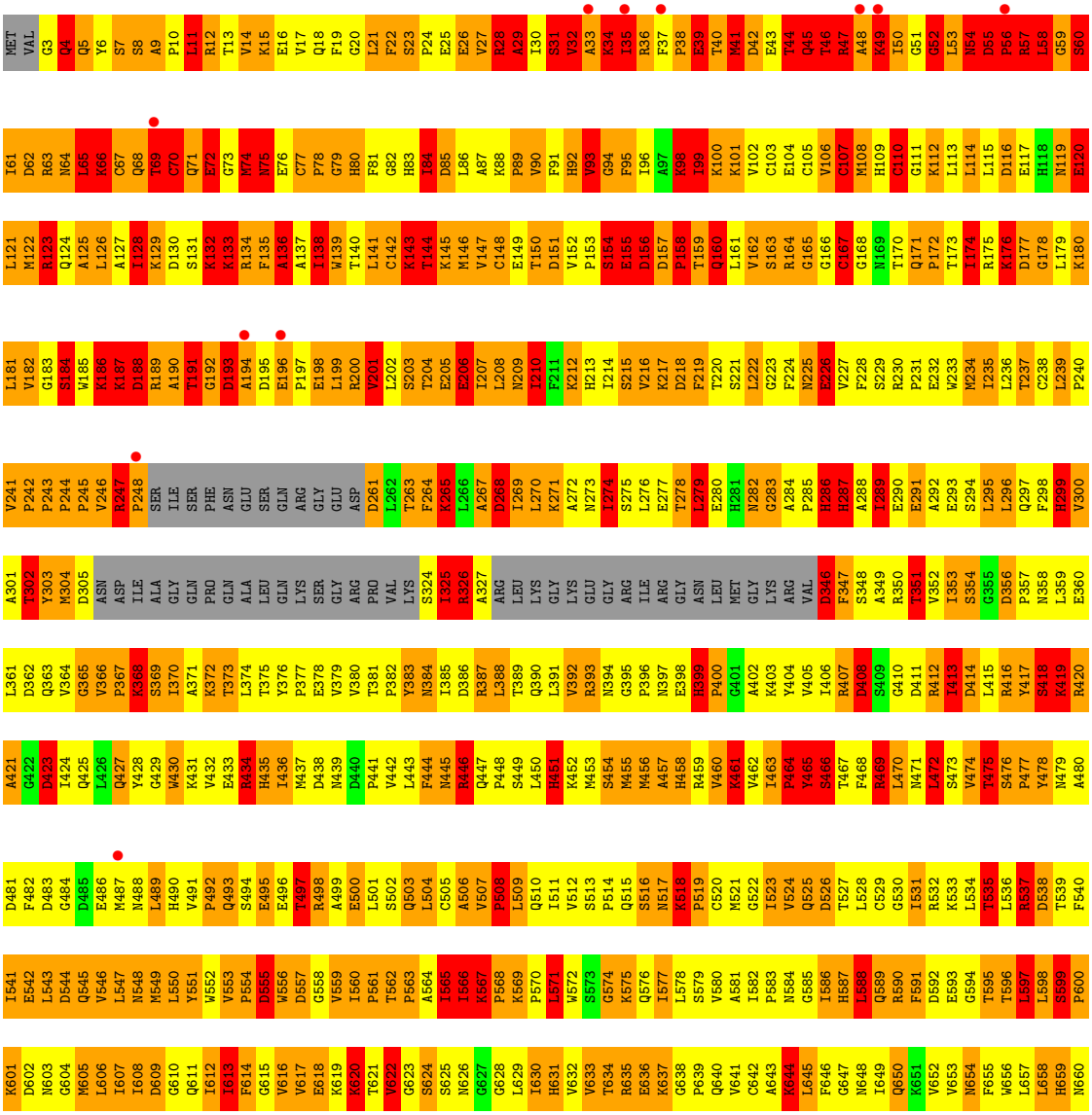
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total O 1 1	0	0

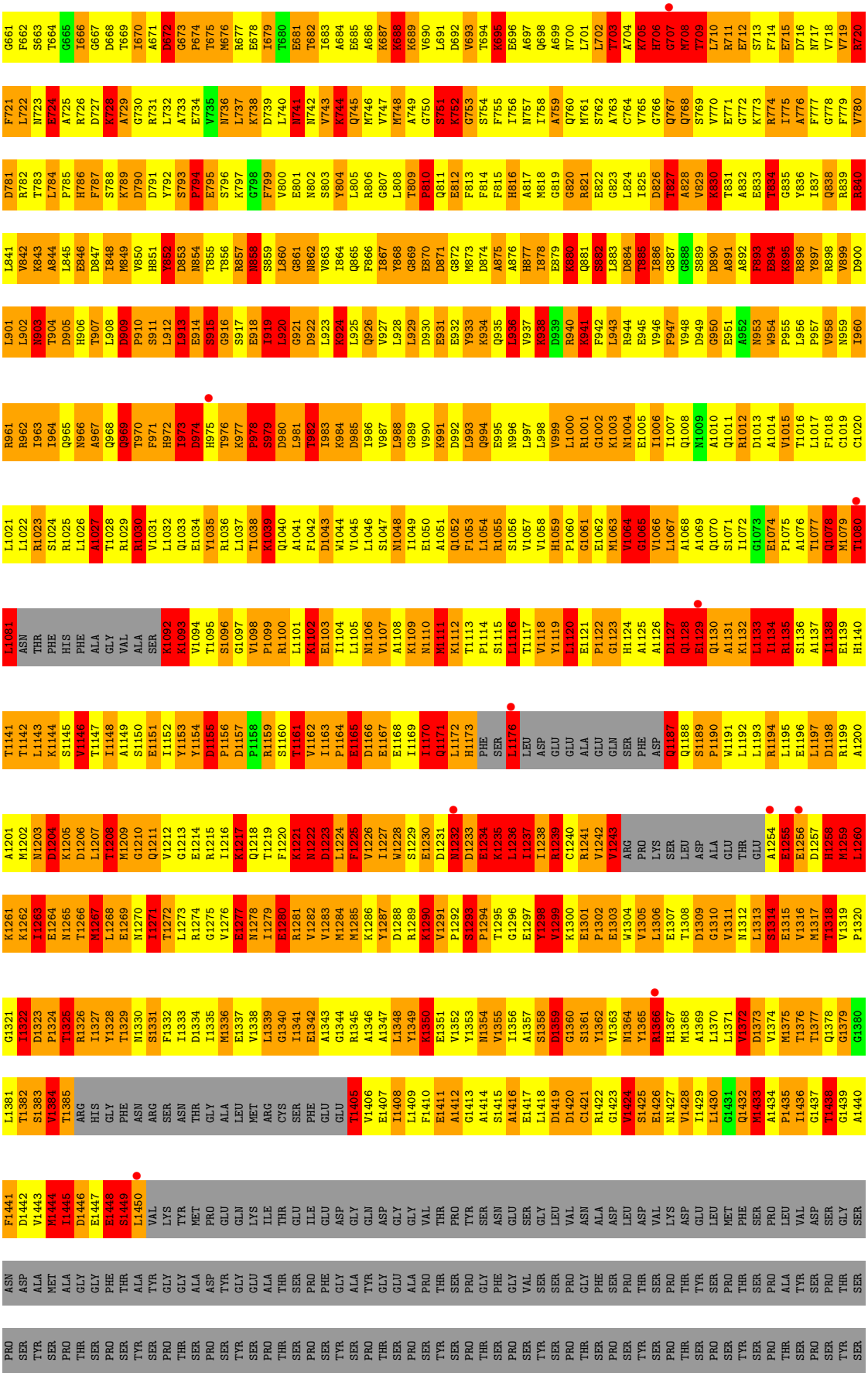
3 Residue-property plots (i)

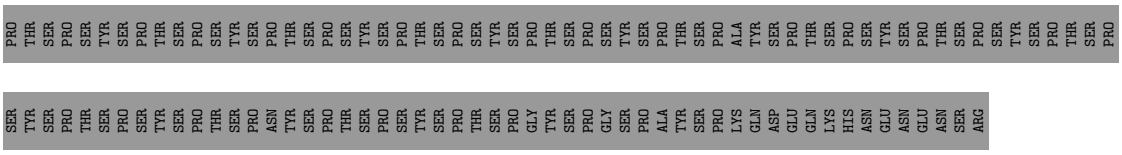
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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

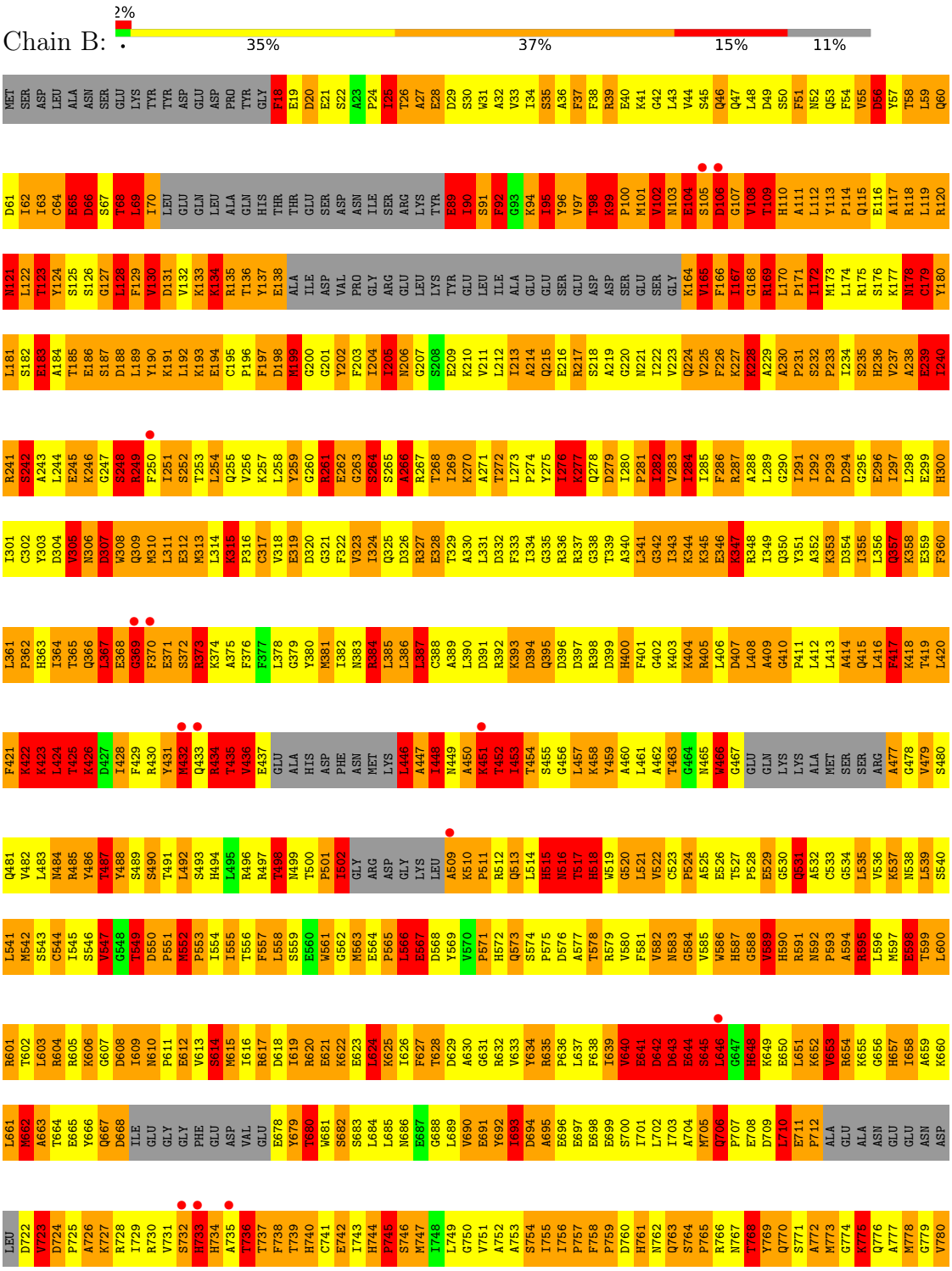
Chain A:

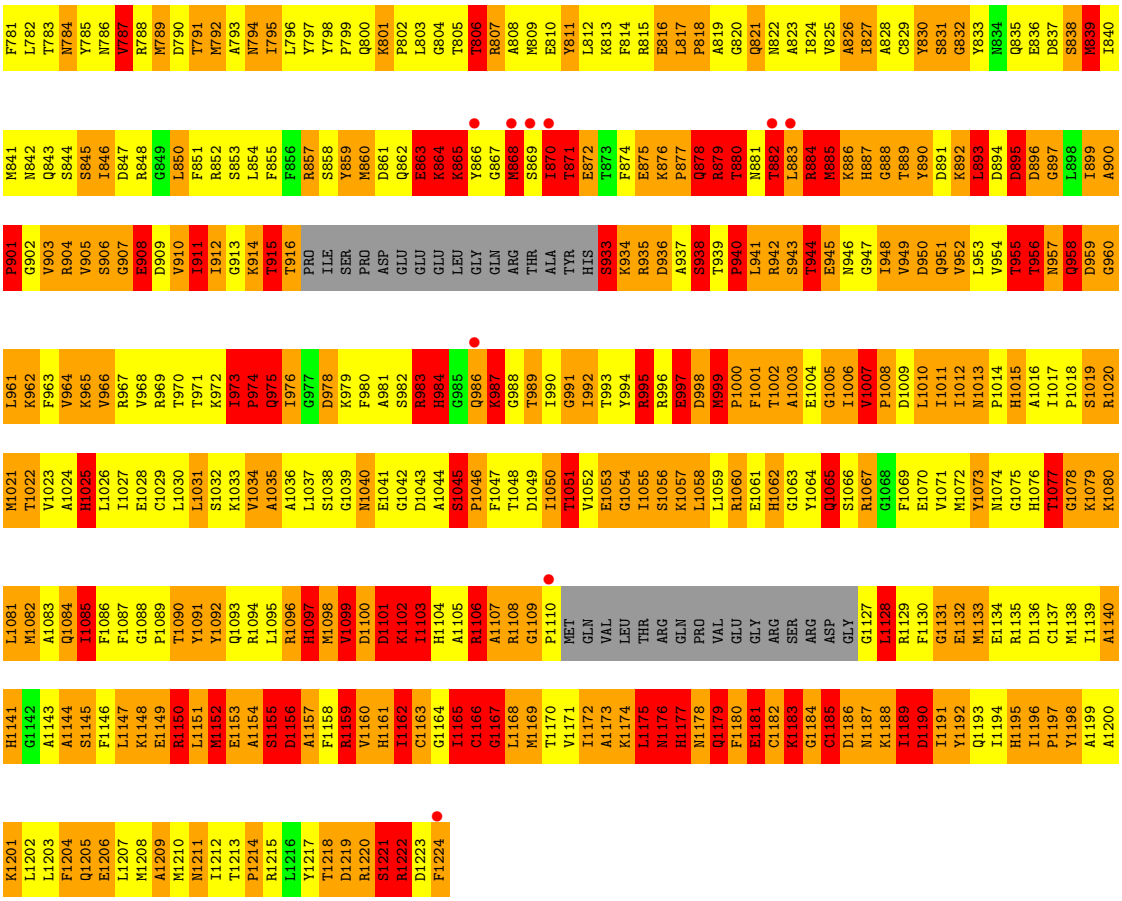






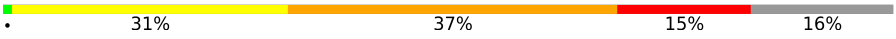
• Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide

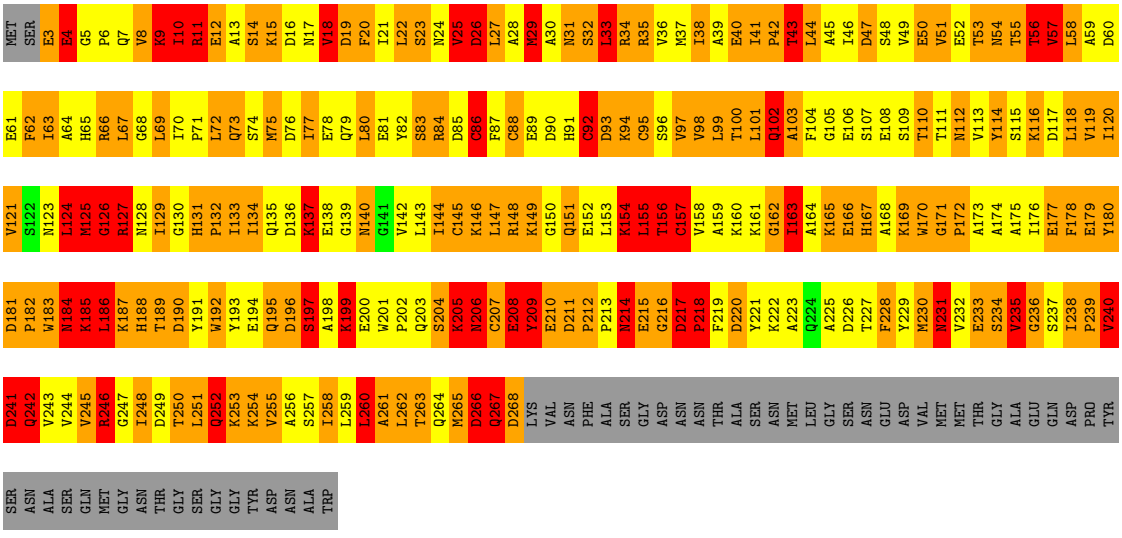




• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide

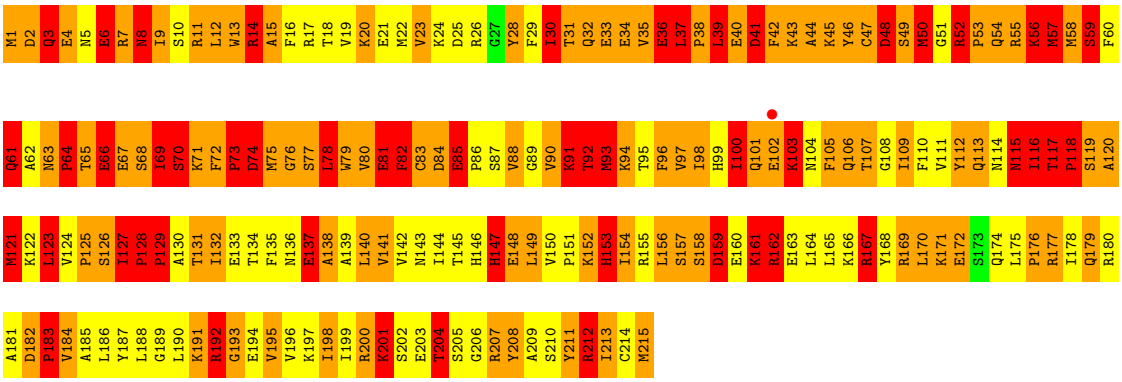
Chain C:





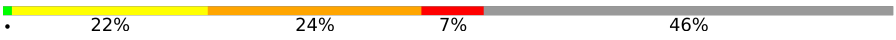
• Molecule 4: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

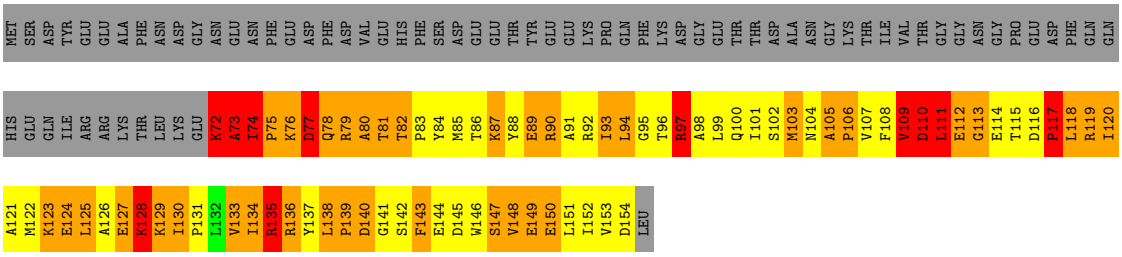
Chain E:



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

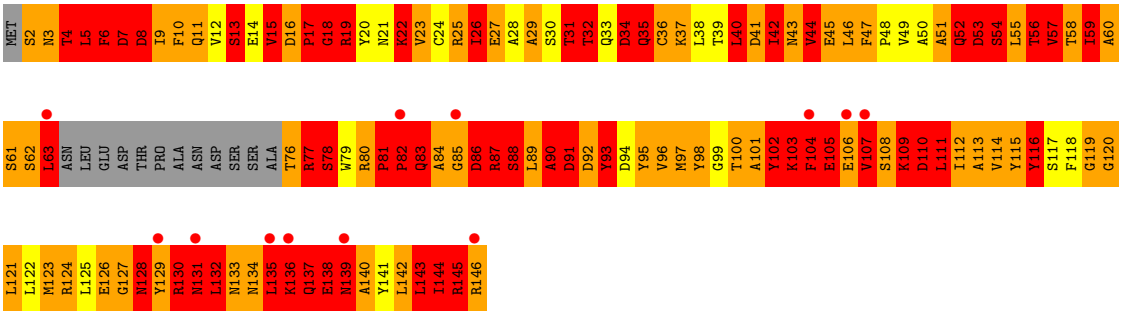
Chain F:





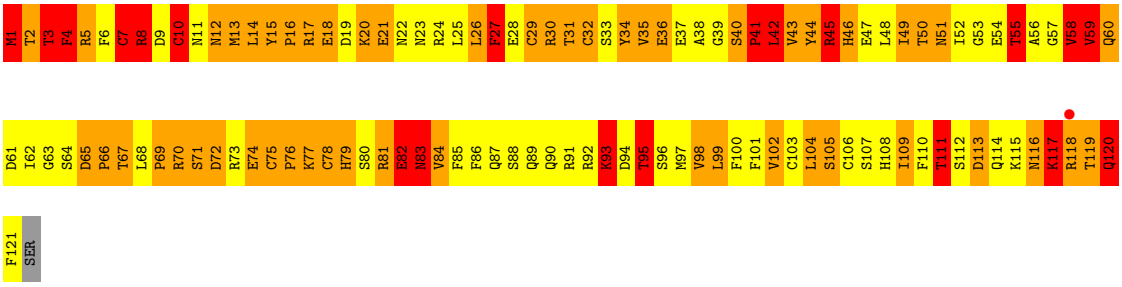
• Molecule 6: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

Chain H:



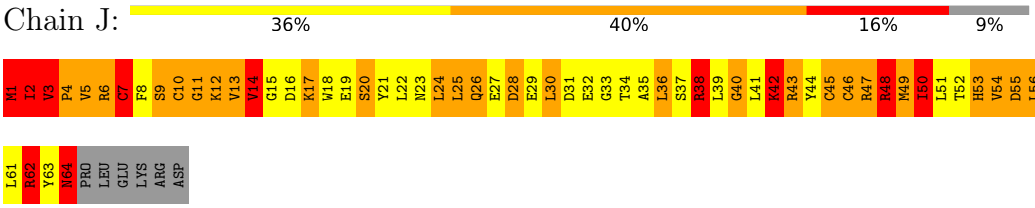
• Molecule 7: DNA-directed RNA polymerase II 14.2 kDa polypeptide

Chain I:



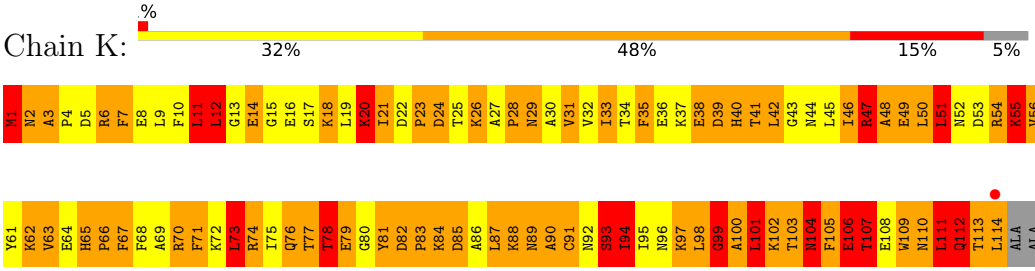
• Molecule 8: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide

Chain J:



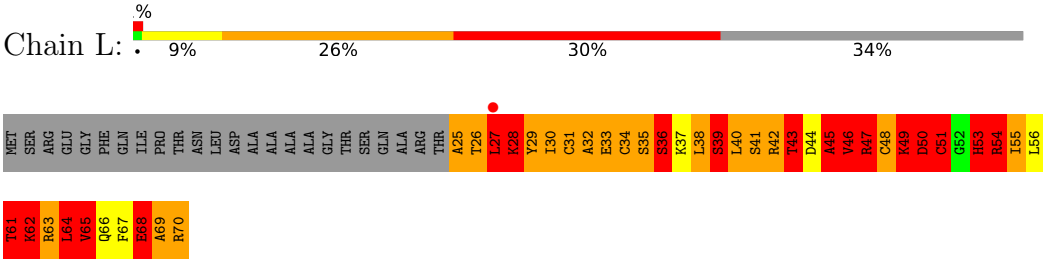
• Molecule 9: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K:



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

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	123.00Å 223.00Å 374.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.40 40.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.40) 97.2 (40.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 3.32Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.262 0.207 , 0.215	Depositor DCC
R_{free} test set	2319 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å^2)	57.9	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 61.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	5.43	3403/10792 (31.5%)	3.43	1848/14601 (12.7%)
2	B	5.33	2843/8860 (32.1%)	3.33	1486/11945 (12.4%)
3	C	5.40	695/2133 (32.6%)	3.41	398/2891 (13.8%)
4	E	5.37	555/1796 (30.9%)	3.35	301/2416 (12.5%)
5	F	4.96	183/682 (26.8%)	3.37	110/922 (11.9%)
6	H	5.31	306/1086 (28.2%)	3.19	178/1470 (12.1%)
7	I	5.54	343/1009 (34.0%)	3.55	203/1357 (15.0%)
8	J	5.10	165/533 (31.0%)	3.58	95/715 (13.3%)
9	K	5.19	305/937 (32.6%)	3.31	161/1265 (12.7%)
10	L	6.23	141/366 (38.5%)	3.65	81/485 (16.7%)
All	All	5.38	8939/28194 (31.7%)	3.39	4861/38067 (12.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	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 (8939) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1064	VAL	CA-C	64.08	2.34	1.52
1	A	1064	VAL	C-O	53.64	1.88	1.24
4	E	57	MET	SD-CE	47.96	2.99	1.79
4	E	50	MET	SD-CE	39.00	2.77	1.79
2	B	552	MET	SD-CE	35.62	2.68	1.79
3	C	75	MET	SD-CE	34.23	2.65	1.79
3	C	267	GLN	CA-C	32.17	1.81	1.53
1	A	44	THR	CA-CB	31.74	2.07	1.53
3	C	125	MET	SD-CE	30.59	2.56	1.79
2	B	101	MET	SD-CE	30.15	2.54	1.79
6	H	104	PHE	CA-C	30.04	1.93	1.52
1	A	1275	GLY	C-O	30.01	1.50	1.23
2	B	552	MET	CG-SD	29.95	2.55	1.80
1	A	464	PRO	C-O	-28.73	0.86	1.24
2	B	1150	ARG	CZ-NH2	27.96	1.69	1.33
1	A	549	MET	SD-CE	-27.61	1.10	1.79
2	B	1164	GLY	C-O	27.15	1.43	1.24
9	K	1	MET	SD-CE	26.69	2.46	1.79
2	B	246	LYS	CA-C	26.54	1.85	1.52
1	A	304	MET	SD-CE	26.46	2.45	1.79
1	A	1285	MET	SD-CE	26.35	2.45	1.79
5	F	103	MET	SD-CE	26.04	2.44	1.79
2	B	885	MET	SD-CE	25.30	2.42	1.79
1	A	1280	GLU	C-O	-25.03	0.92	1.24
2	B	1150	ARG	CZ-NH1	25.03	1.67	1.32
2	B	768	THR	CA-C	24.46	1.85	1.52
10	L	45	ALA	CA-CB	24.17	1.94	1.53
2	B	381	MET	SD-CE	-24.08	1.19	1.79
1	A	227	VAL	C-O	23.95	1.48	1.23
1	A	708	MET	SD-CE	23.85	2.39	1.79
1	A	188	ASP	CA-C	23.79	1.84	1.52
2	B	999	MET	SD-CE	-23.66	1.20	1.79
2	B	1050	ILE	C-O	-23.55	0.96	1.24
6	H	11	GLN	CA-C	-22.97	1.25	1.52
2	B	819	ALA	CA-CB	-22.64	1.35	1.53
10	L	26	THR	CA-CB	22.49	1.91	1.53
1	A	731	ARG	C-O	-22.42	0.97	1.24
9	K	111	LEU	C-O	22.14	1.51	1.24
1	A	880	LYS	C-O	-22.06	0.97	1.24
2	B	436	VAL	CA-CB	22.05	1.84	1.54
1	A	593	GLU	C-O	22.01	1.52	1.24
1	A	670	ILE	CA-CB	-21.93	1.27	1.54
2	B	1171	VAL	C-O	21.84	1.45	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	870	ILE	CA-CB	21.58	1.84	1.53
2	B	792	MET	SD-CE	21.45	2.33	1.79
3	C	198	ALA	CA-CB	-21.38	1.18	1.53
3	C	120	ILE	CA-CB	-21.35	1.30	1.54
2	B	903	VAL	CA-CB	-21.30	1.27	1.54
1	A	1108	ALA	CA-CB	-21.17	1.20	1.53
1	A	1137	ALA	C-O	21.11	1.52	1.24
2	B	705	MET	SD-CE	-20.98	1.27	1.79
2	B	1154	ALA	CA-CB	20.85	1.85	1.53
1	A	74	MET	SD-CE	20.80	2.31	1.79
10	L	48	CYS	CA-C	20.73	1.80	1.52
4	E	1	MET	SD-CE	20.48	2.30	1.79
1	A	40	THR	CA-CB	20.45	1.80	1.53
6	H	146	ARG	NE-CZ	20.33	1.55	1.33
1	A	1291	VAL	C-O	-20.23	1.09	1.24
1	A	274	ILE	CA-CB	20.15	1.80	1.54
1	A	69	THR	CA-C	20.11	1.79	1.52
2	B	1191	ILE	CA-CB	-20.11	1.34	1.55
2	B	699	GLU	N-CA	-20.09	1.19	1.46
2	B	747	MET	SD-CE	-19.88	1.29	1.79
3	C	163	ILE	CA-CB	-19.76	1.26	1.54
1	A	752	LYS	CE-NZ	19.67	2.08	1.49
1	A	864	ILE	C-O	19.63	1.43	1.23
1	A	728	LYS	CD-CE	19.61	2.11	1.52
1	A	45	GLN	CA-C	19.60	1.79	1.52
1	A	1349	TYR	C-O	-19.60	1.00	1.24
1	A	1302	PRO	C-O	19.58	1.46	1.23
2	B	110	HIS	CA-C	19.57	1.75	1.52
3	C	181	ASP	CA-C	-19.57	1.28	1.52
3	C	134	ILE	CA-CB	-19.53	1.29	1.54
1	A	406	ILE	CA-CB	-19.44	1.29	1.54
1	A	1131	ALA	CA-CB	-19.25	1.23	1.53
2	B	1015	HIS	CE1-NE2	19.25	1.51	1.32
3	C	70	ILE	CA-C	-19.23	1.37	1.53
2	B	619	ILE	CA-CB	-19.23	1.27	1.54
1	A	1232	ASN	C-O	19.21	1.48	1.24
10	L	68	GLU	CG-CD	19.21	2.00	1.52
3	C	81	GLU	C-O	19.13	1.47	1.23
1	A	1074	GLU	C-O	-19.08	1.06	1.24
1	A	775	ILE	CA-CB	-19.05	1.34	1.54
6	H	23	VAL	CA-CB	-19.01	1.26	1.55
1	A	938	LYS	CD-CE	18.97	2.09	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	27	ALA	CA-CB	-18.93	1.23	1.53
1	A	620	LYS	CE-NZ	18.88	2.06	1.49
6	H	27	GLU	CA-C	18.83	1.76	1.52
7	I	56	ALA	C-O	-18.77	1.01	1.23
5	F	136	ARG	CZ-NH1	-18.76	1.06	1.32
1	A	1268	LEU	N-CA	-18.73	1.22	1.46
1	A	1422	ARG	NE-CZ	18.73	1.53	1.33
1	A	1135	ARG	CG-CD	18.70	2.08	1.52
5	F	122	MET	SD-CE	-18.62	1.33	1.79
4	E	186	LEU	CA-C	-18.58	1.27	1.52
1	A	1281	ARG	NE-CZ	18.56	1.53	1.33
1	A	752	LYS	CD-CE	18.54	2.08	1.52
4	E	47	CYS	CA-C	18.52	1.75	1.52
2	B	542	MET	SD-CE	-18.50	1.33	1.79
2	B	733	HIS	CA-C	18.50	1.77	1.52
2	B	1091	TYR	CA-C	-18.45	1.30	1.52
1	A	849	MET	SD-CE	-18.44	1.33	1.79
1	A	61	ILE	CA-CB	18.43	1.79	1.54
4	E	49	SER	CA-C	18.38	1.73	1.53
9	K	2	ASN	C-O	18.36	1.48	1.24
2	B	531	GLN	CD-OE1	18.35	1.58	1.23
2	B	204	ILE	CA-CB	-18.28	1.32	1.54
2	B	253	THR	CA-CB	-18.23	1.28	1.53
1	A	1287	TYR	C-O	18.22	1.46	1.23
2	B	409	ALA	CA-CB	-18.18	1.25	1.53
1	A	620	LYS	CD-CE	18.14	2.06	1.52
2	B	531	GLN	CG-CD	18.05	1.97	1.52
1	A	1222	ASN	CB-CG	18.04	1.97	1.52
3	C	127	ARG	N-CA	18.01	1.68	1.46
7	I	17	ARG	CG-CD	17.90	2.06	1.52
2	B	30	SER	C-O	-17.90	1.03	1.24
1	A	111	GLY	C-O	17.88	1.46	1.24
1	A	673	GLY	C-O	-17.85	1.05	1.24
4	E	152	LYS	CD-CE	17.77	2.05	1.52
1	A	616	VAL	CA-CB	-17.72	1.32	1.54
1	A	734	GLU	CD-OE2	17.72	1.59	1.25
1	A	643	ALA	CA-CB	-17.71	1.23	1.53
2	B	703	ILE	C-O	17.70	1.42	1.24
1	A	351	THR	C-O	-17.66	1.01	1.24
1	A	1264	GLU	CA-C	-17.64	1.30	1.52
2	B	646	LEU	CG-CD2	17.59	2.10	1.52
6	H	91	ASP	CA-C	17.59	1.74	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	55	THR	CB-CG2	17.59	2.10	1.52
1	A	738	LYS	C-O	-17.58	1.01	1.23
7	I	1	MET	CG-SD	17.56	2.24	1.80
9	K	56	VAL	CA-CB	17.55	1.74	1.54
2	B	735	ALA	N-CA	17.54	1.67	1.46
1	A	987	VAL	CA-CB	-17.50	1.34	1.54
2	B	817	LEU	N-CA	-17.50	1.28	1.46
2	B	245	GLU	CA-C	17.49	1.75	1.52
3	C	49	VAL	C-O	-17.48	1.06	1.23
2	B	1149	GLU	CA-C	-17.46	1.30	1.52
1	A	1433	MET	CA-C	-17.43	1.30	1.52
1	A	1045	VAL	CA-CB	-17.41	1.33	1.54
2	B	1139	ILE	C-O	-17.38	1.04	1.24
7	I	75	CYS	CA-C	-17.25	1.31	1.53
4	E	147	HIS	CG-CD2	17.25	1.54	1.35
1	A	247	ARG	CA-C	17.23	1.72	1.52
1	A	805	LEU	CA-C	-17.21	1.30	1.52
2	B	949	VAL	CA-CB	-17.20	1.34	1.54
6	H	139	ASN	CB-CG	17.20	1.95	1.52
8	J	24	LEU	C-O	-17.17	1.01	1.24
3	C	154	LYS	CD-CE	17.16	2.04	1.52
10	L	63	ARG	NE-CZ	17.11	1.51	1.33
2	B	1140	ALA	N-CA	-17.07	1.24	1.46
1	A	1347	ALA	C-O	-17.07	1.04	1.24
2	B	1155	SER	N-CA	17.05	1.68	1.46
1	A	476	SER	C-O	-17.03	1.02	1.24
4	E	162	ARG	CG-CD	17.01	2.03	1.52
8	J	49	MET	SD-CE	-17.01	1.37	1.79
2	B	846	ILE	CA-CB	16.98	1.75	1.54
1	A	1259	MET	CG-SD	16.97	2.23	1.80
3	C	51	VAL	C-O	-16.96	1.05	1.24
1	A	843	LYS	C-O	-16.96	1.04	1.24
3	C	66	ARG	NE-CZ	-16.96	1.14	1.33
9	K	39	ASP	CA-C	-16.95	1.33	1.53
1	A	1049	ILE	CA-CB	-16.94	1.33	1.54
2	B	246	LYS	N-CA	16.91	1.66	1.46
1	A	1259	MET	SD-CE	16.86	2.21	1.79
5	F	80	ALA	CA-CB	16.78	1.77	1.54
8	J	57	ILE	CA-CB	-16.76	1.30	1.54
8	J	54	VAL	CA-CB	-16.76	1.32	1.54
2	B	704	ALA	C-O	-16.75	1.02	1.23
2	B	662	MET	SD-CE	16.74	2.21	1.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	941	LYS	CD-CE	16.71	2.02	1.52
2	B	436	VAL	CA-C	16.68	1.74	1.52
1	A	1227	ILE	CA-C	-16.68	1.38	1.52
2	B	414	ALA	CA-CB	-16.66	1.27	1.53
3	C	155	LEU	C-O	16.63	1.44	1.23
1	A	1291	VAL	CA-CB	-16.58	1.27	1.54
1	A	1284	MET	CA-C	-16.56	1.30	1.52
2	B	178	ASN	C-O	-16.55	1.02	1.24
1	A	1102	LYS	CG-CD	16.55	2.02	1.52
1	A	521	MET	SD-CE	-16.54	1.38	1.79
3	C	42	PRO	CA-CB	-16.54	1.30	1.53
1	A	32	VAL	C-O	16.53	1.43	1.24
1	A	1105	LEU	CA-C	-16.51	1.29	1.52
6	H	131	ASN	CA-C	16.51	1.74	1.52
1	A	1311	VAL	N-CA	-16.49	1.26	1.46
2	B	588	GLY	C-O	16.49	1.46	1.23
2	B	1155	SER	CA-CB	16.48	1.81	1.53
1	A	1341	ILE	CA-CB	-16.46	1.33	1.54
6	H	136	LYS	CA-C	16.46	1.74	1.52
1	A	1433	MET	SD-CE	-16.46	1.38	1.79
2	B	266	ALA	C-O	16.46	1.44	1.24
10	L	50	ASP	CA-C	16.45	1.74	1.52
1	A	14	VAL	C-O	-16.44	1.04	1.24
2	B	497	ARG	CZ-NH1	16.44	1.55	1.32
7	I	17	ARG	CA-C	-16.44	1.31	1.52
3	C	64	ALA	CA-CB	-16.40	1.27	1.53
2	B	598	GLU	CG-CD	16.38	1.93	1.52
1	A	1236	LEU	C-O	-16.38	1.04	1.24
4	E	20	LYS	CE-NZ	16.34	1.98	1.49
3	C	181	ASP	C-O	-16.33	1.03	1.24
1	A	1012	ARG	C-O	16.31	1.43	1.24
2	B	435	THR	CA-C	16.28	1.74	1.53
1	A	390	GLN	C-O	16.28	1.43	1.24
2	B	1083	ALA	CA-CB	-16.27	1.25	1.53
1	A	577	ILE	CA-CB	-16.25	1.31	1.54
1	A	187	LYS	CA-C	16.25	1.76	1.52
3	C	179	GLU	C-O	-16.25	1.03	1.23
1	A	1305	VAL	C-O	-16.24	1.07	1.24
1	A	1080	THR	CA-C	16.23	1.74	1.52
1	A	673	GLY	CA-C	-16.22	1.40	1.51
1	A	350	ARG	NE-CZ	-16.22	1.15	1.33
1	A	771	GLU	CA-C	-16.22	1.31	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	93	MET	SD-CE	16.19	2.20	1.79
3	C	255	VAL	CA-CB	-16.15	1.31	1.54
7	I	57	GLY	C-O	-16.15	1.03	1.24
2	B	106	ASP	CA-C	16.14	1.74	1.52
1	A	191	THR	CA-CB	16.12	1.80	1.53
1	A	808	LEU	C-O	-16.12	1.04	1.23
7	I	120	GLN	CB-CG	16.11	2.00	1.52
1	A	1149	ALA	C-O	16.10	1.43	1.23
2	B	523	CYS	CA-C	-16.10	1.34	1.53
2	B	529	GLU	CD-OE1	16.09	1.55	1.25
10	L	68	GLU	CD-OE1	16.07	1.55	1.25
10	L	27	LEU	CA-C	16.07	1.74	1.52
1	A	813	PHE	N-CA	-16.04	1.27	1.46
1	A	912	LEU	CA-C	-16.02	1.31	1.52
7	I	72	ASP	CB-CG	16.02	1.92	1.52
2	B	1106	ARG	CA-C	16.02	1.73	1.52
1	A	469	ARG	CD-NE	-16.02	1.23	1.46
1	A	839	ARG	NE-CZ	15.99	1.50	1.33
4	E	202	SER	C-O	-15.99	1.03	1.24
2	B	1101	ASP	CA-C	15.99	1.75	1.52
3	C	195	GLN	CD-OE1	15.97	1.53	1.23
4	E	162	ARG	NE-CZ	15.97	1.50	1.33
2	B	164	LYS	CD-CE	15.96	2.00	1.52
4	E	30	ILE	C-O	-15.93	1.07	1.24
4	E	131	THR	CB-CG2	15.91	2.05	1.52
9	K	5	ASP	C-O	15.85	1.43	1.23
6	H	52	GLN	CG-CD	15.85	1.91	1.52
4	E	110	PHE	CA-C	-15.82	1.34	1.52
1	A	664	THR	CA-C	-15.81	1.32	1.52
2	B	344	LYS	CB-CG	15.79	1.99	1.52
2	B	364	ILE	CA-CB	-15.79	1.32	1.54
2	B	1048	THR	CA-C	-15.78	1.37	1.53
2	B	1156	ASP	CB-CG	15.78	1.91	1.52
1	A	900	ASP	CA-C	-15.78	1.34	1.53
1	A	728	LYS	CG-CD	15.77	1.99	1.52
2	B	1072	MET	SD-CE	-15.77	1.40	1.79
3	C	154	LYS	CG-CD	15.76	1.99	1.52
1	A	216	VAL	CA-CB	-15.76	1.34	1.54
2	B	529	GLU	CD-OE2	15.74	1.55	1.25
2	B	25	ILE	CA-C	-15.73	1.35	1.52
1	A	209	ASN	CG-OD1	15.72	1.53	1.23
1	A	1109	LYS	CG-CD	15.72	1.99	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	3	VAL	CA-CB	-15.70	1.33	1.54
1	A	896	ARG	CZ-NH1	15.69	1.54	1.32
1	A	974	ASP	CA-C	-15.68	1.33	1.52
2	B	915	THR	CA-CB	15.67	1.83	1.54
1	A	1110	ASN	CB-CG	15.66	1.91	1.52
6	H	15	VAL	C-O	15.63	1.40	1.24
1	A	198	GLU	C-O	-15.63	1.05	1.24
2	B	959	ASP	C-O	15.60	1.44	1.24
1	A	677	ARG	NE-CZ	15.59	1.50	1.33
2	B	130	VAL	CA-C	15.57	1.72	1.52
1	A	695	LYS	CD-CE	15.55	1.99	1.52
1	A	496	GLU	CD-OE1	15.55	1.54	1.25
6	H	139	ASN	CA-CB	15.52	1.79	1.53
1	A	375	THR	C-O	-15.49	1.04	1.23
9	K	4	PRO	C-O	15.48	1.40	1.23
2	B	899	ILE	CA-CB	-15.47	1.33	1.54
1	A	24	PRO	C-O	15.46	1.42	1.24
2	B	184	ALA	C-O	-15.46	1.04	1.23
4	E	23	VAL	C-O	15.46	1.41	1.24
6	H	131	ASN	CA-CB	15.45	1.79	1.53
1	A	885	THR	N-CA	-15.43	1.26	1.46
5	F	105	ALA	CA-CB	-15.43	1.26	1.53
2	B	123	THR	CA-CB	-15.42	1.26	1.53
2	B	993	THR	C-O	-15.41	1.05	1.23
1	A	1232	ASN	CG-OD1	15.40	1.52	1.23
1	A	792	TYR	C-O	-15.39	1.04	1.24
5	F	83	PRO	C-O	15.38	1.43	1.24
2	B	1070	GLU	C-O	-15.37	1.05	1.23
2	B	690	VAL	C-O	-15.35	1.08	1.24
2	B	986	GLN	CA-C	15.34	1.70	1.52
7	I	120	GLN	CA-C	15.34	1.63	1.52
6	H	56	THR	CA-CB	15.33	1.72	1.53
1	A	1326	ARG	C-O	-15.29	1.02	1.24
4	E	162	ARG	CB-CG	15.27	1.98	1.52
1	A	206	GLU	CD-OE2	15.26	1.54	1.25
2	B	245	GLU	C-O	15.25	1.42	1.24
1	A	49	LYS	CD-CE	15.24	1.98	1.52
2	B	871	THR	CA-CB	15.23	1.77	1.53
1	A	1222	ASN	CA-CB	15.21	1.77	1.53
4	E	179	GLN	CD-OE1	15.21	1.52	1.23
1	A	1256	GLU	N-CA	15.21	1.65	1.46
1	A	70	CYS	N-CA	15.18	1.65	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	238	ILE	CA-C	-15.18	1.36	1.52
2	B	1165	ILE	CA-C	15.17	1.68	1.52
5	F	130	ILE	CA-C	-15.17	1.41	1.53
2	B	1086	PHE	CA-C	-15.17	1.33	1.52
1	A	776	ALA	C-O	-15.16	1.03	1.23
6	H	59	ILE	CA-CB	-15.15	1.37	1.54
10	L	65	VAL	CA-C	-15.13	1.34	1.52
2	B	204	ILE	C-O	-15.11	1.07	1.24
2	B	711	GLU	CA-C	15.10	1.71	1.52
2	B	1097	HIS	CA-C	15.09	1.73	1.52
3	C	248	ILE	CA-CB	-15.08	1.35	1.54
2	B	516	ASN	C-O	-15.07	1.05	1.24
1	A	1273	LEU	C-O	15.07	1.40	1.24
1	A	725	ALA	CA-CB	-15.04	1.29	1.53
7	I	99	LEU	C-O	-15.04	1.06	1.23
2	B	598	GLU	CD-OE2	15.03	1.53	1.25
9	K	66	PRO	CA-C	-15.01	1.32	1.52
2	B	184	ALA	CA-CB	-14.99	1.27	1.53
3	C	195	GLN	CG-CD	14.96	1.89	1.52
4	E	1	MET	CG-SD	14.91	2.18	1.80
6	H	88	SER	N-CA	14.91	1.65	1.46
1	A	830	LYS	CG-CD	14.90	1.97	1.52
1	A	746	MET	SD-CE	-14.90	1.42	1.79
7	I	51	ASN	C-O	-14.90	1.04	1.24
2	B	200	GLY	C-O	-14.89	1.04	1.23
2	B	103	ASN	CB-CG	14.88	1.89	1.52
1	A	346	ASP	CB-CG	14.88	1.89	1.52
4	E	98	ILE	CA-CB	14.88	1.74	1.54
1	A	873	MET	C-O	-14.87	1.04	1.23
2	B	1030	LEU	CA-C	-14.87	1.34	1.52
1	A	479	ASN	CA-C	-14.86	1.33	1.53
2	B	285	ILE	CA-CB	-14.86	1.36	1.54
1	A	1162	VAL	CA-C	-14.85	1.33	1.52
7	I	113	ASP	CA-C	-14.84	1.34	1.52
1	A	1223	ASP	CB-CG	14.84	1.89	1.52
3	C	143	LEU	C-O	-14.84	1.05	1.24
1	A	264	PHE	CB-CG	14.82	1.84	1.50
2	B	369	GLY	C-O	14.81	1.40	1.23
1	A	392	VAL	CA-CB	-14.80	1.33	1.54
1	A	1064	VAL	N-CA	-14.79	1.27	1.46
2	B	128	LEU	CA-C	-14.79	1.34	1.52
1	A	1077	THR	C-O	-14.79	1.05	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	833	TYR	CE1-CZ	-14.78	1.02	1.38
2	B	1146	PHE	C-O	-14.78	1.05	1.24
10	L	69	ALA	CA-C	-14.77	1.34	1.53
7	I	37	GLU	CD-OE1	14.76	1.53	1.25
4	E	190	LEU	C-O	14.73	1.43	1.23
1	A	961	ARG	CZ-NH2	14.73	1.52	1.33
7	I	44	TYR	N-CA	14.73	1.63	1.46
7	I	92	ARG	C-O	14.72	1.42	1.23
1	A	1064	VAL	CB-CG1	-14.71	1.04	1.52
2	B	935	ARG	NE-CZ	14.70	1.49	1.33
1	A	1135	ARG	CZ-NH2	14.70	1.52	1.33
1	A	1372	VAL	CA-CB	-14.68	1.35	1.54
4	E	75	MET	C-O	14.66	1.41	1.24
2	B	933	SER	CA-C	14.64	1.83	1.52
2	B	1154	ALA	CA-C	14.64	1.71	1.52
7	I	75	CYS	C-O	-14.64	1.03	1.24
2	B	502	ILE	CA-CB	14.63	1.94	1.54
6	H	6	PHE	CA-C	-14.62	1.34	1.52
2	B	987	LYS	CE-NZ	14.62	1.93	1.49
6	H	131	ASN	CB-CG	14.60	1.88	1.52
1	A	17	VAL	CA-CB	-14.59	1.36	1.54
1	A	555	ASP	CB-CG	14.59	1.88	1.52
6	H	77	ARG	NE-CZ	14.58	1.49	1.33
1	A	491	VAL	CA-CB	-14.58	1.39	1.53
1	A	1448	GLU	CA-C	14.57	1.72	1.52
2	B	546	SER	CA-C	-14.56	1.33	1.52
2	B	563	MET	SD-CE	-14.55	1.43	1.79
3	C	164	ALA	CA-CB	-14.55	1.27	1.53
1	A	416	ARG	CA-C	-14.54	1.32	1.52
2	B	826	ALA	C-O	-14.54	1.06	1.23
2	B	1156	ASP	CA-CB	14.53	1.76	1.53
3	C	230	MET	SD-CE	-14.51	1.43	1.79
3	C	127	ARG	C-O	14.50	1.41	1.24
7	I	86	PHE	C-O	-14.48	1.06	1.23
2	B	368	GLU	CA-CB	14.48	1.75	1.53
1	A	1040	GLN	C-O	-14.48	1.06	1.24
3	C	159	ALA	C-O	-14.47	1.05	1.23
4	E	45	LYS	CD-CE	14.46	1.95	1.52
7	I	29	CYS	C-O	14.45	1.40	1.23
1	A	370	ILE	C-O	-14.45	1.06	1.24
4	E	215	MET	SD-CE	14.44	2.15	1.79
1	A	1331	SER	C-O	14.43	1.40	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	995	ARG	CD-NE	-14.42	1.26	1.46
2	B	60	GLN	C-O	-14.41	1.05	1.24
1	A	35	ILE	CA-C	14.41	1.71	1.52
2	B	194	GLU	CD-OE1	14.40	1.52	1.25
2	B	963	PHE	C-O	14.40	1.42	1.24
4	E	208	TYR	CG-CD2	-14.39	1.09	1.39
1	A	681	GLU	CD-OE2	14.38	1.52	1.25
3	C	39	ALA	CA-CB	-14.35	1.33	1.53
1	A	123	ARG	CB-CG	14.35	1.95	1.52
2	B	434	ARG	CG-CD	14.34	1.95	1.52
2	B	347	LYS	CD-CE	14.34	1.95	1.52
1	A	668	ASP	N-CA	-14.32	1.27	1.46
1	A	1444	MET	SD-CE	14.31	2.15	1.79
1	A	603	ASN	CA-C	-14.31	1.35	1.52
2	B	479	VAL	CA-CB	-14.30	1.35	1.54
4	E	66	GLU	CD-OE2	14.30	1.52	1.25
2	B	239	GLU	CD-OE2	14.30	1.52	1.25
1	A	82	GLY	C-O	-14.29	1.06	1.23
4	E	44	ALA	CA-CB	14.28	1.77	1.53
1	A	421	ALA	N-CA	-14.28	1.29	1.46
6	H	109	LYS	CA-C	14.27	1.71	1.52
6	H	78	SER	CA-C	-14.25	1.33	1.52
1	A	703	THR	CB-CG2	14.25	1.99	1.52
1	A	99	ILE	C-O	14.24	1.41	1.24
4	E	59	SER	C-O	14.24	1.42	1.24
5	F	116	ASP	C-O	-14.24	1.06	1.24
4	E	147	HIS	CD2-NE2	-14.24	1.22	1.37
1	A	462	VAL	C-O	14.23	1.38	1.24
1	A	661	GLY	CA-C	14.23	1.67	1.51
4	E	66	GLU	CA-CB	14.22	1.75	1.53
1	A	1309	ASP	CA-C	-14.22	1.35	1.52
6	H	51	ALA	CA-CB	14.21	1.75	1.53
1	A	1232	ASN	CB-CG	14.21	1.87	1.52
1	A	529	CYS	CA-C	-14.21	1.34	1.52
10	L	33	GLU	CA-C	14.20	1.71	1.52
3	C	199	LYS	C-O	-14.20	1.05	1.24
6	H	32	THR	CA-CB	14.20	1.77	1.53
1	A	597	LEU	CG-CD1	14.20	1.99	1.52
2	B	371	GLU	CD-OE1	14.20	1.52	1.25
1	A	241	VAL	CA-C	-14.19	1.42	1.53
1	A	696	GLU	N-CA	-14.19	1.29	1.46
3	C	240	VAL	CA-C	-14.18	1.34	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	582	ILE	C-O	14.18	1.42	1.24
1	A	699	ALA	C-O	-14.18	1.04	1.24
1	A	1412	ALA	C-O	-14.17	1.07	1.24
2	B	1097	HIS	CA-CB	14.17	1.77	1.53
1	A	1038	THR	CA-C	-14.17	1.34	1.53
1	A	1119	TYR	CE2-CZ	-14.16	1.04	1.38
1	A	1304	TRP	C-O	14.16	1.41	1.23
1	A	920	LEU	CA-C	-14.11	1.35	1.52
2	B	648	HIS	C-O	-14.11	1.05	1.23
2	B	271	ALA	CA-C	-14.11	1.35	1.52
4	E	31	THR	CA-C	-14.09	1.35	1.52
1	A	464	PRO	C-N	-14.09	1.14	1.33
10	L	50	ASP	CB-CG	14.08	1.87	1.52
1	A	427	GLN	CG-CD	14.06	1.87	1.52
3	C	165	LYS	CE-NZ	14.06	1.91	1.49
2	B	975	GLN	CD-NE2	14.06	1.62	1.33
9	K	12	LEU	CG-CD1	14.04	1.98	1.52
1	A	1311	VAL	C-O	14.04	1.38	1.24
7	I	24	ARG	N-CA	14.04	1.64	1.45
1	A	843	LYS	CG-CD	14.04	1.94	1.52
2	B	723	VAL	CA-CB	14.03	1.72	1.54
2	B	951	GLN	CG-CD	14.02	1.87	1.52
1	A	39	GLU	CA-C	14.02	1.69	1.52
2	B	348	ARG	NE-CZ	-14.02	1.17	1.33
1	A	189	ARG	CA-C	14.01	1.70	1.53
2	B	466	TRP	CA-C	14.01	1.71	1.52
2	B	697	GLU	C-O	-14.01	1.05	1.24
1	A	46	THR	CA-CB	14.01	1.77	1.53
1	A	771	GLU	CD-OE2	14.01	1.51	1.25
3	C	12	GLU	N-CA	-13.99	1.28	1.46
2	B	525	ALA	C-O	13.99	1.42	1.23
1	A	1277	GLU	CD-OE2	13.99	1.51	1.25
5	F	148	VAL	C-O	13.99	1.40	1.24
10	L	42	ARG	NE-CZ	13.97	1.48	1.33
4	E	128	PRO	CA-C	13.97	1.65	1.52
2	B	711	GLU	CG-CD	13.96	1.86	1.52
1	A	1290	LYS	CD-CE	13.96	1.94	1.52
2	B	365	THR	C-O	13.91	1.40	1.23
1	A	1118	VAL	C-O	-13.89	1.09	1.24
1	A	1209	MET	N-CA	-13.87	1.29	1.46
4	E	74	ASP	CA-C	13.85	1.71	1.52
1	A	596	THR	C-O	-13.85	1.06	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1262	LYS	CG-CD	13.85	1.94	1.52
2	B	766	ARG	N-CA	-13.84	1.29	1.46
1	A	956	LEU	C-O	-13.83	1.09	1.24
1	A	1110	ASN	CG-ND2	13.83	1.62	1.33
1	A	1198	ASP	C-O	13.83	1.40	1.24
1	A	189	ARG	N-CA	13.82	1.62	1.46
8	J	7	CYS	C-O	13.80	1.40	1.23
2	B	344	LYS	CD-CE	13.80	1.93	1.52
1	A	1196	GLU	CD-OE1	13.78	1.51	1.25
3	C	190	ASP	C-O	-13.78	1.08	1.24
1	A	1303	GLU	C-O	-13.77	1.07	1.23
7	I	84	VAL	CA-CB	-13.77	1.35	1.54
2	B	181	LEU	C-O	13.76	1.42	1.24
2	B	1017	ILE	CG1-CD1	-13.75	0.98	1.51
8	J	42	LYS	CD-CE	13.75	1.93	1.52
2	B	1137	CYS	C-O	-13.74	1.07	1.24
1	A	1350	LYS	CE-NZ	13.73	1.90	1.49
9	K	94	ILE	CA-C	-13.73	1.36	1.52
2	B	912	ILE	CA-CB	-13.72	1.36	1.54
1	A	800	VAL	CA-CB	-13.71	1.37	1.53
3	C	212	PRO	C-O	-13.69	1.09	1.24
2	B	1006	ILE	CA-CB	-13.69	1.37	1.54
2	B	904	ARG	C-O	-13.68	1.06	1.23
1	A	1368	MET	SD-CE	-13.68	1.45	1.79
1	A	922	ASP	N-CA	-13.68	1.29	1.46
1	A	123	ARG	NE-CZ	13.67	1.48	1.33
2	B	804	GLY	C-O	-13.67	1.05	1.23
2	B	595	ARG	NE-CZ	13.65	1.48	1.33
1	A	1080	THR	CA-CB	13.65	1.76	1.53
4	E	79	TRP	C-O	-13.65	1.06	1.24
1	A	898	ARG	C-O	-13.65	1.07	1.24
2	B	357	GLN	CA-C	-13.64	1.34	1.52
7	I	71	SER	C-O	13.64	1.42	1.23
3	C	172	PRO	CA-C	-13.62	1.33	1.52
7	I	8	ARG	CZ-NH1	13.62	1.51	1.32
2	B	957	ASN	CA-C	13.61	1.71	1.52
2	B	1157	ALA	CA-CB	13.60	1.70	1.52
2	B	136	THR	CA-C	13.59	1.69	1.52
2	B	751	VAL	CA-CB	-13.59	1.37	1.54
6	H	87	ARG	CA-C	13.59	1.66	1.52
2	B	220	GLY	CA-C	-13.58	1.37	1.52
1	A	686	ALA	CA-C	-13.57	1.34	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1419	ASP	CA-C	-13.57	1.35	1.52
6	H	35	GLN	CA-C	13.57	1.71	1.52
1	A	986	ILE	CA-C	-13.56	1.36	1.52
7	I	111	THR	C-O	-13.56	1.06	1.23
2	B	824	ILE	C-O	-13.55	1.08	1.24
9	K	22	ASP	C-O	13.56	1.38	1.24
10	L	43	THR	CA-CB	13.54	1.76	1.53
1	A	1374	VAL	C-O	13.53	1.40	1.24
1	A	679	ILE	C-O	13.52	1.39	1.24
2	B	681	TRP	CA-C	-13.52	1.34	1.52
1	A	659	HIS	CA-CB	-13.52	1.33	1.53
1	A	1412	ALA	CA-C	-13.52	1.35	1.52
1	A	1138	ILE	C-O	13.52	1.37	1.23
2	B	657	HIS	CA-CB	-13.52	1.31	1.53
2	B	479	VAL	C-O	-13.52	1.06	1.24
1	A	225	ASN	C-O	13.49	1.38	1.23
1	A	1100	ARG	CA-C	-13.49	1.35	1.52
2	B	870	ILE	CG1-CD1	13.49	2.04	1.51
1	A	1414	ALA	CA-CB	-13.48	1.29	1.53
2	B	525	ALA	N-CA	-13.47	1.29	1.46
1	A	836	TYR	CA-C	13.47	1.71	1.52
1	A	482	PHE	C-N	-13.46	1.17	1.33
1	A	610	GLY	C-O	13.46	1.43	1.24
2	B	793	ALA	C-O	-13.46	1.07	1.23
8	J	24	LEU	CA-C	-13.45	1.33	1.52
3	C	245	VAL	CA-CB	-13.44	1.37	1.54
4	E	91	LYS	CA-CB	13.43	1.74	1.53
1	A	23	SER	C-O	13.43	1.40	1.23
2	B	1018	PRO	CA-C	-13.42	1.33	1.52
4	E	142	VAL	C-O	13.41	1.37	1.24
10	L	44	ASP	C-O	13.41	1.41	1.24
1	A	459	ARG	CD-NE	-13.41	1.27	1.46
1	A	654	ASN	N-CA	-13.40	1.29	1.46
1	A	193	ASP	N-CA	13.38	1.63	1.46
6	H	19	ARG	CZ-NH2	13.37	1.50	1.33
2	B	332	ASP	C-O	-13.37	1.08	1.24
2	B	54	PHE	C-O	-13.37	1.08	1.24
7	I	117	LYS	CE-NZ	13.36	1.89	1.49
2	B	116	GLU	CA-C	-13.36	1.34	1.52
1	A	864	ILE	CA-CB	-13.36	1.38	1.54
9	K	42	LEU	CA-C	-13.35	1.34	1.52
2	B	779	GLY	C-O	-13.35	1.05	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	406	LEU	CA-C	13.35	1.69	1.52
6	H	26	ILE	CA-CB	-13.34	1.38	1.54
1	A	931	GLU	CD-OE2	13.33	1.50	1.25
2	B	1108	ARG	CA-C	13.33	1.70	1.52
1	A	434	ARG	CD-NE	-13.32	1.27	1.46
1	A	177	ASP	CG-OD2	13.32	1.50	1.25
1	A	209	ASN	CG-ND2	13.31	1.61	1.33
1	A	822	GLU	C-O	-13.31	1.07	1.24
10	L	65	VAL	CA-CB	-13.31	1.35	1.54
2	B	266	ALA	CA-CB	13.31	1.75	1.53
6	H	19	ARG	CG-CD	13.30	1.92	1.52
1	A	474	VAL	CA-CB	-13.29	1.36	1.54
1	A	641	VAL	CA-CB	-13.29	1.37	1.54
3	C	13	ALA	C-O	-13.29	1.06	1.23
7	I	82	GLU	CA-C	13.28	1.70	1.53
2	B	323	VAL	CA-CB	-13.27	1.39	1.54
2	B	95	ILE	CA-C	-13.27	1.36	1.52
2	B	827	ILE	N-CA	-13.27	1.30	1.46
1	A	506	ALA	C-O	-13.27	1.07	1.23
1	A	671	ALA	CA-CB	-13.26	1.32	1.53
1	A	677	ARG	CZ-NH1	13.26	1.51	1.32
2	B	626	ILE	C-O	-13.26	1.10	1.24
1	A	347	PHE	N-CA	13.25	1.63	1.46
9	K	21	ILE	C-O	-13.25	1.10	1.24
3	C	261	ALA	C-O	-13.25	1.06	1.24
4	E	194	GLU	C-O	-13.23	1.07	1.23
8	J	38	ARG	CB-CG	13.22	1.92	1.52
1	A	1171	GLN	CG-CD	13.21	1.85	1.52
2	B	1183	LYS	CA-CB	13.20	1.74	1.53
1	A	603	ASN	N-CA	-13.20	1.29	1.45
5	F	137	TYR	CA-C	-13.20	1.35	1.52
4	E	69	ILE	CA-CB	-13.19	1.32	1.54
6	H	86	ASP	CA-C	13.18	1.70	1.52
3	C	256	ALA	CA-CB	-13.18	1.31	1.53
1	A	350	ARG	C-O	-13.17	1.09	1.23
1	A	244	PRO	CA-C	13.16	1.64	1.52
1	A	878	ILE	CA-CB	-13.16	1.38	1.54
9	K	30	ALA	CA-C	-13.16	1.36	1.52
1	A	1228	TRP	CA-C	-13.15	1.36	1.52
3	C	15	LYS	CG-CD	13.14	1.91	1.52
2	B	346	GLU	CG-CD	13.14	1.84	1.52
1	A	1280	GLU	CD-OE2	13.13	1.50	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1155	ASP	CA-CB	-13.13	1.36	1.53
1	A	1001	ARG	C-O	13.12	1.40	1.24
5	F	93	ILE	CA-CB	-13.11	1.40	1.54
2	B	1189	ILE	CG1-CD1	13.11	2.02	1.51
2	B	522	VAL	CA-CB	-13.11	1.35	1.55
9	K	46	ILE	CG1-CD1	-13.10	1.00	1.51
10	L	29	TYR	N-CA	13.10	1.62	1.45
6	H	38	LEU	CA-C	-13.10	1.37	1.52
4	E	201	LYS	CG-CD	13.09	1.91	1.52
2	B	211	VAL	CB-CG1	-13.09	1.09	1.52
3	C	58	LEU	N-CA	-13.09	1.29	1.45
1	A	892	ALA	CA-CB	-13.08	1.31	1.53
1	A	683	ILE	CA-C	-13.07	1.36	1.52
2	B	660	LYS	C-O	13.06	1.39	1.24
1	A	195	ASP	C-O	13.06	1.40	1.23
1	A	1352	VAL	C-O	-13.06	1.06	1.24
1	A	1111	MET	SD-CE	-13.05	1.47	1.79
2	B	592	ASN	CG-OD1	13.05	1.48	1.23
3	C	253	LYS	C-O	13.04	1.39	1.24
1	A	677	ARG	CZ-NH2	13.04	1.50	1.33
1	A	1289	ARG	C-O	-13.04	1.09	1.23
2	B	733	HIS	N-CA	13.04	1.63	1.46
1	A	359	LEU	CA-CB	-13.03	1.30	1.53
2	B	329	THR	N-CA	-13.02	1.30	1.46
1	A	1211	GLN	CA-C	-13.02	1.36	1.52
4	E	46	TYR	C-O	13.01	1.42	1.24
9	K	111	LEU	CA-C	13.01	1.70	1.52
4	E	50	MET	CA-C	13.01	1.70	1.52
7	I	119	THR	N-CA	13.01	1.61	1.46
1	A	462	VAL	CA-CB	-13.00	1.38	1.54
1	A	966	ASN	N-CA	-12.99	1.30	1.46
2	B	766	ARG	CZ-NH1	12.99	1.50	1.32
6	H	9	ILE	CA-CB	12.99	1.72	1.54
2	B	327	ARG	C-O	-12.98	1.07	1.24
4	E	153	HIS	C-O	-12.98	1.08	1.24
4	E	23	VAL	CA-CB	-12.98	1.39	1.54
1	A	187	LYS	C-O	12.97	1.40	1.24
2	B	169	ARG	CZ-NH2	12.97	1.50	1.33
1	A	874	ASP	CG-OD2	12.97	1.50	1.25
2	B	223	VAL	C-O	-12.96	1.08	1.24
2	B	641	GLU	C-O	-12.96	1.08	1.23
2	B	883	LEU	CA-CB	12.96	1.72	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	419	LYS	C-O	-12.96	1.07	1.24
3	C	18	VAL	C-O	-12.96	1.08	1.24
9	K	54	ARG	NE-CZ	12.96	1.47	1.33
1	A	1218	GLN	CA-C	-12.95	1.34	1.52
2	B	1186	ASP	CA-C	12.94	1.69	1.53
8	J	2	ILE	N-CA	-12.94	1.31	1.46
2	B	739	THR	CA-C	-12.93	1.35	1.52
2	B	172	ILE	CA-CB	-12.91	1.37	1.54
2	B	448	ILE	CA-CB	12.91	1.71	1.54
7	I	94	ASP	CA-CB	12.91	1.73	1.53
2	B	595	ARG	CD-NE	12.90	1.64	1.46
1	A	373	THR	C-O	-12.89	1.08	1.24
2	B	887	HIS	C-O	12.89	1.40	1.24
7	I	22	ASN	C-O	12.88	1.42	1.24
1	A	366	VAL	CA-CB	-12.87	1.43	1.54
2	B	1163	CYS	CA-CB	12.87	1.74	1.53
1	A	497	THR	C-O	-12.87	1.07	1.24
1	A	1274	ARG	CZ-NH1	12.87	1.50	1.32
1	A	957	PRO	CA-CB	-12.85	1.33	1.53
2	B	343	ILE	CA-CB	-12.84	1.39	1.54
1	A	1015	VAL	CB-CG2	-12.84	1.10	1.52
2	B	1158	PHE	C-O	-12.82	1.07	1.24
1	A	843	LYS	CD-CE	12.82	1.91	1.52
2	B	993	THR	CA-CB	-12.82	1.31	1.53
7	I	54	GLU	C-O	-12.82	1.08	1.24
6	H	41	ASP	CA-C	-12.81	1.37	1.52
4	E	131	THR	C-O	-12.81	1.07	1.23
2	B	763	GLN	CA-C	-12.80	1.37	1.52
7	I	93	LYS	CD-CE	12.81	1.90	1.52
1	A	882	SER	C-O	-12.80	1.08	1.24
2	B	434	ARG	CB-CG	12.79	1.90	1.52
2	B	40	GLU	CA-C	-12.78	1.35	1.52
1	A	752	LYS	CA-CB	-12.78	1.33	1.53
1	A	9	ALA	CA-C	-12.76	1.35	1.52
4	E	130	ALA	C-O	12.76	1.39	1.23
2	B	724	ASP	C-N	-12.76	1.20	1.34
2	B	1154	ALA	C-O	12.76	1.39	1.24
1	A	660	ASN	CA-C	-12.75	1.36	1.52
2	B	448	ILE	N-CA	12.75	1.60	1.46
1	A	264	PHE	CA-C	12.74	1.70	1.52
2	B	564	GLU	CD-OE1	12.74	1.49	1.25
1	A	1337	GLU	CD-OE1	12.74	1.49	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	73	ALA	N-CA	12.74	1.62	1.46
1	A	1214	GLU	CD-OE1	12.74	1.49	1.25
2	B	702	LEU	N-CA	-12.73	1.30	1.46
2	B	982	SER	CA-C	-12.73	1.36	1.53
2	B	627	PHE	CA-C	-12.72	1.37	1.52
7	I	1	MET	SD-CE	12.70	2.11	1.79
1	A	734	GLU	CD-OE1	12.69	1.49	1.25
2	B	240	ILE	CA-C	-12.69	1.37	1.52
2	B	1023	VAL	CA-CB	-12.69	1.38	1.54
8	J	14	VAL	CA-CB	-12.69	1.37	1.54
1	A	1234	GLU	CD-OE1	12.68	1.49	1.25
1	A	1126	ALA	CA-CB	-12.68	1.32	1.53
1	A	704	ALA	C-O	12.68	1.40	1.23
2	B	667	GLN	CD-OE1	12.68	1.47	1.23
1	A	905	ASP	N-CA	-12.67	1.29	1.46
4	E	208	TYR	CE1-CZ	-12.67	1.07	1.38
1	A	942	PHE	C-N	-12.65	1.16	1.34
2	B	880	THR	CA-C	12.65	1.71	1.53
1	A	368	LYS	CG-CD	12.64	1.90	1.52
1	A	618	GLU	CD-OE2	12.64	1.49	1.25
1	A	858	ASN	CB-CG	-12.63	1.20	1.52
2	B	996	ARG	CZ-NH1	12.63	1.50	1.32
2	B	1085	ILE	CG1-CD1	-12.63	1.02	1.51
1	A	119	ASN	C-O	12.63	1.40	1.24
1	A	1226	VAL	CA-CB	-12.62	1.37	1.54
2	B	174	LEU	C-O	-12.63	1.07	1.23
2	B	1043	ASP	CA-C	-12.62	1.37	1.52
4	E	192	ARG	NE-CZ	12.62	1.47	1.33
7	I	84	VAL	CB-CG2	-12.61	1.10	1.52
1	A	996	ASN	N-CA	-12.61	1.30	1.46
7	I	120	GLN	CA-CB	12.61	1.71	1.53
2	B	914	LYS	C-O	12.60	1.38	1.23
2	B	769	TYR	N-CA	-12.60	1.30	1.46
1	A	676	MET	CG-SD	12.59	2.12	1.80
1	A	1189	SER	C-O	-12.59	1.08	1.24
3	C	13	ALA	CA-C	-12.59	1.36	1.52
6	H	131	ASN	N-CA	12.59	1.62	1.46
1	A	96	ILE	CG1-CD1	-12.58	1.02	1.51
6	H	19	ARG	CB-CG	12.58	1.90	1.52
6	H	132	LEU	CA-C	12.58	1.69	1.52
2	B	1106	ARG	NE-CZ	12.57	1.46	1.33
7	I	1	MET	CA-CB	12.57	1.78	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	345	LYS	C-O	-12.56	1.09	1.24
1	A	413	ILE	C-O	-12.54	1.10	1.24
6	H	63	LEU	CA-C	12.54	1.79	1.52
1	A	1108	ALA	CA-C	-12.54	1.37	1.52
1	A	1080	THR	CB-CG2	12.53	1.93	1.52
1	A	31	SER	C-O	12.53	1.39	1.23
1	A	1256	GLU	CA-C	12.53	1.69	1.52
1	A	1419	ASP	CG-OD1	12.53	1.49	1.25
9	K	111	LEU	CG-CD1	12.53	1.93	1.52
2	B	20	ASP	C-O	-12.52	1.08	1.23
3	C	254	LYS	CA-C	-12.51	1.36	1.52
4	E	131	THR	CA-C	-12.51	1.37	1.52
8	J	42	LYS	CG-CD	12.50	1.90	1.52
1	A	464	PRO	CA-C	-12.50	1.34	1.52
2	B	313	MET	SD-CE	-12.50	1.48	1.79
2	B	732	SER	CA-C	12.48	1.69	1.53
1	A	1153	TYR	C-O	12.48	1.39	1.23
7	I	40	SER	CA-C	-12.48	1.37	1.52
1	A	681	GLU	C-O	12.48	1.39	1.24
1	A	1063	MET	CA-C	12.48	1.67	1.53
1	A	1255	GLU	CA-C	12.48	1.69	1.52
2	B	563	MET	C-O	-12.48	1.08	1.23
2	B	136	THR	CA-CB	12.47	1.71	1.53
1	A	674	PRO	N-CA	-12.47	1.31	1.47
1	A	1267	MET	SD-CE	-12.47	1.48	1.79
7	I	35	VAL	C-O	-12.47	1.08	1.23
2	B	811	TYR	CZ-OH	-12.47	1.11	1.38
2	B	887	HIS	CA-C	12.47	1.69	1.52
1	A	424	ILE	CA-C	-12.46	1.37	1.52
4	E	57	MET	CG-SD	12.46	2.11	1.80
9	K	34	THR	CA-C	-12.45	1.38	1.52
1	A	1318	THR	C-O	-12.44	1.06	1.23
7	I	34	TYR	CA-C	-12.45	1.36	1.52
2	B	310	MET	SD-CE	-12.44	1.48	1.79
1	A	516	SER	CA-CB	-12.44	1.35	1.53
1	A	938	LYS	CA-C	-12.44	1.36	1.52
2	B	63	ILE	CA-C	12.44	1.71	1.52
1	A	795	GLU	CD-OE2	12.43	1.49	1.25
1	A	1320	PRO	CA-C	-12.43	1.35	1.52
2	B	809	MET	C-O	-12.42	1.08	1.24
1	A	457	ALA	N-CA	-12.42	1.31	1.46
1	A	469	ARG	NE-CZ	-12.42	1.19	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	699	GLU	CA-CB	-12.42	1.31	1.53
3	C	15	LYS	CB-CG	12.41	1.89	1.52
4	E	161	LYS	CD-CE	12.41	1.89	1.52
2	B	1188	LYS	CG-CD	12.41	1.89	1.52
6	H	132	LEU	CA-CB	12.40	1.74	1.53
1	A	177	ASP	CG-OD1	12.39	1.48	1.25
1	A	85	ASP	C-O	12.39	1.39	1.23
1	A	655	PHE	CG-CD2	-12.39	1.12	1.38
2	B	580	VAL	CA-CB	-12.39	1.39	1.54
1	A	443	LEU	CA-C	-12.38	1.38	1.52
2	B	19	GLU	N-CA	12.37	1.62	1.46
2	B	105	SER	CA-C	12.37	1.69	1.52
1	A	108	MET	SD-CE	-12.37	1.48	1.79
1	A	123	ARG	CD-NE	12.37	1.63	1.46
2	B	389	ALA	CA-CB	-12.35	1.33	1.53
2	B	265	SER	C-O	12.34	1.39	1.24
2	B	1193	GLN	C-O	-12.34	1.07	1.23
1	A	44	THR	CA-C	12.34	1.69	1.52
1	A	950	GLY	CA-C	12.34	1.69	1.51
1	A	1450	LEU	CG-CD2	12.34	1.93	1.52
3	C	10	ILE	CG1-CD1	-12.34	1.03	1.51
1	A	1075	PRO	C-O	-12.34	1.09	1.24
1	A	4	GLN	CA-C	12.34	1.69	1.52
1	A	393	ARG	CD-NE	12.33	1.63	1.46
7	I	50	THR	CA-C	-12.33	1.38	1.52
4	E	7	ARG	NE-CZ	12.32	1.46	1.33
1	A	1299	VAL	C-O	12.31	1.38	1.23
1	A	1304	TRP	CE2-CZ2	-12.31	1.14	1.39
1	A	1442	ASP	CA-C	-12.31	1.38	1.52
1	A	1107	VAL	C-O	12.31	1.38	1.24
2	B	905	VAL	C-O	-12.30	1.09	1.23
2	B	259	TYR	C-O	-12.30	1.08	1.23
1	A	69	THR	CA-CB	12.30	1.74	1.53
1	A	985	ASP	CA-C	12.30	1.68	1.52
2	B	1102	LYS	N-CA	12.28	1.60	1.46
4	E	7	ARG	CD-NE	12.28	1.63	1.46
1	A	193	ASP	CA-CB	12.28	1.74	1.53
3	C	113	VAL	C-O	-12.28	1.10	1.24
1	A	125	ALA	C-O	-12.27	1.07	1.24
7	I	113	ASP	C-O	-12.26	1.08	1.24
9	K	46	ILE	CA-CB	-12.26	1.40	1.54
1	A	178	GLY	C-O	-12.25	1.07	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	219	ALA	CA-CB	12.25	1.73	1.53
2	B	415	GLN	CB-CG	12.25	1.89	1.52
2	B	396	ASP	CG-OD1	12.25	1.48	1.25
1	A	1338	VAL	CA-CB	-12.24	1.40	1.54
3	C	84	ARG	C-O	-12.24	1.07	1.24
4	E	191	LYS	CD-CE	12.24	1.89	1.52
2	B	1052	VAL	CB-CG2	-12.24	1.12	1.52
5	F	129	LYS	CD-CE	12.24	1.89	1.52
1	A	1023	ARG	NE-CZ	-12.24	1.19	1.33
1	A	1068	ALA	CA-C	-12.24	1.36	1.52
7	I	2	THR	CA-CB	-12.24	1.32	1.53
2	B	785	TYR	CG-CD2	-12.23	1.13	1.39
1	A	919	ILE	CA-CB	12.22	1.68	1.54
8	J	41	LEU	CA-C	-12.21	1.36	1.52
1	A	1017	LEU	CA-C	-12.19	1.36	1.52
1	A	1225	PHE	CB-CG	12.19	1.78	1.50
1	A	787	PHE	CG-CD1	-12.19	1.13	1.38
2	B	1128	LEU	N-CA	12.19	1.61	1.46
7	I	118	ARG	CA-C	12.18	1.69	1.52
2	B	644	GLU	CA-C	12.18	1.69	1.52
7	I	8	ARG	N-CA	12.18	1.61	1.46
1	A	49	LYS	CA-C	12.17	1.67	1.52
2	B	1150	ARG	C-N	-12.16	1.17	1.33
1	A	174	ILE	N-CA	-12.15	1.32	1.46
2	B	758	PHE	CA-CB	-12.14	1.34	1.53
1	A	346	ASP	CG-OD2	12.14	1.48	1.25
1	A	515	GLN	CD-OE1	12.14	1.46	1.23
2	B	1165	ILE	CA-CB	12.14	1.70	1.54
2	B	1193	GLN	C-N	-12.13	1.17	1.33
8	J	22	LEU	CA-C	12.13	1.68	1.52
1	A	949	ASP	C-O	-12.13	1.08	1.24
2	B	1188	LYS	CD-CE	12.13	1.88	1.52
4	E	186	LEU	N-CA	-12.13	1.30	1.46
2	B	1145	SER	N-CA	-12.12	1.30	1.46
3	C	29	MET	SD-CE	12.12	2.09	1.79
1	A	360	GLU	C-O	-12.12	1.06	1.23
2	B	451	LYS	CG-CD	12.12	1.88	1.52
4	E	147	HIS	CA-C	-12.12	1.35	1.53
3	C	95	CYS	C-O	-12.12	1.06	1.24
1	A	1236	LEU	CA-C	-12.12	1.38	1.52
2	B	835	GLN	C-O	-12.12	1.08	1.23
1	A	795	GLU	C-O	-12.10	1.09	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	111	LEU	CA-C	12.10	1.68	1.52
1	A	12	ARG	CZ-NH1	12.09	1.49	1.32
2	B	581	PHE	C-O	12.09	1.39	1.23
4	E	76	GLY	C-O	-12.07	1.12	1.23
2	B	734	HIS	C-N	12.07	1.49	1.33
6	H	34	ASP	CA-C	12.06	1.69	1.52
1	A	912	LEU	C-N	-12.06	1.18	1.33
2	B	644	GLU	CD-OE1	12.06	1.48	1.25
2	B	509	ALA	CA-CB	12.06	1.92	1.52
7	I	92	ARG	CA-C	12.05	1.68	1.52
2	B	1094	ARG	NE-CZ	-12.04	1.19	1.33
1	A	997	LEU	CA-C	-12.04	1.38	1.53
2	B	576	ASP	C-O	12.04	1.41	1.24
2	B	665	GLU	CD-OE2	12.04	1.48	1.25
7	I	30	ARG	CA-C	-12.03	1.35	1.52
1	A	1448	GLU	N-CA	12.03	1.61	1.46
2	B	1022	THR	CA-C	12.02	1.65	1.53
2	B	962	LYS	CD-CE	12.01	1.88	1.52
1	A	511	ILE	CA-C	-12.00	1.38	1.52
1	A	36	ARG	CA-C	-12.00	1.36	1.52
1	A	475	THR	C-O	-12.00	1.09	1.24
1	A	226	GLU	CD-OE2	11.99	1.48	1.25
2	B	312	GLU	CD-OE2	11.99	1.48	1.25
2	B	695	ALA	C-O	-11.99	1.09	1.24
1	A	66	LYS	CA-C	11.99	1.65	1.52
1	A	693	VAL	CA-CB	-11.99	1.37	1.54
1	A	792	TYR	CA-CB	-11.98	1.35	1.53
1	A	821	ARG	CD-NE	-11.98	1.29	1.46
2	B	203	PHE	N-CA	11.98	1.60	1.45
3	C	102	GLN	CA-C	-11.98	1.37	1.52
1	A	172	PRO	CA-C	-11.97	1.36	1.52
2	B	49	ASP	C-O	-11.97	1.10	1.24
7	I	36	GLU	CA-CB	-11.97	1.33	1.53
1	A	190	ALA	CA-CB	11.96	1.73	1.53
1	A	509	LEU	CA-CB	-11.95	1.33	1.53
1	A	1023	ARG	CZ-NH1	-11.96	1.16	1.32
1	A	1132	LYS	CD-CE	11.95	1.88	1.52
1	A	217	LYS	CG-CD	11.95	1.88	1.52
1	A	780	VAL	N-CA	11.94	1.59	1.46
2	B	1155	SER	CA-C	11.93	1.68	1.52
1	A	16	GLU	N-CA	11.93	1.60	1.46
1	A	49	LYS	N-CA	11.93	1.60	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1029	CYS	CA-C	11.93	1.68	1.52
1	A	593	GLU	CA-C	11.92	1.69	1.52
1	A	220	THR	CA-C	-11.92	1.37	1.52
2	B	607	GLY	C-O	-11.92	1.07	1.24
2	B	792	MET	CA-C	-11.92	1.38	1.52
7	I	3	THR	CA-C	-11.91	1.37	1.53
1	A	777	PHE	CG-CD2	-11.90	1.13	1.38
3	C	156	THR	CA-C	-11.89	1.38	1.52
1	A	1350	LYS	CG-CD	11.89	1.88	1.52
1	A	44	THR	N-CA	11.89	1.61	1.46
2	B	411	PRO	C-O	11.89	1.39	1.24
1	A	927	VAL	CA-CB	-11.88	1.39	1.54
2	B	172	ILE	CG1-CD1	11.88	1.98	1.51
2	B	632	ARG	NE-CZ	-11.88	1.20	1.33
2	B	94	LYS	CA-C	11.88	1.68	1.52
1	A	731	ARG	CA-C	-11.87	1.37	1.52
2	B	620	ARG	CZ-NH2	11.87	1.48	1.33
1	A	902	LEU	N-CA	-11.87	1.31	1.46
2	B	105	SER	C-O	11.87	1.39	1.24
8	J	36	LEU	CA-C	-11.86	1.37	1.52
1	A	1327	ILE	CA-CB	11.86	1.66	1.54
1	A	744	LYS	CA-C	-11.86	1.37	1.52
1	A	144	THR	CB-CG2	11.85	1.91	1.52
2	B	1221	SER	CA-C	11.85	1.68	1.52
1	A	724	GLU	N-CA	-11.84	1.31	1.46
1	A	284	ALA	CA-CB	11.84	1.72	1.53
2	B	662	MET	CG-SD	-11.84	1.51	1.80
2	B	759	PRO	C-O	11.84	1.39	1.24
8	J	8	PHE	N-CA	11.84	1.61	1.46
2	B	1079	LYS	CA-C	-11.83	1.38	1.52
1	A	49	LYS	CG-CD	11.82	1.88	1.52
1	A	1128	GLN	CA-C	11.82	1.68	1.52
3	C	232	VAL	CA-CB	-11.82	1.39	1.54
5	F	142	SER	C-O	-11.82	1.08	1.23
7	I	95	THR	C-O	-11.82	1.09	1.23
1	A	1239	ARG	CG-CD	11.81	1.87	1.52
4	E	130	ALA	CA-CB	11.81	1.72	1.53
1	A	895	LYS	CD-CE	11.81	1.87	1.52
1	A	1159	ARG	NE-CZ	11.81	1.46	1.33
2	B	346	GLU	CD-OE2	11.81	1.47	1.25
1	A	864	ILE	CA-C	-11.81	1.40	1.52
1	A	522	GLY	N-CA	11.80	1.56	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	45	ARG	CD-NE	11.80	1.62	1.46
2	B	531	GLN	CD-NE2	11.80	1.58	1.33
1	A	1289	ARG	CA-C	-11.80	1.38	1.52
1	A	1269	GLU	N-CA	11.80	1.61	1.46
1	A	1341	ILE	CA-C	-11.79	1.37	1.52
1	A	934	LYS	CD-CE	11.78	1.87	1.52
1	A	773	LYS	C-O	-11.78	1.08	1.23
2	B	137	TYR	CB-CG	11.78	1.77	1.51
3	C	88	CYS	CA-C	-11.78	1.36	1.53
1	A	52	GLY	C-O	-11.77	1.08	1.23
1	A	469	ARG	C-O	-11.77	1.08	1.23
10	L	40	LEU	CB-CG	11.77	1.76	1.53
1	A	1109	LYS	CD-CE	11.76	1.87	1.52
2	B	660	LYS	N-CA	-11.75	1.31	1.46
7	I	45	ARG	CG-CD	11.73	1.87	1.52
2	B	870	ILE	CA-C	11.73	1.62	1.52
7	I	28	GLU	N-CA	-11.72	1.31	1.45
2	B	587	HIS	N-CA	-11.72	1.31	1.46
3	C	175	ALA	N-CA	-11.72	1.31	1.45
1	A	466	SER	N-CA	11.72	1.61	1.46
6	H	146	ARG	CZ-NH2	11.72	1.48	1.33
2	B	1023	VAL	N-CA	-11.72	1.32	1.46
1	A	1285	MET	CG-SD	11.71	2.10	1.80
1	A	1222	ASN	CA-C	11.71	1.68	1.52
2	B	531	GLN	CB-CG	11.70	1.87	1.52
2	B	324	ILE	C-O	-11.70	1.11	1.24
1	A	455	MET	C-O	-11.70	1.09	1.23
4	E	52	ARG	C-O	11.70	1.39	1.23
2	B	822	ASN	CA-C	-11.69	1.38	1.52
3	C	129	ILE	CA-C	-11.69	1.38	1.52
2	B	699	GLU	CA-C	-11.68	1.36	1.52
3	C	78	GLU	CD-OE2	11.68	1.47	1.25
4	E	35	VAL	CA-CB	-11.68	1.40	1.54
4	E	189	GLY	C-O	11.67	1.39	1.23
1	A	28	ARG	C-O	11.67	1.38	1.24
1	A	1260	LEU	C-O	-11.67	1.10	1.24
1	A	1237	ILE	N-CA	-11.66	1.32	1.46
2	B	249	ARG	C-O	11.65	1.38	1.24
2	B	1183	LYS	CA-C	11.65	1.69	1.52
1	A	304	MET	CG-SD	11.65	2.09	1.80
1	A	1080	THR	N-CA	11.65	1.61	1.46
2	B	248	SER	N-CA	11.65	1.61	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	GLN	CB-CG	11.64	1.87	1.52
1	A	1139	GLU	CA-C	-11.64	1.37	1.52
1	A	1119	TYR	CG-CD1	-11.62	1.15	1.39
7	I	93	LYS	CG-CD	11.62	1.87	1.52
1	A	513	SER	C-O	-11.61	1.12	1.24
2	B	242	SER	C-O	-11.61	1.09	1.23
1	A	602	ASP	CA-CB	-11.61	1.36	1.53
1	A	1263	ILE	CG1-CD1	11.60	1.97	1.51
3	C	12	GLU	CD-OE1	11.60	1.47	1.25
1	A	430	TRP	CA-C	-11.60	1.37	1.53
2	B	512	ARG	CA-C	11.60	1.68	1.52
2	B	706	GLN	CG-CD	11.60	1.81	1.52
3	C	147	LEU	CA-C	-11.60	1.38	1.52
2	B	635	ARG	C-O	-11.60	1.09	1.24
1	A	893	PHE	CA-C	-11.59	1.37	1.52
2	B	813	LYS	C-N	-11.58	1.18	1.34
2	B	1168	LEU	CA-C	-11.58	1.38	1.52
4	E	164	LEU	CA-C	-11.58	1.38	1.52
2	B	1139	ILE	C-N	11.57	1.49	1.33
1	A	196	GLU	CD-OE1	11.56	1.47	1.25
2	B	1069	PHE	C-O	11.56	1.39	1.23
1	A	489	LEU	C-O	-11.55	1.09	1.23
2	B	983	ARG	CZ-NH2	-11.55	1.18	1.33
2	B	870	ILE	C-O	11.55	1.37	1.23
2	B	1146	PHE	CA-C	-11.55	1.37	1.52
1	A	15	LYS	C-O	-11.55	1.09	1.24
3	C	79	GLN	CD-OE1	11.55	1.45	1.23
1	A	891	ALA	C-O	-11.54	1.10	1.24
2	B	347	LYS	CG-CD	11.54	1.87	1.52
2	B	1221	SER	CA-CB	11.54	1.73	1.53
1	A	946	VAL	CA-CB	-11.54	1.38	1.54
1	A	356	ASP	C-N	-11.53	1.22	1.34
8	J	24	LEU	C-N	-11.53	1.15	1.33
1	A	613	ILE	CA-C	-11.52	1.36	1.53
6	H	107	VAL	CA-CB	11.52	1.70	1.54
1	A	1282	VAL	C-O	-11.51	1.12	1.24
1	A	393	ARG	CA-C	-11.51	1.38	1.52
1	A	747	VAL	C-O	-11.51	1.10	1.24
1	A	606	LEU	N-CA	-11.51	1.31	1.46
1	A	560	ILE	CA-CB	-11.50	1.39	1.54
1	A	1144	LYS	C-O	-11.50	1.10	1.24
1	A	705	LYS	CB-CG	11.50	1.86	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	18	LYS	C-O	-11.50	1.10	1.24
1	A	186	LYS	CD-CE	11.49	1.86	1.52
1	A	977	LYS	CB-CG	11.48	1.86	1.52
2	B	272	THR	CA-C	-11.48	1.38	1.52
2	B	566	LEU	C-O	-11.48	1.10	1.24
1	A	1438	THR	CA-CB	-11.47	1.32	1.53
3	C	179	GLU	CA-C	-11.47	1.38	1.52
1	A	1435	PRO	CA-C	-11.47	1.41	1.53
1	A	1137	ALA	CA-CB	-11.46	1.33	1.53
2	B	594	ALA	CA-C	-11.46	1.36	1.52
1	A	163	SER	CA-C	-11.46	1.37	1.52
4	E	39	LEU	C-O	11.46	1.36	1.24
4	E	162	ARG	CZ-NH1	11.46	1.48	1.32
2	B	241	ARG	C-O	-11.46	1.09	1.23
2	B	1153	GLU	CD-OE2	11.46	1.47	1.25
1	A	26	GLU	CA-C	-11.45	1.36	1.52
2	B	935	ARG	CD-NE	11.45	1.62	1.46
2	B	895	ASP	CB-CG	11.45	1.80	1.52
4	E	204	THR	CA-CB	-11.45	1.35	1.53
2	B	966	VAL	C-O	-11.44	1.11	1.24
3	C	197	SER	CB-OG	11.44	1.65	1.42
2	B	263	GLY	C-O	11.44	1.39	1.23
1	A	207	ILE	CA-CB	11.43	1.68	1.54
1	A	149	GLU	CA-C	-11.43	1.37	1.53
1	A	220	THR	N-CA	11.43	1.60	1.46
2	B	132	VAL	CA-C	11.43	1.65	1.52
4	E	54	GLN	CB-CG	11.43	1.86	1.52
1	A	1362	TYR	C-O	-11.43	1.11	1.23
2	B	328	GLU	CD-OE2	11.42	1.47	1.25
1	A	1097	GLY	C-O	-11.42	1.08	1.23
8	J	7	CYS	CA-CB	11.41	1.71	1.53
1	A	1405	THR	CA-CB	11.41	1.85	1.54
6	H	30	SER	C-O	11.41	1.37	1.23
10	L	28	LYS	CA-C	11.41	1.68	1.52
2	B	855	PHE	CG-CD2	-11.40	1.15	1.38
3	C	16	ASP	C-O	-11.39	1.09	1.24
1	A	1188	GLN	C-O	11.38	1.38	1.24
1	A	874	ASP	C-O	-11.38	1.10	1.24
10	L	62	LYS	CD-CE	11.38	1.86	1.52
1	A	1320	PRO	CA-CB	-11.37	1.38	1.53
1	A	844	ALA	N-CA	-11.37	1.31	1.46
1	A	761	MET	CA-C	-11.37	1.38	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	572	HIS	CA-CB	11.37	1.73	1.53
2	B	1055	ILE	C-O	-11.37	1.09	1.24
1	A	1107	VAL	N-CA	-11.37	1.32	1.46
3	C	143	LEU	CA-CB	-11.37	1.38	1.53
2	B	1190	ASP	C-O	-11.37	1.09	1.24
1	A	867	ILE	C-O	-11.36	1.11	1.23
1	A	818	MET	SD-CE	-11.35	1.51	1.79
1	A	1023	ARG	C-O	-11.35	1.09	1.24
10	L	69	ALA	CA-CB	-11.35	1.36	1.53
1	A	576	GLN	CA-C	-11.35	1.37	1.52
2	B	646	LEU	CG-CD1	11.35	1.90	1.52
1	A	109	HIS	CA-CB	11.34	1.67	1.53
1	A	1235	LYS	CD-CE	11.34	1.86	1.52
1	A	183	GLY	CA-C	-11.34	1.40	1.52
1	A	518	LYS	CD-CE	11.34	1.86	1.52
1	A	606	LEU	C-O	-11.34	1.11	1.23
1	A	917	SER	CA-C	-11.34	1.38	1.52
2	B	772	ALA	CA-CB	11.33	1.71	1.53
4	E	178	ILE	CA-C	11.33	1.66	1.52
1	A	787	PHE	CE2-CZ	-11.32	1.04	1.38
2	B	235	SER	CB-OG	-11.32	1.19	1.42
1	A	9	ALA	CA-CB	11.31	1.72	1.52
1	A	620	LYS	CB-CG	11.31	1.86	1.52
2	B	361	LEU	C-N	-11.31	1.21	1.34
1	A	1349	TYR	CG-CD2	-11.30	1.15	1.39
3	C	166	GLU	CD-OE2	11.30	1.46	1.25
4	E	181	ALA	CA-C	-11.30	1.38	1.53
1	A	498	ARG	NE-CZ	-11.30	1.20	1.33
5	F	82	THR	CA-C	-11.30	1.40	1.53
6	H	130	ARG	NE-CZ	-11.30	1.20	1.33
1	A	1434	ALA	CA-CB	-11.29	1.31	1.53
2	B	1132	GLU	CG-CD	11.29	1.80	1.52
1	A	1132	LYS	CE-NZ	11.29	1.83	1.49
6	H	21	ASN	CA-C	-11.29	1.37	1.52
1	A	622	VAL	CA-C	-11.29	1.38	1.52
2	B	970	THR	CA-CB	-11.29	1.25	1.54
1	A	1412	ALA	CA-CB	11.28	1.71	1.53
1	A	1014	ALA	C-N	-11.28	1.20	1.33
2	B	67	SER	CA-CB	11.28	1.70	1.53
1	A	349	ALA	CA-C	-11.28	1.38	1.52
1	A	630	ILE	CG1-CD1	-11.28	1.07	1.51
1	A	461	LYS	C-O	11.28	1.36	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	589	VAL	CA-CB	-11.28	1.38	1.54
9	K	45	LEU	C-O	11.27	1.37	1.24
2	B	104	GLU	CA-C	11.27	1.67	1.52
1	A	649	ILE	CG1-CD1	-11.27	1.07	1.51
1	A	978	PRO	CB-CG	11.26	2.06	1.49
2	B	244	LEU	CA-C	11.26	1.66	1.52
2	B	466	TRP	C-O	11.26	1.38	1.24
1	A	62	ASP	N-CA	11.25	1.60	1.46
2	B	812	LEU	C-O	-11.25	1.08	1.23
2	B	1012	ILE	CB-CG1	-11.25	1.30	1.53
1	A	795	GLU	CG-CD	11.25	1.80	1.52
2	B	639	ILE	C-N	-11.24	1.19	1.33
2	B	650	GLU	CD-OE2	11.24	1.46	1.25
1	A	1270	ASN	C-O	11.24	1.39	1.24
2	B	1046	PRO	N-CD	-11.24	1.32	1.47
5	F	96	THR	C-O	-11.24	1.11	1.24
2	B	620	ARG	CZ-NH1	11.23	1.48	1.32
2	B	1048	THR	C-O	-11.23	1.12	1.24
1	A	57	ARG	C-O	-11.22	1.09	1.24
2	B	1181	GLU	N-CA	11.22	1.59	1.46
2	B	1223	ASP	C-N	11.22	1.49	1.33
4	E	208	TYR	CA-C	-11.22	1.38	1.52
2	B	552	MET	CB-CG	11.22	1.86	1.52
1	A	821	ARG	C-O	-11.21	1.10	1.24
1	A	1208	THR	N-CA	-11.21	1.32	1.46
3	C	26	ASP	CG-OD1	11.21	1.46	1.25
8	J	13	VAL	N-CA	-11.21	1.31	1.46
1	A	591	PHE	CA-C	-11.21	1.39	1.52
1	A	1425	SER	CB-OG	11.21	1.64	1.42
3	C	8	VAL	CA-CB	-11.21	1.38	1.54
1	A	632	VAL	CB-CG1	-11.20	1.15	1.52
9	K	20	LYS	CG-CD	11.20	1.86	1.52
1	A	779	PHE	CA-CB	-11.20	1.36	1.53
2	B	986	GLN	CG-CD	11.19	1.80	1.52
5	F	153	VAL	CA-C	-11.20	1.40	1.52
1	A	744	LYS	CD-CE	11.19	1.86	1.52
10	L	46	VAL	C-O	-11.19	1.10	1.24
1	A	160	GLN	CA-C	-11.19	1.39	1.52
3	C	174	ALA	C-O	-11.19	1.09	1.24
9	K	28	PRO	C-O	-11.19	1.11	1.23
1	A	984	LYS	CE-NZ	11.18	1.82	1.49
1	A	55	ASP	CA-C	-11.18	1.38	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	572	TRP	CZ3-CH2	-11.18	1.12	1.40
2	B	1214	PRO	C-O	11.17	1.38	1.24
2	B	115	GLN	CD-NE2	11.17	1.56	1.33
2	B	736	THR	CB-CG2	11.17	1.89	1.52
2	B	909	ASP	C-O	-11.17	1.10	1.23
1	A	391	LEU	N-CA	11.17	1.60	1.46
7	I	17	ARG	NE-CZ	11.17	1.45	1.33
2	B	124	TYR	CA-CB	-11.16	1.34	1.53
2	B	185	THR	CA-C	-11.16	1.38	1.53
1	A	817	ALA	CA-C	-11.16	1.37	1.52
2	B	884	ARG	NE-CZ	11.16	1.45	1.33
5	F	118	LEU	CG-CD1	-11.16	1.15	1.52
2	B	251	ILE	CB-CG2	11.16	1.89	1.52
1	A	1207	LEU	CA-C	11.15	1.65	1.52
2	B	353	LYS	CG-CD	11.15	1.85	1.52
2	B	999	MET	CA-C	-11.15	1.38	1.52
1	A	750	GLY	C-O	-11.14	1.08	1.24
1	A	885	THR	C-O	11.14	1.38	1.24
2	B	668	ASP	CG-OD1	11.14	1.46	1.25
3	C	103	ALA	C-O	-11.14	1.10	1.23
1	A	1278	ASN	CG-OD1	11.14	1.44	1.23
1	A	961	ARG	NE-CZ	11.13	1.45	1.33
1	A	1130	GLN	CG-CD	11.13	1.79	1.52
2	B	624	LEU	CA-CB	-11.13	1.35	1.53
2	B	649	LYS	C-O	11.13	1.38	1.23
4	E	104	ASN	CG-OD1	11.13	1.44	1.23
3	C	110	THR	CA-C	-11.13	1.39	1.52
2	B	845	SER	C-N	-11.13	1.19	1.33
2	B	1008	PRO	CA-CB	-11.13	1.39	1.53
1	A	840	ARG	NE-CZ	11.12	1.45	1.33
5	F	136	ARG	NE-CZ	-11.12	1.20	1.33
5	F	77	ASP	C-O	11.12	1.38	1.23
6	H	45	GLU	CD-OE2	11.12	1.46	1.25
1	A	549	MET	C-O	-11.12	1.10	1.24
1	A	1237	ILE	CA-CB	-11.12	1.38	1.54
1	A	1167	GLU	CA-CB	11.11	1.70	1.53
2	B	389	ALA	N-CA	-11.11	1.32	1.46
9	K	82	ASP	CA-C	-11.11	1.41	1.53
2	B	1186	ASP	CB-CG	11.11	1.79	1.52
7	I	28	GLU	C-O	-11.11	1.08	1.23
1	A	28	ARG	CZ-NH2	11.10	1.47	1.33
1	A	585	GLY	C-O	11.10	1.43	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1420	ASP	CG-OD2	11.10	1.46	1.25
2	B	996	ARG	N-CA	-11.09	1.32	1.46
6	H	32	THR	C-O	11.09	1.38	1.24
1	A	1359	ASP	CA-C	-11.08	1.38	1.52
1	A	601	LYS	CD-CE	11.08	1.85	1.52
9	K	85	ASP	CA-CB	11.08	1.72	1.53
2	B	103	ASN	C-O	11.07	1.38	1.24
1	A	36	ARG	C-O	-11.07	1.10	1.24
3	C	78	GLU	CD-OE1	11.07	1.46	1.25
7	I	28	GLU	CA-C	-11.07	1.39	1.52
2	B	520	GLY	C-O	-11.07	1.07	1.24
1	A	84	ILE	CG1-CD1	-11.07	1.08	1.51
3	C	267	GLN	C-O	11.07	1.35	1.24
1	A	1149	ALA	CA-CB	-11.06	1.35	1.53
1	A	1076	ALA	C-O	-11.06	1.10	1.24
2	B	361	LEU	CA-C	-11.06	1.38	1.52
10	L	70	ARG	NE-CZ	11.06	1.45	1.33
1	A	1362	TYR	CG-CD2	-11.06	1.16	1.39
1	A	896	ARG	CA-C	-11.06	1.38	1.52
10	L	28	LYS	CE-NZ	11.05	1.82	1.49
2	B	418	LYS	CA-C	-11.05	1.38	1.53
2	B	230	ALA	CA-C	11.05	1.66	1.52
3	C	13	ALA	CA-CB	-11.05	1.35	1.53
2	B	1166	CYS	CA-CB	11.05	1.68	1.53
6	H	77	ARG	CB-CG	11.05	1.85	1.52
6	H	63	LEU	C-O	11.05	1.45	1.23
2	B	482	VAL	CA-CB	-11.04	1.40	1.54
1	A	285	PRO	CA-C	-11.04	1.39	1.52
2	B	316	PRO	C-O	11.04	1.38	1.24
2	B	515	HIS	CG-CD2	-11.04	1.23	1.35
1	A	1116	LEU	C-O	-11.04	1.10	1.24
2	B	416	LEU	CA-C	-11.04	1.39	1.52
6	H	55	LEU	C-O	-11.04	1.11	1.23
1	A	295	LEU	CG-CD2	11.03	1.89	1.52
2	B	265	SER	CA-C	11.03	1.66	1.52
2	B	352	ALA	CA-C	-11.03	1.38	1.52
3	C	28	ALA	C-O	11.03	1.37	1.24
1	A	172	PRO	C-O	-11.03	1.11	1.23
2	B	315	LYS	CA-CB	-11.03	1.38	1.53
2	B	1210	MET	N-CA	-11.03	1.33	1.46
1	A	209	ASN	CA-C	-11.02	1.37	1.52
1	A	1162	VAL	CA-CB	-11.02	1.39	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	796	LEU	C-O	-11.02	1.10	1.23
4	E	34	GLU	CD-OE2	11.02	1.46	1.25
1	A	1315	GLU	C-N	-11.02	1.20	1.34
2	B	246	LYS	CA-CB	11.02	1.70	1.53
3	C	227	THR	CA-CB	11.01	1.73	1.53
1	A	519	PRO	CA-C	-11.01	1.38	1.52
1	A	1359	ASP	CG-OD1	11.01	1.46	1.25
1	A	851	HIS	CA-CB	-11.00	1.36	1.53
1	A	673	GLY	C-N	-11.00	1.20	1.34
1	A	632	VAL	N-CA	10.99	1.59	1.46
1	A	641	VAL	C-O	-10.99	1.11	1.24
3	C	170	TRP	CZ3-CH2	-10.99	1.12	1.40
3	C	220	ASP	CB-CG	10.99	1.79	1.52
1	A	958	VAL	N-CA	10.98	1.60	1.46
3	C	57	VAL	CA-C	10.98	1.66	1.52
9	K	64	GLU	C-O	-10.98	1.09	1.24
9	K	65	HIS	C-N	-10.98	1.23	1.33
1	A	616	VAL	N-CA	-10.97	1.33	1.46
1	A	805	LEU	CA-CB	-10.97	1.36	1.53
1	A	204	THR	C-O	-10.97	1.11	1.24
1	A	571	LEU	CG-CD2	10.97	1.88	1.52
2	B	237	VAL	CA-CB	-10.97	1.35	1.55
2	B	280	ILE	CA-CB	-10.97	1.41	1.54
3	C	97	VAL	CA-CB	-10.97	1.40	1.54
2	B	240	ILE	C-O	-10.96	1.12	1.23
2	B	375	ALA	CA-CB	-10.96	1.36	1.53
10	L	33	GLU	C-O	10.96	1.37	1.24
1	A	282	ASN	CB-CG	10.96	1.79	1.52
1	A	138	ILE	CA-C	10.96	1.67	1.52
1	A	268	ASP	CB-CG	10.96	1.79	1.52
1	A	925	LEU	C-O	-10.95	1.11	1.24
2	B	305	VAL	CB-CG1	10.95	1.88	1.52
6	H	85	GLY	C-O	10.95	1.38	1.23
1	A	579	SER	C-O	10.95	1.38	1.24
2	B	191	LYS	C-O	-10.95	1.11	1.24
2	B	308	TRP	N-CA	-10.95	1.31	1.46
2	B	369	GLY	CA-C	10.95	1.69	1.51
1	A	508	PRO	C-O	10.94	1.38	1.24
5	F	121	ALA	C-O	-10.94	1.10	1.24
3	C	94	LYS	CE-NZ	10.94	1.82	1.49
1	A	751	SER	CB-OG	10.93	1.64	1.42
2	B	1002	THR	CA-C	10.93	1.68	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	195	VAL	N-CA	10.93	1.59	1.46
1	A	432	VAL	C-O	-10.93	1.12	1.24
1	A	1034	GLU	C-O	10.92	1.38	1.23
2	B	1130	PHE	CA-C	-10.92	1.37	1.53
4	E	52	ARG	NE-CZ	10.91	1.45	1.33
1	A	963	ILE	C-O	-10.91	1.11	1.24
2	B	986	GLN	CB-CG	10.91	1.85	1.52
2	B	755	ILE	C-O	10.91	1.36	1.24
9	K	81	TYR	N-CA	10.91	1.59	1.46
2	B	959	ASP	CA-C	10.90	1.67	1.52
2	B	1185	CYS	CA-C	10.88	1.67	1.52
6	H	85	GLY	CA-C	10.88	1.67	1.51
3	C	267	GLN	N-CA	10.88	1.65	1.47
3	C	28	ALA	CA-CB	-10.87	1.35	1.53
1	A	532	ARG	N-CA	-10.87	1.33	1.46
3	C	35	ARG	C-O	10.87	1.38	1.24
1	A	1279	ILE	CA-C	-10.87	1.39	1.52
3	C	65	HIS	N-CA	-10.87	1.32	1.46
10	L	64	LEU	CG-CD1	10.87	1.88	1.52
2	B	947	GLY	CA-C	-10.87	1.40	1.52
2	B	550	ASP	CA-C	-10.86	1.37	1.52
2	B	1219	ASP	CB-CG	10.86	1.79	1.52
1	A	900	ASP	N-CA	10.86	1.59	1.46
3	C	9	LYS	CD-CE	10.85	1.85	1.52
9	K	12	LEU	N-CA	10.85	1.58	1.45
2	B	41	LYS	C-O	10.85	1.38	1.24
4	E	67	GLU	CD-OE1	10.85	1.46	1.25
1	A	1417	GLU	CA-CB	10.84	1.70	1.53
3	C	11	ARG	C-O	10.84	1.37	1.24
6	H	26	ILE	CA-C	-10.84	1.40	1.52
10	L	49	LYS	CA-C	10.84	1.67	1.52
1	A	1065	GLY	N-CA	-10.83	1.29	1.45
2	B	465	ASN	C-O	10.83	1.37	1.23
2	B	1150	ARG	C-O	-10.83	1.11	1.24
10	L	47	ARG	CG-CD	10.83	1.84	1.52
1	A	880	LYS	CG-CD	10.83	1.84	1.52
3	C	120	ILE	CA-C	10.83	1.65	1.52
8	J	4	PRO	CA-CB	-10.83	1.39	1.53
1	A	986	ILE	C-O	-10.83	1.12	1.24
9	K	113	THR	C-O	10.82	1.37	1.23
3	C	196	ASP	CB-CG	10.82	1.79	1.52
3	C	196	ASP	CG-OD1	10.82	1.46	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1229	SER	C-O	10.82	1.37	1.23
1	A	942	PHE	C-O	-10.82	1.11	1.24
3	C	104	PHE	CA-C	-10.82	1.39	1.52
2	B	775	LYS	CB-CG	10.81	1.84	1.52
3	C	97	VAL	C-O	-10.81	1.09	1.24
1	A	563	PRO	C-O	-10.81	1.11	1.23
1	A	363	GLN	CA-C	-10.81	1.38	1.53
2	B	595	ARG	CA-C	-10.81	1.38	1.52
2	B	892	LYS	CD-CE	10.81	1.84	1.52
1	A	1381	LEU	N-CA	10.80	1.59	1.46
2	B	911	ILE	N-CA	-10.80	1.32	1.46
2	B	1219	ASP	N-CA	10.80	1.59	1.46
1	A	1421	CYS	C-O	-10.80	1.08	1.23
2	B	287	ARG	CA-CB	-10.80	1.35	1.53
2	B	489	SER	CA-C	-10.80	1.37	1.52
2	B	48	LEU	N-CA	-10.80	1.33	1.46
1	A	877	HIS	N-CA	-10.79	1.33	1.46
1	A	1420	ASP	CG-OD1	10.79	1.45	1.25
1	A	941	LYS	CG-CD	10.79	1.84	1.52
2	B	986	GLN	C-O	10.79	1.36	1.24
1	A	219	PHE	CA-CB	-10.79	1.35	1.53
3	C	195	GLN	C-O	-10.79	1.10	1.24
3	C	199	LYS	CG-CD	10.78	1.84	1.52
2	B	1096	ARG	C-O	-10.78	1.09	1.23
2	B	658	ILE	CA-CB	-10.78	1.39	1.54
7	I	30	ARG	CA-CB	-10.78	1.34	1.53
1	A	193	ASP	CA-C	10.77	1.67	1.52
1	A	905	ASP	CG-OD2	10.77	1.45	1.25
5	F	91	ALA	CA-CB	-10.77	1.35	1.53
9	K	20	LYS	CD-CE	10.77	1.84	1.52
6	H	12	VAL	C-O	10.77	1.35	1.23
1	A	1277	GLU	N-CA	10.76	1.59	1.46
2	B	210	LYS	C-O	-10.76	1.10	1.24
2	B	1072	MET	C-O	10.76	1.37	1.23
1	A	157	ASP	CB-CG	10.76	1.78	1.52
2	B	1046	PRO	CA-C	10.76	1.66	1.52
1	A	874	ASP	CA-C	-10.76	1.39	1.52
1	A	886	ILE	C-N	-10.76	1.21	1.33
2	B	271	ALA	C-O	-10.76	1.10	1.23
4	E	71	LYS	N-CA	10.75	1.59	1.46
2	B	462	ALA	CA-CB	-10.75	1.35	1.53
8	J	42	LYS	C-O	10.75	1.38	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	302	THR	CA-CB	10.75	1.71	1.53
1	A	553	VAL	C-N	-10.75	1.21	1.33
2	B	418	LYS	CD-CE	10.75	1.84	1.52
2	B	1100	ASP	CA-CB	10.74	1.71	1.53
2	B	789	MET	SD-CE	10.74	2.06	1.79
9	K	61	TYR	C-O	-10.74	1.09	1.23
6	H	25	ARG	CA-C	10.74	1.66	1.52
2	B	18	PHE	CA-CB	10.73	1.75	1.53
2	B	1143	ALA	CA-CB	-10.73	1.38	1.52
1	A	738	LYS	CE-NZ	10.73	1.81	1.49
9	K	69	ALA	CA-C	-10.73	1.39	1.52
1	A	1114	PRO	CA-C	-10.73	1.38	1.52
1	A	430	TRP	CE3-CZ3	-10.71	1.06	1.38
1	A	387	ARG	CA-C	10.71	1.68	1.52
1	A	832	ALA	C-O	10.70	1.36	1.24
1	A	941	LYS	CE-NZ	10.70	1.81	1.49
1	A	1414	ALA	N-CA	-10.70	1.32	1.46
2	B	703	ILE	CA-CB	-10.70	1.40	1.54
4	E	44	ALA	C-O	10.70	1.37	1.24
8	J	26	GLN	CD-OE1	10.70	1.43	1.23
1	A	897	TYR	CG-CD2	-10.70	1.16	1.39
2	B	1181	GLU	CA-CB	10.70	1.73	1.53
1	A	462	VAL	N-CA	10.69	1.58	1.46
1	A	1290	LYS	CE-NZ	10.69	1.81	1.49
1	A	80	HIS	C-O	10.68	1.37	1.23
1	A	840	ARG	CA-C	-10.68	1.38	1.52
2	B	283	VAL	C-O	-10.68	1.10	1.24
3	C	205	LYS	CD-CE	10.68	1.84	1.52
5	F	77	ASP	CG-OD1	10.68	1.45	1.25
1	A	1095	THR	CA-C	-10.68	1.39	1.52
2	B	1106	ARG	CD-NE	10.68	1.61	1.46
1	A	264	PHE	CA-CB	10.67	1.71	1.53
1	A	188	ASP	CB-CG	10.67	1.78	1.52
3	C	125	MET	CG-SD	10.67	2.07	1.80
1	A	578	LEU	N-CA	10.67	1.59	1.46
10	L	59	ALA	N-CA	10.67	1.59	1.46
1	A	922	ASP	C-O	-10.67	1.11	1.24
4	E	56	LYS	CG-CD	10.67	1.84	1.52
1	A	1277	GLU	CD-OE1	10.66	1.45	1.25
9	K	67	PHE	N-CA	-10.66	1.31	1.46
1	A	496	GLU	CD-OE2	10.66	1.45	1.25
3	C	86	CYS	N-CA	10.66	1.60	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1408	ILE	CG1-CD1	10.65	1.93	1.51
2	B	1027	ILE	N-CA	-10.65	1.32	1.46
6	H	44	VAL	C-O	10.65	1.36	1.24
2	B	1090	THR	CB-CG2	-10.65	1.17	1.52
1	A	193	ASP	CB-CG	10.65	1.78	1.52
2	B	1011	ILE	CA-CB	10.65	1.68	1.54
1	A	1126	ALA	CA-C	10.64	1.67	1.52
2	B	350	GLN	N-CA	-10.64	1.32	1.46
6	H	136	LYS	CA-CB	10.64	1.71	1.53
9	K	34	THR	C-N	-10.64	1.18	1.33
1	A	687	LYS	CA-C	10.64	1.67	1.52
4	E	177	ARG	C-O	-10.64	1.10	1.23
1	A	881	GLN	N-CA	-10.63	1.32	1.45
2	B	118	ARG	CD-NE	-10.63	1.31	1.46
3	C	137	LYS	CG-CD	10.63	1.84	1.52
1	A	297	GLN	C-O	-10.63	1.11	1.24
2	B	205	ILE	CG1-CD1	-10.63	1.10	1.51
4	E	108	GLY	C-O	-10.63	1.09	1.23
6	H	104	PHE	C-O	10.63	1.37	1.24
8	J	63	TYR	C-O	-10.63	1.09	1.23
2	B	643	ASP	C-O	-10.62	1.02	1.23
2	B	646	LEU	CB-CG	10.62	1.74	1.53
4	E	52	ARG	CB-CG	10.62	1.84	1.52
2	B	136	THR	C-O	10.62	1.36	1.24
3	C	56	THR	CA-CB	-10.61	1.35	1.53
4	E	185	ALA	CA-CB	-10.61	1.35	1.53
6	H	19	ARG	CZ-NH1	10.61	1.47	1.32
1	A	14	VAL	CA-C	-10.61	1.39	1.52
10	L	38	LEU	N-CA	-10.61	1.32	1.46
2	B	1021	MET	CA-C	-10.60	1.40	1.53
1	A	1019	CYS	CA-C	-10.60	1.38	1.52
1	A	1129	GLU	CD-OE1	10.60	1.45	1.25
2	B	1186	ASP	CA-CB	10.59	1.70	1.53
1	A	964	ILE	CG1-CD1	-10.59	1.10	1.51
3	C	82	TYR	N-CA	10.59	1.59	1.46
4	E	128	PRO	CA-CB	10.59	1.68	1.54
1	A	117	GLU	CA-C	-10.59	1.38	1.52
2	B	868	MET	CA-C	10.58	1.67	1.52
2	B	976	ILE	CA-C	-10.58	1.39	1.52
1	A	629	LEU	C-O	-10.58	1.11	1.24
1	A	793	SER	C-O	-10.58	1.07	1.23
2	B	1154	ALA	N-CA	10.58	1.59	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1103	GLU	C-O	10.57	1.36	1.24
1	A	1277	GLU	CG-CD	10.57	1.78	1.52
2	B	908	GLU	CD-OE2	10.57	1.45	1.25
1	A	1194	ARG	N-CA	-10.57	1.33	1.46
2	B	641	GLU	CG-CD	10.57	1.78	1.52
4	E	138	ALA	CA-CB	-10.57	1.35	1.53
1	A	393	ARG	NE-CZ	10.56	1.44	1.33
2	B	855	PHE	C-O	-10.56	1.12	1.24
8	J	22	LEU	N-CA	-10.56	1.33	1.46
8	J	50	ILE	C-O	10.56	1.36	1.23
1	A	398	GLU	CD-OE2	10.56	1.45	1.25
9	K	50	LEU	C-O	-10.55	1.10	1.24
3	C	102	GLN	CB-CG	10.55	1.84	1.52
8	J	26	GLN	CB-CG	10.55	1.84	1.52
1	A	283	GLY	C-O	10.55	1.38	1.23
7	I	72	ASP	CG-OD1	10.55	1.45	1.25
1	A	1024	SER	CA-C	-10.54	1.38	1.52
5	F	87	LYS	CD-CE	10.54	1.84	1.52
1	A	618	GLU	CD-OE1	10.54	1.45	1.25
1	A	720	ARG	CD-NE	10.54	1.61	1.46
2	B	1223	ASP	C-O	10.54	1.37	1.24
1	A	404	TYR	CG-CD1	-10.54	1.17	1.39
7	I	70	ARG	NE-CZ	-10.54	1.21	1.33
2	B	848	ARG	CZ-NH2	10.54	1.47	1.33
1	A	1119	TYR	CA-C	-10.54	1.40	1.52
2	B	809	MET	CA-C	-10.54	1.37	1.52
2	B	1181	GLU	CA-C	10.54	1.65	1.52
2	B	1061	GLU	CD-OE1	10.53	1.45	1.25
1	A	41	MET	SD-CE	10.53	2.05	1.79
1	A	1139	GLU	N-CA	10.53	1.58	1.46
1	A	1339	LEU	CA-CB	-10.53	1.39	1.54
7	I	20	LYS	CD-CE	10.53	1.84	1.52
1	A	521	MET	CA-C	-10.53	1.39	1.52
1	A	1333	ILE	CA-CB	-10.53	1.41	1.54
2	B	664	THR	N-CA	-10.53	1.33	1.46
6	H	20	TYR	C-O	10.53	1.37	1.23
2	B	987	LYS	CA-CB	-10.53	1.37	1.53
4	E	195	VAL	CA-CB	-10.53	1.41	1.54
1	A	770	VAL	C-O	-10.52	1.12	1.24
2	B	733	HIS	C-O	10.52	1.37	1.24
3	C	162	GLY	C-O	10.52	1.36	1.24
1	A	507	VAL	CA-CB	10.52	1.60	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	220	GLY	C-O	-10.52	1.10	1.23
4	E	179	GLN	CA-CB	-10.52	1.35	1.53
2	B	37	PHE	C-O	10.51	1.36	1.24
2	B	791	THR	N-CA	-10.51	1.33	1.46
1	A	20	GLY	C-O	10.51	1.35	1.23
1	A	1112	LYS	CD-CE	10.51	1.83	1.52
9	K	1	MET	N-CA	10.51	1.66	1.46
7	I	1	MET	CB-CG	10.50	1.83	1.52
2	B	315	LYS	CE-NZ	10.50	1.80	1.49
1	A	1227	ILE	C-O	-10.50	1.10	1.23
1	A	1385	THR	CA-C	10.50	1.75	1.52
2	B	852	ARG	CZ-NH1	-10.50	1.18	1.32
2	B	870	ILE	N-CA	10.50	1.64	1.47
3	C	60	ASP	CA-C	-10.49	1.39	1.52
1	A	217	LYS	CD-CE	10.49	1.83	1.52
6	H	2	SER	CA-C	10.49	1.75	1.52
1	A	499	ALA	CA-C	-10.49	1.39	1.52
2	B	852	ARG	CZ-NH2	-10.48	1.19	1.33
6	H	38	LEU	CG-CD1	-10.48	1.18	1.52
2	B	770	GLN	CD-NE2	10.47	1.55	1.33
1	A	892	ALA	C-O	-10.47	1.10	1.24
3	C	126	GLY	C-O	10.47	1.38	1.23
6	H	61	SER	C-O	10.47	1.37	1.24
3	C	148	ARG	CD-NE	10.47	1.60	1.46
1	A	268	ASP	CA-CB	10.46	1.71	1.53
2	B	401	PHE	C-O	-10.46	1.10	1.24
1	A	36	ARG	NE-CZ	10.46	1.44	1.33
1	A	1195	LEU	C-O	-10.46	1.11	1.23
1	A	326	ARG	CA-C	10.46	1.66	1.52
3	C	116	LYS	C-O	10.46	1.37	1.24
1	A	37	PHE	CE1-CZ	10.45	1.70	1.38
2	B	667	GLN	C-O	10.45	1.35	1.23
5	F	77	ASP	CG-OD2	10.45	1.45	1.25
9	K	99	GLY	C-O	10.45	1.38	1.23
1	A	1012	ARG	CG-CD	10.45	1.83	1.52
4	E	169	ARG	CA-C	10.45	1.67	1.53
9	K	30	ALA	CA-CB	-10.45	1.35	1.53
6	H	91	ASP	C-O	10.44	1.36	1.24
2	B	215	GLN	N-CA	-10.44	1.33	1.46
2	B	706	GLN	CB-CG	10.44	1.83	1.52
2	B	815	ARG	CZ-NH2	10.44	1.47	1.33
2	B	250	PHE	CA-C	10.44	1.67	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	46	HIS	CA-C	-10.44	1.41	1.53
7	I	82	GLU	CA-CB	10.44	1.71	1.53
1	A	1003	LYS	CD-CE	10.44	1.83	1.52
1	A	781	ASP	CA-CB	-10.43	1.37	1.53
2	B	981	ALA	CA-CB	-10.43	1.35	1.53
2	B	1106	ARG	CG-CD	10.43	1.83	1.52
2	B	580	VAL	CA-C	-10.43	1.39	1.52
5	F	116	ASP	CA-C	-10.42	1.40	1.52
5	F	135	ARG	N-CA	-10.42	1.33	1.46
1	A	716	ASP	CG-OD1	10.42	1.45	1.25
2	B	803	LEU	N-CA	-10.41	1.33	1.46
1	A	1194	ARG	CB-CG	10.41	1.83	1.52
1	A	1441	PHE	C-O	-10.41	1.11	1.23
2	B	785	TYR	CE1-CZ	-10.41	1.13	1.38
1	A	720	ARG	NE-CZ	10.40	1.44	1.33
3	C	223	ALA	CA-C	-10.40	1.38	1.53
1	A	1238	ILE	N-CA	-10.40	1.34	1.46
1	A	305	ASP	N-CA	10.40	1.66	1.46
1	A	1269	GLU	CD-OE1	10.39	1.45	1.25
2	B	385	LEU	CA-C	-10.39	1.39	1.52
2	B	414	ALA	CA-C	10.39	1.65	1.52
3	C	193	TYR	CA-C	-10.39	1.40	1.52
8	J	39	LEU	CA-C	-10.39	1.35	1.52
1	A	724	GLU	CD-OE1	10.38	1.45	1.25
2	B	239	GLU	CG-CD	10.38	1.78	1.52
3	C	67	LEU	C-O	10.38	1.36	1.24
2	B	958	GLN	CA-C	10.38	1.66	1.52
2	B	1221	SER	N-CA	10.38	1.59	1.46
7	I	45	ARG	C-O	10.38	1.36	1.23
9	K	72	LYS	CA-C	-10.38	1.40	1.52
3	C	75	MET	CB-CG	-10.38	1.21	1.52
3	C	82	TYR	CZ-OH	10.38	1.59	1.38
4	E	192	ARG	CD-NE	10.37	1.60	1.46
1	A	50	ILE	N-CA	10.37	1.58	1.46
2	B	962	LYS	CG-CD	10.37	1.83	1.52
2	B	356	LEU	C-O	-10.37	1.11	1.24
1	A	1196	GLU	CA-CB	-10.37	1.38	1.53
2	B	106	ASP	CG-OD2	10.37	1.45	1.25
6	H	141	TYR	CE1-CZ	-10.37	1.13	1.38
1	A	1371	LEU	C-O	10.37	1.36	1.24
4	E	43	LYS	CB-CG	10.37	1.83	1.52
2	B	1108	ARG	NE-CZ	10.36	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1139	ILE	CA-CB	-10.36	1.42	1.54
1	A	472	LEU	CG-CD2	-10.36	1.18	1.52
8	J	24	LEU	CG-CD2	-10.36	1.18	1.52
1	A	181	LEU	CA-C	-10.36	1.40	1.52
1	A	940	ARG	C-O	-10.36	1.11	1.24
1	A	519	PRO	C-O	-10.36	1.11	1.23
2	B	958	GLN	CB-CG	10.35	1.83	1.52
2	B	1215	ARG	C-O	-10.35	1.11	1.24
1	A	1265	ASN	CA-CB	10.34	1.69	1.53
2	B	803	LEU	CA-CB	-10.34	1.36	1.53
1	A	529	CYS	C-N	-10.34	1.18	1.33
1	A	1381	LEU	C-O	-10.34	1.11	1.24
2	B	568	ASP	C-O	-10.34	1.10	1.24
10	L	41	SER	N-CA	10.34	1.59	1.46
1	A	944	ARG	CA-CB	-10.34	1.35	1.53
1	A	1206	ASP	CB-CG	10.34	1.77	1.52
6	H	3	ASN	CA-C	10.34	1.65	1.53
1	A	3	GLY	N-CA	10.33	1.62	1.45
1	A	1355	VAL	CA-CB	-10.33	1.42	1.54
3	C	102	GLN	C-O	10.33	1.36	1.23
1	A	34	LYS	C-O	-10.33	1.10	1.24
1	A	1104	ILE	C-O	-10.32	1.12	1.24
2	B	1024	ALA	CA-CB	-10.32	1.37	1.53
7	I	56	ALA	CA-CB	-10.32	1.36	1.53
2	B	191	LYS	CB-CG	10.32	1.83	1.52
1	A	289	ILE	CA-C	-10.31	1.40	1.52
1	A	497	THR	N-CA	-10.31	1.33	1.46
1	A	561	PRO	CA-CB	10.31	1.68	1.53
1	A	808	LEU	N-CA	-10.31	1.32	1.46
1	A	578	LEU	CG-CD1	-10.31	1.18	1.52
7	I	51	ASN	CG-OD1	10.31	1.43	1.23
2	B	1019	SER	C-O	10.30	1.37	1.24
1	A	681	GLU	CD-OE1	10.30	1.45	1.25
2	B	679	TYR	C-O	10.30	1.37	1.24
1	A	996	ASN	CA-C	10.29	1.68	1.52
3	C	251	LEU	C-O	-10.29	1.12	1.24
1	A	810	PRO	C-O	-10.29	1.10	1.24
1	A	995	GLU	CD-OE2	10.29	1.45	1.25
1	A	1372	VAL	CB-CG1	-10.29	1.18	1.52
2	B	1163	CYS	C-N	-10.29	1.22	1.33
4	E	37	LEU	CG-CD1	10.29	1.86	1.52
6	H	9	ILE	CG1-CD1	10.29	1.91	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	VAL	CA-C	-10.28	1.40	1.52
4	E	114	ASN	N-CA	10.28	1.59	1.46
1	A	423	ASP	CB-CG	10.28	1.77	1.52
1	A	722	LEU	CA-C	-10.28	1.38	1.52
1	A	817	ALA	CA-CB	-10.28	1.36	1.53
1	A	1214	GLU	C-O	10.28	1.37	1.24
2	B	39	ARG	C-O	-10.28	1.12	1.24
10	L	50	ASP	CA-CB	10.28	1.70	1.53
5	F	114	GLU	C-O	-10.28	1.10	1.23
8	J	26	GLN	CG-CD	10.28	1.77	1.52
1	A	801	GLU	CD-OE1	10.27	1.44	1.25
1	A	1194	ARG	CD-NE	-10.27	1.31	1.46
1	A	825	ILE	CA-CB	-10.27	1.40	1.54
1	A	1422	ARG	CZ-NH2	10.27	1.46	1.33
1	A	543	LEU	N-CA	-10.26	1.33	1.46
2	B	428	ILE	CG1-CD1	10.26	1.91	1.51
1	A	1003	LYS	C-O	10.26	1.36	1.24
1	A	1129	GLU	CG-CD	10.26	1.77	1.52
7	I	25	LEU	CA-C	10.26	1.65	1.52
1	A	28	ARG	CG-CD	10.26	1.83	1.52
1	A	121	LEU	C-O	-10.26	1.11	1.24
2	B	235	SER	CA-C	-10.25	1.39	1.52
1	A	990	VAL	CA-CB	-10.25	1.39	1.54
1	A	644	LYS	C-O	-10.25	1.12	1.24
2	B	978	ASP	CG-OD2	10.25	1.44	1.25
2	B	859	TYR	CA-CB	-10.24	1.37	1.53
2	B	169	ARG	NE-CZ	10.24	1.44	1.33
6	H	35	GLN	C-O	10.24	1.36	1.24
4	E	113	GLN	CA-CB	10.24	1.69	1.53
6	H	111	LEU	CG-CD1	10.23	1.86	1.52
1	A	1232	ASN	CA-C	10.23	1.66	1.52
7	I	34	TYR	CG-CD2	-10.23	1.17	1.39
2	B	1097	HIS	CD2-NE2	10.22	1.49	1.37
3	C	17	ASN	C-O	-10.22	1.11	1.23
2	B	496	ARG	CA-CB	-10.22	1.38	1.53
4	E	41	ASP	CB-CG	10.22	1.77	1.52
1	A	1419	ASP	CB-CG	10.22	1.77	1.52
2	B	1203	LEU	C-N	-10.22	1.20	1.33
10	L	50	ASP	C-O	10.22	1.36	1.24
1	A	37	PHE	C-O	-10.22	1.10	1.23
1	A	175	ARG	C-O	10.22	1.36	1.23
2	B	958	GLN	N-CA	10.22	1.59	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	871	ASP	C-O	-10.21	1.11	1.24
1	A	1241	ARG	C-O	-10.21	1.11	1.23
2	B	1151	LEU	N-CA	-10.21	1.33	1.46
3	C	266	ASP	CA-C	10.21	1.66	1.52
1	A	188	ASP	N-CA	10.21	1.59	1.46
4	E	23	VAL	N-CA	-10.21	1.34	1.46
1	A	28	ARG	NE-CZ	10.21	1.44	1.33
4	E	109	ILE	CA-C	-10.21	1.40	1.52
1	A	190	ALA	CA-C	10.21	1.66	1.52
1	A	1074	GLU	CD-OE2	10.21	1.44	1.25
2	B	251	ILE	CA-CB	10.21	1.68	1.54
1	A	1155	ASP	N-CA	10.20	1.56	1.46
4	E	16	PHE	CA-C	-10.20	1.39	1.52
1	A	188	ASP	CA-CB	10.20	1.70	1.53
2	B	705	MET	C-O	-10.20	1.10	1.24
4	E	32	GLN	C-O	-10.20	1.12	1.24
4	E	148	GLU	CA-C	-10.20	1.38	1.52
1	A	170	THR	C-O	10.20	1.37	1.23
1	A	1114	PRO	C-O	-10.20	1.12	1.23
9	K	61	TYR	CA-C	-10.20	1.39	1.52
9	K	96	ASN	C-O	10.19	1.36	1.24
2	B	879	ARG	N-CA	10.19	1.59	1.46
9	K	38	GLU	CA-C	10.19	1.65	1.52
1	A	1076	ALA	CA-CB	10.19	1.70	1.53
2	B	1057	LYS	C-O	10.19	1.36	1.24
2	B	768	THR	CB-OG1	10.19	1.60	1.43
1	A	504	LEU	CG-CD1	-10.19	1.19	1.52
2	B	1095	LEU	CA-CB	-10.18	1.37	1.53
1	A	212	LYS	CG-CD	10.18	1.82	1.52
1	A	872	GLY	CA-C	-10.18	1.36	1.51
2	B	56	ASP	C-O	-10.18	1.11	1.24
4	E	66	GLU	CG-CD	10.18	1.77	1.52
10	L	27	LEU	CB-CG	10.18	1.73	1.53
2	B	220	GLY	N-CA	-10.17	1.36	1.44
2	B	656	GLY	C-N	10.17	1.47	1.33
2	B	684	LEU	N-CA	-10.17	1.33	1.46
2	B	959	ASP	CB-CG	10.17	1.77	1.52
1	A	1363	VAL	C-O	10.17	1.34	1.23
3	C	50	GLU	CD-OE1	10.16	1.44	1.25
1	A	1191	TRP	C-O	10.16	1.36	1.24
1	A	1304	TRP	CA-C	-10.16	1.39	1.52
7	I	34	TYR	CE2-CZ	-10.16	1.13	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	605	MET	SD-CE	-10.15	1.54	1.79
1	A	1173	HIS	CA-C	10.15	1.74	1.52
2	B	694	ASP	CG-OD2	10.15	1.44	1.25
1	A	1140	HIS	C-O	-10.15	1.11	1.23
4	E	25	ASP	C-O	10.15	1.37	1.24
8	J	61	LEU	CA-CB	-10.15	1.35	1.53
1	A	1269	GLU	CD-OE2	10.15	1.44	1.25
8	J	38	ARG	N-CA	-10.15	1.33	1.46
1	A	655	PHE	CE1-CZ	-10.14	1.08	1.38
1	A	465	TYR	C-O	-10.14	1.11	1.24
1	A	767	GLN	CA-CB	-10.14	1.37	1.53
2	B	453	ILE	CA-C	-10.14	1.40	1.52
4	E	193	GLY	C-O	10.14	1.39	1.24
1	A	1336	MET	C-O	-10.14	1.11	1.24
1	A	502	SER	CA-C	-10.13	1.38	1.52
3	C	70	ILE	C-N	-10.13	1.20	1.33
8	J	55	ASP	CA-C	-10.13	1.41	1.53
9	K	50	LEU	CA-C	-10.13	1.39	1.52
1	A	1111	MET	CG-SD	10.13	2.06	1.80
4	E	154	ILE	C-O	10.13	1.35	1.24
2	B	805	THR	C-O	-10.12	1.09	1.23
2	B	106	ASP	CB-CG	10.12	1.77	1.52
1	A	920	LEU	CB-CG	-10.12	1.33	1.53
1	A	596	THR	CA-C	-10.12	1.39	1.52
1	A	945	GLU	CD-OE2	10.12	1.44	1.25
3	C	211	ASP	CG-OD2	10.12	1.44	1.25
9	K	59	ALA	CA-CB	-10.12	1.36	1.53
2	B	567	GLU	CA-C	10.11	1.66	1.52
1	A	1116	LEU	CB-CG	-10.11	1.33	1.53
2	B	176	SER	C-O	-10.11	1.10	1.23
3	C	84	ARG	CB-CG	10.11	1.82	1.52
7	I	15	TYR	N-CA	-10.11	1.32	1.45
7	I	36	GLU	CG-CD	10.11	1.77	1.52
2	B	1007	VAL	CB-CG1	-10.11	1.19	1.52
5	F	110	ASP	CG-OD1	10.11	1.44	1.25
2	B	1211	ASN	N-CA	10.10	1.57	1.46
2	B	758	PHE	CE1-CZ	10.10	1.69	1.38
1	A	836	TYR	CZ-OH	10.10	1.59	1.38
1	A	1159	ARG	N-CA	10.10	1.58	1.46
1	A	689	LYS	CD-CE	10.09	1.82	1.52
3	C	79	GLN	CD-NE2	10.09	1.54	1.33
1	A	974	ASP	N-CA	10.09	1.58	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	691	GLU	CA-C	-10.09	1.40	1.52
5	F	128	LYS	CA-C	-10.09	1.38	1.53
1	A	130	ASP	CG-OD1	10.08	1.44	1.25
4	E	186	LEU	C-N	-10.08	1.20	1.33
2	B	546	SER	C-O	-10.08	1.11	1.23
10	L	29	TYR	C-O	-10.08	1.10	1.23
2	B	666	TYR	CE1-CZ	10.07	1.62	1.38
1	A	1111	MET	C-O	-10.07	1.10	1.23
2	B	603	LEU	N-CA	-10.07	1.33	1.46
1	A	1187	GLN	CA-CB	10.07	1.73	1.53
2	B	276	ILE	CG1-CD1	-10.07	1.12	1.51
3	C	3	GLU	CD-OE2	10.07	1.44	1.25
1	A	702	LEU	C-O	10.06	1.36	1.23
1	A	1104	ILE	CA-CB	-10.06	1.43	1.54
1	A	1328	TYR	C-O	-10.06	1.11	1.23
1	A	1337	GLU	CD-OE2	10.06	1.44	1.25
1	A	1198	ASP	N-CA	10.06	1.58	1.46
3	C	199	LYS	CB-CG	10.06	1.82	1.52
5	F	80	ALA	N-CA	-10.06	1.32	1.45
1	A	1268	LEU	CA-CB	-10.06	1.37	1.53
2	B	49	ASP	C-N	-10.05	1.20	1.33
1	A	326	ARG	NE-CZ	10.05	1.44	1.33
5	F	97	ARG	C-O	-10.05	1.11	1.24
7	I	51	ASN	CA-C	-10.05	1.39	1.52
1	A	395	GLY	C-O	-10.04	1.10	1.24
1	A	1288	ASP	N-CA	10.04	1.58	1.46
2	B	327	ARG	CZ-NH1	10.04	1.46	1.32
2	B	1025	HIS	CG-ND1	-10.04	1.27	1.38
7	I	93	LYS	CA-CB	10.04	1.70	1.53
2	B	532	ALA	N-CA	10.04	1.58	1.46
1	A	1235	LYS	CE-NZ	10.04	1.79	1.49
9	K	88	LYS	CG-CD	10.04	1.82	1.52
1	A	161	LEU	CA-C	-10.03	1.40	1.52
1	A	47	ARG	CA-C	10.03	1.66	1.52
2	B	120	ARG	CB-CG	10.03	1.82	1.52
2	B	1128	LEU	CA-C	10.03	1.66	1.52
7	I	43	VAL	CA-C	-10.03	1.38	1.52
7	I	5	ARG	CA-C	-10.02	1.40	1.52
1	A	1114	PRO	CA-CB	-10.01	1.40	1.53
2	B	553	PRO	CA-CB	-10.01	1.39	1.53
3	C	116	LYS	CD-CE	10.01	1.82	1.52
4	E	195	VAL	CA-C	-10.01	1.40	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	112	LEU	C-O	-10.01	1.12	1.24
1	A	177	ASP	CB-CG	10.00	1.77	1.52
1	A	107	CYS	CA-C	-10.00	1.40	1.52
2	B	868	MET	N-CA	10.00	1.59	1.46
1	A	120	GLU	CA-C	10.00	1.66	1.52
1	A	205	GLU	CD-OE1	10.00	1.44	1.25
1	A	1093	LYS	CG-CD	10.00	1.82	1.52
9	K	91	CYS	CA-C	10.00	1.67	1.52
1	A	439	ASN	CA-CB	-9.99	1.40	1.53
3	C	228	PHE	N-CA	-9.98	1.33	1.46
2	B	1101	ASP	CB-CG	9.98	1.77	1.52
2	B	538	ASN	C-O	-9.98	1.12	1.24
2	B	403	LYS	CA-C	-9.98	1.40	1.53
3	C	40	GLU	CA-C	9.98	1.65	1.52
1	A	272	ALA	CA-CB	9.97	1.69	1.53
1	A	870	GLU	CD-OE2	9.97	1.44	1.25
2	B	183	GLU	CG-CD	9.97	1.76	1.52
4	E	99	HIS	N-CA	9.97	1.58	1.46
6	H	103	LYS	CA-C	-9.97	1.39	1.52
1	A	457	ALA	C-O	-9.96	1.11	1.24
4	E	52	ARG	CA-C	9.96	1.65	1.53
2	B	1138	MET	N-CA	-9.96	1.33	1.46
1	A	243	PRO	CA-CB	-9.96	1.40	1.54
1	A	563	PRO	CA-C	-9.95	1.40	1.52
1	A	1278	ASN	C-O	-9.95	1.11	1.24
2	B	54	PHE	CA-C	-9.94	1.40	1.52
2	B	118	ARG	N-CA	-9.94	1.33	1.46
2	B	992	ILE	CA-CB	-9.94	1.48	1.55
4	E	147	HIS	CG-ND1	-9.94	1.27	1.38
1	A	1314	SER	CA-C	-9.93	1.39	1.52
1	A	1359	ASP	CB-CG	9.93	1.76	1.52
2	B	815	ARG	CD-NE	-9.93	1.32	1.46
4	E	91	LYS	CB-CG	9.93	1.82	1.52
1	A	16	GLU	CD-OE1	9.93	1.44	1.25
4	E	200	ARG	NE-CZ	-9.93	1.22	1.33
10	L	68	GLU	CD-OE2	9.93	1.44	1.25
1	A	112	LYS	N-CA	-9.92	1.33	1.46
1	A	510	GLN	CA-CB	-9.92	1.38	1.53
1	A	668	ASP	CA-CB	-9.92	1.36	1.53
1	A	920	LEU	CA-CB	-9.92	1.36	1.53
3	C	200	GLU	C-O	9.92	1.37	1.23
7	I	81	ARG	CA-C	9.92	1.66	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	861	GLY	C-O	-9.92	1.10	1.24
2	B	32	ALA	CA-C	-9.92	1.39	1.52
3	C	68	GLY	N-CA	9.92	1.59	1.45
3	C	230	MET	CG-SD	9.92	2.05	1.80
7	I	62	ILE	C-O	-9.92	1.10	1.24
2	B	869	SER	CA-C	9.92	1.66	1.52
2	B	1135	ARG	CA-C	-9.92	1.40	1.52
3	C	89	GLU	CD-OE2	9.92	1.44	1.25
7	I	109	ILE	CA-CB	9.91	1.67	1.54
1	A	941	LYS	N-CA	-9.91	1.34	1.46
2	B	45	SER	CA-CB	9.91	1.69	1.53
6	H	111	LEU	N-CA	9.91	1.58	1.45
1	A	566	ILE	CB-CG2	9.91	1.85	1.52
1	A	1221	LYS	CG-CD	9.91	1.82	1.52
2	B	657	HIS	C-N	-9.91	1.22	1.33
2	B	33	VAL	C-O	-9.91	1.12	1.24
2	B	191	LYS	CA-C	-9.91	1.39	1.52
2	B	227	LYS	CG-CD	9.91	1.82	1.52
2	B	810	GLU	C-N	-9.91	1.19	1.33
2	B	1182	CYS	N-CA	9.91	1.59	1.46
1	A	1098	VAL	C-N	-9.90	1.21	1.34
2	B	1132	GLU	C-O	9.90	1.36	1.24
1	A	923	LEU	C-O	9.90	1.36	1.24
9	K	39	ASP	CA-CB	-9.90	1.40	1.54
1	A	469	ARG	CG-CD	9.89	1.82	1.52
1	A	1284	MET	CB-CG	-9.89	1.22	1.52
1	A	1118	VAL	N-CA	-9.89	1.34	1.46
2	B	96	TYR	CG-CD1	9.89	1.60	1.39
1	A	1228	TRP	CD2-CE2	-9.89	1.24	1.41
6	H	41	ASP	CB-CG	9.89	1.76	1.52
4	E	147	HIS	CB-CG	9.88	1.64	1.50
1	A	53	LEU	C-O	9.88	1.39	1.24
1	A	1263	ILE	CA-CB	9.88	1.68	1.54
2	B	205	ILE	N-CA	-9.88	1.32	1.46
6	H	126	GLU	CD-OE1	9.88	1.44	1.25
1	A	479	ASN	C-O	-9.88	1.11	1.23
1	A	45	GLN	N-CA	9.87	1.58	1.46
2	B	556	THR	C-O	9.88	1.35	1.24
2	B	624	LEU	CG-CD1	-9.88	1.20	1.52
2	B	1146	PHE	CG-CD1	-9.87	1.18	1.38
2	B	589	VAL	C-O	-9.87	1.14	1.24
1	A	503	GLN	CD-OE1	9.87	1.42	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	593	PRO	C-O	-9.86	1.11	1.24
2	B	124	TYR	CE1-CZ	-9.86	1.14	1.38
1	A	1099	PRO	CA-C	-9.86	1.36	1.52
4	E	192	ARG	CA-C	-9.86	1.40	1.52
5	F	130	ILE	CA-CB	-9.86	1.43	1.53
2	B	118	ARG	C-O	9.85	1.35	1.24
1	A	137	ALA	CA-C	9.85	1.66	1.52
1	A	380	VAL	CA-CB	-9.85	1.42	1.54
3	C	11	ARG	C-N	-9.85	1.21	1.33
10	L	27	LEU	CA-CB	9.85	1.70	1.53
3	C	110	THR	CA-CB	9.85	1.68	1.53
1	A	347	PHE	CA-C	-9.84	1.39	1.52
3	C	50	GLU	CG-CD	9.84	1.76	1.52
6	H	90	ALA	CA-CB	-9.84	1.36	1.53
1	A	1068	ALA	CA-CB	-9.83	1.36	1.53
10	L	43	THR	N-CA	9.83	1.57	1.46
1	A	537	ARG	CA-CB	9.82	1.69	1.53
2	B	496	ARG	CD-NE	-9.82	1.32	1.46
1	A	99	ILE	CA-CB	-9.82	1.42	1.54
1	A	656	TRP	CG-CD2	-9.82	1.26	1.43
1	A	291	GLU	CG-CD	9.82	1.76	1.52
2	B	1099	VAL	C-O	-9.82	1.12	1.24
1	A	656	TRP	CD2-CE3	-9.81	1.24	1.40
2	B	1160	VAL	C-O	9.81	1.35	1.24
2	B	1154	ALA	C-N	9.81	1.47	1.33
1	A	1256	GLU	CA-CB	9.81	1.70	1.53
2	B	324	ILE	CA-CB	-9.80	1.41	1.53
1	A	755	PHE	N-CA	-9.80	1.34	1.46
1	A	43	GLU	CA-C	9.79	1.65	1.52
1	A	669	THR	N-CA	-9.79	1.33	1.46
4	E	111	VAL	CA-CB	-9.79	1.42	1.54
1	A	667	GLY	CA-C	9.79	1.64	1.52
2	B	555	ILE	CA-CB	-9.79	1.41	1.54
2	B	120	ARG	CZ-NH1	9.79	1.46	1.32
2	B	896	ASP	CA-C	-9.79	1.39	1.52
2	B	945	GLU	CD-OE1	9.79	1.44	1.25
1	A	1384	VAL	CA-C	-9.79	1.42	1.52
1	A	1212	VAL	CA-CB	-9.78	1.44	1.54
1	A	1289	ARG	NE-CZ	-9.78	1.22	1.33
2	B	854	LEU	C-O	-9.78	1.11	1.23
2	B	1213	THR	C-O	-9.78	1.12	1.24
1	A	711	ARG	N-CA	-9.78	1.33	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1005	GLU	C-O	-9.78	1.11	1.24
5	F	106	PRO	CA-C	-9.78	1.39	1.52
6	H	36	CYS	N-CA	9.78	1.58	1.46
2	B	692	TYR	CG-CD1	-9.77	1.18	1.39
8	J	3	VAL	C-N	-9.77	1.20	1.33
1	A	1223	ASP	CG-OD1	9.77	1.44	1.25
1	A	635	ARG	C-O	-9.77	1.12	1.24
2	B	499	ASN	CA-C	-9.77	1.40	1.52
2	B	1097	HIS	ND1-CE1	9.77	1.42	1.32
1	A	230	ARG	CZ-NH1	9.77	1.46	1.32
7	I	13	MET	N-CA	-9.76	1.32	1.45
1	A	1141	THR	CA-CB	-9.76	1.37	1.53
2	B	1212	ILE	CA-CB	-9.76	1.42	1.54
1	A	1153	TYR	CG-CD1	-9.76	1.18	1.39
2	B	376	PHE	CA-C	-9.76	1.40	1.52
2	B	630	ALA	C-O	-9.76	1.11	1.23
6	H	30	SER	N-CA	9.76	1.58	1.46
2	B	857	ARG	CA-C	-9.75	1.40	1.52
1	A	445	ASN	CA-C	9.74	1.64	1.52
1	A	1423	GLY	C-N	-9.74	1.21	1.33
9	K	110	ASN	CG-OD1	9.74	1.42	1.23
7	I	27	PHE	CE1-CZ	-9.74	1.09	1.38
3	C	216	GLY	C-O	9.74	1.37	1.23
9	K	62	LYS	C-O	9.74	1.36	1.23
2	B	329	THR	CA-CB	-9.73	1.38	1.53
3	C	127	ARG	CZ-NH1	9.73	1.46	1.32
9	K	73	LEU	C-O	9.73	1.36	1.24
1	A	560	ILE	C-N	-9.73	1.21	1.33
3	C	79	GLN	CA-CB	9.73	1.68	1.53
1	A	1109	LYS	CB-CG	9.73	1.81	1.52
1	A	543	LEU	CA-C	-9.73	1.40	1.52
1	A	652	VAL	CA-C	-9.73	1.40	1.52
2	B	191	LYS	CD-CE	9.73	1.81	1.52
1	A	165	GLY	C-O	9.72	1.37	1.23
7	I	118	ARG	CD-NE	9.72	1.59	1.46
3	C	79	GLN	C-N	-9.72	1.20	1.33
2	B	96	TYR	CE1-CZ	9.72	1.61	1.38
2	B	785	TYR	CG-CD1	-9.72	1.19	1.39
7	I	67	THR	CA-C	-9.72	1.39	1.52
1	A	1025	ARG	CG-CD	-9.71	1.23	1.52
1	A	556	TRP	CD2-CE3	-9.71	1.24	1.40
1	A	1308	THR	C-O	-9.71	1.10	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	74	ARG	NE-CZ	-9.71	1.22	1.33
2	B	96	TYR	CG-CD2	9.71	1.59	1.39
2	B	595	ARG	C-O	-9.71	1.12	1.24
2	B	547	VAL	CA-CB	-9.71	1.41	1.54
2	B	1129	ARG	CZ-NH1	9.71	1.46	1.32
4	E	166	LYS	C-O	9.70	1.35	1.24
2	B	620	ARG	CG-CD	9.70	1.81	1.52
2	B	1181	GLU	C-O	9.70	1.35	1.24
1	A	1001	ARG	CZ-NH2	9.70	1.46	1.33
1	A	191	THR	N-CA	9.70	1.58	1.46
1	A	1195	LEU	C-N	-9.70	1.20	1.33
1	A	1223	ASP	CA-CB	9.69	1.68	1.53
4	E	7	ARG	CB-CG	9.69	1.81	1.52
6	H	136	LYS	N-CA	9.69	1.58	1.46
10	L	55	ILE	C-O	9.69	1.34	1.24
4	E	78	LEU	N-CA	-9.69	1.33	1.45
1	A	748	MET	C-N	-9.69	1.19	1.33
1	A	826	ASP	CA-C	-9.69	1.40	1.52
1	A	1374	VAL	CA-CB	-9.69	1.42	1.54
9	K	49	GLU	C-O	-9.69	1.12	1.24
1	A	206	GLU	CD-OE1	9.68	1.43	1.25
1	A	1048	ASN	CG-ND2	9.68	1.53	1.33
6	H	19	ARG	NE-CZ	9.68	1.43	1.33
9	K	69	ALA	C-O	-9.68	1.10	1.23
9	K	91	CYS	CA-CB	-9.68	1.38	1.53
1	A	826	ASP	C-O	-9.68	1.12	1.24
2	B	60	GLN	CB-CG	-9.68	1.23	1.52
9	K	30	ALA	C-O	-9.68	1.12	1.23
1	A	364	VAL	C-N	-9.68	1.23	1.33
1	A	1136	SER	N-CA	-9.68	1.33	1.46
2	B	656	GLY	C-O	9.68	1.35	1.23
1	A	1134	ILE	C-O	9.67	1.34	1.24
2	B	279	ASP	CB-CG	9.67	1.76	1.52
10	L	47	ARG	CD-NE	9.67	1.59	1.46
2	B	705	MET	CA-C	-9.67	1.39	1.52
1	A	864	ILE	N-CA	-9.67	1.34	1.45
2	B	707	PRO	N-CD	-9.67	1.34	1.47
2	B	773	MET	CG-SD	-9.66	1.56	1.80
2	B	839	MET	C-O	-9.66	1.12	1.23
1	A	1144	LYS	CG-CD	9.66	1.81	1.52
2	B	1146	PHE	CE2-CZ	-9.66	1.09	1.38
4	E	9	ILE	CA-CB	9.66	1.67	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	396	PRO	CB-CG	-9.65	1.01	1.49
5	F	137	TYR	CA-CB	-9.65	1.38	1.53
1	A	830	LYS	CA-C	-9.65	1.40	1.52
2	B	595	ARG	CG-CD	9.65	1.81	1.52
2	B	935	ARG	CG-CD	9.65	1.81	1.52
1	A	708	MET	CA-CB	-9.65	1.37	1.53
1	A	1282	VAL	CA-CB	-9.65	1.41	1.54
1	A	1070	GLN	N-CA	-9.65	1.34	1.46
1	A	1424	VAL	CA-CB	-9.65	1.41	1.54
2	B	333	PHE	CG-CD2	-9.64	1.18	1.38
1	A	176	LYS	C-O	9.64	1.35	1.23
2	B	905	VAL	CA-C	-9.64	1.42	1.52
1	A	186	LYS	CB-CG	9.64	1.81	1.52
2	B	597	MET	SD-CE	-9.64	1.55	1.79
9	K	54	ARG	CD-NE	9.64	1.59	1.46
2	B	288	ALA	C-O	9.63	1.36	1.24
4	E	94	LYS	CG-CD	9.63	1.81	1.52
1	A	527	THR	C-O	-9.63	1.11	1.24
1	A	552	TRP	CD2-CE2	-9.63	1.25	1.41
2	B	219	ALA	CA-C	-9.63	1.40	1.53
5	F	136	ARG	CA-C	-9.62	1.40	1.52
2	B	119	LEU	CA-CB	-9.62	1.38	1.53
1	A	346	ASP	C-O	-9.62	1.04	1.23
1	A	1365	TYR	CA-C	-9.62	1.39	1.52
2	B	706	GLN	CD-NE2	9.62	1.53	1.33
2	B	802	PRO	CA-C	-9.62	1.42	1.52
4	E	171	LYS	C-O	-9.61	1.11	1.23
2	B	341	LEU	CA-C	-9.61	1.40	1.52
2	B	1082	MET	CA-C	-9.61	1.40	1.52
10	L	66	GLN	CD-OE1	9.61	1.41	1.23
2	B	764	SER	C-N	-9.61	1.21	1.33
2	B	1013	ASN	C-N	-9.61	1.22	1.33
2	B	1183	LYS	C-O	9.61	1.36	1.23
7	I	65	ASP	N-CA	9.61	1.59	1.46
1	A	121	LEU	CG-CD1	9.60	1.84	1.52
1	A	948	VAL	CA-CB	-9.60	1.38	1.54
1	A	1108	ALA	N-CA	-9.60	1.34	1.46
5	F	95	GLY	C-O	-9.60	1.10	1.23
7	I	21	GLU	CD-OE2	9.60	1.43	1.25
7	I	100	PHE	CG-CD2	-9.60	1.18	1.38
1	A	821	ARG	N-CA	-9.59	1.34	1.46
1	A	1354	ASN	C-O	-9.59	1.12	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1132	GLU	CD-OE1	9.59	1.43	1.25
2	B	708	GLU	CD-OE2	9.59	1.43	1.25
5	F	148	VAL	N-CA	-9.59	1.35	1.46
1	A	200	ARG	C-O	-9.58	1.11	1.24
1	A	511	ILE	C-O	-9.58	1.13	1.24
1	A	1066	VAL	CA-CB	-9.58	1.43	1.54
2	B	705	MET	CG-SD	9.58	2.04	1.80
3	C	23	SER	CA-CB	9.58	1.69	1.53
9	K	70	ARG	C-O	-9.58	1.12	1.23
2	B	771	SER	CA-C	-9.58	1.39	1.52
3	C	44	LEU	C-O	9.58	1.35	1.23
5	F	79	ARG	NE-CZ	-9.58	1.22	1.33
1	A	491	VAL	C-O	-9.57	1.12	1.24
1	A	589	GLN	CA-C	-9.57	1.41	1.52
2	B	95	ILE	CA-CB	-9.57	1.42	1.54
2	B	274	PRO	CA-CB	9.57	1.66	1.53
5	F	119	ARG	CA-C	-9.57	1.39	1.52
2	B	604	ARG	NE-CZ	-9.57	1.22	1.33
2	B	775	LYS	N-CA	-9.57	1.33	1.46
1	A	1326	ARG	CZ-NH1	-9.57	1.19	1.32
3	C	219	PHE	CE1-CZ	-9.57	1.09	1.38
5	F	103	MET	N-CA	-9.57	1.35	1.46
8	J	64	ASN	CG-OD1	9.57	1.41	1.23
1	A	22	PHE	C-O	9.56	1.35	1.24
2	B	819	ALA	CA-C	-9.56	1.43	1.53
1	A	875	ALA	CA-CB	-9.56	1.36	1.53
1	A	1416	ALA	CA-C	-9.56	1.42	1.53
1	A	717	ASN	CG-OD1	9.56	1.41	1.23
2	B	39	ARG	CB-CG	9.55	1.81	1.52
2	B	579	ARG	NE-CZ	-9.55	1.22	1.33
1	A	942	PHE	CD2-CE2	-9.55	1.09	1.38
7	I	7	CYS	CA-C	-9.55	1.40	1.52
8	J	47	ARG	NE-CZ	-9.55	1.22	1.33
2	B	876	LYS	C-O	-9.55	1.12	1.24
2	B	976	ILE	C-O	-9.55	1.12	1.24
1	A	1036	ARG	CZ-NH1	9.55	1.46	1.32
2	B	105	SER	CA-CB	9.55	1.69	1.53
1	A	652	VAL	N-CA	-9.54	1.34	1.46
2	B	635	ARG	CZ-NH2	-9.54	1.21	1.33
1	A	722	LEU	C-O	-9.54	1.11	1.24
2	B	487	THR	CA-CB	-9.54	1.35	1.54
4	E	185	ALA	N-CA	-9.54	1.34	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	868	TYR	CA-C	-9.54	1.40	1.52
2	B	945	GLU	C-O	9.54	1.35	1.23
1	A	1285	MET	CA-C	-9.53	1.40	1.52
4	E	8	ASN	CG-ND2	9.53	1.53	1.33
7	I	54	GLU	CD-OE2	9.53	1.43	1.25
9	K	32	VAL	CB-CG2	-9.53	1.21	1.52
1	A	33	ALA	C-O	-9.52	1.12	1.23
4	E	16	PHE	C-O	9.52	1.36	1.24
4	E	115	ASN	CB-CG	9.52	1.75	1.52
3	C	226	ASP	C-O	-9.52	1.11	1.24
6	H	140	ALA	CA-CB	-9.52	1.38	1.53
10	L	47	ARG	NE-CZ	9.52	1.43	1.33
1	A	127	ALA	C-O	9.52	1.35	1.24
2	B	401	PHE	CA-C	-9.52	1.39	1.52
1	A	705	LYS	CA-CB	9.52	1.76	1.53
2	B	784	ASN	C-O	-9.52	1.09	1.23
1	A	412	ARG	NE-CZ	-9.51	1.22	1.33
2	B	189	LEU	CA-C	9.51	1.65	1.52
1	A	407	ARG	C-O	9.51	1.38	1.24
1	A	1447	GLU	C-O	9.51	1.35	1.24
2	B	965	LYS	C-O	-9.51	1.13	1.24
1	A	1100	ARG	CZ-NH2	-9.51	1.21	1.33
7	I	104	LEU	CA-C	-9.51	1.40	1.52
4	E	170	LEU	C-O	9.50	1.35	1.23
8	J	56	LEU	N-CA	-9.50	1.34	1.46
1	A	346	ASP	CA-CB	9.50	1.72	1.53
9	K	97	LYS	CA-C	-9.50	1.39	1.52
1	A	813	PHE	CE2-CZ	-9.50	1.10	1.38
2	B	1196	ILE	CA-CB	-9.50	1.39	1.54
4	E	150	VAL	N-CA	-9.50	1.37	1.46
9	K	35	PHE	C-O	-9.50	1.12	1.24
1	A	1010	ALA	CA-C	-9.49	1.40	1.52
1	A	893	PHE	CG-CD1	-9.49	1.19	1.38
1	A	1329	THR	CA-C	-9.49	1.40	1.52
4	E	191	LYS	CE-NZ	9.49	1.77	1.49
9	K	88	LYS	CE-NZ	9.49	1.77	1.49
6	H	2	SER	CA-CB	9.49	1.72	1.53
1	A	615	GLY	C-O	-9.49	1.14	1.24
1	A	813	PHE	C-N	-9.49	1.21	1.34
1	A	1152	ILE	CA-CB	-9.49	1.43	1.54
1	A	1349	TYR	C-N	-9.49	1.20	1.34
1	A	1428	VAL	CA-C	-9.49	1.41	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	195	GLN	CA-C	-9.49	1.43	1.52
1	A	1222	ASN	CG-OD1	9.48	1.41	1.23
7	I	66	PRO	CA-CB	-9.48	1.38	1.53
1	A	546	VAL	CA-C	-9.48	1.41	1.52
2	B	486	TYR	CA-CB	-9.48	1.38	1.53
6	H	96	VAL	N-CA	-9.48	1.34	1.46
8	J	38	ARG	CA-C	-9.48	1.39	1.52
10	L	39	SER	CA-C	9.48	1.65	1.52
1	A	788	SER	C-O	-9.47	1.11	1.23
1	A	1110	ASN	CG-OD1	9.47	1.41	1.23
1	A	1204	ASP	CB-CG	9.47	1.75	1.52
2	B	235	SER	CA-CB	-9.47	1.40	1.54
4	E	162	ARG	CD-NE	9.47	1.59	1.46
1	A	1024	SER	N-CA	-9.47	1.34	1.46
1	A	1187	GLN	CB-CG	9.47	1.80	1.52
2	B	328	GLU	C-N	-9.47	1.21	1.33
5	F	123	LYS	CE-NZ	9.47	1.77	1.49
3	C	268	ASP	CA-C	9.47	1.72	1.52
1	A	69	THR	C-N	9.47	1.46	1.33
1	A	827	THR	N-CA	-9.47	1.35	1.46
2	B	623	GLU	C-O	-9.47	1.11	1.23
4	E	172	GLU	CA-CB	9.47	1.68	1.53
1	A	912	LEU	C-O	-9.46	1.12	1.24
2	B	822	ASN	C-O	-9.46	1.12	1.24
3	C	27	LEU	C-O	-9.46	1.12	1.24
9	K	54	ARG	CZ-NH1	9.46	1.46	1.32
1	A	486	GLU	CA-C	9.46	1.64	1.52
2	B	557	PHE	N-CA	-9.46	1.34	1.46
4	E	118	PRO	CB-CG	9.46	1.97	1.49
5	F	144	GLU	N-CA	-9.46	1.33	1.45
1	A	927	VAL	C-O	9.46	1.35	1.24
8	J	18	TRP	CA-CB	-9.46	1.38	1.53
1	A	457	ALA	CA-C	-9.46	1.41	1.52
7	I	41	PRO	C-N	-9.46	1.20	1.33
1	A	883	LEU	N-CA	-9.45	1.34	1.46
1	A	931	GLU	CG-CD	9.45	1.75	1.52
1	A	1239	ARG	CZ-NH2	-9.45	1.21	1.33
1	A	71	GLN	CG-CD	9.45	1.75	1.52
1	A	840	ARG	CG-CD	9.45	1.80	1.52
7	I	93	LYS	CE-NZ	9.45	1.77	1.49
10	L	29	TYR	CG-CD2	-9.45	1.19	1.39
1	A	838	GLN	N-CA	-9.45	1.35	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1419	ASP	CG-OD2	9.45	1.43	1.25
2	B	697	GLU	CD-OE2	9.45	1.43	1.25
3	C	88	CYS	C-O	-9.45	1.11	1.23
1	A	545	GLN	C-O	-9.44	1.13	1.24
2	B	645	SER	C-O	-9.45	1.12	1.24
2	B	1176	ASN	CB-CG	9.44	1.75	1.52
3	C	12	GLU	CA-CB	-9.44	1.37	1.53
2	B	281	PRO	N-CA	-9.44	1.36	1.47
2	B	337	ARG	CD-NE	-9.44	1.33	1.46
3	C	33	LEU	CA-C	9.44	1.65	1.52
2	B	1043	ASP	CG-OD2	9.44	1.43	1.25
1	A	734	GLU	CA-C	-9.44	1.40	1.52
2	B	554	ILE	CA-CB	-9.44	1.42	1.54
3	C	219	PHE	C-O	9.43	1.35	1.23
2	B	265	SER	CA-CB	9.43	1.67	1.53
1	A	1055	ARG	CG-CD	9.43	1.80	1.52
2	B	650	GLU	CD-OE1	9.43	1.43	1.25
2	B	743	ILE	N-CA	-9.43	1.35	1.46
1	A	1013	ASP	CA-C	9.43	1.65	1.52
1	A	1021	LEU	CA-C	-9.43	1.40	1.52
3	C	253	LYS	CD-CE	9.42	1.80	1.52
5	F	120	ILE	N-CA	-9.42	1.35	1.46
4	E	138	ALA	C-O	-9.42	1.12	1.24
5	F	108	PHE	CA-C	-9.42	1.40	1.52
9	K	100	ALA	N-CA	-9.42	1.35	1.46
2	B	131	ASP	CA-CB	9.42	1.65	1.52
7	I	105	SER	N-CA	9.42	1.58	1.46
1	A	1408	ILE	CA-CB	-9.41	1.42	1.54
2	B	318	VAL	C-O	9.41	1.35	1.24
2	B	651	LEU	CG-CD2	-9.41	1.21	1.52
9	K	102	LYS	CG-CD	9.41	1.80	1.52
1	A	92	HIS	CA-C	-9.41	1.41	1.52
1	A	493	GLN	CA-CB	-9.41	1.39	1.54
1	A	1274	ARG	CZ-NH2	9.41	1.45	1.33
2	B	1045	SER	CA-C	-9.41	1.40	1.53
1	A	1281	ARG	CZ-NH2	9.41	1.45	1.33
2	B	527	THR	CA-CB	-9.41	1.40	1.54
1	A	819	GLY	C-N	-9.40	1.20	1.33
1	A	1067	LEU	CG-CD1	-9.40	1.21	1.52
2	B	750	GLY	C-O	-9.40	1.15	1.23
3	C	123	ASN	CA-CB	9.40	1.64	1.53
10	L	54	ARG	CG-CD	9.40	1.80	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	747	VAL	CA-CB	-9.39	1.41	1.54
3	C	34	ARG	NE-CZ	-9.39	1.22	1.33
6	H	3	ASN	CG-OD1	9.39	1.41	1.23
2	B	39	ARG	NE-CZ	9.39	1.43	1.33
1	A	206	GLU	CA-C	-9.39	1.40	1.52
1	A	381	THR	C-O	-9.39	1.12	1.24
2	B	532	ALA	CA-C	-9.39	1.38	1.52
4	E	208	TYR	CB-CG	9.39	1.72	1.51
1	A	87	ALA	C-N	-9.39	1.21	1.32
2	B	186	GLU	CD-OE2	9.39	1.43	1.25
5	F	97	ARG	N-CA	-9.39	1.34	1.46
6	H	87	ARG	CD-NE	9.39	1.59	1.46
3	C	201	TRP	CD2-CE3	-9.38	1.25	1.40
2	B	594	ALA	C-O	-9.38	1.11	1.24
7	I	31	THR	CA-C	9.38	1.64	1.52
2	B	1080	LYS	CA-C	9.38	1.65	1.52
1	A	326	ARG	CG-CD	9.38	1.80	1.52
1	A	820	GLY	C-N	-9.37	1.21	1.33
3	C	170	TRP	CD2-CE3	-9.37	1.25	1.40
1	A	423	ASP	C-O	9.37	1.36	1.23
2	B	1177	HIS	N-CA	9.36	1.59	1.46
2	B	31	TRP	CD2-CE2	-9.36	1.25	1.41
2	B	734	HIS	CA-C	9.36	1.67	1.52
1	A	781	ASP	C-O	9.36	1.39	1.24
1	A	941	LYS	C-O	9.36	1.34	1.24
1	A	1050	GLU	C-O	9.35	1.35	1.24
2	B	870	ILE	CB-CG1	9.35	1.72	1.53
4	E	31	THR	CB-CG2	9.35	1.83	1.52
5	F	94	LEU	CA-C	-9.35	1.39	1.52
2	B	665	GLU	CD-OE1	9.35	1.43	1.25
4	E	103	LYS	CD-CE	9.35	1.80	1.52
1	A	1070	GLN	C-O	-9.35	1.13	1.24
6	H	135	LEU	CA-C	9.35	1.65	1.52
2	B	205	ILE	CA-CB	-9.34	1.41	1.54
4	E	35	VAL	N-CA	-9.34	1.35	1.46
1	A	1034	GLU	CD-OE2	9.34	1.43	1.25
9	K	110	ASN	CB-CG	9.34	1.75	1.52
1	A	483	ASP	N-CA	9.34	1.56	1.46
1	A	551	TYR	CG-CD2	-9.34	1.19	1.39
2	B	178	ASN	CG-OD1	9.34	1.41	1.23
2	B	394	ASP	CG-OD2	9.34	1.43	1.25
1	A	366	VAL	C-N	-9.34	1.21	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1148	ILE	C-O	-9.34	1.13	1.24
2	B	809	MET	N-CA	-9.34	1.34	1.46
4	E	172	GLU	CA-C	-9.33	1.41	1.52
2	B	584	GLY	C-O	9.33	1.37	1.24
2	B	605	ARG	NE-CZ	-9.33	1.22	1.33
2	B	899	ILE	C-O	-9.33	1.12	1.24
3	C	180	TYR	C-O	-9.33	1.11	1.23
2	B	963	PHE	CB-CG	-9.32	1.29	1.50
2	B	833	TYR	CG-CD2	-9.32	1.19	1.39
3	C	56	THR	C-O	-9.32	1.12	1.24
1	A	165	GLY	CA-C	9.32	1.65	1.51
1	A	1159	ARG	CZ-NH1	9.32	1.45	1.32
2	B	615	MET	N-CA	-9.32	1.35	1.46
1	A	733	ALA	C-O	-9.31	1.13	1.24
4	E	156	LEU	C-O	9.31	1.35	1.23
1	A	176	LYS	CG-CD	9.31	1.80	1.52
1	A	664	THR	C-O	-9.30	1.12	1.23
4	E	210	SER	CA-CB	-9.30	1.40	1.53
5	F	86	THR	C-O	-9.30	1.12	1.23
1	A	908	LEU	CA-C	-9.30	1.41	1.52
1	A	1206	ASP	C-O	9.29	1.34	1.23
4	E	136	ASN	CA-C	-9.29	1.40	1.52
2	B	668	ASP	CB-CG	9.29	1.75	1.52
4	E	191	LYS	C-O	-9.29	1.12	1.24
2	B	489	SER	C-O	-9.29	1.11	1.24
2	B	515	HIS	CA-C	-9.29	1.41	1.52
2	B	950	ASP	C-N	-9.29	1.22	1.33
1	A	980	ASP	C-O	9.29	1.36	1.24
1	A	795	GLU	C-N	-9.28	1.21	1.34
1	A	1072	ILE	C-O	-9.28	1.12	1.23
10	L	62	LYS	CE-NZ	9.28	1.77	1.49
2	B	19	GLU	CA-C	9.28	1.65	1.52
2	B	581	PHE	CG-CD1	-9.28	1.19	1.38
1	A	4	GLN	CB-CG	9.27	1.80	1.52
1	A	842	VAL	CA-CB	-9.27	1.43	1.54
2	B	316	PRO	CA-CB	-9.27	1.40	1.53
1	A	506	ALA	CA-C	-9.27	1.40	1.52
6	H	2	SER	N-CA	9.27	1.63	1.46
7	I	88	SER	CA-C	-9.27	1.40	1.52
1	A	186	LYS	CG-CD	9.26	1.80	1.52
1	A	299	HIS	CA-CB	9.26	1.68	1.53
1	A	556	TRP	CE2-CZ2	-9.26	1.20	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	200	GLU	CD-OE2	9.26	1.43	1.25
1	A	1155	ASP	CB-CG	-9.26	1.28	1.52
3	C	230	MET	C-O	-9.26	1.11	1.23
4	E	41	ASP	C-O	9.26	1.35	1.24
1	A	711	ARG	C-O	-9.26	1.12	1.24
1	A	1141	THR	C-O	9.26	1.34	1.23
2	B	1168	LEU	N-CA	9.26	1.57	1.45
1	A	100	LYS	N-CA	9.25	1.57	1.46
2	B	1143	ALA	C-O	-9.25	1.13	1.23
1	A	1264	GLU	C-N	-9.25	1.22	1.33
1	A	687	LYS	CE-NZ	9.25	1.77	1.49
2	B	781	PHE	N-CA	-9.25	1.33	1.46
2	B	31	TRP	CZ3-CH2	-9.25	1.17	1.40
2	B	1175	LEU	N-CA	9.25	1.57	1.46
7	I	43	VAL	CA-CB	-9.25	1.43	1.54
2	B	773	MET	N-CA	-9.24	1.35	1.46
3	C	138	GLU	CA-C	-9.24	1.39	1.52
2	B	889	THR	C-O	-9.24	1.12	1.23
3	C	50	GLU	CA-C	-9.24	1.41	1.52
1	A	1288	ASP	CG-OD1	9.24	1.42	1.25
2	B	362	PRO	N-CD	-9.24	1.34	1.47
2	B	1135	ARG	N-CA	-9.24	1.34	1.46
1	A	34	LYS	CG-CD	9.23	1.80	1.52
5	F	83	PRO	N-CA	-9.23	1.35	1.47
7	I	19	ASP	CG-OD2	9.23	1.42	1.25
8	J	27	GLU	CD-OE1	9.23	1.42	1.25
10	L	68	GLU	N-CA	-9.23	1.33	1.46
1	A	105	CYS	N-CA	9.23	1.57	1.45
1	A	1071	SER	N-CA	-9.23	1.34	1.46
1	A	1203	ASN	CG-ND2	9.23	1.52	1.33
3	C	142	VAL	CA-CB	-9.23	1.42	1.54
4	E	211	TYR	CE1-CZ	-9.23	1.16	1.38
4	E	211	TYR	CG-CD2	-9.23	1.20	1.39
5	F	121	ALA	C-N	-9.23	1.20	1.33
2	B	601	ARG	CZ-NH2	9.23	1.45	1.33
3	C	192	TRP	CA-C	9.23	1.65	1.52
1	A	1162	VAL	N-CA	-9.22	1.34	1.46
2	B	282	ILE	CA-CB	-9.22	1.41	1.54
6	H	137	GLN	CG-CD	9.22	1.75	1.52
10	L	31	CYS	C-O	9.22	1.35	1.24
1	A	589	GLN	CD-OE1	9.22	1.41	1.23
1	A	731	ARG	CA-CB	-9.22	1.39	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	133	ILE	C-O	9.22	1.35	1.24
1	A	559	VAL	CA-CB	-9.21	1.43	1.54
1	A	1029	ARG	NE-CZ	-9.22	1.23	1.33
1	A	1030	ARG	C-N	-9.22	1.24	1.34
1	A	247	ARG	C-O	9.21	1.36	1.24
1	A	880	LYS	N-CA	-9.21	1.34	1.46
1	A	1445	ILE	CA-CB	-9.21	1.42	1.54
1	A	1138	ILE	CA-CB	-9.21	1.43	1.54
1	A	684	ALA	CA-CB	9.20	1.69	1.53
1	A	636	GLU	C-O	9.20	1.36	1.24
1	A	850	VAL	C-O	-9.20	1.12	1.24
4	E	208	TYR	CG-CD1	-9.20	1.20	1.39
1	A	793	SER	CA-C	-9.20	1.41	1.52
1	A	898	ARG	NE-CZ	9.19	1.43	1.33
1	A	1315	GLU	CD-OE2	9.19	1.42	1.25
9	K	54	ARG	CZ-NH2	9.19	1.45	1.33
1	A	1268	LEU	CG-CD2	-9.19	1.22	1.52
6	H	130	ARG	CA-C	9.19	1.66	1.53
1	A	1120	LEU	CG-CD1	9.19	1.82	1.52
2	B	976	ILE	C-N	-9.19	1.20	1.33
2	B	1044	ALA	N-CA	9.19	1.56	1.46
3	C	18	VAL	CA-C	-9.18	1.41	1.52
3	C	154	LYS	C-O	-9.18	1.12	1.23
2	B	711	GLU	CA-CB	-9.18	1.39	1.53
1	A	364	VAL	CA-C	-9.17	1.41	1.52
3	C	100	THR	CA-CB	-9.17	1.34	1.54
3	C	194	GLU	C-O	9.17	1.36	1.23
4	E	85	GLU	CA-CB	9.17	1.69	1.53
9	K	36	GLU	CA-CB	-9.17	1.39	1.53
1	A	1004	ASN	CA-C	9.16	1.66	1.53
1	A	70	CYS	CA-CB	9.16	1.67	1.53
1	A	965	GLN	C-O	-9.16	1.12	1.24
2	B	742	GLU	N-CA	-9.16	1.34	1.46
6	H	131	ASN	C-O	9.16	1.35	1.24
2	B	702	LEU	CG-CD2	-9.16	1.22	1.52
3	C	18	VAL	CB-CG2	-9.16	1.22	1.52
2	B	572	HIS	C-O	-9.15	1.12	1.24
5	F	150	GLU	CA-C	-9.15	1.39	1.52
6	H	17	PRO	C-O	-9.15	1.12	1.24
2	B	723	VAL	CB-CG2	9.15	1.82	1.52
1	A	904	THR	C-O	-9.15	1.11	1.24
1	A	302	THR	CB-CG2	9.15	1.82	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	762	SER	C-O	-9.15	1.11	1.24
2	B	763	GLN	C-N	-9.15	1.20	1.33
1	A	1144	LYS	CD-CE	9.14	1.79	1.52
2	B	958	GLN	CG-CD	9.14	1.75	1.52
1	A	839	ARG	CZ-NH2	9.14	1.45	1.33
1	A	969	GLN	CD-OE1	9.14	1.41	1.23
1	A	1344	GLY	C-O	-9.14	1.11	1.23
2	B	403	LYS	C-O	-9.14	1.11	1.23
9	K	35	PHE	CG-CD1	-9.14	1.19	1.38
1	A	123	ARG	CA-C	-9.14	1.40	1.52
1	A	353	ILE	CB-CG1	-9.14	1.35	1.53
2	B	809	MET	C-N	-9.14	1.22	1.33
2	B	1186	ASP	N-CA	9.14	1.60	1.46
3	C	78	GLU	C-O	-9.13	1.10	1.24
3	C	263	THR	C-O	-9.14	1.12	1.24
1	A	110	CYS	CA-CB	9.13	1.67	1.53
1	A	241	VAL	C-O	-9.13	1.12	1.24
2	B	92	PHE	CA-CB	9.13	1.67	1.53
2	B	1065	GLN	N-CA	9.13	1.57	1.45
1	A	524	VAL	C-O	-9.13	1.12	1.23
3	C	123	ASN	C-O	-9.13	1.12	1.24
2	B	767	ASN	N-CA	-9.12	1.35	1.46
2	B	1106	ARG	CZ-NH2	9.12	1.45	1.33
1	A	350	ARG	CZ-NH2	-9.12	1.21	1.33
1	A	977	LYS	CE-NZ	9.12	1.76	1.49
1	A	1322	ILE	CG1-CD1	-9.12	1.16	1.51
9	K	26	LYS	CE-NZ	9.12	1.76	1.49
9	K	94	ILE	CA-CB	9.12	1.65	1.54
1	A	634	THR	CA-C	-9.12	1.41	1.52
6	H	52	GLN	CA-C	9.12	1.65	1.52
8	J	51	LEU	C-O	9.12	1.35	1.24
2	B	864	LYS	CA-C	9.12	1.65	1.52
7	I	119	THR	CA-C	9.11	1.64	1.52
2	B	20	ASP	N-CA	9.11	1.57	1.46
2	B	312	GLU	CD-OE1	9.11	1.42	1.25
2	B	592	ASN	CA-C	9.11	1.64	1.52
2	B	483	LEU	CG-CD1	-9.11	1.22	1.52
4	E	77	SER	N-CA	-9.11	1.33	1.46
1	A	498	ARG	N-CA	-9.10	1.35	1.46
1	A	1230	GLU	CA-C	-9.10	1.40	1.53
7	I	119	THR	CA-CB	9.10	1.67	1.53
2	B	586	TRP	C-N	-9.10	1.20	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	153	HIS	CG-ND1	-9.10	1.28	1.38
7	I	82	GLU	CG-CD	9.10	1.74	1.52
2	B	249	ARG	NE-CZ	9.10	1.43	1.33
1	A	1225	PHE	CA-CB	9.10	1.67	1.53
6	H	43	ASN	C-O	-9.10	1.12	1.23
1	A	949	ASP	CA-C	-9.10	1.40	1.52
1	A	37	PHE	CG-CD2	9.09	1.57	1.38
1	A	381	THR	N-CA	-9.09	1.33	1.46
2	B	622	LYS	CE-NZ	9.09	1.76	1.49
2	B	362	PRO	N-CA	-9.09	1.35	1.47
1	A	106	VAL	CA-C	9.09	1.64	1.52
1	A	1423	GLY	C-O	-9.09	1.10	1.23
2	B	249	ARG	CG-CD	9.09	1.79	1.52
2	B	328	GLU	CA-CB	9.09	1.68	1.53
1	A	994	GLN	N-CA	-9.09	1.35	1.46
1	A	1117	THR	CA-CB	-9.09	1.40	1.53
2	B	1176	ASN	CG-OD1	9.09	1.40	1.23
1	A	66	LYS	CA-CB	9.08	1.68	1.53
2	B	1149	GLU	C-N	-9.08	1.21	1.33
1	A	167	CYS	CA-C	9.08	1.65	1.52
1	A	1094	VAL	CA-C	9.08	1.63	1.52
6	H	85	GLY	N-CA	9.08	1.58	1.45
1	A	180	LYS	CA-C	-9.08	1.41	1.52
1	A	589	GLN	CD-NE2	9.07	1.52	1.33
1	A	925	LEU	CA-C	-9.07	1.41	1.52
2	B	908	GLU	CA-CB	9.07	1.65	1.53
8	J	1	MET	SD-CE	9.07	2.02	1.79
5	F	133	VAL	CA-CB	-9.07	1.41	1.55
9	K	61	TYR	CG-CD2	-9.07	1.20	1.39
4	E	153	HIS	CA-CB	-9.07	1.39	1.53
10	L	40	LEU	CA-CB	9.07	1.66	1.53
2	B	554	ILE	C-O	-9.06	1.13	1.24
4	E	79	TRP	C-N	-9.06	1.22	1.33
4	E	206	GLY	CA-C	-9.06	1.39	1.51
1	A	688	LYS	CD-CE	9.05	1.79	1.52
1	A	725	ALA	CA-C	-9.05	1.41	1.52
1	A	1296	GLY	N-CA	9.05	1.55	1.45
2	B	333	PHE	CA-C	-9.05	1.40	1.52
3	C	260	LEU	CA-C	-9.05	1.40	1.52
7	I	66	PRO	CA-C	-9.05	1.36	1.52
1	A	66	LYS	N-CA	9.05	1.57	1.46
1	A	649	ILE	N-CA	-9.05	1.35	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	995	ARG	CA-C	9.05	1.65	1.53
2	B	1173	ALA	C-O	9.05	1.34	1.23
1	A	155	GLU	CD-OE2	9.05	1.42	1.25
1	A	446	ARG	CZ-NH1	9.04	1.45	1.32
2	B	186	GLU	N-CA	9.04	1.57	1.46
2	B	1223	ASP	CA-C	9.04	1.65	1.52
2	B	195	CYS	CA-C	-9.04	1.42	1.53
8	J	53	HIS	CG-ND1	-9.04	1.28	1.38
2	B	219	ALA	C-N	-9.04	1.24	1.33
7	I	41	PRO	C-O	-9.04	1.12	1.24
1	A	466	SER	CB-OG	-9.04	1.24	1.42
1	A	806	ARG	CA-C	-9.04	1.40	1.52
1	A	1041	ALA	N-CA	-9.04	1.35	1.46
1	A	1440	ALA	CA-C	9.04	1.66	1.52
6	H	141	TYR	CA-CB	-9.04	1.38	1.53
9	K	58	PHE	CB-CG	9.04	1.71	1.50
3	C	19	ASP	CB-CG	-9.03	1.29	1.52
1	A	1318	THR	CB-CG2	9.03	1.82	1.52
1	A	185	TRP	CG-CD2	-9.02	1.27	1.43
1	A	900	ASP	C-O	9.02	1.34	1.23
1	A	1274	ARG	N-CA	9.02	1.57	1.45
2	B	916	THR	CA-C	9.02	1.71	1.52
2	B	1018	PRO	N-CA	-9.02	1.35	1.47
1	A	432	VAL	CA-CB	-9.02	1.43	1.54
1	A	738	LYS	N-CA	-9.02	1.34	1.45
2	B	393	LYS	CG-CD	9.02	1.79	1.52
3	C	249	ASP	CG-OD2	9.02	1.42	1.25
2	B	606	LYS	C-O	9.02	1.35	1.24
2	B	1032	SER	CB-OG	9.02	1.60	1.42
3	C	168	ALA	C-O	-9.02	1.12	1.24
2	B	1050	ILE	C-N	-9.02	1.21	1.33
2	B	1198	TYR	CA-C	-9.01	1.41	1.52
9	K	17	SER	N-CA	9.01	1.56	1.45
8	J	43	ARG	CG-CD	9.01	1.79	1.52
1	A	105	CYS	C-O	-9.01	1.12	1.23
1	A	805	LEU	CB-CG	-9.01	1.35	1.53
2	B	968	VAL	CB-CG2	-9.01	1.22	1.52
3	C	22	LEU	CA-CB	-9.01	1.39	1.53
2	B	89	GLU	CA-C	9.00	1.71	1.52
10	L	43	THR	CB-CG2	9.00	1.82	1.52
2	B	128	LEU	N-CA	-9.00	1.35	1.46
4	E	155	ARG	C-O	9.00	1.34	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	233	PRO	CB-CG	9.00	1.94	1.49
2	B	491	THR	N-CA	-9.00	1.35	1.46
1	A	1112	LYS	CG-CD	9.00	1.79	1.52
1	A	666	ILE	CA-CB	-8.99	1.41	1.54
4	E	198	ILE	C-N	-8.99	1.22	1.33
2	B	384	ARG	CD-NE	8.99	1.58	1.46
10	L	30	ILE	CA-CB	-8.99	1.39	1.55
1	A	544	ASP	CB-CG	8.98	1.74	1.52
3	C	177	GLU	C-O	-8.98	1.12	1.23
4	E	11	ARG	NE-CZ	-8.98	1.23	1.33
1	A	199	LEU	CG-CD1	8.98	1.82	1.52
9	K	26	LYS	CG-CD	8.98	1.79	1.52
2	B	944	THR	CB-CG2	8.97	1.82	1.52
6	H	110	ASP	N-CA	8.97	1.56	1.46
2	B	853	SER	CB-OG	8.97	1.60	1.42
7	I	60	GLN	CA-C	-8.97	1.40	1.52
1	A	87	ALA	CA-CB	-8.97	1.39	1.53
1	A	274	ILE	CB-CG2	8.97	1.82	1.52
4	E	103	LYS	C-O	8.97	1.35	1.24
2	B	211	VAL	CA-C	-8.96	1.42	1.52
2	B	336	ARG	CZ-NH1	8.96	1.45	1.32
9	K	88	LYS	CD-CE	8.96	1.79	1.52
1	A	944	ARG	CZ-NH2	-8.96	1.21	1.33
1	A	1188	GLN	CA-C	8.96	1.63	1.52
2	B	829	CYS	CA-C	-8.96	1.41	1.52
7	I	98	VAL	CA-CB	-8.95	1.44	1.54
2	B	135	ARG	NE-CZ	8.95	1.42	1.33
2	B	25	ILE	CB-CG2	8.95	1.82	1.52
7	I	82	GLU	CD-OE1	8.94	1.42	1.25
1	A	271	LYS	CG-CD	8.94	1.79	1.52
1	A	913	LEU	CA-CB	8.94	1.69	1.53
1	A	1013	ASP	CG-OD2	8.94	1.42	1.25
2	B	1012	ILE	CG1-CD1	-8.94	1.16	1.51
6	H	87	ARG	CG-CD	8.93	1.79	1.52
1	A	461	LYS	CA-CB	-8.93	1.39	1.53
2	B	1030	LEU	C-O	-8.93	1.13	1.24
1	A	433	GLU	CD-OE1	8.93	1.42	1.25
2	B	961	LEU	C-O	8.93	1.35	1.24
9	K	35	PHE	CG-CD2	-8.93	1.20	1.38
2	B	169	ARG	CZ-NH1	8.93	1.45	1.32
2	B	1041	GLU	CD-OE2	8.93	1.42	1.25
2	B	1224	PHE	N-CA	8.92	1.63	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	806	ARG	CZ-NH2	8.92	1.45	1.33
2	B	642	ASP	C-O	8.92	1.35	1.23
1	A	998	LEU	C-O	-8.92	1.13	1.23
2	B	308	TRP	CA-C	-8.92	1.40	1.52
4	E	43	LYS	C-O	8.92	1.35	1.24
4	E	90	VAL	CB-CG1	8.92	1.81	1.52
2	B	1137	CYS	CA-C	8.92	1.64	1.52
1	A	1379	GLY	N-CA	-8.91	1.30	1.44
2	B	568	ASP	CB-CG	8.91	1.74	1.52
6	H	32	THR	CA-C	8.91	1.64	1.52
1	A	644	LYS	CE-NZ	8.91	1.76	1.49
2	B	291	ILE	CG1-CD1	-8.91	1.17	1.51
7	I	58	VAL	CA-C	-8.91	1.41	1.52
8	J	21	TYR	CG-CD2	-8.90	1.20	1.39
2	B	415	GLN	CA-CB	8.90	1.67	1.53
1	A	1221	LYS	CB-CG	8.90	1.79	1.52
2	B	328	GLU	CB-CG	8.90	1.79	1.52
2	B	1100	ASP	C-O	8.90	1.34	1.24
2	B	996	ARG	C-O	8.89	1.34	1.24
5	F	107	VAL	CA-C	8.89	1.64	1.52
2	B	583	ASN	CG-OD1	-8.89	1.06	1.23
1	A	728	LYS	CA-C	-8.89	1.41	1.52
1	A	782	ARG	C-O	-8.89	1.12	1.23
1	A	931	GLU	CA-C	-8.89	1.40	1.52
5	F	151	LEU	CA-C	-8.88	1.41	1.52
2	B	410	GLY	C-N	-8.88	1.22	1.33
1	A	904	THR	CB-OG1	8.88	1.57	1.43
1	A	1008	GLN	CD-OE1	8.88	1.40	1.23
4	E	143	ASN	C-O	-8.88	1.13	1.24
6	H	21	ASN	C-O	-8.88	1.12	1.24
2	B	345	LYS	CD-CE	8.87	1.79	1.52
2	B	528	PRO	CA-CB	-8.88	1.40	1.53
4	E	196	VAL	N-CA	8.88	1.57	1.46
9	K	14	GLU	CA-C	8.88	1.63	1.52
2	B	728	ARG	NE-CZ	-8.87	1.23	1.33
1	A	648	ASN	CB-CG	-8.87	1.29	1.52
3	C	29	MET	CG-SD	-8.87	1.58	1.80
1	A	649	ILE	CA-C	8.87	1.64	1.52
3	C	199	LYS	CA-C	-8.87	1.40	1.52
1	A	174	ILE	CG1-CD1	-8.87	1.17	1.51
9	K	65	HIS	CA-C	-8.87	1.42	1.52
2	B	447	ALA	C-O	8.86	1.35	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	188	HIS	CA-C	8.86	1.64	1.52
7	I	28	GLU	CD-OE1	8.86	1.42	1.25
9	K	79	GLU	CD-OE1	8.86	1.42	1.25
1	A	818	MET	C-N	-8.86	1.20	1.33
5	F	129	LYS	CE-NZ	8.86	1.75	1.49
9	K	48	ALA	CA-CB	-8.86	1.38	1.53
1	A	1230	GLU	CD-OE1	8.85	1.42	1.25
6	H	121	LEU	C-O	8.85	1.34	1.24
1	A	1021	LEU	N-CA	-8.85	1.35	1.46
2	B	68	THR	CA-CB	8.85	1.69	1.53
10	L	27	LEU	N-CA	8.85	1.57	1.46
2	B	165	VAL	N-CA	8.85	1.57	1.46
2	B	825	VAL	N-CA	-8.85	1.35	1.46
2	B	1047	PHE	N-CA	-8.85	1.33	1.46
4	E	188	LEU	CA-C	8.85	1.68	1.52
2	B	1183	LYS	CG-CD	8.85	1.78	1.52
8	J	30	LEU	CA-CB	-8.85	1.39	1.53
9	K	93	SER	CA-CB	8.85	1.69	1.53
1	A	293	GLU	CD-OE2	8.85	1.42	1.25
2	B	634	TYR	C-N	-8.85	1.23	1.33
3	C	16	ASP	CG-OD2	8.85	1.42	1.25
1	A	16	GLU	CD-OE2	8.84	1.42	1.25
5	F	74	ILE	C-N	-8.84	1.22	1.33
1	A	404	TYR	CA-C	-8.84	1.41	1.52
3	C	3	GLU	CD-OE1	8.84	1.42	1.25
5	F	108	PHE	N-CA	-8.83	1.33	1.45
1	A	837	ILE	CA-CB	-8.83	1.43	1.54
2	B	954	VAL	CA-CB	8.83	1.66	1.54
3	C	202	PRO	C-O	-8.83	1.14	1.23
2	B	729	ILE	C-O	-8.83	1.14	1.24
4	E	213	ILE	CA-C	-8.83	1.41	1.52
2	B	1171	VAL	CA-CB	-8.82	1.40	1.53
1	A	89	PRO	CA-C	-8.82	1.40	1.52
4	E	60	PHE	C-O	-8.82	1.14	1.23
1	A	87	ALA	N-CA	-8.82	1.35	1.46
2	B	961	LEU	CA-C	8.82	1.64	1.52
3	C	206	ASN	C-O	-8.82	1.12	1.24
1	A	653	VAL	C-N	-8.81	1.22	1.33
3	C	87	PHE	C-O	-8.81	1.12	1.24
1	A	774	ARG	NE-CZ	8.81	1.42	1.33
2	B	232	SER	CA-C	-8.81	1.42	1.53
1	A	983	ILE	C-O	-8.81	1.13	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1280	GLU	CG-CD	8.81	1.74	1.52
9	K	107	THR	CA-C	-8.81	1.41	1.52
2	B	869	SER	C-N	8.81	1.41	1.33
1	A	537	ARG	N-CA	8.80	1.57	1.46
1	A	851	HIS	CB-CG	-8.80	1.37	1.50
2	B	511	PRO	CA-CB	-8.80	1.41	1.53
5	F	148	VAL	CA-C	-8.80	1.42	1.52
10	L	63	ARG	CD-NE	8.80	1.58	1.46
2	B	736	THR	CB-OG1	-8.80	1.29	1.43
3	C	260	LEU	CG-CD2	8.80	1.81	1.52
8	J	55	ASP	N-CA	8.80	1.58	1.46
1	A	792	TYR	CG-CD2	-8.80	1.20	1.39
2	B	296	GLU	CA-C	-8.80	1.40	1.52
1	A	99	ILE	N-CA	-8.79	1.36	1.46
1	A	618	GLU	C-O	8.80	1.32	1.24
1	A	471	ASN	CA-C	-8.79	1.41	1.52
2	B	136	THR	N-CA	8.79	1.56	1.46
1	A	264	PHE	CG-CD1	8.79	1.57	1.38
2	B	858	SER	N-CA	8.79	1.56	1.46
4	E	159	ASP	CG-OD1	8.79	1.42	1.25
2	B	692	TYR	CG-CD2	-8.79	1.20	1.39
1	A	1112	LYS	CE-NZ	8.79	1.75	1.49
1	A	640	GLN	CD-OE1	8.78	1.40	1.23
1	A	810	PRO	C-N	-8.78	1.22	1.33
2	B	135	ARG	CA-C	8.78	1.63	1.52
6	H	41	ASP	C-O	-8.78	1.13	1.24
4	E	40	GLU	CD-OE1	8.78	1.42	1.25
7	I	79	HIS	CA-C	8.78	1.64	1.52
1	A	1003	LYS	CG-CD	8.78	1.78	1.52
2	B	459	TYR	CA-CB	-8.78	1.39	1.53
9	K	97	LYS	C-O	-8.78	1.12	1.24
2	B	24	PRO	CA-CB	-8.78	1.43	1.53
2	B	515	HIS	CB-CG	-8.78	1.37	1.50
2	B	734	HIS	C-O	8.78	1.37	1.24
2	B	771	SER	C-O	-8.78	1.12	1.24
2	B	836	GLU	CA-CB	-8.77	1.40	1.53
1	A	446	ARG	NE-CZ	-8.77	1.23	1.33
2	B	537	LYS	CA-C	-8.77	1.41	1.52
2	B	578	THR	C-O	-8.77	1.13	1.24
2	B	1027	ILE	C-N	-8.77	1.22	1.33
2	B	1091	TYR	C-O	-8.77	1.13	1.24
3	C	28	ALA	CA-C	-8.77	1.41	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	149	GLU	CG-CD	8.77	1.74	1.52
2	B	722	ASP	CB-CG	8.76	1.74	1.52
4	E	122	LYS	CA-CB	8.76	1.68	1.53
10	L	34	CYS	CB-SG	-8.76	1.52	1.81
1	A	1130	GLN	CD-NE2	8.76	1.51	1.33
2	B	777	ALA	CA-CB	-8.76	1.39	1.53
1	A	271	LYS	CD-CE	8.76	1.78	1.52
2	B	399	ASP	CA-C	8.76	1.64	1.52
7	I	91	ARG	C-O	-8.76	1.11	1.23
1	A	1332	PHE	N-CA	-8.76	1.34	1.46
1	A	1367	HIS	CA-C	-8.76	1.43	1.52
3	C	265	MET	SD-CE	8.76	2.01	1.79
2	B	278	GLN	CB-CG	-8.75	1.26	1.52
1	A	157	ASP	CA-CB	8.75	1.67	1.53
3	C	190	ASP	CA-C	8.75	1.63	1.52
1	A	992	ASP	CB-CG	8.75	1.74	1.52
2	B	700	SER	C-O	-8.75	1.11	1.24
6	H	88	SER	CA-C	8.75	1.64	1.52
9	K	6	ARG	CA-CB	-8.75	1.38	1.53
2	B	833	TYR	C-O	-8.74	1.12	1.24
2	B	564	GLU	CA-C	-8.74	1.40	1.52
7	I	8	ARG	CA-C	8.74	1.64	1.52
1	A	411	ASP	N-CA	8.74	1.56	1.46
2	B	707	PRO	C-N	-8.74	1.21	1.33
9	K	61	TYR	N-CA	-8.74	1.34	1.45
2	B	279	ASP	CG-OD2	8.73	1.42	1.25
3	C	210	GLU	C-O	-8.73	1.12	1.23
2	B	1058	LEU	CA-C	8.73	1.64	1.52
1	A	72	GLU	CA-C	8.73	1.64	1.52
1	A	569	LYS	C-O	-8.73	1.14	1.24
2	B	1062	HIS	CB-CG	-8.73	1.38	1.50
6	H	95	TYR	C-N	-8.73	1.22	1.33
8	J	2	ILE	C-O	-8.73	1.13	1.23
2	B	519	TRP	CZ3-CH2	-8.73	1.18	1.40
2	B	436	VAL	N-CA	8.73	1.57	1.46
4	E	211	TYR	CE2-CZ	-8.73	1.17	1.38
3	C	202	PRO	N-CD	-8.72	1.35	1.47
5	F	154	ASP	CB-CG	8.72	1.73	1.52
1	A	361	LEU	C-O	-8.72	1.13	1.24
1	A	1242	VAL	CA-CB	-8.72	1.42	1.54
2	B	426	LYS	CD-CE	8.72	1.78	1.52
1	A	863	VAL	C-O	-8.72	1.14	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1087	PHE	CD2-CE2	-8.72	1.12	1.38
2	B	21	GLU	C-O	-8.71	1.12	1.24
1	A	640	GLN	CD-NE2	8.71	1.51	1.33
2	B	723	VAL	CB-CG1	8.71	1.81	1.52
2	B	1086	PHE	CG-CD2	-8.71	1.20	1.38
5	F	151	LEU	N-CA	8.71	1.56	1.46
1	A	618	GLU	CA-CB	-8.70	1.41	1.54
6	H	11	GLN	CA-CB	8.70	1.67	1.53
9	K	114	LEU	CA-CB	8.70	1.70	1.53
1	A	544	ASP	CG-OD1	8.70	1.41	1.25
2	B	132	VAL	C-O	8.70	1.35	1.23
2	B	518	HIS	CE1-NE2	-8.70	1.23	1.32
1	A	542	GLU	C-O	-8.70	1.12	1.23
3	C	205	LYS	CG-CD	8.70	1.78	1.52
4	E	205	SER	C-O	-8.70	1.12	1.24
1	A	94	GLY	C-O	8.70	1.35	1.23
1	A	202	LEU	CA-C	-8.70	1.42	1.52
2	B	406	LEU	C-O	8.70	1.34	1.24
1	A	1134	ILE	CA-C	8.69	1.63	1.52
2	B	1102	LYS	C-O	8.69	1.34	1.24
2	B	875	GLU	CG-CD	8.69	1.73	1.52
1	A	141	LEU	N-CA	-8.69	1.34	1.46
2	B	1147	LEU	CA-C	-8.69	1.41	1.52
4	E	95	THR	CA-CB	8.69	1.68	1.53
8	J	63	TYR	CA-C	-8.69	1.42	1.52
9	K	41	THR	CB-CG2	-8.69	1.23	1.52
4	E	136	ASN	CG-ND2	8.69	1.51	1.33
7	I	69	PRO	CA-C	-8.69	1.41	1.52
10	L	39	SER	C-O	8.69	1.34	1.24
1	A	237	THR	CA-CB	-8.68	1.38	1.53
1	A	386	ASP	CA-CB	8.68	1.67	1.53
1	A	19	PHE	CA-CB	-8.68	1.40	1.53
1	A	552	TRP	CZ3-CH2	-8.68	1.18	1.40
2	B	709	ASP	C-O	-8.68	1.11	1.23
1	A	811	GLN	N-CA	-8.68	1.35	1.46
2	B	320	ASP	CG-OD1	8.68	1.41	1.25
5	F	146	TRP	CA-C	8.68	1.62	1.52
3	C	90	ASP	C-O	-8.68	1.13	1.24
1	A	54	ASN	CA-C	8.68	1.64	1.52
2	B	653	VAL	CB-CG2	-8.67	1.24	1.52
1	A	926	GLN	C-O	8.67	1.34	1.24
2	B	787	VAL	N-CA	-8.67	1.35	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	629	ASP	C-N	-8.67	1.21	1.33
10	L	38	LEU	CG-CD1	8.67	1.81	1.52
1	A	515	GLN	CA-C	-8.66	1.42	1.52
1	A	747	VAL	CA-C	-8.66	1.40	1.52
3	C	219	PHE	CG-CD2	-8.66	1.20	1.38
4	E	17	ARG	NE-CZ	8.66	1.42	1.33
1	A	650	GLN	CD-OE1	-8.66	1.07	1.23
2	B	462	ALA	CA-C	-8.66	1.41	1.52
2	B	563	MET	CG-SD	8.66	2.02	1.80
4	E	98	ILE	CB-CG2	8.66	1.81	1.52
1	A	821	ARG	CA-C	-8.66	1.41	1.52
1	A	1261	LYS	CD-CE	8.66	1.78	1.52
9	K	32	VAL	C-O	8.66	1.33	1.24
1	A	520	CYS	CA-C	8.65	1.64	1.52
2	B	209	GLU	C-O	-8.65	1.13	1.24
2	B	791	THR	CA-CB	-8.65	1.40	1.53
1	A	1036	ARG	CZ-NH2	8.65	1.44	1.33
3	C	9	LYS	CG-CD	8.65	1.78	1.52
1	A	560	ILE	C-O	-8.65	1.13	1.24
1	A	736	ASN	C-N	-8.65	1.20	1.33
1	A	819	GLY	CA-C	-8.65	1.39	1.51
2	B	783	THR	CA-C	-8.65	1.40	1.52
3	C	242	GLN	CD-OE1	8.65	1.40	1.23
1	A	1144	LYS	CA-C	-8.64	1.41	1.52
5	F	76	LYS	CG-CD	8.64	1.78	1.52
1	A	153	PRO	C-O	8.64	1.35	1.24
2	B	174	LEU	C-N	-8.64	1.21	1.33
4	E	70	SER	N-CA	-8.64	1.35	1.46
2	B	137	TYR	CA-C	8.64	1.64	1.52
6	H	11	GLN	CB-CG	8.64	1.78	1.52
7	I	23	ASN	CA-C	-8.64	1.42	1.53
1	A	412	ARG	N-CA	-8.64	1.35	1.46
2	B	846	ILE	C-O	8.64	1.34	1.24
2	B	883	LEU	CB-CG	8.64	1.70	1.53
1	A	915	SER	C-N	-8.63	1.23	1.33
2	B	1095	LEU	CB-CG	-8.63	1.36	1.53
2	B	187	SER	N-CA	-8.63	1.35	1.46
1	A	529	CYS	C-O	-8.63	1.14	1.24
1	A	1118	VAL	CB-CG2	-8.63	1.24	1.52
9	K	103	THR	N-CA	-8.63	1.37	1.46
1	A	995	GLU	CD-OE1	8.63	1.41	1.25
1	A	1222	ASN	CG-ND2	8.63	1.51	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	296	GLU	CD-OE2	8.63	1.41	1.25
2	B	348	ARG	CA-CB	-8.63	1.40	1.53
2	B	382	ILE	N-CA	-8.63	1.35	1.46
3	C	13	ALA	C-N	-8.63	1.21	1.33
1	A	514	PRO	N-CA	-8.63	1.36	1.47
2	B	699	GLU	C-N	-8.63	1.22	1.33
2	B	785	TYR	CD1-CE1	-8.62	1.12	1.38
2	B	855	PHE	CA-C	-8.62	1.42	1.52
2	B	1102	LYS	CB-CG	8.62	1.78	1.52
6	H	120	GLY	C-O	8.63	1.36	1.24
1	A	90	VAL	C-O	-8.62	1.14	1.23
3	C	49	VAL	CB-CG2	-8.62	1.24	1.52
5	F	98	ALA	CA-CB	-8.62	1.39	1.53
1	A	710	LEU	C-O	-8.62	1.14	1.24
9	K	5	ASP	CG-OD2	8.62	1.41	1.25
2	B	18	PHE	CB-CG	8.62	1.70	1.50
2	B	769	TYR	CB-CG	8.62	1.70	1.51
6	H	106	GLU	CA-C	8.61	1.64	1.52
7	I	78	CYS	CA-CB	8.61	1.68	1.53
9	K	11	LEU	CG-CD1	8.62	1.80	1.52
1	A	523	ILE	N-CA	-8.61	1.36	1.46
2	B	778	MET	SD-CE	-8.61	1.58	1.79
2	B	989	THR	CA-CB	-8.61	1.40	1.53
1	A	163	SER	N-CA	8.61	1.56	1.45
1	A	1350	LYS	N-CA	-8.61	1.35	1.46
2	B	697	GLU	N-CA	8.61	1.57	1.46
10	L	32	ALA	C-O	8.61	1.34	1.24
1	A	292	ALA	CA-C	-8.60	1.41	1.52
2	B	664	THR	CA-C	-8.60	1.41	1.52
4	E	177	ARG	CA-C	-8.60	1.42	1.52
1	A	264	PHE	CD2-CE2	8.60	1.64	1.38
1	A	1278	ASN	C-N	-8.60	1.22	1.33
2	B	358	LYS	CB-CG	8.60	1.78	1.52
4	E	24	LYS	CA-C	-8.60	1.41	1.52
6	H	115	TYR	CZ-OH	8.60	1.56	1.38
1	A	590	ARG	CZ-NH2	-8.60	1.22	1.33
5	F	85	MET	SD-CE	-8.60	1.58	1.79
2	B	865	LYS	CA-CB	8.60	1.68	1.53
1	A	1383	SER	CA-CB	-8.59	1.39	1.53
2	B	134	LYS	CB-CG	8.59	1.78	1.52
3	C	9	LYS	C-O	-8.59	1.13	1.24
3	C	210	GLU	CD-OE2	8.59	1.41	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	731	ARG	C-N	-8.59	1.23	1.33
1	A	1092	LYS	CB-CG	8.59	1.78	1.52
2	B	743	ILE	CG1-CD1	-8.59	1.18	1.51
2	B	874	PHE	CA-C	-8.59	1.42	1.52
2	B	837	ASP	CA-C	8.59	1.64	1.53
2	B	959	ASP	CG-OD2	8.59	1.41	1.25
2	B	1103	ILE	N-CA	8.59	1.57	1.46
1	A	1287	TYR	CG-CD1	8.59	1.57	1.39
7	I	65	ASP	CB-CG	-8.59	1.30	1.52
10	L	26	THR	CB-CG2	8.59	1.80	1.52
4	E	168	TYR	CA-C	-8.58	1.41	1.52
2	B	1153	GLU	CA-C	8.58	1.64	1.52
1	A	385	ILE	C-O	-8.58	1.12	1.24
2	B	604	ARG	CD-NE	-8.58	1.34	1.46
2	B	138	GLU	N-CA	8.58	1.62	1.46
1	A	1237	ILE	CG1-CD1	-8.57	1.18	1.51
1	A	1375	MET	SD-CE	-8.57	1.58	1.79
2	B	617	ARG	CZ-NH2	-8.57	1.22	1.33
7	I	93	LYS	C-N	8.57	1.45	1.33
1	A	460	VAL	CA-C	-8.57	1.42	1.52
1	A	1154	TYR	C-N	8.57	1.43	1.33
3	C	137	LYS	CD-CE	8.57	1.78	1.52
2	B	904	ARG	NE-CZ	-8.56	1.23	1.33
4	E	31	THR	CA-CB	8.56	1.67	1.53
2	B	758	PHE	C-O	-8.56	1.13	1.24
6	H	47	PHE	CA-C	-8.56	1.42	1.52
7	I	94	ASP	CB-CG	8.56	1.73	1.52
7	I	120	GLN	C-O	8.56	1.35	1.23
2	B	961	LEU	CG-CD1	8.56	1.80	1.52
1	A	368	LYS	CD-CE	8.56	1.78	1.52
3	C	239	PRO	C-N	-8.55	1.23	1.33
1	A	965	GLN	CD-NE2	8.55	1.51	1.33
2	B	545	ILE	N-CA	-8.55	1.36	1.46
9	K	47	ARG	N-CA	-8.55	1.36	1.46
1	A	987	VAL	N-CA	-8.55	1.36	1.46
2	B	283	VAL	CA-CB	-8.55	1.42	1.54
2	B	1076	HIS	CG-ND1	-8.54	1.28	1.38
7	I	89	GLN	CG-CD	-8.54	1.30	1.52
5	F	108	PHE	CA-CB	-8.54	1.41	1.53
2	B	1005	GLY	C-O	8.54	1.35	1.24
3	C	145	CYS	CA-CB	-8.54	1.39	1.53
1	A	116	ASP	C-O	-8.54	1.13	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	490	HIS	N-CA	-8.54	1.36	1.46
3	C	156	THR	C-O	-8.54	1.12	1.23
2	B	988	GLY	C-O	-8.53	1.12	1.23
6	H	57	VAL	CA-C	8.53	1.62	1.52
1	A	16	GLU	C-O	8.53	1.34	1.23
1	A	801	GLU	CD-OE2	8.53	1.41	1.25
2	B	320	ASP	CA-C	-8.53	1.41	1.52
2	B	197	PHE	CG-CD1	-8.53	1.21	1.38
2	B	991	GLY	C-O	-8.53	1.12	1.23
2	B	1051	THR	N-CA	-8.53	1.34	1.45
4	E	139	ALA	CA-CB	8.53	1.68	1.53
1	A	960	ILE	CB-CG1	-8.53	1.36	1.53
2	B	434	ARG	CA-CB	8.53	1.64	1.53
2	B	343	ILE	CG1-CD1	8.53	1.85	1.51
2	B	344	LYS	CG-CD	8.53	1.78	1.52
2	B	772	ALA	CA-C	8.53	1.63	1.52
5	F	149	GLU	CD-OE2	8.53	1.41	1.25
1	A	1291	VAL	N-CA	-8.53	1.37	1.46
1	A	990	VAL	CB-CG1	-8.52	1.24	1.52
1	A	1262	LYS	CD-CE	8.52	1.78	1.52
1	A	987	VAL	C-O	8.52	1.33	1.24
1	A	1002	GLY	C-O	8.52	1.35	1.23
2	B	167	ILE	C-O	8.52	1.34	1.23
1	A	568	PRO	CB-CG	-8.52	1.07	1.49
1	A	614	PHE	C-O	-8.52	1.13	1.23
1	A	80	HIS	CG-CD2	8.52	1.45	1.35
3	C	196	ASP	CG-OD2	8.52	1.41	1.25
1	A	1133	LEU	CA-C	-8.51	1.41	1.52
2	B	1069	PHE	CE1-CZ	-8.51	1.13	1.38
1	A	943	LEU	N-CA	-8.51	1.35	1.46
1	A	191	THR	CA-C	8.51	1.64	1.52
1	A	993	LEU	C-O	-8.51	1.13	1.24
3	C	22	LEU	CA-C	-8.51	1.41	1.52
4	E	93	MET	CG-SD	8.51	2.02	1.80
1	A	1305	VAL	CA-CB	-8.51	1.42	1.54
2	B	745	PRO	CG-CD	8.51	1.79	1.50
2	B	1134	GLU	CA-C	8.51	1.64	1.52
3	C	238	ILE	CG1-CD1	-8.50	1.18	1.51
1	A	737	LEU	C-O	8.50	1.34	1.23
7	I	60	GLN	C-N	-8.50	1.23	1.33
9	K	56	VAL	C-O	-8.50	1.14	1.24
1	A	970	THR	CA-C	-8.50	1.41	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1064	TYR	CZ-OH	8.50	1.55	1.38
4	E	118	PRO	CA-CB	8.50	1.65	1.53
2	B	1004	GLU	C-O	8.50	1.34	1.24
9	K	109	TRP	C-O	8.50	1.35	1.24
4	E	63	ASN	CA-CB	8.50	1.64	1.54
1	A	1230	GLU	CD-OE2	8.49	1.41	1.25
1	A	1325	THR	CA-CB	-8.49	1.39	1.53
7	I	42	LEU	CA-C	-8.49	1.41	1.52
1	A	1060	PRO	C-O	-8.49	1.13	1.23
1	A	427	GLN	CD-OE1	8.49	1.39	1.23
1	A	580	VAL	CA-CB	-8.49	1.42	1.54
9	K	16	GLU	CD-OE2	8.49	1.41	1.25
10	L	42	ARG	CD-NE	8.49	1.58	1.46
1	A	1063	MET	C-O	-8.48	1.12	1.23
6	H	43	ASN	CG-ND2	8.48	1.51	1.33
1	A	1127	ASP	CG-OD2	8.48	1.41	1.25
2	B	380	TYR	C-O	-8.48	1.13	1.24
1	A	384	ASN	CA-C	8.48	1.63	1.52
2	B	868	MET	CA-CB	8.48	1.67	1.53
1	A	961	ARG	C-O	-8.48	1.13	1.24
3	C	154	LYS	CB-CG	8.48	1.77	1.52
3	C	183	TRP	C-O	-8.48	1.12	1.23
9	K	108	GLU	CD-OE2	8.48	1.41	1.25
3	C	261	ALA	CA-CB	-8.47	1.41	1.54
2	B	454	THR	CA-CB	-8.47	1.40	1.53
2	B	1192	TYR	CG-CD1	-8.47	1.21	1.39
1	A	1105	LEU	C-O	-8.47	1.13	1.24
2	B	661	LEU	CA-C	-8.47	1.41	1.52
4	E	104	ASN	C-O	8.47	1.36	1.23
8	J	23	ASN	CG-ND2	8.47	1.51	1.33
1	A	574	GLY	CA-C	-8.46	1.42	1.52
1	A	792	TYR	CE1-CZ	-8.46	1.18	1.38
8	J	63	TYR	CG-CD2	-8.46	1.21	1.39
2	B	826	ALA	N-CA	-8.46	1.35	1.46
1	A	130	ASP	CB-CG	8.46	1.73	1.52
1	A	715	GLU	CA-C	-8.46	1.42	1.52
2	B	954	VAL	CA-C	-8.46	1.42	1.52
9	K	83	PRO	C-O	-8.46	1.12	1.24
1	A	1308	THR	N-CA	-8.46	1.35	1.45
2	B	1008	PRO	CG-CD	-8.46	1.22	1.50
1	A	1329	THR	N-CA	-8.46	1.35	1.45
2	B	1106	ARG	CA-CB	8.46	1.63	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	42	ARG	N-CA	8.46	1.56	1.46
1	A	806	ARG	CZ-NH1	8.45	1.44	1.32
2	B	24	PRO	N-CA	-8.45	1.37	1.46
2	B	453	ILE	CB-CG2	-8.45	1.24	1.52
1	A	427	GLN	CD-NE2	8.45	1.50	1.33
1	A	441	PRO	CA-CB	-8.45	1.42	1.53
1	A	1223	ASP	CG-OD2	8.45	1.41	1.25
1	A	884	ASP	CA-CB	8.45	1.67	1.53
3	C	136	ASP	CG-OD1	-8.45	1.09	1.25
9	K	75	ILE	C-O	-8.45	1.15	1.24
1	A	62	ASP	CA-C	8.45	1.64	1.52
1	A	470	LEU	N-CA	-8.45	1.35	1.45
1	A	1162	VAL	C-O	-8.45	1.14	1.24
2	B	889	THR	CA-C	-8.45	1.42	1.52
10	L	56	LEU	C-O	-8.45	1.13	1.23
1	A	555	ASP	CA-CB	8.44	1.67	1.53
1	A	109	HIS	CA-C	8.44	1.60	1.53
1	A	373	THR	CB-CG2	-8.44	1.24	1.52
2	B	520	GLY	C-N	-8.44	1.22	1.33
2	B	841	MET	SD-CE	-8.44	1.58	1.79
1	A	833	GLU	C-O	8.44	1.33	1.24
9	K	73	LEU	CB-CG	-8.44	1.36	1.53
1	A	132	LYS	CG-CD	8.44	1.77	1.52
1	A	180	LYS	CB-CG	8.44	1.77	1.52
1	A	244	PRO	C-O	8.44	1.33	1.24
4	E	186	LEU	C-O	-8.44	1.13	1.24
7	I	42	LEU	C-O	-8.44	1.13	1.24
8	J	44	TYR	CG-CD2	-8.44	1.21	1.39
1	A	895	LYS	CG-CD	8.43	1.77	1.52
2	B	459	TYR	C-O	-8.43	1.14	1.24
2	B	1087	PHE	CA-CB	-8.43	1.39	1.53
2	B	1130	PHE	N-CA	-8.43	1.32	1.47
4	E	8	ASN	CG-OD1	8.43	1.39	1.23
1	A	45	GLN	CA-CB	8.43	1.67	1.53
1	A	1190	PRO	CB-CG	8.43	1.91	1.49
2	B	116	GLU	C-N	-8.43	1.21	1.33
6	H	86	ASP	N-CA	8.43	1.57	1.46
1	A	425	GLN	CG-CD	8.43	1.73	1.52
1	A	159	THR	CA-CB	8.43	1.67	1.53
2	B	226	PHE	CD1-CE1	8.43	1.64	1.38
2	B	227	LYS	CD-CE	8.43	1.77	1.52
2	B	655	LYS	CA-C	-8.43	1.41	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	981	LEU	C-N	-8.42	1.21	1.33
3	C	46	ILE	C-O	-8.42	1.15	1.24
1	A	455	MET	N-CA	8.42	1.58	1.46
2	B	629	ASP	C-O	-8.42	1.13	1.23
6	H	57	VAL	N-CA	8.42	1.56	1.46
6	H	76	THR	CB-CG2	8.42	1.80	1.52
1	A	759	ALA	C-N	-8.41	1.21	1.33
1	A	1112	LYS	C-O	-8.41	1.14	1.24
6	H	96	VAL	CA-C	8.41	1.63	1.52
8	J	2	ILE	C-N	8.41	1.42	1.33
1	A	1427	ASN	N-CA	-8.41	1.35	1.46
2	B	192	LEU	CG-CD2	8.41	1.80	1.52
6	H	112	ILE	CB-CG2	-8.41	1.24	1.52
1	A	978	PRO	CA-C	8.41	1.62	1.52
1	A	681	GLU	CG-CD	8.41	1.73	1.52
6	H	29	ALA	CA-CB	-8.41	1.40	1.53
9	K	55	LYS	C-O	8.41	1.35	1.24
2	B	336	ARG	CZ-NH2	8.41	1.44	1.33
1	A	519	PRO	N-CA	-8.41	1.36	1.47
1	A	844	ALA	CA-C	-8.41	1.41	1.52
9	K	83	PRO	CB-CG	-8.40	1.07	1.49
2	B	301	ILE	C-O	-8.40	1.14	1.23
7	I	14	LEU	CG-CD1	-8.40	1.24	1.52
10	L	61	THR	CB-CG2	8.40	1.80	1.52
1	A	512	VAL	C-O	-8.40	1.14	1.24
1	A	747	VAL	CB-CG1	-8.40	1.24	1.52
2	B	1057	LYS	CG-CD	8.40	1.77	1.52
2	B	754	SER	CA-CB	-8.39	1.39	1.53
10	L	47	ARG	C-O	-8.39	1.13	1.24
1	A	1234	GLU	CG-CD	8.39	1.73	1.52
2	B	183	GLU	CD-OE1	8.39	1.41	1.25
4	E	139	ALA	CA-C	-8.39	1.41	1.52
3	C	59	ALA	C-O	-8.39	1.13	1.23
1	A	997	LEU	C-O	-8.38	1.13	1.23
1	A	1290	LYS	CA-CB	-8.39	1.40	1.53
2	B	848	ARG	CA-CB	-8.39	1.39	1.53
2	B	608	ASP	CG-OD1	8.38	1.41	1.25
2	B	1171	VAL	C-N	8.38	1.43	1.33
3	C	234	SER	N-CA	-8.38	1.35	1.45
1	A	1214	GLU	CD-OE2	8.38	1.41	1.25
2	B	65	GLU	CG-CD	8.38	1.73	1.52
2	B	1042	GLY	CA-C	-8.38	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	191	LYS	CG-CD	8.38	1.77	1.52
1	A	924	LYS	CA-C	8.38	1.64	1.52
1	A	1447	GLU	CD-OE1	8.38	1.41	1.25
2	B	479	VAL	CA-C	-8.38	1.40	1.52
7	I	111	THR	CA-C	-8.38	1.42	1.52
1	A	855	THR	C-O	-8.37	1.12	1.23
6	H	126	GLU	CG-CD	8.38	1.73	1.52
2	B	165	VAL	CA-CB	8.37	1.65	1.54
2	B	496	ARG	N-CA	-8.37	1.37	1.46
1	A	357	PRO	C-O	8.37	1.35	1.24
1	A	451	HIS	CA-C	-8.37	1.42	1.52
1	A	4	GLN	CG-CD	8.37	1.73	1.52
1	A	795	GLU	CD-OE1	8.37	1.41	1.25
2	B	1108	ARG	C-O	8.37	1.34	1.24
1	A	969	GLN	CD-NE2	8.36	1.50	1.33
9	K	66	PRO	N-CA	-8.36	1.37	1.47
1	A	388	LEU	CB-CG	-8.36	1.36	1.53
2	B	193	LYS	CD-CE	8.36	1.77	1.52
2	B	275	TYR	CA-C	-8.36	1.41	1.52
2	B	406	LEU	CG-CD2	-8.36	1.25	1.52
2	B	738	PHE	C-O	8.36	1.34	1.23
2	B	972	LYS	CA-CB	-8.36	1.41	1.53
2	B	1099	VAL	CA-CB	-8.36	1.43	1.54
1	A	507	VAL	CB-CG2	-8.36	1.25	1.52
2	B	216	GLU	CD-OE2	8.36	1.41	1.25
2	B	1008	PRO	CA-C	-8.36	1.42	1.52
2	B	1086	PHE	CG-CD1	-8.36	1.21	1.38
2	B	807	ARG	CB-CG	8.35	1.77	1.52
1	A	195	ASP	CA-C	8.35	1.64	1.52
3	C	167	HIS	CA-CB	-8.35	1.39	1.53
1	A	467	THR	C-O	-8.35	1.13	1.23
1	A	1416	ALA	C-O	-8.35	1.11	1.23
2	B	94	LYS	C-N	8.35	1.45	1.33
1	A	11	LEU	CA-C	-8.35	1.42	1.52
1	A	517	ASN	CA-C	-8.35	1.41	1.53
6	H	107	VAL	CB-CG1	8.35	1.80	1.52
1	A	1345	ARG	CZ-NH2	-8.35	1.22	1.33
2	B	995	ARG	NE-CZ	-8.35	1.23	1.33
2	B	895	ASP	CG-OD2	8.34	1.41	1.25
2	B	969	ARG	NE-CZ	-8.34	1.23	1.33
1	A	527	THR	N-CA	-8.34	1.35	1.46
7	I	50	THR	C-O	-8.34	1.13	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	114	PRO	CG-CD	-8.34	1.22	1.50
2	B	411	PRO	CA-CB	-8.34	1.42	1.53
2	B	962	LYS	CE-NZ	8.34	1.74	1.49
1	A	966	ASN	CA-C	-8.33	1.42	1.52
2	B	330	ALA	CA-CB	-8.33	1.40	1.53
2	B	778	MET	CA-C	-8.33	1.42	1.52
5	F	136	ARG	C-O	-8.33	1.13	1.24
7	I	69	PRO	N-CA	-8.33	1.37	1.47
8	J	21	TYR	CA-CB	8.33	1.67	1.53
1	A	1113	THR	C-N	-8.33	1.22	1.33
2	B	561	TRP	C-N	-8.33	1.23	1.33
2	B	759	PRO	CA-C	-8.33	1.38	1.52
4	E	166	LYS	CA-C	-8.33	1.42	1.52
2	B	325	GLN	CD-OE1	8.33	1.39	1.23
2	B	627	PHE	CD1-CE1	-8.32	1.13	1.38
2	B	785	TYR	CA-C	-8.32	1.41	1.52
2	B	535	LEU	CA-C	-8.32	1.41	1.52
7	I	100	PHE	CE1-CZ	-8.32	1.13	1.38
9	K	74	ARG	C-O	8.32	1.33	1.24
9	K	90	ALA	CA-CB	-8.32	1.40	1.53
1	A	835	GLY	C-O	8.32	1.35	1.23
2	B	211	VAL	N-CA	-8.32	1.36	1.46
1	A	1199	ARG	C-O	8.32	1.33	1.24
1	A	22	PHE	CA-CB	-8.32	1.42	1.53
1	A	767	GLN	CB-CG	-8.32	1.27	1.52
2	B	994	TYR	CA-C	-8.32	1.42	1.52
3	C	60	ASP	CG-OD2	8.32	1.41	1.25
3	C	252	GLN	CG-CD	8.32	1.72	1.52
1	A	463	ILE	CB-CG1	-8.31	1.36	1.53
1	A	852	TYR	CA-CB	-8.31	1.39	1.53
2	B	189	LEU	CB-CG	-8.31	1.36	1.53
2	B	586	TRP	C-O	-8.31	1.14	1.24
2	B	896	ASP	C-O	-8.31	1.13	1.24
6	H	84	ALA	C-O	8.31	1.34	1.24
3	C	252	GLN	CD-OE1	8.31	1.39	1.23
1	A	1129	GLU	CA-CB	8.31	1.67	1.53
1	A	1335	ILE	CA-CB	-8.31	1.44	1.54
1	A	471	ASN	CA-CB	8.31	1.66	1.53
3	C	187	LYS	CE-NZ	8.31	1.74	1.49
1	A	843	LYS	CA-CB	8.30	1.66	1.53
1	A	937	VAL	CA-CB	-8.31	1.43	1.54
10	L	26	THR	C-O	8.31	1.34	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	828	ALA	CA-CB	-8.30	1.40	1.53
9	K	83	PRO	C-N	-8.30	1.22	1.33
1	A	1208	THR	CA-C	8.30	1.63	1.52
1	A	1221	LYS	CA-CB	8.30	1.67	1.53
2	B	164	LYS	CG-CD	8.30	1.77	1.52
3	C	109	SER	CA-CB	8.30	1.65	1.53
3	C	135	GLN	CA-C	8.30	1.62	1.52
7	I	9	ASP	C-O	8.30	1.33	1.24
1	A	1384	VAL	CA-CB	-8.30	1.45	1.54
2	B	118	ARG	CA-C	8.30	1.63	1.52
1	A	451	HIS	N-CA	-8.30	1.35	1.46
2	B	620	ARG	CB-CG	8.30	1.77	1.52
3	C	231	ASN	CB-CG	8.30	1.72	1.52
1	A	137	ALA	CA-CB	-8.29	1.39	1.53
1	A	755	PHE	C-O	8.29	1.33	1.24
1	A	403	LYS	N-CA	-8.29	1.34	1.46
1	A	1279	ILE	N-CA	-8.29	1.36	1.46
2	B	31	TRP	CG-CD1	-8.29	1.16	1.36
4	E	119	SER	C-O	8.29	1.34	1.24
1	A	814	PHE	C-O	-8.29	1.13	1.24
2	B	1108	ARG	N-CA	8.29	1.56	1.46
1	A	19	PHE	C-O	-8.29	1.13	1.23
1	A	537	ARG	CZ-NH1	8.29	1.44	1.32
6	H	34	ASP	C-O	8.28	1.34	1.24
1	A	404	TYR	CA-CB	-8.28	1.38	1.54
1	A	551	TYR	CG-CD1	-8.28	1.22	1.39
2	B	189	LEU	C-O	8.28	1.33	1.24
7	I	93	LYS	C-O	8.28	1.34	1.24
2	B	536	VAL	N-CA	8.28	1.56	1.46
8	J	29	GLU	CD-OE1	8.28	1.41	1.25
1	A	205	GLU	CG-CD	8.28	1.72	1.52
1	A	444	PHE	CA-C	-8.28	1.42	1.52
1	A	720	ARG	CG-CD	8.28	1.77	1.52
1	A	918	GLU	N-CA	-8.28	1.34	1.46
2	B	121	ASN	CB-CG	8.27	1.72	1.52
2	B	899	ILE	CA-C	-8.27	1.42	1.52
3	C	158	VAL	C-O	-8.27	1.15	1.24
1	A	99	ILE	CG1-CD1	-8.27	1.19	1.51
2	B	622	LYS	CB-CG	8.27	1.77	1.52
1	A	143	LYS	CE-NZ	8.27	1.74	1.49
1	A	1018	PHE	CG-CD1	-8.27	1.21	1.38
3	C	263	THR	CB-CG2	8.27	1.79	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1347	ALA	N-CA	-8.27	1.36	1.46
9	K	71	PHE	CD2-CE2	-8.27	1.13	1.38
1	A	1322	ILE	N-CA	8.27	1.56	1.46
2	B	646	LEU	N-CA	8.27	1.56	1.46
4	E	181	ALA	CA-CB	-8.27	1.42	1.53
2	B	92	PHE	N-CA	8.26	1.56	1.46
2	B	336	ARG	C-O	8.26	1.34	1.24
3	C	203	GLN	CD-NE2	8.26	1.50	1.33
4	E	127	ILE	CA-C	-8.26	1.44	1.52
1	A	65	LEU	CA-CB	8.26	1.67	1.53
2	B	340	ALA	N-CA	-8.26	1.35	1.45
2	B	1012	ILE	CB-CG2	-8.26	1.25	1.52
6	H	103	LYS	C-O	-8.26	1.13	1.24
2	B	828	ALA	C-O	-8.26	1.13	1.23
4	E	56	LYS	CA-CB	8.26	1.67	1.53
1	A	151	ASP	N-CA	-8.26	1.36	1.46
3	C	100	THR	CA-C	-8.26	1.42	1.52
9	K	3	ALA	CA-C	8.26	1.62	1.52
9	K	84	LYS	N-CA	-8.26	1.35	1.46
1	A	44	THR	CB-CG2	8.25	1.79	1.52
2	B	346	GLU	CD-OE1	8.25	1.41	1.25
2	B	708	GLU	N-CA	-8.25	1.35	1.46
1	A	1160	SER	CB-OG	8.25	1.58	1.42
1	A	1283	VAL	CA-CB	-8.25	1.43	1.54
2	B	348	ARG	C-O	-8.25	1.14	1.24
3	C	150	GLY	N-CA	8.25	1.56	1.45
3	C	199	LYS	CD-CE	8.25	1.77	1.52
4	E	167	ARG	CZ-NH2	8.25	1.44	1.33
6	H	116	TYR	CG-CD1	8.25	1.56	1.39
10	L	29	TYR	CE2-CZ	-8.25	1.18	1.38
1	A	868	TYR	CE2-CZ	-8.25	1.18	1.38
1	A	1062	GLU	C-O	8.25	1.33	1.23
2	B	642	ASP	CA-C	-8.25	1.42	1.52
1	A	962	ARG	C-O	-8.25	1.13	1.24
2	B	381	MET	CG-SD	8.25	2.01	1.80
2	B	459	TYR	CG-CD1	8.25	1.56	1.39
1	A	413	ILE	CA-C	-8.24	1.42	1.52
1	A	511	ILE	N-CA	8.24	1.56	1.46
1	A	1447	GLU	CD-OE2	8.24	1.41	1.25
2	B	404	LYS	CA-C	-8.24	1.42	1.52
3	C	189	THR	CA-C	-8.24	1.42	1.52
1	A	1066	VAL	CA-C	-8.24	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	133	ASN	C-O	8.24	1.34	1.24
2	B	1076	HIS	N-CA	-8.24	1.35	1.46
1	A	943	LEU	C-O	-8.24	1.13	1.24
1	A	1429	ILE	CA-C	-8.24	1.42	1.52
1	A	1319	VAL	CA-C	-8.24	1.44	1.52
8	J	21	TYR	CA-C	-8.24	1.42	1.53
1	A	1421	CYS	N-CA	-8.23	1.34	1.46
2	B	933	SER	C-O	8.23	1.40	1.23
1	A	106	VAL	CB-CG2	-8.23	1.25	1.52
1	A	179	LEU	CA-CB	8.23	1.67	1.53
3	C	79	GLN	CG-CD	8.23	1.72	1.52
4	E	106	GLN	CA-C	8.23	1.64	1.52
1	A	934	LYS	CA-C	-8.22	1.42	1.52
4	E	167	ARG	NE-CZ	-8.22	1.24	1.33
4	E	179	GLN	CD-NE2	8.22	1.50	1.33
7	I	59	VAL	C-O	-8.22	1.14	1.23
2	B	1148	LYS	CD-CE	8.22	1.77	1.52
7	I	95	THR	CA-C	-8.22	1.42	1.52
2	B	423	LYS	CG-CD	8.22	1.77	1.52
6	H	20	TYR	CG-CD2	-8.22	1.22	1.39
6	H	30	SER	CA-C	8.22	1.63	1.52
1	A	961	ARG	CA-C	-8.21	1.41	1.52
2	B	367	LEU	CA-CB	8.22	1.66	1.53
2	B	916	THR	CB-CG2	8.21	1.79	1.52
6	H	8	ASP	CA-C	8.21	1.63	1.52
8	J	6	ARG	C-O	8.21	1.34	1.23
4	E	15	ALA	N-CA	-8.21	1.35	1.46
4	E	187	TYR	CG-CD1	-8.21	1.22	1.39
2	B	542	MET	CA-CB	8.21	1.66	1.53
1	A	77	CYS	CA-C	-8.21	1.43	1.52
9	K	87	LEU	C-O	8.21	1.34	1.24
1	A	285	PRO	C-O	-8.21	1.12	1.23
1	A	1159	ARG	CZ-NH2	8.21	1.44	1.33
2	B	228	LYS	CD-CE	8.21	1.77	1.52
2	B	234	ILE	CA-CB	-8.21	1.44	1.54
2	B	1189	ILE	CB-CG2	8.20	1.79	1.52
2	B	1210	MET	CA-C	-8.20	1.39	1.52
2	B	974	PRO	CA-C	-8.20	1.42	1.52
1	A	599	SER	C-O	-8.20	1.13	1.24
1	A	1347	ALA	CA-C	-8.20	1.42	1.52
2	B	20	ASP	CG-OD1	8.20	1.41	1.25
2	B	213	ILE	N-CA	-8.20	1.36	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	625	LYS	CE-NZ	8.20	1.74	1.49
4	E	211	TYR	C-O	8.20	1.33	1.23
1	A	110	CYS	C-O	8.20	1.33	1.24
1	A	468	PHE	CE2-CZ	-8.20	1.14	1.38
1	A	496	GLU	CG-CD	8.20	1.72	1.52
1	A	1324	PRO	N-CD	-8.20	1.36	1.47
1	A	1353	TYR	CG-CD1	-8.20	1.22	1.39
1	A	1449	SER	C-O	8.20	1.34	1.23
2	B	934	LYS	C-O	8.20	1.34	1.24
1	A	1106	ASN	C-N	-8.20	1.22	1.33
1	A	1197	LEU	CA-CB	-8.20	1.40	1.53
1	A	1440	ALA	C-O	8.20	1.34	1.24
3	C	214	ASN	CB-CG	8.20	1.72	1.52
1	A	196	GLU	CD-OE2	8.19	1.41	1.25
1	A	755	PHE	CB-CG	8.19	1.69	1.50
1	A	911	SER	C-O	8.19	1.34	1.24
2	B	459	TYR	CD2-CE2	8.20	1.63	1.38
2	B	726	ALA	C-O	-8.19	1.12	1.24
2	B	256	VAL	C-O	-8.19	1.15	1.24
4	E	54	GLN	CG-CD	8.19	1.72	1.52
1	A	12	ARG	NE-CZ	8.19	1.42	1.33
1	A	1214	GLU	CG-CD	8.19	1.72	1.52
1	A	516	SER	CB-OG	8.19	1.58	1.42
1	A	857	ARG	CA-C	-8.19	1.42	1.52
2	B	831	SER	CA-CB	-8.19	1.39	1.53
2	B	1224	PHE	CD2-CE2	8.19	1.63	1.38
5	F	79	ARG	CA-C	8.19	1.63	1.52
1	A	390	GLN	CD-OE1	8.18	1.39	1.23
1	A	860	LEU	C-O	-8.18	1.13	1.24
2	B	950	ASP	CA-C	-8.18	1.41	1.52
7	I	101	PHE	CB-CG	-8.18	1.31	1.50
2	B	1040	ASN	CB-CG	-8.18	1.31	1.52
6	H	129	TYR	CE1-CZ	8.18	1.57	1.38
2	B	137	TYR	N-CA	8.18	1.56	1.46
1	A	269	ILE	CA-CB	8.18	1.65	1.54
1	A	901	LEU	CG-CD2	-8.18	1.25	1.52
9	K	23	PRO	CB-CG	8.18	1.90	1.49
2	B	115	GLN	CG-CD	8.18	1.72	1.52
1	A	551	TYR	CE2-CZ	-8.18	1.18	1.38
1	A	1188	GLN	CG-CD	8.18	1.72	1.52
9	K	67	PHE	CG-CD2	-8.18	1.21	1.38
1	A	828	ALA	C-O	8.18	1.33	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	244	VAL	C-O	8.18	1.33	1.24
5	F	145	ASP	C-O	8.18	1.33	1.24
1	A	631	HIS	CA-C	-8.17	1.41	1.52
1	A	1188	GLN	CD-OE1	8.17	1.39	1.23
2	B	626	ILE	CA-CB	-8.17	1.41	1.55
1	A	609	ASP	CG-OD1	8.17	1.40	1.25
5	F	97	ARG	NE-CZ	-8.17	1.24	1.33
7	I	56	ALA	CA-C	-8.17	1.42	1.52
5	F	92	ARG	CB-CG	-8.17	1.27	1.52
1	A	1345	ARG	NE-CZ	-8.17	1.24	1.33
1	A	1040	GLN	CG-CD	8.16	1.72	1.52
5	F	89	GLU	C-N	-8.16	1.23	1.33
1	A	92	HIS	CA-CB	8.16	1.63	1.53
1	A	388	LEU	C-O	-8.16	1.14	1.24
1	A	604	GLY	C-O	-8.16	1.08	1.23
1	A	840	ARG	CD-NE	8.16	1.57	1.46
2	B	823	ALA	CA-C	-8.16	1.42	1.52
1	A	929	LEU	N-CA	-8.16	1.36	1.46
5	F	106	PRO	CA-CB	-8.16	1.42	1.53
1	A	601	LYS	CG-CD	8.16	1.76	1.52
1	A	865	GLN	CG-CD	8.16	1.72	1.52
3	C	174	ALA	CA-CB	-8.16	1.39	1.53
3	C	175	ALA	CA-CB	-8.16	1.39	1.53
10	L	37	LYS	C-O	-8.16	1.13	1.24
1	A	1314	SER	N-CA	-8.15	1.36	1.46
2	B	387	LEU	N-CA	-8.15	1.35	1.46
2	B	510	LYS	C-N	-8.15	1.24	1.33
2	B	624	LEU	C-O	-8.15	1.14	1.23
2	B	899	ILE	CB-CG1	-8.15	1.37	1.53
2	B	1098	MET	CG-SD	8.15	2.01	1.80
2	B	1186	ASP	C-O	8.15	1.34	1.23
7	I	18	GLU	CD-OE1	8.15	1.40	1.25
1	A	233	TRP	CA-C	-8.15	1.41	1.52
1	A	1385	THR	CB-CG2	8.15	1.79	1.52
3	C	52	GLU	CA-CB	8.15	1.66	1.53
4	E	174	GLN	CD-OE1	8.15	1.39	1.23
1	A	1105	LEU	N-CA	-8.15	1.35	1.46
1	A	1229	SER	C-N	8.15	1.44	1.33
2	B	1183	LYS	CD-CE	8.15	1.76	1.52
3	C	256	ALA	N-CA	-8.15	1.35	1.46
1	A	834	THR	CA-CB	-8.14	1.40	1.53
3	C	163	ILE	C-O	-8.14	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	75	PRO	CA-C	-8.14	1.41	1.52
1	A	414	ASP	C-O	-8.14	1.14	1.24
1	A	963	ILE	CB-CG2	-8.14	1.25	1.52
1	A	370	ILE	CA-C	-8.14	1.41	1.52
3	C	46	ILE	CG1-CD1	-8.14	1.20	1.51
1	A	368	LYS	CA-C	-8.14	1.42	1.52
1	A	1034	GLU	CG-CD	8.14	1.72	1.52
2	B	777	ALA	N-CA	-8.14	1.36	1.45
1	A	163	SER	CA-CB	8.14	1.66	1.53
1	A	644	LYS	CA-CB	-8.13	1.40	1.53
1	A	700	ASN	CA-CB	-8.13	1.41	1.53
1	A	711	ARG	CA-C	-8.13	1.41	1.52
4	E	53	PRO	CB-CG	8.13	1.90	1.49
1	A	1018	PHE	CG-CD2	-8.13	1.21	1.38
1	A	782	ARG	N-CA	8.13	1.55	1.46
2	B	1101	ASP	CA-CB	8.13	1.68	1.53
1	A	838	GLN	CB-CG	8.13	1.76	1.52
1	A	858	ASN	N-CA	8.13	1.56	1.45
2	B	668	ASP	CG-OD2	8.13	1.40	1.25
4	E	57	MET	CB-CG	8.13	1.76	1.52
4	E	67	GLU	CD-OE2	8.13	1.40	1.25
9	K	92	ASN	CA-CB	8.13	1.66	1.53
1	A	1053	PHE	CE1-CZ	-8.13	1.14	1.38
1	A	194	ALA	N-CA	8.12	1.56	1.46
2	B	499	ASN	CG-ND2	8.12	1.50	1.33
1	A	386	ASP	CA-C	8.12	1.62	1.52
1	A	1359	ASP	CG-OD2	8.12	1.40	1.25
2	B	104	GLU	C-O	8.12	1.34	1.23
2	B	723	VAL	N-CA	8.12	1.56	1.46
2	B	1161	HIS	CG-CD2	8.12	1.44	1.35
3	C	240	VAL	N-CA	-8.12	1.36	1.46
4	E	118	PRO	CG-CD	8.12	1.78	1.50
1	A	349	ALA	C-O	-8.12	1.14	1.23
1	A	53	LEU	CA-C	8.12	1.65	1.53
1	A	1217	LYS	C-O	8.12	1.34	1.24
2	B	707	PRO	CA-CB	-8.12	1.41	1.53
2	B	1084	GLN	C-O	-8.12	1.13	1.23
3	C	20	PHE	C-O	-8.12	1.15	1.23
6	H	146	ARG	CZ-NH1	8.12	1.44	1.32
1	A	376	TYR	CG-CD1	-8.12	1.22	1.39
1	A	1417	GLU	CD-OE1	8.12	1.40	1.25
2	B	327	ARG	CZ-NH2	8.12	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	730	ARG	N-CA	-8.11	1.36	1.45
1	A	171	GLN	CD-NE2	8.11	1.50	1.33
2	B	1059	LEU	N-CA	-8.11	1.35	1.46
3	C	225	ALA	CA-CB	-8.11	1.42	1.53
7	I	27	PHE	CA-CB	-8.11	1.42	1.53
2	B	242	SER	CB-OG	8.11	1.58	1.42
1	A	911	SER	N-CA	8.11	1.56	1.46
2	B	1015	HIS	C-O	-8.11	1.13	1.24
2	B	1183	LYS	CB-CG	8.11	1.76	1.52
2	B	299	GLU	C-O	-8.11	1.13	1.24
2	B	1082	MET	N-CA	-8.11	1.36	1.46
1	A	1445	ILE	CG1-CD1	8.10	1.83	1.51
2	B	1074	ASN	C-N	-8.10	1.23	1.33
1	A	718	VAL	CA-CB	-8.10	1.43	1.54
2	B	635	ARG	CA-C	-8.10	1.42	1.52
2	B	494	HIS	C-O	-8.10	1.14	1.24
1	A	511	ILE	CG1-CD1	-8.10	1.20	1.51
1	A	1450	LEU	CB-CG	8.10	1.69	1.53
3	C	48	SER	CA-C	-8.10	1.42	1.52
2	B	477	ALA	CA-CB	8.09	1.79	1.52
1	A	477	PRO	CA-C	-8.09	1.39	1.52
2	B	40	GLU	N-CA	-8.09	1.36	1.46
2	B	357	GLN	C-O	-8.09	1.13	1.24
1	A	296	LEU	N-CA	8.09	1.55	1.46
1	A	460	VAL	CB-CG2	-8.09	1.25	1.52
1	A	1418	LEU	CA-C	-8.09	1.42	1.52
2	B	709	ASP	CA-C	-8.09	1.41	1.52
3	C	76	ASP	CG-OD1	8.09	1.40	1.25
7	I	18	GLU	C-O	8.09	1.33	1.23
7	I	62	ILE	C-N	-8.09	1.20	1.33
3	C	35	ARG	CD-NE	-8.08	1.34	1.46
9	K	63	VAL	C-O	8.08	1.33	1.24
1	A	524	VAL	CB-CG2	-8.08	1.25	1.52
1	A	860	LEU	CG-CD1	8.08	1.79	1.52
2	B	652	LYS	C-O	8.08	1.33	1.24
2	B	1010	LEU	CA-C	-8.08	1.42	1.52
1	A	921	GLY	CA-C	8.08	1.63	1.51
2	B	337	ARG	NE-CZ	-8.08	1.24	1.33
1	A	393	ARG	CG-CD	8.08	1.76	1.52
1	A	37	PHE	CA-C	8.07	1.62	1.53
2	B	784	ASN	N-CA	-8.07	1.37	1.46
3	C	37	MET	N-CA	-8.07	1.36	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	276	ILE	N-CA	-8.07	1.36	1.46
1	A	770	VAL	CA-CB	-8.06	1.43	1.54
1	A	897	TYR	CE1-CZ	-8.06	1.18	1.38
2	B	173	MET	C-O	-8.06	1.14	1.24
1	A	691	LEU	CA-CB	-8.06	1.40	1.53
1	A	1267	MET	CA-C	-8.06	1.42	1.52
2	B	358	LYS	CA-C	-8.06	1.41	1.52
2	B	458	LYS	CD-CE	8.06	1.76	1.52
2	B	1000	PRO	N-CA	-8.06	1.37	1.46
2	B	1014	PRO	CA-C	-8.06	1.38	1.52
2	B	1034	VAL	CA-CB	-8.06	1.44	1.54
2	B	1161	HIS	ND1-CE1	8.06	1.40	1.32
4	E	71	LYS	CA-C	-8.06	1.41	1.52
1	A	1242	VAL	N-CA	-8.05	1.36	1.46
2	B	1106	ARG	N-CA	8.05	1.56	1.46
1	A	187	LYS	N-CA	8.05	1.57	1.46
1	A	198	GLU	CA-C	-8.05	1.42	1.52
6	H	142	LEU	CA-CB	-8.05	1.37	1.53
6	H	145	ARG	NE-CZ	8.05	1.42	1.33
1	A	408	ASP	CG-OD2	8.05	1.40	1.25
2	B	204	ILE	CG1-CD1	-8.05	1.20	1.51
1	A	155	GLU	CA-C	8.04	1.63	1.52
1	A	734	GLU	CG-CD	8.04	1.72	1.52
2	B	1194	ILE	CA-C	-8.05	1.43	1.52
9	K	43	GLY	CA-C	8.05	1.60	1.52
1	A	1408	ILE	C-O	-8.04	1.14	1.24
2	B	268	THR	N-CA	-8.04	1.35	1.45
7	I	8	ARG	CB-CG	8.04	1.76	1.52
1	A	347	PHE	C-O	-8.04	1.13	1.24
1	A	934	LYS	CG-CD	8.04	1.76	1.52
2	B	1067	ARG	CZ-NH2	-8.04	1.23	1.33
2	B	535	LEU	N-CA	-8.04	1.35	1.46
2	B	852	ARG	C-O	-8.04	1.14	1.23
1	A	756	ILE	N-CA	8.04	1.56	1.46
8	J	53	HIS	CG-CD2	-8.04	1.27	1.35
1	A	782	ARG	NE-CZ	8.04	1.41	1.33
7	I	74	GLU	CD-OE2	8.04	1.40	1.25
4	E	133	GLU	C-O	8.03	1.34	1.24
9	K	58	PHE	C-O	8.04	1.33	1.23
8	J	1	MET	CA-CB	-8.03	1.37	1.53
2	B	681	TRP	CG-CD1	-8.03	1.16	1.36
1	A	427	GLN	CB-CG	8.03	1.76	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	31	TRP	C-N	-8.03	1.22	1.33
7	I	91	ARG	CA-C	-8.03	1.41	1.53
9	K	95	ILE	CA-CB	-8.03	1.44	1.54
1	A	717	ASN	C-O	-8.02	1.14	1.24
1	A	810	PRO	CA-C	8.02	1.64	1.52
3	C	199	LYS	N-CA	8.02	1.56	1.46
5	F	136	ARG	N-CA	-8.02	1.36	1.46
2	B	426	LYS	CE-NZ	8.02	1.73	1.49
2	B	908	GLU	CB-CG	8.02	1.76	1.52
2	B	945	GLU	CA-C	8.02	1.63	1.52
2	B	965	LYS	CD-CE	8.02	1.76	1.52
2	B	658	ILE	N-CA	-8.02	1.35	1.46
1	A	65	LEU	CA-C	8.02	1.63	1.52
1	A	1216	ILE	CA-CB	-8.02	1.44	1.54
2	B	536	VAL	CA-C	-8.02	1.43	1.52
2	B	739	THR	CA-CB	-8.02	1.42	1.54
2	B	788	ARG	CD-NE	-8.02	1.35	1.46
2	B	1148	LYS	C-O	-8.01	1.14	1.24
1	A	177	ASP	C-O	8.01	1.34	1.24
2	B	102	VAL	CA-CB	8.01	1.65	1.54
1	A	369	SER	C-O	8.01	1.34	1.24
1	A	879	GLU	CD-OE1	8.01	1.40	1.25
6	H	92	ASP	CA-CB	8.01	1.64	1.53
2	B	975	GLN	C-O	-8.01	1.14	1.23
2	B	418	LYS	CG-CD	8.01	1.76	1.52
2	B	998	ASP	CA-CB	-8.01	1.40	1.53
5	F	78	GLN	CG-CD	8.01	1.72	1.52
4	E	129	PRO	CB-CG	8.00	1.82	1.51
7	I	94	ASP	CG-OD2	8.00	1.40	1.25
9	K	44	ASN	C-O	8.00	1.34	1.24
1	A	214	ILE	C-O	8.00	1.34	1.24
2	B	1185	CYS	CA-CB	8.00	1.67	1.53
7	I	54	GLU	CD-OE1	8.00	1.40	1.25
1	A	750	GLY	C-N	-8.00	1.21	1.33
1	A	1435	PRO	CA-CB	-8.00	1.44	1.53
10	L	50	ASP	N-CA	8.00	1.56	1.46
1	A	833	GLU	CD-OE1	8.00	1.40	1.25
7	I	11	ASN	CG-OD1	-8.00	1.08	1.23
2	B	254	LEU	N-CA	-8.00	1.35	1.46
2	B	727	LYS	CA-C	-8.00	1.41	1.53
2	B	1061	GLU	CD-OE2	8.00	1.40	1.25
1	A	1202	MET	SD-CE	7.99	1.99	1.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	LYS	CG-CD	7.99	1.76	1.52
1	A	759	ALA	CA-C	-7.99	1.42	1.52
2	B	879	ARG	CD-NE	7.99	1.57	1.46
8	J	54	VAL	N-CA	-7.99	1.36	1.46
9	K	2	ASN	CA-C	7.99	1.64	1.52
2	B	187	SER	CA-C	7.99	1.63	1.52
1	A	130	ASP	C-O	-7.99	1.14	1.24
1	A	923	LEU	CA-C	-7.98	1.41	1.52
1	A	167	CYS	CA-CB	7.98	1.67	1.53
1	A	408	ASP	C-O	7.98	1.34	1.24
1	A	1311	VAL	CA-C	-7.98	1.42	1.52
1	A	126	LEU	C-O	7.98	1.34	1.24
1	A	568	PRO	CA-C	-7.98	1.39	1.52
1	A	1098	VAL	CA-CB	-7.97	1.43	1.54
6	H	86	ASP	CA-CB	7.97	1.67	1.53
6	H	96	VAL	C-O	7.97	1.32	1.24
7	I	30	ARG	CG-CD	7.97	1.76	1.52
2	B	782	LEU	CG-CD2	-7.97	1.26	1.52
4	E	78	LEU	CA-C	-7.97	1.42	1.52
4	E	91	LYS	C-O	7.97	1.33	1.24
1	A	1127	ASP	CA-CB	7.97	1.64	1.52
1	A	12	ARG	C-O	-7.97	1.14	1.23
1	A	601	LYS	CE-NZ	7.97	1.73	1.49
1	A	1159	ARG	CA-CB	7.97	1.65	1.53
2	B	125	SER	CA-C	7.97	1.62	1.52
2	B	177	LYS	C-O	7.97	1.34	1.24
2	B	501	PRO	CA-C	-7.97	1.43	1.52
4	E	129	PRO	CG-CD	7.97	1.73	1.51
9	K	5	ASP	CA-C	7.97	1.62	1.52
2	B	254	LEU	CA-C	-7.96	1.43	1.52
9	K	81	TYR	C-O	-7.96	1.15	1.24
1	A	586	ILE	CA-C	-7.96	1.42	1.52
1	A	53	LEU	CG-CD1	7.96	1.78	1.52
2	B	306	ASN	N-CA	7.96	1.56	1.46
2	B	811	TYR	CE2-CZ	-7.96	1.19	1.38
4	E	106	GLN	CA-CB	7.96	1.68	1.53
2	B	795	ILE	C-O	-7.96	1.16	1.24
10	L	41	SER	C-O	7.96	1.34	1.24
2	B	489	SER	C-N	-7.96	1.23	1.34
8	J	14	VAL	N-CA	-7.96	1.36	1.46
2	B	434	ARG	NE-CZ	7.95	1.41	1.33
1	A	248	PRO	CB-CG	7.95	1.89	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	102	GLU	C-O	7.95	1.34	1.24
9	K	21	ILE	CB-CG2	-7.95	1.26	1.52
1	A	47	ARG	N-CA	7.95	1.56	1.46
1	A	301	ALA	C-O	-7.95	1.14	1.24
1	A	305	ASP	CA-C	7.95	1.69	1.52
1	A	1204	ASP	CA-C	-7.95	1.42	1.52
2	B	169	ARG	CA-C	7.95	1.61	1.52
2	B	225	VAL	CA-CB	-7.95	1.44	1.54
1	A	999	VAL	CA-C	-7.95	1.45	1.52
1	A	1034	GLU	CA-CB	-7.95	1.41	1.53
1	A	1435	PRO	N-CA	-7.95	1.38	1.47
2	B	979	LYS	CB-CG	-7.95	1.28	1.52
2	B	742	GLU	CD-OE2	-7.95	1.10	1.25
1	A	1230	GLU	N-CA	7.95	1.56	1.45
2	B	38	PHE	CG-CD1	-7.95	1.22	1.38
4	E	183	PRO	N-CA	-7.95	1.37	1.47
1	A	222	LEU	C-O	7.94	1.34	1.24
1	A	1136	SER	C-O	7.94	1.34	1.24
2	B	769	TYR	CA-C	-7.94	1.42	1.52
3	C	103	ALA	CA-C	-7.94	1.42	1.52
5	F	81	THR	CA-C	7.94	1.64	1.53
1	A	792	TYR	CA-C	-7.94	1.41	1.52
1	A	999	VAL	N-CA	-7.94	1.37	1.46
2	B	1163	CYS	N-CA	7.94	1.55	1.46
1	A	690	VAL	CA-CB	7.93	1.63	1.54
2	B	21	GLU	CD-OE2	7.93	1.40	1.25
4	E	51	GLY	CA-C	7.93	1.62	1.51
1	A	412	ARG	CG-CD	7.93	1.76	1.52
2	B	573	GLN	N-CA	7.93	1.56	1.45
3	C	210	GLU	CD-OE1	7.93	1.40	1.25
2	B	502	ILE	N-CA	7.93	1.61	1.46
1	A	1238	ILE	C-O	-7.93	1.15	1.24
1	A	1449	SER	CA-C	7.93	1.62	1.52
5	F	87	LYS	CE-NZ	7.93	1.73	1.49
1	A	1066	VAL	C-N	-7.93	1.23	1.33
1	A	1378	GLN	C-N	-7.93	1.20	1.33
10	L	51	CYS	N-CA	7.93	1.56	1.46
2	B	298	LEU	N-CA	-7.92	1.35	1.46
2	B	523	CYS	C-O	-7.92	1.13	1.23
2	B	423	LYS	CD-CE	7.92	1.76	1.52
2	B	811	TYR	CA-CB	7.92	1.66	1.53
5	F	90	ARG	CD-NE	7.92	1.57	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	14	LEU	C-O	-7.92	1.14	1.23
1	A	1092	LYS	CG-CD	7.92	1.76	1.52
2	B	213	ILE	CA-CB	-7.92	1.44	1.54
2	B	995	ARG	N-CA	7.92	1.56	1.45
1	A	112	LYS	CA-C	-7.92	1.43	1.52
3	C	136	ASP	N-CA	-7.92	1.35	1.46
2	B	31	TRP	CD2-CE3	-7.92	1.27	1.40
2	B	1132	GLU	N-CA	-7.92	1.35	1.46
1	A	1214	GLU	CA-CB	7.91	1.66	1.53
4	E	20	LYS	CD-CE	7.91	1.76	1.52
2	B	209	GLU	CA-CB	-7.91	1.41	1.53
1	A	917	SER	CA-CB	-7.91	1.41	1.53
1	A	1005	GLU	CD-OE1	7.91	1.40	1.25
1	A	1305	VAL	CA-C	-7.91	1.42	1.52
2	B	833	TYR	CA-C	-7.91	1.41	1.52
3	C	207	CYS	CA-C	7.91	1.62	1.52
3	C	211	ASP	CG-OD1	7.91	1.40	1.25
3	C	255	VAL	CB-CG2	-7.91	1.26	1.52
2	B	804	GLY	CA-C	-7.91	1.40	1.51
2	B	954	VAL	C-O	7.91	1.31	1.24
1	A	962	ARG	CG-CD	7.91	1.76	1.52
2	B	838	SER	CB-OG	-7.91	1.26	1.42
7	I	102	VAL	N-CA	7.91	1.56	1.46
1	A	120	GLU	CD-OE1	7.90	1.40	1.25
1	A	633	VAL	CB-CG2	7.90	1.78	1.52
2	B	754	SER	C-N	-7.90	1.24	1.34
7	I	51	ASN	CB-CG	7.90	1.71	1.52
1	A	1293	SER	CB-OG	-7.90	1.26	1.42
2	B	540	SER	C-O	-7.90	1.12	1.23
2	B	565	PRO	C-O	-7.90	1.15	1.23
5	F	79	ARG	CD-NE	-7.90	1.35	1.46
1	A	1226	VAL	N-CA	7.90	1.56	1.46
1	A	1080	THR	C-O	7.89	1.33	1.24
4	E	106	GLN	CG-CD	7.89	1.71	1.52
1	A	705	LYS	CG-CD	7.89	1.76	1.52
1	A	694	THR	C-O	7.89	1.33	1.24
1	A	1239	ARG	N-CA	-7.89	1.36	1.46
1	A	1281	ARG	N-CA	7.89	1.56	1.45
1	A	1340	GLY	C-O	-7.89	1.15	1.23
1	A	363	GLN	C-N	-7.89	1.22	1.33
1	A	448	PRO	CG-CD	-7.89	1.30	1.51
1	A	1225	PHE	CG-CD1	7.89	1.55	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	CYS	N-CA	7.89	1.56	1.46
1	A	397	ASN	N-CA	-7.88	1.35	1.45
1	A	1114	PRO	N-CD	-7.88	1.36	1.47
2	B	90	ILE	N-CA	7.88	1.56	1.46
1	A	109	HIS	CG-ND1	7.88	1.47	1.38
1	A	1111	MET	CA-C	-7.88	1.41	1.53
3	C	86	CYS	CA-C	-7.88	1.42	1.52
6	H	126	GLU	C-O	7.88	1.33	1.23
1	A	599	SER	CA-C	-7.88	1.43	1.52
1	A	731	ARG	N-CA	-7.88	1.36	1.46
1	A	408	ASP	N-CA	-7.88	1.36	1.46
1	A	720	ARG	CA-CB	7.88	1.65	1.53
2	B	113	TYR	CA-C	7.88	1.63	1.52
3	C	220	ASP	CG-OD1	7.88	1.40	1.25
3	C	174	ALA	N-CA	-7.88	1.36	1.46
7	I	86	PHE	N-CA	-7.88	1.35	1.46
4	E	158	SER	N-CA	-7.88	1.35	1.46
1	A	116	ASP	CA-C	-7.87	1.42	1.52
1	A	1156	PRO	C-O	7.87	1.33	1.24
1	A	1238	ILE	CB-CG2	7.87	1.78	1.52
1	A	1059	HIS	CG-ND1	-7.87	1.29	1.38
9	K	44	ASN	CA-C	7.87	1.63	1.52
4	E	154	ILE	CA-CB	-7.87	1.44	1.54
9	K	73	LEU	N-CA	7.87	1.55	1.46
1	A	1323	ASP	C-N	-7.87	1.25	1.34
2	B	568	ASP	CA-CB	7.87	1.67	1.53
2	B	815	ARG	C-O	-7.87	1.13	1.24
2	B	1045	SER	CA-CB	-7.87	1.41	1.53
3	C	71	PRO	C-O	-7.87	1.15	1.23
4	E	202	SER	CA-C	-7.87	1.42	1.52
1	A	40	THR	C-O	7.86	1.33	1.24
1	A	167	CYS	N-CA	7.86	1.56	1.46
1	A	1262	LYS	CB-CG	7.86	1.76	1.52
8	J	21	TYR	C-O	-7.86	1.14	1.23
10	L	67	PHE	CA-C	-7.86	1.42	1.52
1	A	623	GLY	C-O	7.86	1.31	1.23
7	I	90	GLN	C-O	-7.86	1.12	1.23
1	A	640	GLN	C-O	-7.86	1.14	1.24
1	A	1121	GLU	C-O	-7.86	1.14	1.24
2	B	592	ASN	CG-ND2	7.86	1.49	1.33
2	B	782	LEU	CG-CD1	-7.86	1.26	1.52
4	E	138	ALA	CA-C	-7.86	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	42	PRO	CA-C	-7.86	1.42	1.52
3	C	252	GLN	C-O	-7.86	1.14	1.24
1	A	137	ALA	C-O	7.85	1.33	1.24
1	A	142	CYS	C-O	7.85	1.33	1.23
3	C	169	LYS	C-O	-7.85	1.14	1.24
10	L	40	LEU	CG-CD2	7.85	1.78	1.52
1	A	1368	MET	C-O	-7.85	1.13	1.24
2	B	326	ASP	N-CA	-7.85	1.35	1.45
9	K	94	ILE	CB-CG2	-7.85	1.26	1.52
2	B	801	LYS	CA-C	-7.85	1.42	1.52
1	A	1027	ALA	N-CA	-7.84	1.35	1.45
3	C	55	THR	C-O	7.84	1.34	1.24
4	E	135	PHE	CG-CD1	-7.84	1.22	1.38
4	E	208	TYR	CZ-OH	7.84	1.54	1.38
3	C	171	GLY	N-CA	7.84	1.55	1.44
4	E	122	LYS	CA-C	7.84	1.63	1.52
1	A	1301	GLU	CA-CB	7.84	1.65	1.53
5	F	82	THR	C-O	-7.84	1.13	1.23
1	A	263	THR	C-O	7.84	1.33	1.23
1	A	981	LEU	C-O	-7.84	1.14	1.23
2	B	948	ILE	C-O	-7.84	1.14	1.24
1	A	736	ASN	N-CA	-7.83	1.35	1.46
2	B	1019	SER	CB-OG	-7.83	1.26	1.42
1	A	652	VAL	CA-CB	-7.83	1.44	1.54
2	B	178	ASN	CA-C	-7.83	1.41	1.52
2	B	1030	LEU	CA-CB	-7.83	1.41	1.53
6	H	93	TYR	N-CA	7.83	1.54	1.45
1	A	1325	THR	CB-OG1	7.83	1.56	1.43
2	B	592	ASN	CB-CG	7.83	1.71	1.52
3	C	249	ASP	CA-C	7.83	1.62	1.52
3	C	12	GLU	CD-OE2	7.83	1.40	1.25
4	E	103	LYS	CA-CB	7.83	1.64	1.53
2	B	103	ASN	CA-CB	7.83	1.66	1.53
2	B	277	LYS	CA-C	-7.83	1.42	1.52
1	A	827	THR	CA-C	-7.82	1.42	1.52
1	A	491	VAL	CB-CG1	-7.82	1.26	1.52
1	A	628	GLY	N-CA	7.82	1.53	1.45
1	A	604	GLY	CA-C	-7.82	1.40	1.52
1	A	1351	GLU	CD-OE2	7.82	1.40	1.25
2	B	1064	TYR	CG-CD2	-7.82	1.23	1.39
1	A	207	ILE	C-O	-7.82	1.15	1.24
1	A	223	GLY	C-O	7.82	1.35	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	942	PHE	CA-C	-7.82	1.41	1.52
2	B	65	GLU	CD-OE2	7.82	1.40	1.25
4	E	213	ILE	CA-CB	-7.82	1.44	1.54
1	A	1288	ASP	C-O	7.82	1.33	1.23
2	B	385	LEU	C-O	-7.82	1.15	1.24
2	B	514	LEU	CA-C	-7.81	1.43	1.52
2	B	569	TYR	CE1-CZ	-7.81	1.19	1.38
1	A	893	PHE	CE1-CZ	-7.81	1.15	1.38
2	B	573	GLN	CG-CD	7.81	1.71	1.52
1	A	920	LEU	CG-CD2	-7.81	1.26	1.52
2	B	802	PRO	C-O	-7.81	1.15	1.23
3	C	37	MET	CG-SD	-7.81	1.61	1.80
4	E	111	VAL	N-CA	7.81	1.56	1.46
1	A	751	SER	C-O	-7.81	1.13	1.24
2	B	710	LEU	CG-CD1	-7.81	1.26	1.52
1	A	531	ILE	CA-CB	-7.81	1.44	1.54
2	B	270	LYS	CE-NZ	7.81	1.72	1.49
2	B	530	GLY	C-O	7.80	1.33	1.24
2	B	1083	ALA	N-CA	7.80	1.55	1.46
4	E	3	GLN	N-CA	7.80	1.55	1.46
1	A	658	LEU	CG-CD1	-7.80	1.26	1.52
2	B	993	THR	N-CA	7.80	1.55	1.45
3	C	15	LYS	CE-NZ	7.80	1.72	1.49
1	A	298	PHE	N-CA	7.80	1.56	1.46
1	A	572	TRP	CZ2-CH2	-7.80	1.22	1.37
1	A	827	THR	C-N	-7.80	1.23	1.33
1	A	1193	LEU	N-CA	7.80	1.55	1.46
1	A	1267	MET	N-CA	7.80	1.55	1.46
2	B	324	ILE	N-CA	-7.80	1.36	1.46
2	B	373	ARG	CZ-NH1	7.80	1.43	1.32
4	E	82	PHE	CE2-CZ	7.80	1.62	1.38
4	E	45	LYS	CG-CD	7.80	1.75	1.52
2	B	411	PRO	N-CA	-7.80	1.37	1.47
8	J	62	ARG	C-N	-7.80	1.22	1.33
1	A	1264	GLU	CD-OE2	-7.79	1.10	1.25
7	I	117	LYS	CD-CE	7.79	1.75	1.52
2	B	371	GLU	CG-CD	7.79	1.71	1.52
2	B	556	THR	CA-C	7.79	1.62	1.52
1	A	802	ASN	C-O	-7.79	1.14	1.23
1	A	646	PHE	N-CA	7.79	1.55	1.46
1	A	1129	GLU	CD-OE2	7.79	1.40	1.25
1	A	1169	ILE	CA-C	-7.79	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	420	ARG	C-N	-7.79	1.23	1.33
6	H	130	ARG	C-O	7.79	1.32	1.23
2	B	412	LEU	CA-C	-7.79	1.42	1.52
2	B	536	VAL	CB-CG1	-7.79	1.26	1.52
9	K	71	PHE	C-O	7.79	1.33	1.23
2	B	831	SER	C-O	-7.78	1.14	1.24
1	A	1305	VAL	C-N	-7.78	1.22	1.33
1	A	382	PRO	CA-C	-7.78	1.40	1.52
1	A	983	ILE	C-N	-7.78	1.22	1.33
3	C	209	TYR	CE2-CZ	7.78	1.56	1.38
2	B	292	ILE	CA-CB	-7.78	1.44	1.54
3	C	214	ASN	CA-C	7.78	1.62	1.52
1	A	801	GLU	CA-C	-7.78	1.42	1.52
1	A	895	LYS	CE-NZ	7.77	1.72	1.49
1	A	286	HIS	CB-CG	7.77	1.61	1.50
1	A	569	LYS	CE-NZ	7.77	1.72	1.49
2	B	60	GLN	N-CA	-7.77	1.36	1.46
5	F	90	ARG	CZ-NH2	-7.77	1.23	1.33
1	A	430	TRP	CE2-CZ2	-7.77	1.23	1.39
2	B	611	PRO	C-O	-7.77	1.13	1.24
1	A	1426	GLU	CD-OE1	7.77	1.40	1.25
2	B	1129	ARG	C-O	7.77	1.33	1.23
3	C	56	THR	CB-CG2	-7.77	1.26	1.52
3	C	267	GLN	CG-CD	7.77	1.71	1.52
1	A	1269	GLU	C-N	-7.77	1.24	1.33
1	A	1337	GLU	CG-CD	7.76	1.71	1.52
1	A	1367	HIS	C-O	-7.76	1.12	1.23
2	B	180	TYR	N-CA	-7.76	1.35	1.46
2	B	1127	GLY	N-CA	7.76	1.57	1.45
2	B	459	TYR	N-CA	-7.76	1.36	1.46
1	A	1103	GLU	CD-OE2	7.76	1.40	1.25
2	B	59	LEU	N-CA	-7.76	1.38	1.46
2	B	1096	ARG	CA-C	-7.76	1.42	1.53
7	I	31	THR	CA-CB	-7.76	1.42	1.53
10	L	53	HIS	CA-C	7.76	1.62	1.52
10	L	63	ARG	CA-CB	7.76	1.66	1.53
1	A	1267	MET	C-N	-7.75	1.22	1.33
2	B	1074	ASN	CA-C	-7.75	1.42	1.52
2	B	1138	MET	CG-SD	-7.75	1.61	1.80
4	E	21	GLU	CA-CB	-7.75	1.41	1.53
1	A	1144	LYS	N-CA	-7.75	1.36	1.46
2	B	1039	GLY	C-O	-7.75	1.13	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	LEU	CA-C	7.75	1.61	1.52
1	A	1112	LYS	CB-CG	7.75	1.75	1.52
2	B	459	TYR	CD1-CE1	7.75	1.61	1.38
5	F	80	ALA	C-N	-7.75	1.23	1.33
2	B	599	THR	C-O	-7.75	1.15	1.24
3	C	21	ILE	CA-CB	-7.75	1.44	1.54
1	A	553	VAL	CA-CB	-7.74	1.44	1.54
1	A	1093	LYS	N-CA	7.74	1.56	1.46
4	E	207	ARG	CA-C	-7.74	1.43	1.52
1	A	143	LYS	CG-CD	7.74	1.75	1.52
2	B	435	THR	C-O	7.74	1.32	1.23
2	B	658	ILE	CA-C	-7.74	1.41	1.52
2	B	800	GLN	CD-NE2	7.74	1.49	1.33
2	B	982	SER	C-O	-7.74	1.15	1.23
3	C	254	LYS	C-O	-7.74	1.15	1.24
1	A	1038	THR	C-O	-7.74	1.13	1.23
2	B	261	ARG	N-CA	7.74	1.54	1.45
2	B	1031	LEU	CA-CB	-7.74	1.40	1.53
2	B	1064	TYR	N-CA	7.74	1.55	1.45
1	A	264	PHE	CG-CD2	7.74	1.55	1.38
1	A	1218	GLN	CG-CD	7.74	1.71	1.52
2	B	345	LYS	CA-CB	-7.74	1.41	1.53
4	E	132	ILE	N-CA	-7.74	1.37	1.46
2	B	792	MET	CG-SD	7.73	2.00	1.80
6	H	116	TYR	CA-C	7.73	1.63	1.52
1	A	1301	GLU	CD-OE1	7.73	1.40	1.25
1	A	1383	SER	N-CA	-7.73	1.35	1.45
2	B	737	THR	CB-CG2	-7.73	1.27	1.52
1	A	713	SER	N-CA	-7.73	1.36	1.46
2	B	214	ALA	N-CA	-7.73	1.36	1.46
2	B	641	GLU	CD-OE2	7.73	1.40	1.25
2	B	135	ARG	CD-NE	7.72	1.57	1.46
2	B	1045	SER	C-N	-7.72	1.23	1.33
3	C	86	CYS	CA-CB	7.72	1.64	1.53
4	E	137	GLU	CD-OE1	7.72	1.40	1.25
3	C	145	CYS	N-CA	-7.72	1.35	1.46
2	B	842	ASN	CG-ND2	-7.72	1.17	1.33
1	A	753	GLY	C-O	-7.72	1.12	1.23
2	B	865	LYS	CA-C	7.72	1.63	1.52
1	A	682	THR	CA-C	-7.72	1.42	1.52
6	H	20	TYR	CE2-CZ	-7.72	1.19	1.38
1	A	1067	LEU	CB-CG	-7.71	1.38	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	57	TYR	C-O	-7.71	1.14	1.24
2	B	838	SER	N-CA	-7.71	1.35	1.45
3	C	75	MET	CG-SD	-7.71	1.61	1.80
1	A	220	THR	CB-OG1	7.71	1.56	1.43
1	A	567	LYS	CD-CE	7.71	1.75	1.52
2	B	309	GLN	C-O	-7.71	1.15	1.24
1	A	592	ASP	CA-C	7.71	1.63	1.52
1	A	708	MET	CB-CG	-7.71	1.29	1.52
1	A	1145	SER	C-O	-7.71	1.14	1.24
2	B	628	THR	C-O	7.71	1.34	1.24
9	K	102	LYS	CA-C	7.71	1.63	1.52
3	C	180	TYR	CG-CD1	-7.71	1.23	1.39
4	E	168	TYR	CE2-CZ	-7.71	1.19	1.38
9	K	52	ASN	N-CA	-7.70	1.36	1.46
1	A	87	ALA	C-O	-7.70	1.15	1.24
1	A	429	GLY	C-O	7.70	1.35	1.24
1	A	1239	ARG	CZ-NH1	7.70	1.43	1.32
2	B	1078	GLY	C-N	-7.70	1.23	1.33
9	K	19	LEU	CB-CG	-7.70	1.38	1.53
4	E	9	ILE	C-O	7.70	1.32	1.24
1	A	885	THR	CA-C	7.69	1.63	1.52
2	B	166	PHE	CB-CG	-7.69	1.32	1.50
2	B	695	ALA	N-CA	-7.69	1.36	1.46
4	E	121	MET	CG-SD	7.69	2.00	1.80
1	A	143	LYS	C-O	7.69	1.33	1.24
2	B	48	LEU	CG-CD2	-7.69	1.27	1.52
1	A	387	ARG	C-O	7.69	1.33	1.24
7	I	37	GLU	CA-C	-7.69	1.42	1.53
2	B	21	GLU	CA-C	-7.69	1.42	1.52
2	B	271	ALA	CA-CB	-7.69	1.34	1.54
2	B	551	PRO	N-CD	-7.69	1.36	1.47
2	B	1102	LYS	C-N	7.69	1.44	1.33
1	A	117	GLU	CD-OE1	7.69	1.40	1.25
5	F	81	THR	C-O	-7.69	1.13	1.23
6	H	20	TYR	CG-CD1	-7.69	1.23	1.39
2	B	794	ASN	N-CA	-7.68	1.36	1.46
4	E	31	THR	N-CA	-7.68	1.36	1.45
4	E	127	ILE	C-O	7.68	1.34	1.24
4	E	209	ALA	CA-C	-7.68	1.43	1.52
8	J	41	LEU	CG-CD2	-7.68	1.27	1.52
6	H	7	ASP	CA-C	-7.68	1.42	1.52
1	A	1283	VAL	CA-C	7.68	1.62	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	463	THR	CA-CB	-7.68	1.41	1.53
2	B	700	SER	C-N	-7.68	1.23	1.33
1	A	1147	THR	C-N	-7.68	1.24	1.33
1	A	1360	GLY	CA-C	7.68	1.63	1.51
1	A	423	ASP	CG-OD1	7.68	1.40	1.25
1	A	934	LYS	CE-NZ	7.68	1.72	1.49
1	A	994	GLN	CA-C	-7.68	1.42	1.52
2	B	379	GLY	CA-C	-7.68	1.43	1.52
1	A	66	LYS	CB-CG	7.67	1.75	1.52
1	A	686	ALA	C-N	-7.67	1.23	1.34
5	F	153	VAL	CA-CB	-7.67	1.44	1.53
2	B	360	PHE	CG-CD2	-7.67	1.22	1.38
5	F	122	MET	C-O	7.67	1.33	1.24
1	A	77	CYS	C-O	7.67	1.34	1.24
1	A	649	ILE	C-O	7.67	1.33	1.24
2	B	264	SER	CA-C	7.67	1.63	1.52
7	I	73	ARG	NE-CZ	7.67	1.41	1.33
5	F	108	PHE	C-O	-7.67	1.14	1.24
6	H	3	ASN	CB-CG	7.67	1.71	1.52
2	B	54	PHE	C-N	-7.67	1.24	1.33
2	B	1177	HIS	CB-CG	-7.67	1.39	1.50
1	A	617	VAL	CA-CB	-7.66	1.45	1.53
2	B	585	VAL	N-CA	7.66	1.55	1.46
2	B	694	ASP	CB-CG	7.66	1.71	1.52
4	E	161	LYS	CA-CB	-7.66	1.41	1.53
1	A	482	PHE	CE1-CZ	-7.66	1.15	1.38
1	A	1047	SER	C-O	7.66	1.33	1.24
2	B	487	THR	CA-C	-7.66	1.43	1.52
4	E	209	ALA	C-O	-7.66	1.14	1.24
1	A	783	THR	C-O	-7.66	1.14	1.24
2	B	1043	ASP	C-N	-7.66	1.23	1.33
1	A	61	ILE	CB-CG2	7.65	1.77	1.52
2	B	370	PHE	CA-CB	7.65	1.66	1.53
2	B	906	SER	N-CA	-7.65	1.37	1.46
2	B	965	LYS	CE-NZ	7.65	1.72	1.49
1	A	472	LEU	CB-CG	-7.65	1.38	1.53
2	B	969	ARG	CD-NE	-7.65	1.35	1.46
4	E	52	ARG	CZ-NH1	7.65	1.43	1.32
2	B	228	LYS	CB-CG	7.65	1.75	1.52
9	K	19	LEU	CA-C	7.65	1.61	1.52
2	B	1035	ALA	CA-C	-7.64	1.42	1.52
2	B	1220	ARG	CA-C	7.64	1.63	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	23	ASN	CB-CG	7.64	1.71	1.52
1	A	596	THR	CB-CG2	7.64	1.77	1.52
2	B	1197	PRO	C-O	-7.64	1.14	1.23
10	L	66	GLN	CD-NE2	7.64	1.49	1.33
1	A	359	LEU	CG-CD2	-7.64	1.27	1.52
1	A	836	TYR	CA-CB	-7.64	1.40	1.53
1	A	1056	SER	CA-CB	-7.64	1.40	1.53
2	B	61	ASP	N-CA	-7.64	1.36	1.46
4	E	1	MET	CB-CG	7.64	1.75	1.52
5	F	129	LYS	CG-CD	7.64	1.75	1.52
1	A	878	ILE	CB-CG1	-7.64	1.38	1.53
3	C	194	GLU	CD-OE2	7.64	1.39	1.25
3	C	4	GLU	CA-C	-7.63	1.42	1.52
1	A	192	GLY	CA-C	7.63	1.64	1.52
2	B	388	CYS	C-O	-7.63	1.14	1.24
4	E	137	GLU	N-CA	7.63	1.55	1.46
2	B	1026	LEU	N-CA	-7.63	1.36	1.46
1	A	215	SER	C-N	7.63	1.43	1.33
1	A	764	CYS	CA-CB	-7.63	1.41	1.53
1	A	933	TYR	CE2-CZ	-7.63	1.20	1.38
2	B	515	HIS	N-CA	7.63	1.55	1.46
2	B	904	ARG	CD-NE	-7.63	1.35	1.46
9	K	93	SER	CB-OG	7.63	1.57	1.42
3	C	79	GLN	N-CA	-7.63	1.36	1.46
3	C	132	PRO	C-O	-7.63	1.14	1.24
2	B	781	PHE	CA-CB	-7.62	1.40	1.53
2	B	956	THR	CA-CB	-7.62	1.39	1.53
1	A	1147	THR	CB-CG2	-7.62	1.27	1.52
4	E	14	ARG	CA-CB	-7.62	1.41	1.53
7	I	4	PHE	CA-C	-7.62	1.42	1.52
1	A	179	LEU	C-O	7.62	1.34	1.24
2	B	884	ARG	CG-CD	7.62	1.75	1.52
3	C	47	ASP	CG-OD2	7.62	1.39	1.25
8	J	50	ILE	CG1-CD1	-7.62	1.22	1.51
2	B	914	LYS	C-N	7.62	1.43	1.33
4	E	41	ASP	CA-C	7.62	1.62	1.52
3	C	4	GLU	CD-OE1	7.62	1.39	1.25
7	I	3	THR	CB-CG2	7.62	1.77	1.52
1	A	1417	GLU	CG-CD	7.61	1.71	1.52
4	E	62	ALA	CA-C	-7.61	1.42	1.52
7	I	24	ARG	CD-NE	7.61	1.56	1.46
8	J	52	THR	CA-CB	-7.61	1.42	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	240	ILE	CA-CB	-7.61	1.41	1.55
2	B	862	GLN	CA-C	-7.61	1.42	1.53
2	B	880	THR	CB-CG2	7.61	1.77	1.52
2	B	1217	TYR	CA-C	7.61	1.62	1.52
4	E	17	ARG	CZ-NH2	7.61	1.43	1.33
1	A	787	PHE	N-CA	-7.61	1.35	1.45
2	B	757	PRO	N-CA	-7.61	1.38	1.47
2	B	803	LEU	CA-C	-7.61	1.42	1.52
1	A	784	LEU	C-O	-7.61	1.16	1.24
4	E	2	ASP	CA-C	7.61	1.62	1.52
1	A	600	PRO	CA-C	-7.61	1.41	1.52
1	A	1164	PRO	C-O	7.61	1.33	1.24
1	A	1196	GLU	N-CA	-7.60	1.37	1.46
2	B	970	THR	C-O	-7.60	1.14	1.23
4	E	179	GLN	CA-C	7.60	1.63	1.53
1	A	914	GLU	CD-OE1	7.60	1.39	1.25
2	B	694	ASP	N-CA	7.60	1.55	1.45
2	B	1096	ARG	NE-CZ	-7.60	1.24	1.33
7	I	7	CYS	N-CA	7.60	1.56	1.46
1	A	1298	TYR	CG-CD2	-7.60	1.23	1.39
9	K	70	ARG	CA-CB	-7.60	1.40	1.53
2	B	745	PRO	N-CD	-7.60	1.37	1.47
2	B	1036	ALA	C-O	-7.60	1.14	1.24
9	K	17	SER	C-O	-7.59	1.14	1.23
2	B	380	TYR	CE2-CZ	-7.59	1.20	1.38
2	B	997	GLU	N-CA	7.59	1.55	1.46
1	A	37	PHE	CD2-CE2	7.59	1.61	1.38
1	A	412	ARG	CA-CB	-7.59	1.43	1.53
2	B	325	GLN	CA-C	7.59	1.62	1.52
2	B	1206	GLU	CD-OE1	7.59	1.39	1.25
1	A	74	MET	CA-C	-7.59	1.42	1.52
1	A	420	ARG	CB-CG	-7.59	1.29	1.52
1	A	757	ASN	CA-CB	-7.59	1.41	1.53
1	A	928	LEU	CA-C	-7.59	1.43	1.52
1	A	1030	ARG	CA-C	-7.59	1.43	1.52
2	B	456	GLY	N-CA	7.59	1.57	1.45
2	B	1095	LEU	C-O	7.59	1.33	1.23
3	C	117	ASP	N-CA	-7.59	1.35	1.46
1	A	387	ARG	CZ-NH2	-7.59	1.23	1.33
1	A	896	ARG	NE-CZ	-7.59	1.24	1.33
2	B	493	SER	N-CA	-7.59	1.37	1.46
4	E	63	ASN	CG-OD1	7.59	1.38	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1224	PHE	CD1-CE1	7.58	1.61	1.38
3	C	51	VAL	C-N	-7.58	1.23	1.33
1	A	909	ASP	C-N	-7.58	1.26	1.33
2	B	43	LEU	C-O	-7.58	1.14	1.24
3	C	76	ASP	CA-C	7.58	1.63	1.52
9	K	97	LYS	C-N	-7.58	1.23	1.33
2	B	479	VAL	CB-CG1	-7.58	1.27	1.52
2	B	1222	ARG	CD-NE	-7.58	1.35	1.46
2	B	731	VAL	CA-C	-7.58	1.42	1.52
6	H	34	ASP	CA-CB	7.58	1.66	1.53
4	E	175	LEU	C-N	-7.58	1.24	1.33
6	H	43	ASN	CB-CG	7.58	1.71	1.52
1	A	987	VAL	CA-C	-7.57	1.44	1.52
2	B	116	GLU	C-O	-7.57	1.14	1.24
2	B	319	GLU	CD-OE1	7.57	1.39	1.25
2	B	841	MET	CA-C	7.56	1.61	1.52
1	A	552	TRP	C-O	-7.56	1.14	1.24
1	A	1018	PHE	CD1-CE1	7.56	1.61	1.38
2	B	1100	ASP	N-CA	7.56	1.55	1.46
2	B	1131	GLY	C-O	7.56	1.30	1.23
4	E	13	TRP	C-O	7.56	1.33	1.24
4	E	26	ARG	CZ-NH2	-7.56	1.23	1.33
8	J	2	ILE	CA-C	-7.56	1.43	1.52
9	K	85	ASP	CB-CG	7.56	1.71	1.52
2	B	362	PRO	CB-CG	-7.56	1.11	1.49
4	E	2	ASP	C-O	7.56	1.33	1.24
7	I	80	SER	CA-C	-7.56	1.43	1.52
2	B	165	VAL	CA-C	7.56	1.62	1.52
6	H	21	ASN	CA-CB	-7.56	1.41	1.53
1	A	149	GLU	CD-OE2	7.56	1.39	1.25
2	B	458	LYS	C-O	-7.56	1.14	1.24
1	A	452	LYS	C-O	-7.55	1.14	1.24
1	A	666	ILE	CG1-CD1	-7.55	1.22	1.51
1	A	1162	VAL	CB-CG1	7.55	1.77	1.52
3	C	154	LYS	N-CA	-7.55	1.36	1.46
4	E	34	GLU	CG-CD	7.55	1.71	1.52
8	J	43	ARG	N-CA	7.55	1.55	1.46
1	A	897	TYR	C-O	-7.55	1.14	1.24
2	B	1156	ASP	N-CA	7.55	1.55	1.45
8	J	26	GLN	CD-NE2	7.55	1.49	1.33
1	A	953	ASN	CG-OD1	7.55	1.37	1.23
9	K	20	LYS	CA-C	-7.55	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	545	ILE	CA-C	7.55	1.61	1.52
1	A	368	LYS	C-O	-7.55	1.15	1.24
2	B	99	LYS	CD-CE	7.55	1.75	1.52
1	A	1372	VAL	CA-C	7.54	1.62	1.52
2	B	250	PHE	N-CA	7.54	1.55	1.46
2	B	776	GLN	C-N	-7.54	1.22	1.33
4	E	200	ARG	C-O	-7.54	1.14	1.23
7	I	16	PRO	CA-CB	7.54	1.63	1.53
1	A	1255	GLU	CD-OE2	7.54	1.39	1.25
2	B	770	GLN	CG-CD	-7.54	1.33	1.52
2	B	839	MET	CG-SD	7.54	1.99	1.80
2	B	1217	TYR	C-N	7.54	1.45	1.33
1	A	1196	GLU	CD-OE2	7.54	1.39	1.25
2	B	131	ASP	CB-CG	7.54	1.70	1.52
1	A	829	VAL	CB-CG2	7.54	1.77	1.52
1	A	1012	ARG	NE-CZ	7.54	1.41	1.33
1	A	1357	ALA	C-O	7.53	1.33	1.24
9	K	24	ASP	CA-C	-7.53	1.43	1.52
1	A	1206	ASP	CG-OD1	7.53	1.39	1.25
2	B	1097	HIS	CE1-NE2	7.53	1.40	1.32
4	E	165	LEU	C-O	7.53	1.33	1.24
1	A	1384	VAL	C-O	-7.53	1.16	1.23
2	B	1035	ALA	CA-CB	-7.53	1.41	1.53
6	H	39	THR	N-CA	7.53	1.55	1.46
1	A	1280	GLU	CD-OE1	7.53	1.39	1.25
2	B	870	ILE	CB-CG2	7.53	1.77	1.52
10	L	30	ILE	CG1-CD1	7.52	1.81	1.51
1	A	745	GLN	CD-OE1	7.52	1.37	1.23
1	A	138	ILE	N-CA	-7.52	1.37	1.46
2	B	644	GLU	N-CA	-7.52	1.36	1.46
7	I	104	LEU	C-O	-7.52	1.13	1.24
1	A	678	GLU	N-CA	-7.52	1.37	1.46
4	E	113	GLN	CB-CG	7.52	1.75	1.52
1	A	721	PHE	C-O	7.52	1.32	1.24
2	B	875	GLU	CB-CG	7.52	1.75	1.52
4	E	198	ILE	CA-C	-7.52	1.43	1.52
1	A	475	THR	CA-C	-7.51	1.43	1.52
1	A	1443	VAL	C-O	-7.51	1.15	1.24
2	B	201	GLY	C-O	7.51	1.33	1.24
2	B	434	ARG	CD-NE	7.51	1.56	1.46
2	B	1024	ALA	C-O	-7.51	1.15	1.24
7	I	9	ASP	N-CA	-7.51	1.37	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1225	PHE	N-CA	-7.51	1.37	1.46
2	B	199	MET	C-O	-7.51	1.14	1.24
5	F	116	ASP	C-N	-7.51	1.23	1.33
2	B	569	TYR	CA-CB	7.51	1.65	1.53
2	B	307	ASP	N-CA	7.51	1.55	1.46
2	B	525	ALA	C-N	-7.51	1.23	1.33
9	K	14	GLU	N-CA	7.51	1.55	1.46
2	B	262	GLU	CD-OE1	7.50	1.39	1.25
9	K	26	LYS	CB-CG	7.50	1.75	1.52
1	A	369	SER	CA-CB	-7.50	1.41	1.53
7	I	59	VAL	CA-CB	-7.50	1.42	1.54
2	B	855	PHE	CG-CD1	-7.50	1.23	1.38
3	C	15	LYS	CA-CB	7.50	1.66	1.53
6	H	132	LEU	N-CA	7.50	1.55	1.46
2	B	892	LYS	C-O	-7.50	1.14	1.24
3	C	249	ASP	CA-CB	7.50	1.65	1.53
1	A	425	GLN	CA-C	7.50	1.62	1.52
1	A	452	LYS	N-CA	7.50	1.56	1.46
1	A	727	ASP	CA-CB	-7.50	1.41	1.53
1	A	1019	CYS	CA-CB	-7.50	1.40	1.53
2	B	190	TYR	CE2-CZ	-7.50	1.20	1.38
3	C	70	ILE	CA-CB	7.50	1.64	1.53
1	A	913	LEU	CA-C	7.50	1.61	1.52
2	B	521	LEU	C-O	-7.50	1.13	1.23
2	B	743	ILE	C-O	7.50	1.31	1.24
3	C	100	THR	C-O	7.50	1.33	1.23
1	A	447	GLN	CA-C	-7.50	1.43	1.53
1	A	1103	GLU	CA-C	7.50	1.62	1.52
2	B	94	LYS	CB-CG	7.50	1.75	1.52
3	C	71	PRO	N-CD	-7.50	1.37	1.47
8	J	21	TYR	C-N	-7.50	1.23	1.33
1	A	279	LEU	CA-C	-7.49	1.42	1.52
2	B	258	LEU	CA-CB	-7.49	1.43	1.53
3	C	54	ASN	CB-CG	-7.49	1.33	1.52
1	A	685	GLU	N-CA	-7.49	1.36	1.46
1	A	1002	GLY	CA-C	7.49	1.62	1.51
4	E	85	GLU	CD-OE1	7.49	1.39	1.25
9	K	114	LEU	CB-CG	7.49	1.68	1.53
1	A	824	LEU	C-O	-7.49	1.15	1.24
2	B	617	ARG	CA-C	-7.49	1.43	1.52
7	I	97	MET	C-O	7.49	1.33	1.24
1	A	25	GLU	CD-OE1	7.49	1.39	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	142	VAL	N-CA	-7.49	1.37	1.46
1	A	196	GLU	C-O	-7.48	1.14	1.24
1	A	1081	LEU	CG-CD2	7.48	1.77	1.52
3	C	234	SER	CB-OG	7.48	1.57	1.42
1	A	93	VAL	C-N	-7.48	1.22	1.33
1	A	162	VAL	C-O	-7.48	1.16	1.23
1	A	1304	TRP	CE3-CZ3	-7.48	1.16	1.38
3	C	29	MET	C-O	-7.48	1.15	1.24
1	A	348	SER	CA-CB	-7.48	1.40	1.53
2	B	824	ILE	N-CA	-7.48	1.37	1.46
2	B	1053	GLU	CA-C	-7.48	1.43	1.52
1	A	947	PHE	CG-CD1	-7.48	1.23	1.38
1	A	940	ARG	NE-CZ	7.48	1.41	1.33
2	B	106	ASP	CA-CB	7.48	1.66	1.53
5	F	135	ARG	CG-CD	7.48	1.74	1.52
9	K	70	ARG	N-CA	-7.48	1.36	1.45
1	A	274	ILE	CG1-CD1	7.47	1.80	1.51
1	A	581	ALA	CA-CB	-7.47	1.42	1.53
1	A	638	GLY	C-O	-7.47	1.13	1.24
2	B	628	THR	C-N	7.47	1.43	1.33
3	C	68	GLY	CA-C	-7.47	1.41	1.51
3	C	88	CYS	N-CA	7.47	1.55	1.45
2	B	289	LEU	CA-CB	-7.47	1.40	1.53
2	B	400	HIS	CB-CG	-7.47	1.39	1.50
1	A	49	LYS	CE-NZ	7.47	1.71	1.49
1	A	1000	LEU	CA-C	7.47	1.61	1.52
6	H	127	GLY	N-CA	7.47	1.56	1.45
9	K	66	PRO	CA-CB	-7.47	1.41	1.54
9	K	74	ARG	CZ-NH1	-7.47	1.22	1.32
1	A	295	LEU	CA-C	-7.46	1.43	1.52
9	K	36	GLU	CD-OE2	7.46	1.39	1.25
3	C	125	MET	C-O	7.46	1.33	1.24
1	A	388	LEU	CG-CD1	-7.46	1.27	1.52
2	B	987	LYS	CA-C	-7.46	1.42	1.53
3	C	214	ASN	C-O	7.46	1.33	1.24
5	F	93	ILE	C-O	-7.46	1.15	1.24
2	B	770	GLN	CD-OE1	7.46	1.37	1.23
4	E	212	ARG	NE-CZ	-7.46	1.24	1.33
6	H	121	LEU	CA-C	7.46	1.62	1.52
1	A	385	ILE	CA-C	-7.46	1.41	1.52
1	A	1159	ARG	CB-CG	7.46	1.74	1.52
6	H	134	ASN	CA-C	-7.46	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	977	LYS	CG-CD	7.45	1.74	1.52
2	B	284	ILE	CG1-CD1	-7.45	1.22	1.51
2	B	709	ASP	N-CA	-7.45	1.36	1.46
4	E	109	ILE	CB-CG2	-7.45	1.27	1.52
1	A	372	LYS	CD-CE	-7.45	1.30	1.52
2	B	1063	GLY	CA-C	-7.45	1.41	1.51
4	E	195	VAL	C-O	-7.45	1.16	1.24
1	A	120	GLU	CA-CB	7.45	1.66	1.53
3	C	196	ASP	CA-CB	7.45	1.64	1.53
1	A	963	ILE	N-CA	7.45	1.55	1.46
2	B	373	ARG	CA-C	7.45	1.62	1.52
1	A	1203	ASN	CG-OD1	7.44	1.37	1.23
2	B	684	LEU	CA-CB	-7.44	1.41	1.53
1	A	65	LEU	C-O	7.44	1.33	1.24
2	B	115	GLN	CA-C	7.44	1.62	1.52
2	B	899	ILE	N-CA	-7.44	1.37	1.46
10	L	57	LEU	CG-CD2	-7.44	1.27	1.52
1	A	698	GLN	CD-OE1	7.44	1.37	1.23
2	B	617	ARG	C-O	-7.44	1.15	1.24
2	B	667	GLN	CD-NE2	7.44	1.48	1.33
2	B	1223	ASP	N-CA	7.44	1.55	1.46
3	C	12	GLU	CA-C	-7.44	1.43	1.52
7	I	118	ARG	NE-CZ	7.44	1.41	1.33
1	A	514	PRO	CG-CD	-7.44	1.25	1.50
2	B	212	LEU	CB-CG	7.44	1.68	1.53
2	B	903	VAL	C-O	-7.44	1.15	1.24
2	B	1109	GLY	CA-C	7.44	1.62	1.51
8	J	24	LEU	CA-CB	-7.44	1.40	1.53
4	E	71	LYS	CB-CG	7.44	1.74	1.52
2	B	999	MET	C-O	-7.43	1.13	1.23
3	C	90	ASP	CA-C	7.43	1.62	1.52
9	K	61	TYR	CE1-CZ	-7.43	1.20	1.38
2	B	1011	ILE	C-O	-7.43	1.16	1.24
6	H	110	ASP	C-N	7.43	1.44	1.33
4	E	58	MET	SD-CE	7.43	1.98	1.79
9	K	7	PHE	CB-CG	-7.43	1.33	1.50
1	A	41	MET	CA-C	7.43	1.62	1.52
1	A	413	ILE	CB-CG1	-7.43	1.38	1.53
1	A	527	THR	C-N	-7.43	1.23	1.33
3	C	41	ILE	CA-CB	-7.42	1.44	1.54
1	A	678	GLU	CG-CD	7.42	1.70	1.52
1	A	771	GLU	C-O	-7.42	1.13	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	CYS	CA-C	-7.42	1.43	1.53
3	C	61	GLU	N-CA	7.42	1.55	1.46
1	A	28	ARG	CA-C	7.42	1.62	1.52
1	A	29	ALA	CA-C	7.42	1.62	1.52
3	C	193	TYR	C-O	7.42	1.31	1.23
1	A	1349	TYR	CZ-OH	7.42	1.53	1.38
2	B	983	ARG	N-CA	-7.42	1.38	1.46
3	C	27	LEU	CG-CD1	-7.41	1.28	1.52
3	C	252	GLN	CD-NE2	7.41	1.48	1.33
6	H	14	GLU	CA-C	-7.41	1.43	1.52
7	I	25	LEU	CA-CB	7.41	1.63	1.53
1	A	84	ILE	CA-CB	7.41	1.64	1.54
1	A	787	PHE	CA-CB	-7.41	1.42	1.53
1	A	724	GLU	C-N	-7.41	1.23	1.33
2	B	561	TRP	C-O	-7.41	1.14	1.24
2	B	764	SER	CB-OG	-7.41	1.27	1.42
2	B	1060	ARG	CB-CG	-7.41	1.30	1.52
3	C	241	ASP	CB-CG	7.41	1.70	1.52
1	A	971	PHE	C-O	-7.41	1.14	1.24
2	B	310	MET	CA-CB	-7.40	1.41	1.53
2	B	342	GLY	CA-C	-7.40	1.44	1.52
4	E	38	PRO	CA-C	-7.40	1.41	1.52
1	A	87	ALA	CA-C	-7.40	1.43	1.52
1	A	706	HIS	CA-C	-7.40	1.42	1.52
2	B	417	PHE	C-O	7.40	1.34	1.24
2	B	809	MET	SD-CE	-7.40	1.61	1.79
1	A	352	VAL	CA-CB	-7.40	1.46	1.54
1	A	729	ALA	CA-CB	-7.39	1.40	1.53
1	A	794	PRO	N-CD	-7.39	1.37	1.47
1	A	961	ARG	C-N	-7.39	1.23	1.33
2	B	618	ASP	CG-OD1	7.39	1.39	1.25
3	C	70	ILE	CB-CG1	7.39	1.68	1.53
3	C	191	TYR	N-CA	-7.39	1.36	1.46
7	I	28	GLU	CD-OE2	7.39	1.39	1.25
1	A	1068	ALA	C-N	-7.39	1.23	1.33
2	B	344	LYS	C-O	7.39	1.33	1.23
2	B	1065	GLN	CB-CG	-7.39	1.30	1.52
3	C	156	THR	CB-CG2	7.39	1.76	1.52
3	C	252	GLN	CA-C	-7.39	1.43	1.52
6	H	20	TYR	CE1-CZ	-7.39	1.20	1.38
1	A	613	ILE	CA-CB	7.39	1.61	1.55
1	A	1120	LEU	N-CA	7.39	1.54	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	973	ILE	N-CA	-7.39	1.37	1.46
4	E	102	GLU	CG-CD	7.39	1.70	1.52
9	K	26	LYS	CD-CE	7.39	1.74	1.52
1	A	817	ALA	C-N	-7.39	1.24	1.33
6	H	121	LEU	N-CA	-7.39	1.36	1.46
8	J	1	MET	CG-SD	-7.39	1.62	1.80
9	K	109	TRP	CZ3-CH2	-7.39	1.22	1.40
2	B	533	CYS	CA-CB	-7.39	1.41	1.53
2	B	1046	PRO	CB-CG	-7.39	1.12	1.49
3	C	217	ASP	CA-C	7.39	1.62	1.52
1	A	458	HIS	C-O	7.38	1.33	1.23
3	C	94	LYS	CB-CG	7.38	1.74	1.52
4	E	159	ASP	CA-C	7.38	1.62	1.52
2	B	994	TYR	C-O	-7.38	1.14	1.24
7	I	22	ASN	N-CA	-7.38	1.37	1.46
1	A	92	HIS	C-O	-7.38	1.15	1.24
1	A	170	THR	CA-CB	7.38	1.65	1.53
2	B	128	LEU	CA-CB	-7.38	1.40	1.53
4	E	61	GLN	CA-CB	7.38	1.66	1.54
2	B	51	PHE	CD2-CE2	-7.38	1.16	1.38
1	A	407	ARG	NE-CZ	-7.37	1.25	1.33
1	A	1022	LEU	C-O	-7.37	1.15	1.24
2	B	558	LEU	C-N	-7.37	1.23	1.33
2	B	780	VAL	CA-CB	7.37	1.64	1.54
3	C	238	ILE	C-O	-7.37	1.15	1.24
1	A	264	PHE	CE1-CZ	7.37	1.60	1.38
2	B	364	ILE	C-O	7.37	1.32	1.24
1	A	189	ARG	NE-CZ	7.37	1.41	1.33
1	A	425	GLN	CD-NE2	7.37	1.48	1.33
2	B	1162	ILE	CB-CG1	-7.37	1.38	1.53
6	H	110	ASP	CG-OD2	7.37	1.39	1.25
7	I	109	ILE	CB-CG2	-7.37	1.28	1.52
2	B	541	LEU	N-CA	-7.37	1.37	1.46
3	C	267	GLN	CA-CB	7.37	1.67	1.52
1	A	940	ARG	CA-CB	-7.37	1.41	1.53
2	B	67	SER	CA-C	7.36	1.62	1.52
2	B	651	LEU	C-O	-7.36	1.15	1.23
1	A	635	ARG	CD-NE	-7.36	1.35	1.46
1	A	214	ILE	C-N	7.36	1.43	1.33
2	B	609	ILE	CA-C	-7.36	1.44	1.52
4	E	7	ARG	CG-CD	7.36	1.74	1.52
4	E	207	ARG	CG-CD	7.36	1.74	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	104	PHE	CG-CD1	7.36	1.54	1.38
1	A	588	LEU	CA-C	7.36	1.61	1.52
7	I	83	ASN	CG-OD1	7.36	1.37	1.23
2	B	367	LEU	CA-C	7.36	1.64	1.53
7	I	95	THR	C-N	-7.36	1.24	1.33
1	A	868	TYR	CA-CB	-7.36	1.42	1.53
5	F	74	ILE	CA-C	-7.36	1.45	1.52
3	C	89	GLU	CG-CD	7.35	1.70	1.52
2	B	328	GLU	CG-CD	7.35	1.70	1.52
2	B	1151	LEU	CA-C	7.35	1.63	1.52
3	C	195	GLN	C-N	-7.35	1.23	1.33
4	E	161	LYS	CG-CD	-7.35	1.30	1.52
6	H	135	LEU	CG-CD2	7.35	1.76	1.52
1	A	1120	LEU	C-O	-7.35	1.14	1.23
2	B	730	ARG	NE-CZ	-7.35	1.25	1.33
2	B	882	THR	C-O	7.35	1.33	1.24
2	B	1206	GLU	C-O	-7.35	1.15	1.24
3	C	55	THR	CB-CG2	-7.35	1.28	1.52
5	F	154	ASP	CG-OD2	7.35	1.39	1.25
1	A	101	LYS	CE-NZ	7.35	1.71	1.49
1	A	276	LEU	C-O	-7.35	1.14	1.24
2	B	246	LYS	C-O	7.35	1.32	1.23
7	I	20	LYS	CG-CD	7.35	1.74	1.52
1	A	468	PHE	CA-C	-7.34	1.43	1.52
2	B	1162	ILE	CA-CB	7.34	1.64	1.54
7	I	30	ARG	CZ-NH1	7.34	1.43	1.32
7	I	50	THR	N-CA	7.34	1.54	1.45
2	B	772	ALA	C-O	7.34	1.32	1.24
1	A	430	TRP	CD2-CE2	-7.34	1.28	1.41
3	C	148	ARG	C-O	7.34	1.33	1.23
7	I	118	ARG	CG-CD	7.34	1.74	1.52
1	A	508	PRO	N-CD	-7.34	1.37	1.47
1	A	977	LYS	CA-C	7.34	1.61	1.52
2	B	397	ASP	CA-CB	7.34	1.62	1.52
6	H	60	ALA	CA-C	-7.34	1.44	1.52
1	A	218	ASP	CG-OD2	7.34	1.39	1.25
1	A	893	PHE	CA-CB	-7.34	1.41	1.53
1	A	1342	GLU	C-O	-7.34	1.15	1.24
2	B	186	GLU	CA-C	-7.34	1.43	1.52
2	B	1057	LYS	N-CA	-7.33	1.36	1.46
1	A	189	ARG	C-O	7.33	1.33	1.23
1	A	612	ILE	CA-CB	-7.33	1.45	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	886	ILE	CB-CG2	-7.33	1.28	1.52
2	B	446	LEU	CA-C	7.33	1.68	1.52
5	F	149	GLU	CA-C	7.33	1.62	1.52
2	B	486	TYR	N-CA	-7.33	1.37	1.46
2	B	39	ARG	CA-C	-7.33	1.43	1.52
4	E	81	GLU	CD-OE1	7.33	1.39	1.25
5	F	109	VAL	CA-C	7.33	1.62	1.52
1	A	1064	VAL	C-N	7.33	1.44	1.33
2	B	643	ASP	CA-C	-7.33	1.37	1.52
1	A	659	HIS	CG-CD2	7.32	1.44	1.35
1	A	819	GLY	C-O	-7.32	1.14	1.23
2	B	769	TYR	CD2-CE2	-7.32	1.16	1.38
1	A	1132	LYS	CG-CD	7.32	1.74	1.52
2	B	102	VAL	C-O	7.32	1.31	1.24
2	B	232	SER	C-O	-7.32	1.14	1.23
2	B	431	TYR	N-CA	7.32	1.55	1.46
2	B	812	LEU	N-CA	-7.32	1.36	1.46
2	B	366	GLN	N-CA	7.32	1.55	1.46
2	B	1219	ASP	CA-CB	7.32	1.64	1.53
9	K	47	ARG	C-O	-7.32	1.15	1.24
1	A	1430	LEU	C-N	-7.32	1.24	1.33
2	B	624	LEU	CB-CG	-7.32	1.38	1.53
9	K	106	GLU	C-O	7.32	1.33	1.24
1	A	1293	SER	CA-C	-7.31	1.41	1.52
1	A	829	VAL	CA-C	7.31	1.62	1.52
1	A	1138	ILE	CA-C	-7.31	1.45	1.52
2	B	690	VAL	CB-CG1	-7.31	1.28	1.52
2	B	743	ILE	CA-C	-7.31	1.44	1.52
2	B	1156	ASP	CG-OD2	7.31	1.39	1.25
2	B	387	LEU	CA-C	7.31	1.62	1.52
1	A	228	PHE	CA-C	7.31	1.61	1.52
1	A	813	PHE	CA-CB	-7.31	1.42	1.53
1	A	1211	GLN	CG-CD	7.31	1.70	1.52
2	B	990	ILE	C-O	-7.31	1.16	1.24
2	B	1088	GLY	CA-C	-7.31	1.41	1.51
3	C	38	ILE	CB-CG2	-7.31	1.28	1.52
3	C	138	GLU	CD-OE1	7.31	1.39	1.25
1	A	191	THR	CB-CG2	7.31	1.76	1.52
1	A	134	ARG	CB-CG	-7.30	1.30	1.52
1	A	377	PRO	N-CA	-7.30	1.38	1.47
6	H	3	ASN	CA-CB	7.30	1.63	1.53
1	A	155	GLU	CG-CD	7.30	1.70	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	243	VAL	C-O	-7.30	1.14	1.24
7	I	44	TYR	CA-C	-7.30	1.43	1.52
1	A	50	ILE	C-O	-7.30	1.16	1.24
1	A	69	THR	C-O	7.30	1.33	1.24
1	A	1119	TYR	N-CA	-7.30	1.36	1.45
1	A	1308	THR	CB-CG2	-7.30	1.28	1.52
1	A	1326	ARG	N-CA	7.30	1.55	1.46
2	B	599	THR	CA-CB	-7.30	1.42	1.53
3	C	114	TYR	CE2-CZ	-7.30	1.20	1.38
2	B	234	ILE	N-CA	-7.30	1.38	1.46
7	I	98	VAL	C-O	7.30	1.34	1.24
10	L	59	ALA	CA-C	-7.30	1.43	1.52
3	C	57	VAL	C-N	-7.30	1.23	1.33
4	E	188	LEU	N-CA	-7.30	1.35	1.46
2	B	692	TYR	C-O	-7.30	1.15	1.24
2	B	785	TYR	CE2-CZ	-7.30	1.20	1.38
8	J	20	SER	C-O	-7.30	1.14	1.24
2	B	575	PRO	C-O	7.29	1.32	1.24
1	A	191	THR	C-O	7.29	1.33	1.24
2	B	549	THR	C-O	7.29	1.32	1.23
2	B	866	TYR	CA-C	7.29	1.62	1.52
3	C	169	LYS	CA-CB	-7.29	1.41	1.53
8	J	8	PHE	C-O	-7.29	1.15	1.24
1	A	743	VAL	CA-CB	-7.29	1.44	1.54
1	A	748	MET	CA-C	-7.29	1.43	1.52
2	B	1090	THR	C-O	-7.29	1.15	1.23
1	A	441	PRO	CG-CD	-7.29	1.25	1.50
9	K	50	LEU	CA-CB	-7.29	1.41	1.53
2	B	310	MET	N-CA	-7.29	1.37	1.46
2	B	696	GLU	N-CA	-7.29	1.36	1.46
1	A	246	VAL	C-O	7.29	1.32	1.24
2	B	667	GLN	CA-C	7.28	1.61	1.53
2	B	1056	SER	C-O	-7.28	1.15	1.24
2	B	1208	MET	C-O	-7.28	1.15	1.24
7	I	119	THR	C-O	7.28	1.32	1.24
1	A	1385	THR	C-O	7.28	1.38	1.23
2	B	485	ARG	N-CA	-7.28	1.37	1.46
1	A	63	ARG	CA-C	7.28	1.62	1.52
1	A	383	TYR	CA-C	7.28	1.62	1.52
1	A	1132	LYS	C-O	-7.28	1.15	1.24
1	A	1113	THR	C-O	-7.28	1.15	1.24
2	B	1137	CYS	CB-SG	-7.28	1.57	1.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	14	SER	N-CA	-7.28	1.37	1.46
3	C	253	LYS	CA-C	7.28	1.62	1.52
1	A	14	VAL	CA-CB	-7.28	1.45	1.54
2	B	1097	HIS	CG-ND1	7.27	1.46	1.38
1	A	822	GLU	N-CA	7.27	1.55	1.46
2	B	966	VAL	N-CA	-7.27	1.37	1.46
3	C	87	PHE	CA-CB	-7.27	1.41	1.53
2	B	18	PHE	CA-C	7.27	1.68	1.52
1	A	133	LYS	CE-NZ	7.27	1.71	1.49
1	A	741	ASN	C-O	-7.27	1.15	1.24
1	A	760	GLN	C-O	-7.27	1.14	1.24
3	C	222	LYS	CG-CD	7.27	1.74	1.52
5	F	134	ILE	C-O	-7.27	1.16	1.24
1	A	208	LEU	CG-CD1	-7.27	1.28	1.52
6	H	12	VAL	CA-C	7.27	1.61	1.53
2	B	663	ALA	CA-C	-7.27	1.42	1.52
1	A	597	LEU	CA-C	-7.26	1.39	1.52
4	E	75	MET	N-CA	-7.26	1.36	1.46
1	A	645	LEU	C-N	-7.26	1.24	1.33
9	K	39	ASP	C-N	-7.26	1.24	1.34
1	A	734	GLU	C-O	-7.26	1.15	1.24
2	B	709	ASP	C-N	-7.26	1.23	1.33
4	E	184	VAL	CA-CB	7.26	1.64	1.54
1	A	27	VAL	CA-C	7.26	1.61	1.52
1	A	532	ARG	CZ-NH1	7.26	1.43	1.32
1	A	784	LEU	CA-CB	-7.26	1.44	1.53
1	A	1040	GLN	C-N	-7.26	1.24	1.33
2	B	1055	ILE	C-N	-7.26	1.23	1.33
3	C	186	LEU	CA-C	7.26	1.63	1.52
10	L	67	PHE	CG-CD1	-7.26	1.23	1.38
2	B	215	GLN	CB-CG	-7.26	1.30	1.52
1	A	482	PHE	C-O	-7.26	1.12	1.23
10	L	69	ALA	N-CA	7.25	1.57	1.46
1	A	192	GLY	C-O	7.25	1.33	1.23
1	A	521	MET	CG-SD	-7.25	1.62	1.80
1	A	234	MET	SD-CE	-7.25	1.61	1.79
2	B	1155	SER	CB-OG	7.25	1.56	1.42
6	H	27	GLU	N-CA	7.25	1.55	1.46
6	H	123	MET	SD-CE	-7.25	1.61	1.79
7	I	12	ASN	N-CA	-7.25	1.37	1.45
7	I	44	TYR	CA-CB	7.25	1.65	1.53
1	A	526	ASP	C-N	-7.25	1.24	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	GLU	CB-CG	7.25	1.74	1.52
2	B	908	GLU	CG-CD	7.25	1.70	1.52
3	C	30	ALA	C-O	-7.25	1.15	1.24
2	B	31	TRP	NE1-CE2	-7.25	1.29	1.37
2	B	393	LYS	CD-CE	7.25	1.74	1.52
3	C	215	GLU	CG-CD	7.25	1.70	1.52
4	E	213	ILE	CG1-CD1	7.25	1.80	1.51
1	A	1036	ARG	CA-C	-7.25	1.43	1.53
2	B	317	CYS	N-CA	-7.25	1.37	1.46
8	J	45	CYS	CA-C	7.25	1.62	1.52
1	A	1367	HIS	N-CA	7.24	1.55	1.46
2	B	124	TYR	CA-C	-7.24	1.43	1.52
2	B	614	SER	N-CA	7.24	1.54	1.46
2	B	833	TYR	CE2-CZ	-7.24	1.20	1.38
5	F	106	PRO	C-O	-7.24	1.15	1.23
6	H	79	TRP	CA-CB	-7.24	1.41	1.53
9	K	108	GLU	CD-OE1	7.24	1.39	1.25
2	B	984	HIS	CG-ND1	-7.24	1.30	1.38
1	A	121	LEU	C-N	-7.24	1.24	1.33
1	A	895	LYS	C-N	-7.24	1.23	1.33
2	B	914	LYS	CA-CB	-7.24	1.41	1.53
1	A	593	GLU	CD-OE2	7.24	1.39	1.25
1	A	936	LEU	CA-CB	-7.24	1.41	1.53
1	A	1448	GLU	C-N	7.24	1.43	1.33
2	B	589	VAL	CB-CG2	-7.24	1.28	1.52
2	B	983	ARG	C-O	7.24	1.33	1.24
8	J	44	TYR	C-O	-7.24	1.14	1.24
10	L	70	ARG	CZ-NH2	-7.23	1.24	1.33
1	A	655	PHE	CG-CD1	-7.23	1.23	1.38
2	B	756	ILE	C-N	-7.23	1.24	1.33
1	A	1350	LYS	CD-CE	7.23	1.74	1.52
8	J	12	LYS	CA-C	7.23	1.61	1.52
1	A	98	LYS	CD-CE	7.23	1.74	1.52
1	A	734	GLU	CA-CB	7.23	1.64	1.53
1	A	813	PHE	CG-CD1	-7.23	1.23	1.38
1	A	1023	ARG	CA-C	-7.23	1.42	1.52
1	A	1162	VAL	C-N	-7.23	1.25	1.33
4	E	12	LEU	CB-CG	7.23	1.68	1.53
1	A	109	HIS	CD2-NE2	7.22	1.45	1.37
1	A	921	GLY	C-N	-7.22	1.23	1.33
1	A	1078	GLN	CD-NE2	7.22	1.48	1.33
2	B	801	LYS	C-N	-7.22	1.25	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1193	GLN	CD-OE1	7.22	1.37	1.23
4	E	214	CYS	C-O	-7.22	1.15	1.23
9	K	100	ALA	CA-C	-7.22	1.44	1.52
1	A	371	ALA	CA-C	-7.22	1.42	1.52
3	C	81	GLU	CA-C	7.22	1.62	1.52
3	C	161	LYS	N-CA	7.22	1.55	1.45
1	A	988	LEU	N-CA	7.22	1.55	1.46
1	A	1187	GLN	C-O	7.22	1.38	1.23
2	B	305	VAL	CA-C	-7.22	1.41	1.52
2	B	1215	ARG	CG-CD	7.22	1.74	1.52
1	A	957	PRO	N-CA	-7.22	1.39	1.47
1	A	1291	VAL	CB-CG1	-7.22	1.28	1.52
2	B	851	PHE	C-O	-7.22	1.12	1.24
2	B	882	THR	CA-C	7.22	1.62	1.52
3	C	205	LYS	N-CA	7.22	1.54	1.46
2	B	698	GLU	N-CA	-7.21	1.36	1.46
4	E	169	ARG	CG-CD	7.21	1.74	1.52
6	H	22	LYS	CB-CG	7.21	1.74	1.52
2	B	854	LEU	CB-CG	-7.21	1.39	1.53
3	C	41	ILE	CA-C	7.21	1.60	1.52
2	B	179	CYS	C-O	-7.21	1.15	1.23
2	B	187	SER	C-O	7.21	1.33	1.24
4	E	189	GLY	N-CA	-7.21	1.34	1.45
1	A	1023	ARG	N-CA	-7.21	1.37	1.46
2	B	627	PHE	CA-CB	-7.21	1.41	1.53
1	A	125	ALA	C-N	-7.21	1.24	1.34
1	A	954	TRP	CA-CB	-7.21	1.41	1.53
2	B	538	ASN	CA-C	7.21	1.61	1.52
2	B	884	ARG	CZ-NH1	7.21	1.42	1.32
2	B	961	LEU	N-CA	-7.21	1.36	1.46
2	B	1102	LYS	CD-CE	7.21	1.74	1.52
3	C	21	ILE	CA-C	-7.21	1.43	1.52
1	A	860	LEU	CG-CD2	7.20	1.76	1.52
2	B	336	ARG	CA-C	-7.20	1.42	1.52
2	B	1008	PRO	N-CA	-7.20	1.38	1.47
7	I	21	GLU	C-O	-7.20	1.15	1.24
2	B	745	PRO	CA-C	-7.20	1.39	1.52
2	B	190	TYR	CA-CB	-7.20	1.42	1.53
2	B	318	VAL	CA-CB	-7.20	1.45	1.54
2	B	486	TYR	CA-C	-7.20	1.43	1.52
2	B	596	LEU	CG-CD1	-7.20	1.28	1.52
2	B	961	LEU	CB-CG	7.20	1.67	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	57	VAL	CA-CB	-7.20	1.44	1.54
2	B	1134	GLU	CD-OE1	7.20	1.39	1.25
1	A	702	LEU	N-CA	-7.20	1.36	1.46
3	C	259	LEU	C-O	-7.20	1.15	1.24
8	J	60	PHE	C-O	7.20	1.33	1.24
9	K	91	CYS	CB-SG	-7.20	1.57	1.81
8	J	2	ILE	CG1-CD1	-7.19	1.23	1.51
1	A	54	ASN	CA-CB	7.19	1.65	1.53
1	A	1417	GLU	C-O	7.19	1.32	1.23
1	A	114	LEU	CA-C	-7.19	1.42	1.52
1	A	551	TYR	CE1-CZ	-7.19	1.21	1.38
2	B	261	ARG	CZ-NH1	7.19	1.42	1.32
3	C	123	ASN	CG-ND2	7.19	1.48	1.33
9	K	16	GLU	CD-OE1	7.19	1.39	1.25
1	A	403	LYS	CD-CE	7.19	1.74	1.52
1	A	656	TRP	CA-C	-7.19	1.43	1.52
3	C	46	ILE	CA-C	-7.19	1.45	1.52
1	A	210	ILE	CB-CG2	-7.19	1.28	1.52
2	B	46	GLN	CG-CD	-7.19	1.34	1.52
2	B	242	SER	N-CA	-7.19	1.36	1.46
2	B	967	ARG	CB-CG	-7.19	1.30	1.52
6	H	58	THR	CA-C	7.19	1.61	1.52
1	A	1199	ARG	CZ-NH1	7.19	1.42	1.32
1	A	601	LYS	CA-C	7.18	1.62	1.52
2	B	989	THR	CB-CG2	-7.18	1.28	1.52
3	C	133	ILE	C-N	7.18	1.43	1.33
1	A	371	ALA	CA-CB	-7.18	1.41	1.53
2	B	705	MET	CB-CG	-7.18	1.30	1.52
1	A	750	GLY	CA-C	-7.18	1.41	1.51
1	A	971	PHE	CG-CD1	-7.18	1.23	1.38
2	B	403	LYS	C-N	-7.18	1.23	1.33
2	B	500	THR	C-N	-7.18	1.25	1.33
4	E	52	ARG	CD-NE	7.18	1.56	1.46
2	B	391	ASP	C-O	-7.18	1.15	1.24
1	A	877	HIS	CA-CB	-7.18	1.42	1.53
1	A	958	VAL	CB-CG1	-7.18	1.28	1.52
1	A	1040	GLN	CD-NE2	7.18	1.48	1.33
1	A	787	PHE	CG-CD2	-7.17	1.23	1.38
1	A	847	ASP	CG-OD2	7.17	1.39	1.25
1	A	931	GLU	CD-OE1	7.17	1.39	1.25
1	A	1199	ARG	N-CA	7.17	1.54	1.46
2	B	604	ARG	CZ-NH2	-7.17	1.24	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1172	ILE	CB-CG2	7.17	1.76	1.52
3	C	93	ASP	CA-C	-7.17	1.42	1.52
4	E	42	PHE	CB-CG	-7.17	1.34	1.50
1	A	934	LYS	C-O	7.17	1.32	1.24
1	A	938	LYS	C-O	7.17	1.32	1.24
1	A	976	THR	N-CA	7.17	1.54	1.46
1	A	1422	ARG	CZ-NH1	7.17	1.42	1.32
2	B	1098	MET	SD-CE	7.17	1.97	1.79
9	K	25	THR	CA-CB	-7.17	1.41	1.53
1	A	180	LYS	CG-CD	7.17	1.74	1.52
2	B	527	THR	C-O	-7.17	1.16	1.24
2	B	627	PHE	CD2-CE2	-7.17	1.17	1.38
3	C	116	LYS	CA-C	7.17	1.63	1.52
3	C	249	ASP	CG-OD1	7.17	1.39	1.25
1	A	1131	ALA	C-O	-7.17	1.14	1.24
3	C	173	ALA	CA-CB	-7.17	1.42	1.53
4	E	97	VAL	CA-CB	-7.17	1.44	1.54
1	A	407	ARG	CA-CB	-7.16	1.41	1.53
1	A	1067	LEU	CG-CD2	-7.16	1.28	1.52
2	B	449	ASN	CG-OD1	7.16	1.37	1.23
2	B	1058	LEU	CG-CD1	7.16	1.76	1.52
5	F	146	TRP	CB-CG	-7.16	1.28	1.50
1	A	866	PHE	C-O	7.16	1.33	1.24
2	B	500	THR	N-CA	-7.16	1.38	1.46
3	C	105	GLY	CA-C	-7.16	1.41	1.51
1	A	149	GLU	CD-OE1	7.16	1.39	1.25
1	A	770	VAL	CB-CG1	-7.16	1.28	1.52
2	B	285	ILE	CA-C	7.16	1.61	1.52
2	B	328	GLU	CD-OE1	7.16	1.39	1.25
10	L	49	LYS	N-CA	7.16	1.55	1.46
2	B	325	GLN	CA-CB	-7.16	1.42	1.53
4	E	110	PHE	N-CA	-7.16	1.37	1.46
6	H	34	ASP	CB-CG	7.16	1.70	1.52
3	C	80	LEU	CA-C	7.15	1.61	1.52
1	A	326	ARG	CD-NE	7.15	1.56	1.46
1	A	779	PHE	CE1-CZ	-7.15	1.17	1.38
2	B	44	VAL	C-O	-7.15	1.15	1.24
2	B	411	PRO	N-CD	-7.15	1.37	1.47
2	B	552	MET	C-N	-7.15	1.25	1.34
2	B	951	GLN	CD-NE2	7.15	1.48	1.33
2	B	534	GLY	N-CA	-7.15	1.33	1.44
1	A	194	ALA	CA-CB	7.15	1.65	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	341	LEU	C-N	-7.15	1.26	1.34
4	E	43	LYS	CE-NZ	7.15	1.70	1.49
1	A	474	VAL	CB-CG1	-7.15	1.28	1.52
3	C	120	ILE	CG1-CD1	7.15	1.79	1.51
1	A	488	ASN	CA-CB	-7.15	1.41	1.53
3	C	85	ASP	N-CA	-7.15	1.36	1.46
1	A	1450	LEU	CG-CD1	7.14	1.76	1.52
1	A	992	ASP	N-CA	-7.14	1.37	1.46
2	B	463	THR	C-O	7.14	1.33	1.24
3	C	136	ASP	C-O	-7.14	1.15	1.23
1	A	537	ARG	CZ-NH2	7.14	1.42	1.33
1	A	776	ALA	N-CA	-7.14	1.36	1.45
1	A	45	GLN	CB-CG	7.14	1.73	1.52
1	A	734	GLU	C-N	-7.14	1.24	1.33
1	A	985	ASP	CG-OD1	7.14	1.39	1.25
1	A	1327	ILE	N-CA	-7.14	1.37	1.46
2	B	879	ARG	NE-CZ	7.14	1.41	1.33
1	A	979	SER	CA-CB	7.13	1.64	1.53
2	B	965	LYS	CA-C	-7.13	1.44	1.52
1	A	1446	ASP	CB-CG	7.13	1.69	1.52
1	A	1001	ARG	N-CA	-7.13	1.35	1.45
1	A	1161	THR	C-O	7.13	1.32	1.23
2	B	515	HIS	CG-ND1	-7.13	1.30	1.38
2	B	878	GLN	CG-CD	7.13	1.69	1.52
4	E	66	GLU	CD-OE1	7.13	1.38	1.25
7	I	74	GLU	CB-CG	7.13	1.73	1.52
2	B	752	ALA	CA-CB	7.13	1.64	1.53
2	B	1197	PRO	CA-CB	-7.13	1.44	1.53
4	E	191	LYS	N-CA	-7.13	1.37	1.46
1	A	28	ARG	CZ-NH1	7.13	1.42	1.32
1	A	731	ARG	CZ-NH1	7.13	1.42	1.32
1	A	1015	VAL	CB-CG1	-7.13	1.29	1.52
1	A	1092	LYS	C-O	7.12	1.37	1.23
2	B	362	PRO	CA-CB	-7.12	1.43	1.53
2	B	862	GLN	CD-OE1	7.12	1.37	1.23
1	A	944	ARG	N-CA	-7.12	1.36	1.46
1	A	990	VAL	CA-C	-7.12	1.43	1.53
2	B	112	LEU	CB-CG	-7.12	1.39	1.53
4	E	155	ARG	CZ-NH1	7.12	1.42	1.32
1	A	889	SER	N-CA	7.12	1.55	1.45
1	A	1111	MET	C-N	-7.12	1.23	1.33
2	B	1032	SER	CA-C	7.12	1.62	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	169	ARG	N-CA	-7.12	1.37	1.46
2	B	529	GLU	CA-C	-7.12	1.43	1.53
7	I	70	ARG	C-O	-7.12	1.14	1.23
1	A	209	ASN	C-N	-7.12	1.25	1.33
1	A	1355	VAL	CA-C	-7.12	1.43	1.52
2	B	851	PHE	CB-CG	7.12	1.67	1.50
5	F	91	ALA	CA-C	-7.12	1.43	1.52
1	A	209	ASN	N-CA	-7.11	1.37	1.46
2	B	420	LEU	CA-C	-7.11	1.42	1.52
8	J	21	TYR	CE1-CZ	-7.11	1.21	1.38
10	L	70	ARG	CZ-NH1	7.11	1.42	1.32
1	A	1209	MET	SD-CE	-7.11	1.61	1.79
3	C	92	CYS	N-CA	-7.11	1.37	1.46
4	E	181	ALA	C-O	7.11	1.33	1.23
1	A	518	LYS	CB-CG	-7.11	1.31	1.52
2	B	35	SER	CA-CB	-7.11	1.42	1.53
2	B	941	LEU	N-CA	-7.11	1.36	1.46
1	A	938	LYS	CG-CD	7.11	1.73	1.52
2	B	1182	CYS	CA-C	7.11	1.61	1.53
2	B	983	ARG	CD-NE	-7.11	1.36	1.46
4	E	65	THR	CA-C	-7.11	1.43	1.52
6	H	14	GLU	CD-OE1	7.11	1.38	1.25
6	H	53	ASP	N-CA	7.11	1.55	1.46
1	A	815	PHE	C-O	-7.11	1.14	1.24
2	B	395	GLN	N-CA	7.11	1.54	1.46
1	A	1221	LYS	N-CA	7.10	1.55	1.46
2	B	827	ILE	CB-CG1	-7.10	1.39	1.53
7	I	51	ASN	CG-ND2	7.10	1.48	1.33
1	A	396	PRO	N-CD	-7.10	1.37	1.47
1	A	572	TRP	CE2-CZ2	-7.10	1.25	1.39
1	A	827	THR	CB-CG2	7.10	1.75	1.52
1	A	960	ILE	CG1-CD1	-7.10	1.24	1.51
2	B	866	TYR	N-CA	7.10	1.55	1.46
2	B	882	THR	CA-CB	7.10	1.65	1.53
6	H	127	GLY	CA-C	7.10	1.61	1.51
2	B	948	ILE	CB-CG1	-7.10	1.39	1.53
2	B	406	LEU	CA-CB	-7.10	1.43	1.53
1	A	432	VAL	N-CA	-7.10	1.37	1.46
1	A	539	THR	CA-CB	-7.10	1.44	1.53
2	B	171	PRO	C-O	-7.10	1.15	1.23
2	B	352	ALA	C-O	7.10	1.32	1.24
2	B	567	GLU	CD-OE2	7.10	1.38	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	195	GLN	CD-NE2	7.10	1.48	1.33
2	B	527	THR	C-N	7.10	1.42	1.33
2	B	754	SER	CB-OG	7.10	1.56	1.42
1	A	746	MET	C-O	-7.09	1.15	1.24
1	A	754	SER	N-CA	-7.09	1.37	1.46
1	A	1270	ASN	CA-CB	7.09	1.62	1.53
2	B	556	THR	CA-CB	-7.09	1.42	1.53
2	B	805	THR	C-N	-7.09	1.23	1.33
1	A	836	TYR	N-CA	-7.09	1.37	1.46
2	B	861	ASP	C-O	7.09	1.32	1.23
1	A	498	ARG	CB-CG	-7.09	1.31	1.52
2	B	1192	TYR	CG-CD2	-7.09	1.24	1.39
1	A	790	ASP	CA-CB	-7.09	1.41	1.53
2	B	188	ASP	C-O	7.09	1.33	1.24
2	B	518	HIS	CA-CB	-7.09	1.41	1.53
6	H	104	PHE	CA-CB	7.09	1.65	1.53
8	J	63	TYR	CG-CD1	-7.09	1.24	1.39
1	A	842	VAL	N-CA	-7.08	1.38	1.46
1	A	1279	ILE	CA-CB	7.08	1.62	1.53
2	B	567	GLU	CD-OE1	7.08	1.38	1.25
3	C	249	ASP	C-N	-7.08	1.24	1.33
8	J	51	LEU	CA-CB	-7.08	1.40	1.53
2	B	450	ALA	CA-CB	-7.08	1.44	1.53
2	B	996	ARG	CA-CB	-7.08	1.42	1.53
1	A	109	HIS	CB-CG	7.08	1.60	1.50
1	A	805	LEU	CG-CD1	-7.08	1.29	1.52
2	B	43	LEU	CA-CB	-7.08	1.41	1.53
2	B	1010	LEU	CB-CG	-7.08	1.39	1.53
2	B	1047	PHE	CG-CD1	-7.08	1.24	1.38
2	B	1199	ALA	C-O	7.08	1.32	1.24
1	A	1420	ASP	CB-CG	7.08	1.69	1.52
2	B	952	VAL	CA-CB	-7.08	1.44	1.54
2	B	173	MET	CB-CG	7.08	1.73	1.52
1	A	125	ALA	N-CA	-7.07	1.36	1.46
1	A	958	VAL	CA-CB	-7.07	1.44	1.54
1	A	1154	TYR	CE2-CZ	7.07	1.55	1.38
3	C	152	GLU	CD-OE1	7.07	1.38	1.25
1	A	125	ALA	CA-CB	-7.07	1.42	1.53
1	A	427	GLN	C-O	-7.07	1.15	1.23
6	H	92	ASP	CB-CG	7.07	1.69	1.52
2	B	265	SER	CB-OG	7.07	1.56	1.42
3	C	132	PRO	N-CD	-7.07	1.37	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	96	THR	C-N	-7.07	1.24	1.34
7	I	112	SER	CA-CB	-7.07	1.41	1.53
2	B	653	VAL	C-O	7.07	1.32	1.24
5	F	142	SER	CB-OG	-7.07	1.28	1.42
2	B	47	GLN	C-O	-7.06	1.15	1.24
1	A	1153	TYR	CA-C	-7.06	1.44	1.52
2	B	306	ASN	CG-ND2	7.06	1.48	1.33
1	A	1362	TYR	CZ-OH	7.06	1.52	1.38
2	B	790	ASP	CB-CG	7.06	1.69	1.52
3	C	92	CYS	C-O	-7.06	1.15	1.24
2	B	446	LEU	CG-CD2	7.06	1.75	1.52
2	B	601	ARG	CD-NE	7.06	1.56	1.46
2	B	818	PRO	N-CA	-7.06	1.39	1.47
2	B	1160	VAL	C-N	7.06	1.43	1.33
3	C	209	TYR	C-N	-7.06	1.24	1.33
6	H	6	PHE	CA-CB	-7.06	1.42	1.53
1	A	1211	GLN	CB-CG	7.06	1.73	1.52
3	C	137	LYS	CB-CG	7.06	1.73	1.52
1	A	187	LYS	C-N	7.05	1.43	1.33
1	A	473	SER	CA-C	7.05	1.62	1.52
1	A	722	LEU	CG-CD1	-7.05	1.29	1.52
2	B	804	GLY	C-N	-7.05	1.21	1.33
2	B	894	ASP	CB-CG	7.05	1.69	1.52
6	H	31	THR	CA-C	7.05	1.61	1.52
9	K	46	ILE	C-N	-7.05	1.25	1.33
2	B	968	VAL	N-CA	-7.05	1.37	1.46
2	B	1100	ASP	CB-CG	7.05	1.69	1.52
1	A	188	ASP	C-N	7.05	1.43	1.33
8	J	48	ARG	CZ-NH2	-7.05	1.24	1.33
1	A	433	GLU	CA-CB	-7.05	1.44	1.52
1	A	471	ASN	CG-ND2	-7.05	1.18	1.33
1	A	917	SER	C-O	-7.05	1.16	1.24
2	B	627	PHE	CE2-CZ	-7.05	1.17	1.38
6	H	132	LEU	CB-CG	7.05	1.67	1.53
1	A	845	LEU	C-O	-7.05	1.14	1.24
2	B	115	GLN	C-O	-7.05	1.15	1.24
2	B	1102	LYS	CA-C	7.05	1.59	1.52
3	C	176	ILE	C-O	-7.05	1.16	1.24
2	B	757	PRO	C-O	-7.04	1.16	1.23
3	C	5	GLY	CA-C	7.04	1.61	1.51
6	H	19	ARG	CD-NE	7.04	1.56	1.46
1	A	85	ASP	CA-C	7.04	1.62	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	483	LEU	CA-CB	-7.04	1.41	1.53
2	B	795	ILE	CG1-CD1	-7.04	1.24	1.51
6	H	55	LEU	CA-C	-7.04	1.44	1.52
7	I	9	ASP	CG-OD2	7.04	1.38	1.25
1	A	504	LEU	CG-CD2	-7.04	1.29	1.52
1	A	599	SER	C-N	-7.04	1.24	1.33
1	A	650	GLN	CD-NE2	-7.04	1.18	1.33
1	A	976	THR	CB-OG1	7.04	1.55	1.43
1	A	1153	TYR	CA-CB	-7.04	1.40	1.53
2	B	652	LYS	CD-CE	7.04	1.73	1.52
1	A	848	ILE	C-O	-7.04	1.14	1.24
2	B	233	PRO	C-O	-7.04	1.15	1.24
8	J	8	PHE	CG-CD2	-7.04	1.24	1.38
1	A	361	LEU	N-CA	7.04	1.55	1.46
1	A	611	GLN	CD-OE1	7.04	1.36	1.23
1	A	1446	ASP	CA-CB	7.04	1.62	1.52
2	B	449	ASN	CG-ND2	7.04	1.48	1.33
1	A	826	ASP	CG-OD2	7.04	1.38	1.25
1	A	1315	GLU	CA-C	-7.04	1.43	1.52
2	B	538	ASN	CA-CB	-7.04	1.40	1.53
2	B	547	VAL	CB-CG1	-7.04	1.29	1.52
3	C	19	ASP	C-O	-7.04	1.15	1.23
6	H	18	GLY	C-O	-7.03	1.14	1.23
2	B	1002	THR	C-O	-7.03	1.14	1.23
4	E	200	ARG	CB-CG	-7.03	1.31	1.52
2	B	488	TYR	N-CA	7.03	1.54	1.46
1	A	588	LEU	CG-CD1	-7.03	1.29	1.52
1	A	1159	ARG	CG-CD	7.03	1.73	1.52
7	I	120	GLN	N-CA	7.03	1.53	1.46
1	A	1355	VAL	C-O	-7.02	1.15	1.24
2	B	587	HIS	CA-C	7.02	1.62	1.52
1	A	481	ASP	CA-C	-7.02	1.45	1.53
2	B	106	ASP	N-CA	7.02	1.55	1.46
2	B	403	LYS	CB-CG	7.02	1.73	1.52
2	B	958	GLN	CA-CB	7.02	1.65	1.53
1	A	449	SER	CA-C	-7.02	1.44	1.53
1	A	546	VAL	N-CA	-7.02	1.38	1.46
1	A	1163	ILE	CB-CG2	-7.02	1.29	1.52
1	A	325	ILE	C-O	-7.02	1.16	1.24
1	A	572	TRP	CA-C	7.02	1.62	1.52
6	H	56	THR	C-O	7.02	1.32	1.23
9	K	76	GLN	CA-C	7.02	1.61	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1217	LYS	CE-NZ	7.02	1.70	1.49
2	B	579	ARG	CG-CD	7.02	1.73	1.52
3	C	144	ILE	CB-CG1	-7.02	1.39	1.53
6	H	117	SER	C-O	7.02	1.31	1.24
7	I	96	SER	CA-CB	7.02	1.63	1.53
1	A	838	GLN	C-O	-7.01	1.16	1.24
2	B	415	GLN	CD-OE1	7.01	1.36	1.23
4	E	91	LYS	N-CA	7.01	1.54	1.46
9	K	89	ASN	N-CA	-7.01	1.37	1.46
4	E	28	TYR	CG-CD1	-7.01	1.24	1.39
8	J	54	VAL	CA-C	7.01	1.61	1.52
1	A	1414	ALA	CA-C	-7.01	1.43	1.52
2	B	173	MET	SD-CE	-7.01	1.62	1.79
2	B	1061	GLU	CA-CB	7.01	1.64	1.53
2	B	137	TYR	CG-CD1	7.01	1.54	1.39
2	B	249	ARG	CB-CG	7.01	1.73	1.52
2	B	291	ILE	CB-CG2	-7.01	1.29	1.52
2	B	343	ILE	C-O	-7.01	1.16	1.24
3	C	35	ARG	NE-CZ	-7.01	1.25	1.33
3	C	185	LYS	CB-CG	7.01	1.73	1.52
4	E	100	ILE	CA-CB	-7.01	1.46	1.54
6	H	40	LEU	CG-CD1	-7.01	1.29	1.52
8	J	27	GLU	CD-OE2	7.01	1.38	1.25
1	A	575	LYS	CG-CD	-7.00	1.31	1.52
1	A	1336	MET	CG-SD	-7.00	1.63	1.80
2	B	1133	MET	CA-C	-7.00	1.43	1.52
3	C	103	ALA	CA-CB	-7.00	1.41	1.53
1	A	1312	ASN	C-O	-7.00	1.15	1.23
2	B	303	TYR	CD2-CE2	-7.00	1.17	1.38
2	B	1153	GLU	N-CA	7.00	1.55	1.45
3	C	138	GLU	C-O	7.00	1.33	1.23
2	B	352	ALA	CA-CB	-7.00	1.42	1.53
7	I	53	GLY	C-O	7.00	1.33	1.24
3	C	78	GLU	CG-CD	7.00	1.69	1.52
1	A	188	ASP	C-O	7.00	1.32	1.24
1	A	909	ASP	C-O	-7.00	1.15	1.24
1	A	1340	GLY	CA-C	-7.00	1.43	1.52
2	B	342	GLY	C-O	7.00	1.32	1.24
2	B	401	PHE	CD2-CE2	-7.00	1.17	1.38
2	B	693	ILE	C-O	-7.00	1.16	1.24
1	A	369	SER	N-CA	-7.00	1.37	1.46
1	A	841	LEU	CB-CG	-7.00	1.39	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1314	SER	CB-OG	7.00	1.56	1.42
2	B	446	LEU	C-O	7.00	1.37	1.23
2	B	1075	GLY	CA-C	7.00	1.59	1.51
1	A	1446	ASP	CG-OD2	6.99	1.38	1.25
2	B	1057	LYS	CD-CE	6.99	1.73	1.52
3	C	55	THR	CA-C	6.99	1.62	1.52
7	I	6	PHE	C-O	-6.99	1.15	1.23
1	A	787	PHE	CA-C	-6.99	1.44	1.52
1	A	901	LEU	N-CA	6.99	1.55	1.46
8	J	13	VAL	CA-CB	-6.99	1.46	1.54
1	A	152	VAL	N-CA	6.99	1.55	1.46
3	C	235	VAL	CA-C	-6.99	1.43	1.52
6	H	16	ASP	CG-OD2	6.99	1.38	1.25
1	A	602	ASP	C-O	-6.99	1.13	1.23
1	A	848	ILE	CA-CB	-6.99	1.45	1.54
1	A	1164	PRO	CA-CB	6.99	1.63	1.53
2	B	455	SER	N-CA	-6.99	1.37	1.46
4	E	52	ARG	CG-CD	6.99	1.73	1.52
1	A	1428	VAL	CA-CB	-6.98	1.46	1.54
2	B	875	GLU	C-O	-6.98	1.15	1.24
2	B	1099	VAL	CA-C	-6.98	1.43	1.52
2	B	1222	ARG	CA-C	6.98	1.62	1.52
2	B	423	LYS	C-O	-6.98	1.16	1.23
2	B	782	LEU	CB-CG	-6.98	1.39	1.53
3	C	214	ASN	CG-OD1	6.98	1.36	1.23
1	A	831	THR	CB-OG1	6.98	1.54	1.43
1	A	1306	LEU	N-CA	-6.98	1.37	1.45
3	C	111	THR	C-O	-6.98	1.15	1.24
3	C	183	TRP	N-CA	6.98	1.54	1.45
1	A	1144	LYS	C-N	-6.98	1.24	1.33
5	F	108	PHE	C-N	-6.98	1.24	1.33
1	A	513	SER	CA-C	-6.98	1.44	1.52
2	B	524	PRO	C-O	6.98	1.32	1.24
3	C	91	HIS	CA-CB	6.98	1.66	1.53
1	A	736	ASN	CA-C	-6.97	1.43	1.52
1	A	915	SER	CA-CB	6.97	1.65	1.53
1	A	935	GLN	CA-CB	-6.97	1.41	1.53
2	B	887	HIS	CB-CG	6.97	1.59	1.50
1	A	12	ARG	N-CA	6.97	1.54	1.45
1	A	470	LEU	CA-C	-6.97	1.44	1.52
1	A	549	MET	CA-C	-6.97	1.43	1.52
1	A	932	GLU	CD-OE2	6.97	1.38	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	24	LYS	CA-CB	-6.97	1.42	1.53
6	H	105	GLU	C-O	6.97	1.32	1.24
3	C	53	THR	C-O	-6.97	1.15	1.23
4	E	74	ASP	C-O	6.97	1.32	1.24
4	E	161	LYS	N-CA	-6.97	1.38	1.46
1	A	669	THR	C-O	6.97	1.33	1.23
7	I	21	GLU	CD-OE1	6.97	1.38	1.25
2	B	967	ARG	CA-CB	-6.97	1.43	1.53
9	K	27	ALA	CA-CB	6.97	1.63	1.53
1	A	13	THR	CA-C	-6.96	1.43	1.53
1	A	1163	ILE	CA-C	-6.96	1.46	1.52
2	B	814	PHE	CG-CD2	-6.96	1.24	1.38
5	F	119	ARG	N-CA	-6.96	1.37	1.46
7	I	85	PHE	C-N	-6.96	1.24	1.33
2	B	97	VAL	C-O	6.96	1.31	1.24
2	B	203	PHE	C-O	6.96	1.32	1.23
1	A	1255	GLU	C-O	6.96	1.32	1.24
1	A	1346	ALA	C-O	-6.96	1.15	1.24
2	B	756	ILE	C-O	-6.96	1.14	1.24
2	B	1074	ASN	N-CA	-6.96	1.37	1.46
3	C	123	ASN	CB-CG	6.96	1.69	1.52
3	C	240	VAL	C-O	-6.96	1.15	1.24
4	E	169	ARG	C-O	6.96	1.32	1.23
2	B	1006	ILE	N-CA	-6.96	1.38	1.46
3	C	98	VAL	C-O	-6.96	1.16	1.24
8	J	18	TRP	CE2-CZ2	-6.96	1.25	1.39
7	I	57	GLY	C-N	-6.96	1.24	1.33
2	B	183	GLU	CB-CG	6.96	1.73	1.52
2	B	304	ASP	CG-OD2	6.96	1.38	1.25
2	B	662	MET	C-N	-6.96	1.23	1.33
2	B	868	MET	SD-CE	6.96	1.97	1.79
2	B	994	TYR	CE2-CZ	-6.96	1.21	1.38
1	A	1071	SER	C-N	-6.95	1.24	1.33
1	A	1370	LEU	C-N	-6.95	1.24	1.33
1	A	1381	LEU	C-N	-6.95	1.23	1.33
2	B	457	LEU	N-CA	-6.95	1.38	1.46
2	B	744	HIS	CG-CD2	-6.95	1.28	1.35
9	K	73	LEU	CG-CD2	-6.95	1.29	1.52
2	B	1184	GLY	CA-C	-6.95	1.45	1.52
1	A	139	TRP	CD2-CE2	-6.95	1.29	1.41
2	B	366	GLN	CA-C	-6.95	1.43	1.52
7	I	13	MET	SD-CE	6.95	1.97	1.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	583	PRO	CA-C	6.95	1.60	1.52
4	E	99	HIS	CA-C	-6.95	1.43	1.52
8	J	53	HIS	CE1-NE2	-6.95	1.25	1.32
2	B	810	GLU	CA-C	-6.95	1.44	1.52
4	E	7	ARG	CZ-NH1	6.95	1.42	1.32
2	B	629	ASP	CA-C	-6.95	1.43	1.52
2	B	655	LYS	N-CA	-6.95	1.37	1.46
2	B	18	PHE	C-N	6.94	1.43	1.33
2	B	855	PHE	CE1-CZ	-6.94	1.17	1.38
2	B	1091	TYR	CG-CD2	-6.94	1.24	1.39
3	C	243	VAL	CA-C	-6.94	1.42	1.52
2	B	1144	ALA	N-CA	-6.94	1.37	1.46
1	A	1408	ILE	CA-C	-6.94	1.43	1.52
2	B	135	ARG	CG-CD	6.94	1.73	1.52
1	A	133	LYS	CA-CB	-6.94	1.41	1.53
1	A	1153	TYR	CE2-CZ	-6.94	1.21	1.38
1	A	482	PHE	N-CA	-6.94	1.37	1.46
1	A	1337	GLU	C-N	6.94	1.40	1.33
2	B	551	PRO	CA-CB	-6.94	1.42	1.54
4	E	163	GLU	N-CA	6.94	1.54	1.46
7	I	95	THR	CB-CG2	-6.94	1.29	1.52
2	B	874	PHE	CD2-CE2	-6.94	1.17	1.38
2	B	633	VAL	C-O	-6.93	1.14	1.24
4	E	179	GLN	CB-CG	-6.93	1.31	1.52
1	A	1130	GLN	CA-CB	6.93	1.65	1.53
1	A	1378	GLN	CG-CD	6.93	1.69	1.52
9	K	28	PRO	N-CA	-6.93	1.39	1.46
2	B	680	THR	CA-C	-6.93	1.43	1.52
1	A	1038	THR	CA-CB	-6.93	1.43	1.53
3	C	132	PRO	CA-C	-6.93	1.42	1.52
2	B	1144	ALA	C-O	6.93	1.32	1.24
9	K	79	GLU	CG-CD	6.93	1.69	1.52
1	A	1241	ARG	C-N	-6.93	1.24	1.33
1	A	1271	ILE	CA-C	-6.93	1.44	1.52
2	B	769	TYR	CD1-CE1	-6.93	1.17	1.38
3	C	17	ASN	CB-CG	6.93	1.69	1.52
3	C	33	LEU	CG-CD1	-6.93	1.29	1.52
3	C	50	GLU	C-N	-6.93	1.24	1.33
2	B	171	PRO	C-N	-6.92	1.23	1.33
1	A	690	VAL	CA-C	-6.92	1.44	1.52
2	B	641	GLU	N-CA	6.92	1.54	1.46
7	I	58	VAL	CA-CB	-6.92	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	606	LYS	N-CA	-6.92	1.36	1.45
2	B	1178	ASN	CG-ND2	6.92	1.47	1.33
2	B	542	MET	C-N	-6.92	1.24	1.33
2	B	1133	MET	C-O	-6.92	1.15	1.24
3	C	54	ASN	CA-CB	-6.92	1.41	1.53
1	A	1050	GLU	CD-OE1	6.92	1.38	1.25
2	B	1151	LEU	CG-CD1	-6.92	1.29	1.52
6	H	88	SER	C-O	6.92	1.32	1.24
2	B	836	GLU	C-N	6.92	1.43	1.33
7	I	48	LEU	CA-CB	-6.92	1.42	1.53
2	B	70	ILE	CA-CB	6.91	1.73	1.54
2	B	1049	ASP	CB-CG	6.91	1.69	1.52
1	A	626	ASN	CG-ND2	6.91	1.47	1.33
2	B	60	GLN	CG-CD	-6.91	1.34	1.52
1	A	212	LYS	CA-C	6.91	1.62	1.52
1	A	289	ILE	CB-CG2	-6.91	1.29	1.52
6	H	82	PRO	CA-C	6.91	1.62	1.52
1	A	133	LYS	CG-CD	6.91	1.73	1.52
4	E	16	PHE	CD1-CE1	-6.91	1.18	1.38
3	C	144	ILE	CB-CG2	-6.91	1.29	1.52
6	H	102	TYR	CG-CD2	-6.91	1.24	1.39
1	A	48	ALA	C-N	6.91	1.42	1.33
1	A	148	CYS	CA-CB	6.91	1.62	1.52
1	A	866	PHE	CG-CD1	-6.91	1.24	1.38
6	H	84	ALA	C-N	6.91	1.43	1.33
8	J	20	SER	CA-C	-6.90	1.43	1.52
2	B	351	TYR	CG-CD1	-6.90	1.24	1.39
2	B	1076	HIS	CE1-NE2	-6.90	1.25	1.32
5	F	145	ASP	CA-CB	-6.90	1.43	1.53
6	H	3	ASN	N-CA	6.90	1.56	1.46
2	B	587	HIS	CB-CG	-6.90	1.40	1.50
7	I	119	THR	C-N	6.90	1.41	1.33
4	E	102	GLU	N-CA	-6.90	1.37	1.46
10	L	30	ILE	C-O	6.90	1.31	1.23
2	B	19	GLU	CD-OE2	6.90	1.38	1.25
1	A	233	TRP	CA-CB	6.89	1.65	1.53
2	B	137	TYR	CA-CB	6.89	1.65	1.53
3	C	3	GLU	N-CA	6.89	1.59	1.46
7	I	63	GLY	N-CA	-6.89	1.35	1.45
4	E	5	ASN	CA-CB	6.89	1.65	1.53
1	A	81	PHE	CG-CD1	-6.89	1.24	1.38
1	A	1155	ASP	C-O	-6.89	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	62	ARG	CZ-NH1	6.89	1.42	1.32
10	L	25	ALA	CA-CB	6.89	1.75	1.52
1	A	58	LEU	CG-CD2	-6.89	1.29	1.52
1	A	264	PHE	CD1-CE1	6.89	1.59	1.38
1	A	369	SER	CA-C	-6.89	1.43	1.52
2	B	245	GLU	N-CA	6.89	1.54	1.46
2	B	992	ILE	CB-CG1	-6.89	1.39	1.53
1	A	532	ARG	C-O	-6.88	1.16	1.24
4	E	168	TYR	CD2-CE2	6.88	1.59	1.38
2	B	766	ARG	NE-CZ	-6.88	1.25	1.33
1	A	538	ASP	CA-C	-6.88	1.43	1.52
1	A	1187	GLN	CG-CD	6.88	1.69	1.52
2	B	1019	SER	C-N	-6.88	1.23	1.33
1	A	940	ARG	CG-CD	6.88	1.73	1.52
2	B	798	TYR	C-O	-6.88	1.16	1.24
1	A	300	VAL	CA-CB	-6.88	1.45	1.54
1	A	444	PHE	C-O	-6.88	1.15	1.23
1	A	1024	SER	CB-OG	6.88	1.55	1.42
1	A	1315	GLU	CA-CB	6.88	1.64	1.53
2	B	254	LEU	CA-CB	-6.88	1.43	1.53
4	E	98	ILE	N-CA	-6.88	1.38	1.46
2	B	1003	ALA	N-CA	-6.88	1.37	1.46
2	B	407	ASP	CA-C	6.87	1.61	1.52
7	I	73	ARG	CZ-NH2	6.87	1.42	1.33
1	A	207	ILE	CG1-CD1	-6.87	1.25	1.51
1	A	922	ASP	CA-C	-6.87	1.44	1.52
2	B	380	TYR	N-CA	-6.87	1.37	1.46
2	B	640	VAL	CB-CG1	-6.87	1.29	1.52
2	B	1055	ILE	N-CA	-6.87	1.37	1.46
1	A	847	ASP	N-CA	-6.87	1.37	1.46
1	A	884	ASP	CG-OD1	6.87	1.38	1.25
7	I	84	VAL	CA-C	6.87	1.61	1.52
1	A	4	GLN	C-N	6.87	1.42	1.33
2	B	569	TYR	CG-CD2	-6.87	1.25	1.39
2	B	872	GLU	CG-CD	6.87	1.69	1.52
2	B	1171	VAL	CA-C	6.87	1.60	1.52
6	H	124	ARG	NE-CZ	-6.87	1.25	1.33
2	B	236	HIS	CA-C	-6.86	1.44	1.52
2	B	860	MET	CA-CB	-6.86	1.42	1.53
2	B	1089	PRO	CA-CB	6.86	1.62	1.53
2	B	1026	LEU	CB-CG	-6.86	1.39	1.53
4	E	56	LYS	C-O	6.86	1.32	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	174	GLN	N-CA	6.86	1.55	1.46
1	A	1029	ARG	C-O	-6.86	1.15	1.24
1	A	1217	LYS	CA-CB	-6.86	1.41	1.53
3	C	267	GLN	CD-OE1	6.86	1.36	1.23
1	A	361	LEU	CA-C	-6.86	1.43	1.52
4	E	212	ARG	CD-NE	-6.86	1.36	1.46
1	A	76	GLU	C-O	6.86	1.33	1.24
1	A	907	THR	CA-CB	6.86	1.64	1.53
2	B	394	ASP	CB-CG	6.86	1.69	1.52
2	B	825	VAL	CA-CB	-6.86	1.45	1.54
9	K	65	HIS	CG-ND1	-6.85	1.30	1.38
1	A	1312	ASN	CA-C	-6.85	1.45	1.53
2	B	620	ARG	CA-C	-6.85	1.43	1.52
2	B	836	GLU	CA-C	-6.85	1.45	1.53
3	C	43	THR	CA-CB	-6.85	1.42	1.53
1	A	129	LYS	C-O	6.85	1.33	1.23
1	A	367	PRO	CA-C	-6.85	1.44	1.52
1	A	419	LYS	CE-NZ	-6.85	1.28	1.49
1	A	773	LYS	CA-C	-6.85	1.44	1.52
2	B	813	LYS	CD-CE	6.85	1.73	1.52
2	B	1153	GLU	CD-OE1	6.85	1.38	1.25
6	H	35	GLN	CA-CB	6.85	1.65	1.53
8	J	3	VAL	C-O	-6.85	1.15	1.24
1	A	737	LEU	CG-CD1	-6.85	1.29	1.52
2	B	350	GLN	CD-OE1	6.85	1.36	1.23
9	K	35	PHE	CA-CB	6.85	1.62	1.53
9	K	102	LYS	CD-CE	6.85	1.73	1.52
1	A	676	MET	N-CA	-6.85	1.37	1.46
2	B	44	VAL	CA-CB	-6.85	1.45	1.54
1	A	494	SER	CA-C	-6.84	1.43	1.52
2	B	195	CYS	C-N	-6.84	1.24	1.33
2	B	766	ARG	CD-NE	6.84	1.55	1.46
2	B	936	ASP	CA-CB	6.84	1.62	1.53
9	K	14	GLU	CA-CB	6.84	1.64	1.53
2	B	1074	ASN	CA-CB	-6.84	1.42	1.53
2	B	1157	ALA	C-O	6.84	1.31	1.23
6	H	100	THR	CA-CB	-6.84	1.42	1.53
1	A	133	LYS	N-CA	-6.84	1.37	1.46
1	A	276	LEU	CA-C	-6.84	1.43	1.52
1	A	1294	PRO	CG-CD	-6.84	1.27	1.50
2	B	948	ILE	CG1-CD1	-6.84	1.25	1.51
3	C	139	GLY	N-CA	6.84	1.55	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	701	LEU	N-CA	-6.84	1.36	1.46
2	B	315	LYS	CB-CG	-6.84	1.31	1.52
2	B	637	LEU	N-CA	-6.84	1.37	1.45
4	E	144	ILE	C-O	-6.84	1.14	1.24
7	I	107	SER	C-O	6.84	1.33	1.23
3	C	15	LYS	CD-CE	6.83	1.73	1.52
1	A	1287	TYR	CD2-CE2	6.83	1.59	1.38
1	A	1336	MET	CB-CG	-6.83	1.31	1.52
2	B	213	ILE	CG1-CD1	-6.83	1.25	1.51
2	B	401	PHE	CG-CD2	-6.83	1.24	1.38
1	A	657	LEU	CA-C	-6.83	1.43	1.52
2	B	482	VAL	CA-C	-6.83	1.45	1.52
8	J	42	LYS	N-CA	-6.83	1.37	1.46
9	K	61	TYR	CZ-OH	-6.83	1.23	1.38
1	A	683	ILE	N-CA	-6.83	1.38	1.46
1	A	984	LYS	N-CA	-6.83	1.37	1.46
2	B	662	MET	C-O	-6.83	1.15	1.24
4	E	135	PHE	C-O	-6.83	1.15	1.23
3	C	89	GLU	C-O	6.83	1.32	1.24
1	A	135	PHE	CG-CD1	-6.83	1.24	1.38
1	A	659	HIS	C-N	-6.83	1.24	1.33
2	B	268	THR	CA-CB	-6.83	1.43	1.53
2	B	288	ALA	CA-C	-6.83	1.43	1.52
2	B	348	ARG	CB-CG	-6.83	1.31	1.52
3	C	23	SER	CB-OG	6.83	1.55	1.42
3	C	31	ASN	C-N	-6.83	1.25	1.34
7	I	16	PRO	CG-CD	6.82	1.74	1.50
7	I	54	GLU	CA-C	-6.82	1.43	1.52
1	A	1262	LYS	CA-CB	6.82	1.64	1.53
4	E	40	GLU	N-CA	6.82	1.54	1.46
4	E	183	PRO	CB-CG	-6.82	1.15	1.49
1	A	406	ILE	CA-C	-6.82	1.44	1.52
1	A	1050	GLU	N-CA	-6.82	1.38	1.46
1	A	1049	ILE	C-N	-6.82	1.24	1.33
2	B	747	MET	CA-C	6.82	1.62	1.52
1	A	772	GLY	CA-C	-6.82	1.41	1.51
1	A	176	LYS	CA-C	6.81	1.61	1.52
1	A	964	ILE	C-O	6.81	1.32	1.24
1	A	613	ILE	N-CA	-6.81	1.37	1.46
1	A	945	GLU	CD-OE1	6.81	1.38	1.25
2	B	451	LYS	CD-CE	6.81	1.72	1.52
2	B	1054	GLY	CA-C	-6.81	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	170	TRP	C-N	-6.81	1.23	1.33
10	L	67	PHE	N-CA	-6.81	1.37	1.45
1	A	905	ASP	CA-CB	-6.81	1.42	1.53
2	B	1055	ILE	CG1-CD1	-6.81	1.25	1.51
1	A	19	PHE	CD1-CE1	-6.81	1.18	1.38
2	B	98	THR	CA-C	6.81	1.61	1.52
2	B	571	PRO	C-O	-6.81	1.15	1.24
2	B	729	ILE	CA-CB	-6.81	1.45	1.54
1	A	1074	GLU	CA-C	-6.81	1.46	1.52
2	B	1051	THR	C-N	-6.81	1.25	1.33
2	B	900	ALA	CA-C	-6.81	1.46	1.52
2	B	367	LEU	CG-CD1	6.80	1.75	1.52
3	C	168	ALA	CA-CB	-6.80	1.41	1.53
1	A	213	HIS	C-O	6.80	1.33	1.24
2	B	186	GLU	CD-OE1	6.80	1.38	1.25
1	A	739	ASP	C-N	-6.80	1.23	1.33
2	B	37	PHE	CD2-CE2	6.80	1.59	1.38
2	B	90	ILE	C-O	6.80	1.32	1.24
2	B	689	LEU	C-O	-6.80	1.15	1.24
2	B	739	THR	N-CA	6.80	1.55	1.45
2	B	63	ILE	CB-CG2	-6.80	1.30	1.52
2	B	69	LEU	C-O	6.80	1.32	1.24
2	B	564	GLU	C-O	-6.80	1.15	1.24
2	B	655	LYS	C-N	-6.80	1.25	1.33
1	A	1110	ASN	C-N	-6.79	1.23	1.33
3	C	211	ASP	CA-CB	6.79	1.62	1.53
1	A	21	LEU	CA-CB	-6.79	1.41	1.53
1	A	1219	THR	C-O	6.79	1.32	1.24
1	A	1272	THR	CB-CG2	6.79	1.75	1.52
2	B	710	LEU	C-O	-6.79	1.15	1.23
9	K	86	ALA	CA-CB	-6.79	1.42	1.53
2	B	49	ASP	CB-CG	6.79	1.69	1.52
2	B	449	ASN	CB-CG	6.79	1.69	1.52
3	C	170	TRP	N-CA	-6.79	1.37	1.46
3	C	143	LEU	CA-C	-6.79	1.44	1.52
1	A	617	VAL	N-CA	6.79	1.54	1.46
1	A	1239	ARG	CD-NE	6.79	1.55	1.46
2	B	658	ILE	CG1-CD1	-6.79	1.25	1.51
2	B	963	PHE	CE2-CZ	6.79	1.59	1.38
3	C	203	GLN	CA-C	-6.79	1.43	1.52
4	E	159	ASP	CA-CB	6.79	1.64	1.53
1	A	759	ALA	C-O	-6.79	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1023	ARG	CA-CB	-6.79	1.42	1.53
2	B	665	GLU	CA-C	-6.78	1.44	1.52
1	A	125	ALA	CA-C	-6.78	1.43	1.52
2	B	307	ASP	CA-C	6.78	1.61	1.52
2	B	430	ARG	NE-CZ	6.78	1.40	1.33
2	B	973	ILE	C-N	-6.78	1.25	1.33
2	B	975	GLN	CA-C	-6.78	1.44	1.52
1	A	1241	ARG	CA-C	-6.78	1.44	1.52
8	J	59	LYS	CA-C	-6.78	1.43	1.52
2	B	964	VAL	N-CA	-6.78	1.38	1.46
2	B	397	ASP	C-N	-6.78	1.23	1.33
3	C	209	TYR	N-CA	-6.78	1.37	1.46
1	A	463	ILE	C-O	-6.78	1.15	1.24
1	A	728	LYS	CE-NZ	6.78	1.69	1.49
2	B	500	THR	CA-C	-6.78	1.43	1.52
2	B	891	ASP	CB-CG	6.78	1.69	1.52
10	L	69	ALA	C-O	6.78	1.32	1.23
4	E	4	GLU	CA-CB	6.77	1.63	1.53
7	I	67	THR	C-O	-6.77	1.15	1.24
2	B	1148	LYS	CG-CD	6.77	1.72	1.52
2	B	1220	ARG	C-O	6.77	1.32	1.24
7	I	19	ASP	C-N	6.77	1.43	1.33
9	K	15	GLY	C-O	6.77	1.33	1.23
7	I	83	ASN	C-O	6.77	1.32	1.23
2	B	325	GLN	CB-CG	-6.77	1.32	1.52
3	C	228	PHE	CG-CD1	-6.77	1.24	1.38
1	A	273	ASN	CG-ND2	6.77	1.47	1.33
1	A	689	LYS	C-O	-6.77	1.16	1.24
1	A	1261	LYS	CG-CD	6.77	1.72	1.52
2	B	28	GLU	CA-C	-6.77	1.43	1.52
2	B	1159	ARG	CB-CG	6.77	1.72	1.52
2	B	310	MET	CB-CG	-6.77	1.32	1.52
3	C	117	ASP	CA-CB	-6.77	1.42	1.53
2	B	341	LEU	CB-CG	-6.76	1.40	1.53
2	B	1100	ASP	CA-C	6.76	1.61	1.52
2	B	216	GLU	CA-C	-6.76	1.44	1.52
2	B	630	ALA	CA-C	-6.76	1.44	1.53
1	A	705	LYS	CE-NZ	6.76	1.69	1.49
1	A	1066	VAL	C-O	-6.76	1.16	1.24
2	B	239	GLU	CD-OE1	6.76	1.38	1.25
4	E	54	GLN	N-CA	-6.76	1.37	1.46
1	A	55	ASP	CG-OD2	6.76	1.38	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	439	ASN	CB-CG	-6.76	1.35	1.52
1	A	1240	CYS	CA-C	6.76	1.60	1.52
3	C	247	GLY	CA-C	-6.76	1.44	1.52
6	H	104	PHE	CE2-CZ	6.76	1.58	1.38
2	B	186	GLU	CA-CB	6.76	1.64	1.53
3	C	4	GLU	CA-CB	6.76	1.64	1.53
7	I	8	ARG	C-O	-6.76	1.16	1.24
1	A	1310	GLY	C-O	-6.75	1.15	1.23
2	B	896	ASP	N-CA	6.75	1.55	1.46
3	C	90	ASP	N-CA	6.75	1.54	1.46
1	A	95	PHE	C-N	6.75	1.42	1.34
1	A	960	ILE	CB-CG2	-6.75	1.30	1.52
1	A	1059	HIS	C-O	-6.75	1.15	1.24
1	A	1407	GLU	CA-C	6.75	1.61	1.52
1	A	1438	THR	CB-CG2	-6.75	1.30	1.52
2	B	20	ASP	CA-C	-6.75	1.44	1.52
2	B	353	LYS	C-O	-6.75	1.16	1.24
4	E	180	ARG	C-O	6.75	1.32	1.24
7	I	23	ASN	CG-ND2	6.75	1.47	1.33
8	J	48	ARG	CA-C	-6.75	1.43	1.52
1	A	397	ASN	CA-CB	-6.75	1.43	1.53
2	B	194	GLU	C-O	-6.75	1.15	1.24
2	B	846	ILE	CA-C	6.75	1.61	1.52
2	B	1093	GLN	N-CA	-6.75	1.37	1.46
2	B	1100	ASP	CG-OD1	6.75	1.38	1.25
9	K	35	PHE	CE1-CZ	-6.75	1.18	1.38
1	A	429	GLY	CA-C	6.75	1.61	1.51
1	A	527	THR	CB-OG1	6.75	1.54	1.43
2	B	771	SER	C-N	-6.75	1.25	1.33
2	B	996	ARG	NE-CZ	-6.75	1.25	1.33
2	B	1109	GLY	C-O	6.75	1.33	1.24
3	C	16	ASP	CA-C	6.75	1.61	1.52
1	A	1157	ASP	N-CA	-6.75	1.39	1.46
2	B	166	PHE	CA-C	-6.75	1.44	1.52
2	B	565	PRO	CA-CB	-6.75	1.46	1.54
1	A	498	ARG	C-O	6.74	1.32	1.24
2	B	70	ILE	CG1-CD1	6.74	1.78	1.51
2	B	798	TYR	CG-CD1	-6.74	1.25	1.39
3	C	111	THR	CB-OG1	6.74	1.54	1.43
10	L	70	ARG	C-OXT	-6.74	1.10	1.23
3	C	220	ASP	C-O	6.74	1.32	1.23
1	A	739	ASP	N-CA	-6.74	1.37	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	10	ILE	CA-CB	-6.74	1.45	1.54
3	C	129	ILE	CG1-CD1	-6.74	1.25	1.51
7	I	72	ASP	CG-OD2	6.74	1.38	1.25
1	A	1176	LEU	CG-CD2	6.74	1.74	1.52
1	A	1353	TYR	CG-CD2	-6.74	1.25	1.39
2	B	276	ILE	C-O	6.74	1.31	1.24
2	B	359	GLU	C-O	-6.74	1.15	1.24
6	H	77	ARG	CG-CD	6.74	1.72	1.52
10	L	65	VAL	CB-CG2	6.74	1.74	1.52
1	A	1218	GLN	CB-CG	6.74	1.72	1.52
3	C	152	GLU	C-O	-6.74	1.15	1.23
3	C	214	ASN	N-CA	6.74	1.54	1.46
7	I	63	GLY	C-N	-6.74	1.23	1.33
10	L	33	GLU	N-CA	6.74	1.54	1.46
1	A	692	ASP	CB-CG	6.73	1.68	1.52
1	A	1115	SER	CB-OG	6.73	1.55	1.42
2	B	872	GLU	CA-C	6.73	1.61	1.52
1	A	61	ILE	C-O	6.73	1.32	1.24
1	A	402	ALA	CA-CB	-6.73	1.42	1.53
1	A	697	ALA	CA-C	-6.73	1.43	1.52
1	A	1356	ILE	CA-CB	-6.73	1.45	1.54
1	A	1092	LYS	C-N	6.73	1.43	1.33
1	A	1326	ARG	CZ-NH2	-6.73	1.24	1.33
2	B	221	ASN	CA-CB	-6.73	1.44	1.53
6	H	93	TYR	CA-C	6.73	1.62	1.53
1	A	674	PRO	C-O	6.73	1.32	1.24
7	I	15	TYR	C-O	-6.73	1.17	1.24
9	K	61	TYR	CE2-CZ	-6.73	1.22	1.38
1	A	84	ILE	CB-CG1	-6.72	1.40	1.53
1	A	1138	ILE	N-CA	-6.72	1.37	1.45
2	B	40	GLU	C-O	6.72	1.32	1.24
1	A	101	LYS	CB-CG	6.72	1.72	1.52
2	B	848	ARG	NE-CZ	-6.72	1.25	1.33
3	C	191	TYR	CG-CD2	-6.72	1.25	1.39
1	A	897	TYR	N-CA	6.72	1.54	1.46
1	A	900	ASP	C-N	-6.72	1.24	1.33
2	B	780	VAL	C-O	-6.72	1.16	1.24
3	C	81	GLU	CD-OE2	6.72	1.38	1.25
3	C	87	PHE	CA-C	-6.72	1.42	1.52
1	A	499	ALA	C-N	-6.72	1.25	1.33
2	B	1018	PRO	CA-CB	-6.72	1.44	1.53
2	B	745	PRO	C-O	-6.72	1.15	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	616	ILE	CA-C	-6.71	1.44	1.52
4	E	11	ARG	CZ-NH2	6.71	1.42	1.33
1	A	1340	GLY	N-CA	6.71	1.51	1.45
6	H	41	ASP	N-CA	-6.71	1.38	1.46
2	B	992	ILE	CB-CG2	-6.71	1.30	1.52
4	E	120	ALA	C-O	-6.71	1.16	1.24
7	I	74	GLU	CG-CD	6.71	1.68	1.52
1	A	1014	ALA	CA-CB	-6.71	1.41	1.53
2	B	320	ASP	CB-CG	6.71	1.68	1.52
3	C	186	LEU	C-O	6.71	1.32	1.24
9	K	55	LYS	CG-CD	6.71	1.72	1.52
4	E	46	TYR	CD2-CE2	6.71	1.58	1.38
1	A	446	ARG	C-O	-6.70	1.15	1.24
1	A	503	GLN	C-O	-6.70	1.15	1.24
2	B	738	PHE	CD2-CE2	-6.70	1.18	1.38
2	B	1209	ALA	CA-CB	-6.70	1.42	1.53
1	A	56	PRO	C-O	6.70	1.32	1.24
2	B	127	GLY	CA-C	-6.70	1.42	1.51
3	C	233	GLU	C-O	-6.70	1.15	1.24
1	A	63	ARG	NE-CZ	6.70	1.40	1.33
1	A	497	THR	CB-CG2	-6.70	1.30	1.52
1	A	11	LEU	C-O	-6.70	1.16	1.24
1	A	1034	GLU	CA-C	6.70	1.60	1.52
1	A	353	ILE	CA-C	-6.70	1.44	1.52
1	A	684	ALA	CA-C	6.70	1.61	1.52
1	A	796	SER	N-CA	-6.70	1.37	1.46
2	B	1176	ASN	CG-ND2	6.70	1.47	1.33
5	F	128	LYS	CG-CD	6.70	1.72	1.52
9	K	45	LEU	C-N	6.70	1.42	1.33
1	A	1165	GLU	C-O	-6.69	1.15	1.24
1	A	1433	MET	CB-CG	-6.69	1.32	1.52
2	B	488	TYR	C-N	-6.69	1.23	1.33
2	B	611	PRO	N-CD	-6.69	1.38	1.47
2	B	1034	VAL	CA-C	-6.69	1.44	1.52
4	E	125	PRO	CA-C	-6.69	1.46	1.52
7	I	22	ASN	CG-OD1	6.69	1.36	1.23
1	A	948	VAL	N-CA	-6.69	1.36	1.46
1	A	1052	GLN	N-CA	-6.69	1.38	1.46
1	A	994	GLN	C-O	6.69	1.31	1.24
1	A	1012	ARG	CD-NE	6.69	1.55	1.46
6	H	8	ASP	C-O	6.69	1.32	1.24
6	H	136	LYS	CB-CG	6.69	1.72	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	587	HIS	CA-CB	6.69	1.70	1.53
2	B	420	LEU	N-CA	-6.69	1.37	1.46
2	B	620	ARG	NE-CZ	-6.69	1.25	1.33
2	B	837	ASP	N-CA	-6.69	1.36	1.46
5	F	131	PRO	CA-CB	-6.69	1.45	1.53
1	A	411	ASP	CG-OD1	6.69	1.38	1.25
1	A	1339	LEU	N-CA	-6.69	1.36	1.45
3	C	67	LEU	CG-CD1	-6.69	1.30	1.52
7	I	104	LEU	CG-CD2	-6.69	1.30	1.52
1	A	1092	LYS	CD-CE	6.68	1.72	1.52
4	E	18	THR	CB-OG1	6.68	1.54	1.43
4	E	75	MET	SD-CE	6.68	1.96	1.79
7	I	90	GLN	CG-CD	-6.68	1.35	1.52
8	J	39	LEU	CA-CB	-6.68	1.43	1.53
1	A	397	ASN	C-O	6.68	1.33	1.24
1	A	698	GLN	CD-NE2	6.68	1.47	1.33
1	A	815	PHE	CG-CD2	-6.68	1.24	1.38
2	B	287	ARG	CG-CD	6.68	1.72	1.52
1	A	1255	GLU	CG-CD	6.68	1.68	1.52
1	A	1311	VAL	CA-CB	-6.68	1.45	1.54
2	B	40	GLU	CD-OE1	6.68	1.38	1.25
2	B	776	GLN	CA-CB	-6.68	1.44	1.53
3	C	98	VAL	CA-CB	-6.68	1.46	1.54
4	E	39	LEU	N-CA	-6.68	1.38	1.46
1	A	552	TRP	CD2-CE3	-6.68	1.29	1.40
1	A	953	ASN	C-N	-6.68	1.24	1.33
1	A	994	GLN	C-N	-6.68	1.24	1.33
3	C	231	ASN	C-O	-6.68	1.15	1.24
1	A	991	LYS	CE-NZ	6.68	1.69	1.49
3	C	94	LYS	CG-CD	6.68	1.72	1.52
1	A	367	PRO	C-N	-6.68	1.25	1.33
1	A	412	ARG	CZ-NH1	6.68	1.42	1.32
1	A	563	PRO	C-N	-6.68	1.23	1.33
2	B	701	ILE	CA-C	6.68	1.61	1.52
3	C	71	PRO	CA-C	-6.68	1.43	1.52
5	F	78	GLN	CA-C	6.68	1.61	1.52
7	I	59	VAL	CA-C	6.68	1.60	1.52
3	C	197	SER	C-O	-6.67	1.16	1.24
2	B	666	TYR	CD2-CE2	6.67	1.58	1.38
1	A	1019	CYS	N-CA	-6.67	1.37	1.46
2	B	304	ASP	CB-CG	6.67	1.68	1.52
4	E	49	SER	C-O	6.67	1.32	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	66	GLU	CB-CG	6.67	1.72	1.52
4	E	204	THR	CB-CG2	-6.67	1.30	1.52
6	H	15	VAL	CA-CB	-6.67	1.45	1.54
6	H	92	ASP	N-CA	-6.67	1.38	1.46
1	A	837	ILE	C-N	-6.67	1.25	1.33
9	K	66	PRO	N-CD	-6.67	1.38	1.47
2	B	573	GLN	CD-OE1	6.67	1.36	1.23
2	B	667	GLN	N-CA	6.67	1.55	1.46
1	A	1239	ARG	NE-CZ	-6.67	1.25	1.33
2	B	284	ILE	N-CA	-6.67	1.38	1.46
2	B	312	GLU	N-CA	-6.67	1.37	1.46
4	E	178	ILE	N-CA	6.67	1.54	1.46
7	I	94	ASP	CG-OD1	6.67	1.38	1.25
1	A	241	VAL	N-CA	-6.66	1.41	1.46
1	A	1171	GLN	CB-CG	6.66	1.72	1.52
2	B	364	ILE	N-CA	-6.66	1.38	1.46
1	A	1405	THR	CA-C	6.66	1.67	1.52
2	B	577	ALA	CA-CB	-6.66	1.43	1.53
3	C	237	SER	CA-CB	-6.66	1.42	1.53
3	C	250	THR	C-O	-6.66	1.16	1.24
5	F	103	MET	CA-CB	-6.66	1.43	1.53
6	H	94	ASP	CA-C	6.66	1.61	1.52
1	A	1376	THR	CB-CG2	-6.66	1.30	1.52
2	B	1013	ASN	C-O	-6.66	1.13	1.24
9	K	15	GLY	CA-C	6.66	1.61	1.51
1	A	490	HIS	C-O	-6.66	1.16	1.24
1	A	728	LYS	C-N	-6.66	1.24	1.33
1	A	845	LEU	CG-CD2	-6.66	1.30	1.52
1	A	853	ASP	CA-C	-6.66	1.41	1.52
2	B	1047	PHE	CA-CB	-6.66	1.43	1.53
1	A	848	ILE	C-N	-6.66	1.25	1.33
2	B	221	ASN	CG-ND2	6.66	1.47	1.33
2	B	949	VAL	N-CA	-6.66	1.38	1.46
3	C	157	CYS	CB-SG	-6.66	1.59	1.81
6	H	136	LYS	CD-CE	6.65	1.72	1.52
1	A	709	THR	CA-CB	-6.65	1.42	1.53
2	B	901	PRO	C-O	-6.65	1.15	1.24
7	I	58	VAL	C-N	-6.65	1.24	1.33
2	B	681	TRP	CD2-CE2	-6.65	1.30	1.41
8	J	9	SER	N-CA	-6.65	1.37	1.46
2	B	381	MET	CA-C	-6.65	1.43	1.52
2	B	710	LEU	CA-CB	-6.65	1.42	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	150	VAL	CA-CB	-6.65	1.46	1.54
6	H	80	ARG	CA-CB	6.65	1.61	1.53
1	A	72	GLU	N-CA	6.65	1.54	1.46
1	A	813	PHE	CD2-CE2	6.64	1.58	1.38
1	A	1063	MET	C-N	-6.64	1.24	1.33
1	A	1258	HIS	CA-CB	6.64	1.63	1.53
2	B	222	ILE	N-CA	-6.64	1.38	1.46
2	B	766	ARG	C-N	-6.64	1.25	1.33
1	A	630	ILE	C-O	-6.64	1.15	1.24
1	A	786	HIS	CB-CG	-6.64	1.40	1.50
2	B	652	LYS	CG-CD	6.64	1.72	1.52
2	B	966	VAL	CA-CB	-6.64	1.46	1.54
4	E	110	PHE	CE2-CZ	-6.64	1.18	1.38
2	B	1224	PHE	CA-C	6.64	1.66	1.52
1	A	516	SER	C-O	-6.64	1.14	1.23
1	A	859	SER	N-CA	-6.64	1.37	1.46
5	F	84	TYR	CG-CD1	-6.64	1.25	1.39
7	I	103	CYS	CA-C	-6.64	1.44	1.52
1	A	21	LEU	N-CA	6.63	1.53	1.45
9	K	31	VAL	C-O	6.63	1.32	1.23
1	A	1005	GLU	CD-OE2	6.63	1.38	1.25
2	B	262	GLU	CA-CB	6.63	1.64	1.53
2	B	275	TYR	C-N	-6.63	1.25	1.33
3	C	65	HIS	CA-C	6.63	1.61	1.52
4	E	212	ARG	CG-CD	6.63	1.72	1.52
1	A	1103	GLU	N-CA	-6.63	1.38	1.46
3	C	73	GLN	C-O	-6.63	1.15	1.23
1	A	438	ASP	C-O	-6.63	1.16	1.23
1	A	622	VAL	CB-CG1	-6.63	1.30	1.52
7	I	14	LEU	CA-CB	6.63	1.65	1.53
1	A	709	THR	CB-CG2	-6.63	1.30	1.52
2	B	316	PRO	CA-C	-6.62	1.43	1.52
4	E	187	TYR	CE1-CZ	-6.62	1.22	1.38
6	H	122	LEU	CA-C	6.62	1.60	1.52
7	I	55	THR	CA-CB	-6.62	1.43	1.53
1	A	803	SER	C-O	-6.62	1.15	1.23
1	A	1428	VAL	CB-CG1	-6.62	1.30	1.52
1	A	662	PHE	CE1-CZ	-6.62	1.18	1.38
2	B	1195	HIS	CA-C	6.62	1.60	1.52
9	K	47	ARG	CZ-NH1	6.62	1.42	1.32
1	A	1290	LYS	C-O	6.62	1.31	1.24
3	C	47	ASP	CB-CG	6.62	1.68	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	191	TYR	CG-CD1	6.62	1.53	1.39
4	E	95	THR	CB-CG2	6.62	1.74	1.52
1	A	198	GLU	CD-OE2	6.62	1.38	1.25
2	B	652	LYS	CE-NZ	6.62	1.69	1.49
7	I	39	GLY	C-O	6.62	1.32	1.23
1	A	1426	GLU	CG-CD	6.61	1.68	1.52
2	B	1210	MET	SD-CE	6.61	1.96	1.79
8	J	4	PRO	N-CA	-6.61	1.39	1.47
2	B	345	LYS	CG-CD	6.61	1.72	1.52
1	A	698	GLN	CG-CD	6.61	1.68	1.52
2	B	196	PRO	N-CD	-6.61	1.38	1.47
8	J	31	ASP	CG-OD1	6.61	1.38	1.25
10	L	62	LYS	CB-CG	6.61	1.72	1.52
1	A	279	LEU	CB-CG	6.61	1.66	1.53
3	C	35	ARG	CG-CD	6.61	1.72	1.52
4	E	106	GLN	CD-NE2	6.61	1.47	1.33
2	B	895	ASP	CA-CB	6.60	1.65	1.53
3	C	148	ARG	CB-CG	-6.60	1.32	1.52
3	C	259	LEU	CG-CD2	-6.60	1.30	1.52
1	A	1191	TRP	N-CA	6.60	1.54	1.46
4	E	152	LYS	CG-CD	6.60	1.72	1.52
1	A	1221	LYS	CE-NZ	6.60	1.69	1.49
2	B	1037	LEU	N-CA	-6.60	1.38	1.46
10	L	61	THR	CB-OG1	-6.60	1.33	1.43
1	A	129	LYS	CB-CG	6.60	1.72	1.52
1	A	1038	THR	CB-OG1	-6.60	1.33	1.43
1	A	1121	GLU	CD-OE2	6.60	1.37	1.25
1	A	1328	TYR	CA-C	-6.60	1.44	1.52
2	B	811	TYR	CG-CD1	-6.60	1.25	1.39
1	A	264	PHE	CE2-CZ	6.60	1.58	1.38
1	A	1121	GLU	CA-C	-6.60	1.45	1.53
2	B	810	GLU	CD-OE1	6.60	1.37	1.25
2	B	1198	TYR	CD2-CE2	6.60	1.58	1.38
8	J	45	CYS	C-O	6.60	1.32	1.24
7	I	120	GLN	CG-CD	6.60	1.68	1.52
1	A	435	HIS	C-O	-6.59	1.14	1.23
1	A	593	GLU	CD-OE1	6.59	1.37	1.25
2	B	1140	ALA	C-O	6.59	1.32	1.24
2	B	557	PHE	CA-CB	-6.59	1.42	1.53
1	A	491	VAL	CB-CG2	-6.59	1.30	1.52
1	A	498	ARG	CZ-NH2	-6.59	1.24	1.33
1	A	842	VAL	C-O	-6.59	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	982	THR	CA-C	6.59	1.62	1.53
2	B	287	ARG	NE-CZ	-6.59	1.25	1.33
2	B	955	THR	CA-CB	6.59	1.62	1.53
1	A	591	PHE	CE1-CZ	-6.59	1.18	1.38
2	B	218	SER	C-N	-6.59	1.24	1.33
2	B	482	VAL	C-N	-6.59	1.24	1.33
3	C	126	GLY	N-CA	6.59	1.54	1.45
2	B	225	VAL	C-O	-6.58	1.15	1.24
1	A	1070	GLN	CA-C	-6.58	1.44	1.52
1	A	1256	GLU	CD-OE2	6.58	1.37	1.25
2	B	130	VAL	CA-CB	6.58	1.63	1.54
2	B	188	ASP	N-CA	-6.58	1.37	1.46
2	B	230	ALA	C-O	6.58	1.32	1.24
3	C	121	VAL	CA-CB	-6.58	1.45	1.54
9	K	5	ASP	CG-OD1	6.58	1.37	1.25
1	A	187	LYS	CA-CB	6.58	1.63	1.54
1	A	616	VAL	CB-CG1	-6.58	1.30	1.52
1	A	642	CYS	N-CA	-6.58	1.38	1.46
2	B	416	LEU	CB-CG	-6.58	1.40	1.53
1	A	1281	ARG	CD-NE	6.58	1.55	1.46
1	A	1345	ARG	CZ-NH1	-6.58	1.23	1.32
1	A	1060	PRO	CA-C	-6.57	1.44	1.52
3	C	84	ARG	CG-CD	6.57	1.72	1.52
1	A	469	ARG	CB-CG	6.57	1.72	1.52
1	A	269	ILE	C-O	-6.57	1.15	1.24
1	A	511	ILE	CB-CG2	-6.57	1.30	1.52
1	A	1368	MET	CA-C	-6.57	1.43	1.52
2	B	581	PHE	CA-C	6.57	1.60	1.52
2	B	951	GLN	CD-OE1	6.57	1.36	1.23
1	A	228	PHE	C-O	6.57	1.33	1.23
1	A	468	PHE	CG-CD1	-6.57	1.25	1.38
1	A	1354	ASN	CB-CG	6.57	1.68	1.52
2	B	480	SER	CA-C	-6.57	1.44	1.52
3	C	32	SER	N-CA	-6.57	1.38	1.46
2	B	778	MET	CB-CG	-6.57	1.32	1.52
4	E	183	PRO	CA-C	-6.57	1.41	1.52
9	K	65	HIS	CE1-NE2	-6.57	1.25	1.32
2	B	18	PHE	C-O	6.56	1.36	1.23
2	B	522	VAL	CA-C	6.56	1.60	1.52
5	F	119	ARG	C-O	6.56	1.32	1.24
3	C	57	VAL	CB-CG2	-6.56	1.30	1.52
6	H	109	LYS	C-O	6.56	1.32	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	387	LEU	CA-CB	-6.56	1.42	1.53
2	B	710	LEU	CG-CD2	-6.56	1.30	1.52
7	I	17	ARG	CD-NE	6.56	1.55	1.46
1	A	91	PHE	CG-CD1	-6.56	1.25	1.38
1	A	290	GLU	CD-OE1	6.56	1.37	1.25
1	A	705	LYS	C-O	6.56	1.31	1.23
2	B	246	LYS	CB-CG	6.56	1.72	1.52
2	B	733	HIS	CB-CG	6.56	1.59	1.50
5	F	116	ASP	N-CA	6.56	1.56	1.46
6	H	41	ASP	CG-OD1	6.56	1.37	1.25
6	H	87	ARG	CA-CB	6.56	1.65	1.54
2	B	253	THR	CA-C	-6.55	1.44	1.52
2	B	995	ARG	CZ-NH2	6.55	1.42	1.33
4	E	55	ARG	CZ-NH1	-6.55	1.23	1.32
2	B	1135	ARG	CG-CD	-6.55	1.32	1.52
1	A	1197	LEU	C-N	-6.55	1.24	1.33
2	B	137	TYR	CG-CD2	6.55	1.53	1.39
4	E	201	LYS	C-N	-6.55	1.24	1.33
1	A	117	GLU	CD-OE2	6.55	1.37	1.25
3	C	215	GLU	CA-C	6.55	1.61	1.52
4	E	64	PRO	C-O	-6.55	1.15	1.24
6	H	54	SER	CA-C	-6.55	1.44	1.52
2	B	130	VAL	CB-CG2	-6.55	1.30	1.52
7	I	105	SER	CB-OG	6.55	1.55	1.42
2	B	322	PHE	CD2-CE2	-6.55	1.19	1.38
1	A	1164	PRO	CG-CD	6.54	1.73	1.50
2	B	370	PHE	CG-CD1	6.54	1.52	1.38
2	B	990	ILE	N-CA	-6.54	1.38	1.46
1	A	1147	THR	CA-CB	6.54	1.62	1.53
8	J	64	ASN	CB-CG	6.54	1.68	1.52
2	B	59	LEU	C-N	-6.54	1.25	1.33
2	B	394	ASP	CG-OD1	6.54	1.37	1.25
2	B	459	TYR	CE1-CZ	6.54	1.53	1.38
2	B	953	LEU	N-CA	-6.54	1.38	1.46
1	A	36	ARG	CB-CG	6.54	1.72	1.52
1	A	556	TRP	CE3-CZ3	-6.54	1.19	1.38
1	A	571	LEU	CG-CD1	-6.54	1.30	1.52
2	B	272	THR	CA-CB	-6.54	1.44	1.53
2	B	572	HIS	CA-C	-6.54	1.43	1.52
1	A	434	ARG	NE-CZ	-6.54	1.25	1.33
2	B	29	ASP	C-N	-6.54	1.25	1.33
2	B	107	GLY	CA-C	6.54	1.60	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	211	ASP	CA-C	6.54	1.61	1.52
1	A	1155	ASP	CA-C	-6.54	1.43	1.52
3	C	54	ASN	CG-ND2	6.54	1.47	1.33
1	A	74	MET	CB-CG	6.54	1.72	1.52
1	A	119	ASN	CA-CB	6.54	1.63	1.53
1	A	1101	LEU	N-CA	-6.54	1.38	1.46
1	A	1446	ASP	CG-OD1	6.54	1.37	1.25
2	B	835	GLN	CD-OE1	-6.54	1.11	1.23
4	E	52	ARG	CA-CB	6.54	1.66	1.53
1	A	25	GLU	CA-CB	-6.53	1.42	1.53
1	A	210	ILE	N-CA	6.53	1.54	1.46
1	A	1324	PRO	C-O	6.53	1.33	1.24
1	A	104	GLU	C-O	6.53	1.33	1.24
1	A	1026	LEU	CA-CB	-6.53	1.44	1.53
1	A	1078	GLN	CA-CB	6.53	1.64	1.53
2	B	248	SER	CA-CB	6.53	1.64	1.53
2	B	254	LEU	CG-CD1	-6.53	1.30	1.52
2	B	1069	PHE	CE2-CZ	-6.53	1.19	1.38
1	A	1093	LYS	CA-C	6.53	1.61	1.52
1	A	423	ASP	CG-OD2	6.53	1.37	1.25
1	A	699	ALA	C-N	-6.53	1.24	1.33
4	E	135	PHE	CE1-CZ	-6.53	1.19	1.38
1	A	770	VAL	C-N	-6.53	1.24	1.33
1	A	1173	HIS	N-CA	6.53	1.58	1.46
2	B	465	ASN	CA-C	6.53	1.61	1.52
2	B	478	GLY	N-CA	6.53	1.54	1.45
2	B	790	ASP	CA-CB	6.53	1.64	1.53
1	A	1025	ARG	NE-CZ	-6.53	1.25	1.33
2	B	498	THR	CA-CB	6.53	1.66	1.54
2	B	959	ASP	CA-CB	6.53	1.65	1.53
2	B	1133	MET	C-N	-6.53	1.25	1.34
1	A	577	ILE	C-O	-6.52	1.15	1.24
1	A	1280	GLU	CA-C	-6.52	1.44	1.52
3	C	228	PHE	C-O	-6.52	1.16	1.24
8	J	39	LEU	C-O	-6.52	1.15	1.24
1	A	1426	GLU	CA-C	6.52	1.62	1.52
1	A	1104	ILE	CG1-CD1	-6.52	1.26	1.51
1	A	891	ALA	C-N	-6.52	1.25	1.34
2	B	847	ASP	CG-OD2	6.52	1.37	1.25
2	B	887	HIS	C-N	6.52	1.40	1.34
2	B	946	ASN	C-O	-6.52	1.16	1.23
4	E	116	ILE	CA-C	6.52	1.61	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	164	LEU	C-N	-6.52	1.25	1.34
1	A	23	SER	CA-C	6.52	1.61	1.53
1	A	1153	TYR	N-CA	-6.52	1.37	1.45
1	A	175	ARG	CB-CG	6.51	1.72	1.52
1	A	1224	LEU	CA-C	-6.51	1.44	1.52
3	C	196	ASP	N-CA	6.51	1.54	1.46
6	H	80	ARG	CA-C	-6.51	1.46	1.52
3	C	247	GLY	N-CA	-6.51	1.37	1.45
1	A	900	ASP	CA-CB	6.51	1.64	1.53
1	A	1080	THR	C-N	6.51	1.42	1.33
1	A	1292	PRO	N-CA	-6.51	1.39	1.46
1	A	1427	ASN	C-O	6.51	1.32	1.24
1	A	1337	GLU	CA-C	-6.51	1.43	1.52
2	B	451	LYS	C-O	-6.51	1.15	1.24
1	A	1210	GLY	C-N	6.51	1.43	1.33
1	A	1322	ILE	C-O	6.51	1.32	1.24
4	E	136	ASN	C-O	-6.51	1.16	1.23
4	E	157	SER	C-O	6.50	1.31	1.23
1	A	381	THR	CA-CB	-6.50	1.43	1.53
1	A	554	PRO	N-CD	-6.50	1.38	1.47
2	B	245	GLU	C-N	6.50	1.42	1.33
2	B	302	CYS	C-O	6.50	1.31	1.23
2	B	347	LYS	CA-CB	-6.50	1.43	1.53
2	B	806	THR	CA-C	-6.50	1.44	1.52
9	K	68	PHE	CG-CD2	-6.50	1.25	1.38
1	A	226	GLU	C-O	6.50	1.32	1.24
1	A	810	PRO	CB-CG	-6.50	1.17	1.49
4	E	83	CYS	C-O	-6.50	1.16	1.23
4	E	207	ARG	N-CA	-6.50	1.37	1.45
1	A	748	MET	CG-SD	6.50	1.97	1.80
1	A	949	ASP	CB-CG	-6.50	1.35	1.52
3	C	220	ASP	N-CA	-6.50	1.38	1.46
1	A	121	LEU	CB-CG	6.50	1.66	1.53
1	A	956	LEU	CA-CB	-6.50	1.45	1.53
1	A	239	LEU	N-CA	-6.49	1.34	1.45
1	A	571	LEU	C-O	6.49	1.31	1.23
2	B	535	LEU	CG-CD2	-6.49	1.31	1.52
5	F	130	ILE	CG1-CD1	-6.49	1.26	1.51
2	B	279	ASP	CG-OD1	6.49	1.37	1.25
2	B	907	GLY	CA-C	6.49	1.61	1.51
2	B	65	GLU	CA-CB	6.49	1.62	1.53
3	C	148	ARG	N-CA	-6.49	1.37	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	256	ALA	CA-C	-6.49	1.43	1.52
1	A	96	ILE	CA-CB	-6.49	1.45	1.54
1	A	1108	ALA	C-N	6.49	1.43	1.33
1	A	1297	GLU	N-CA	-6.49	1.37	1.45
2	B	481	GLN	C-O	6.49	1.32	1.23
2	B	491	THR	CA-CB	-6.49	1.43	1.53
9	K	40	HIS	CD2-NE2	-6.49	1.30	1.37
2	B	172	ILE	N-CA	-6.48	1.38	1.46
7	I	15	TYR	CD1-CE1	6.48	1.58	1.38
7	I	70	ARG	CZ-NH2	-6.48	1.25	1.33
1	A	424	ILE	C-O	-6.48	1.16	1.24
1	A	1233	ASP	CA-C	-6.48	1.43	1.52
2	B	517	THR	C-N	-6.48	1.24	1.33
4	E	30	ILE	CA-CB	6.48	1.64	1.54
2	B	322	PHE	CG-CD2	-6.48	1.25	1.38
1	A	138	ILE	C-O	6.48	1.31	1.24
1	A	501	LEU	CA-CB	-6.48	1.43	1.53
2	B	120	ARG	CD-NE	6.48	1.55	1.46
2	B	585	VAL	CA-C	6.48	1.60	1.52
2	B	627	PHE	C-O	-6.48	1.16	1.23
2	B	1189	ILE	CB-CG1	6.48	1.66	1.53
2	B	1224	PHE	CG-CD2	6.48	1.52	1.38
4	E	203	GLU	C-O	-6.48	1.15	1.24
4	E	212	ARG	C-O	-6.48	1.15	1.23
1	A	325	ILE	N-CA	6.48	1.54	1.46
2	B	457	LEU	CG-CD2	6.47	1.74	1.52
2	B	814	PHE	CE1-CZ	-6.47	1.19	1.38
4	E	116	ILE	CG1-CD1	6.47	1.77	1.51
1	A	229	SER	CA-C	6.47	1.60	1.53
1	A	670	ILE	C-O	-6.47	1.16	1.24
1	A	768	GLN	CA-CB	-6.47	1.43	1.53
4	E	151	PRO	CA-C	-6.47	1.46	1.53
6	H	88	SER	CA-CB	6.47	1.64	1.53
1	A	713	SER	CA-C	-6.47	1.44	1.52
2	B	804	GLY	N-CA	6.47	1.54	1.45
2	B	1008	PRO	C-O	-6.47	1.16	1.23
2	B	1106	ARG	CB-CG	6.47	1.71	1.52
1	A	1225	PHE	C-O	-6.47	1.16	1.24
1	A	5	GLN	CD-NE2	6.47	1.46	1.33
1	A	305	ASP	CB-CG	6.47	1.68	1.52
2	B	231	PRO	CA-C	6.47	1.64	1.52
2	B	641	GLU	CD-OE1	6.47	1.37	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	643	ASP	CG-OD2	6.47	1.37	1.25
2	B	1169	MET	C-O	6.47	1.32	1.23
1	A	523	ILE	CA-CB	-6.46	1.46	1.54
1	A	604	GLY	C-N	-6.46	1.25	1.33
1	A	776	ALA	CA-C	-6.46	1.44	1.53
2	B	1077	THR	C-O	-6.46	1.16	1.24
8	J	18	TRP	CZ3-CH2	-6.46	1.24	1.40
6	H	110	ASP	C-O	6.46	1.30	1.24
1	A	362	ASP	C-O	-6.46	1.15	1.24
1	A	675	THR	C-O	-6.46	1.16	1.24
2	B	398	ARG	CZ-NH1	6.46	1.41	1.32
2	B	1191	ILE	CB-CG2	-6.46	1.31	1.52
2	B	368	GLU	N-CA	6.46	1.54	1.46
3	C	15	LYS	N-CA	6.46	1.54	1.46
7	I	80	SER	N-CA	6.46	1.53	1.46
9	K	104	ASN	CG-ND2	6.46	1.46	1.33
3	C	106	GLU	CD-OE2	6.46	1.37	1.25
1	A	37	PHE	CD1-CE1	6.46	1.58	1.38
2	B	276	ILE	CA-CB	-6.46	1.46	1.54
2	B	915	THR	CA-C	-6.46	1.44	1.52
2	B	944	THR	CA-C	-6.46	1.43	1.52
9	K	9	LEU	C-O	6.46	1.32	1.24
1	A	1281	ARG	CZ-NH1	6.45	1.41	1.32
2	B	212	LEU	C-O	-6.45	1.16	1.24
9	K	14	GLU	C-O	6.45	1.31	1.23
1	A	155	GLU	CD-OE1	6.45	1.37	1.25
1	A	658	LEU	CA-CB	-6.45	1.42	1.53
9	K	22	ASP	N-CA	-6.45	1.37	1.46
10	L	40	LEU	C-N	6.45	1.42	1.33
1	A	190	ALA	C-O	6.45	1.32	1.24
2	B	305	VAL	CA-CB	-6.45	1.45	1.54
6	H	87	ARG	CB-CG	6.45	1.71	1.52
7	I	94	ASP	N-CA	6.45	1.54	1.46
1	A	162	VAL	CB-CG2	6.45	1.73	1.52
2	B	875	GLU	CA-C	-6.45	1.44	1.52
4	E	204	THR	CB-OG1	-6.45	1.33	1.43
1	A	1196	GLU	CG-CD	6.45	1.68	1.52
1	A	679	ILE	N-CA	-6.45	1.39	1.46
2	B	617	ARG	CA-CB	-6.45	1.44	1.53
2	B	747	MET	CB-CG	-6.45	1.33	1.52
2	B	1139	ILE	CA-C	-6.45	1.45	1.52
7	I	15	TYR	CA-CB	6.45	1.63	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	106	GLU	N-CA	-6.45	1.37	1.46
1	A	127	ALA	C-N	6.44	1.42	1.33
1	A	525	GLN	CD-OE1	6.44	1.35	1.23
2	B	698	GLU	CA-C	6.44	1.61	1.52
2	B	96	TYR	N-CA	6.44	1.53	1.45
2	B	321	GLY	C-O	6.44	1.32	1.23
2	B	358	LYS	CE-NZ	6.44	1.68	1.49
2	B	620	ARG	CD-NE	-6.44	1.37	1.46
2	B	1110	PRO	N-CA	6.44	1.56	1.47
4	E	84	ASP	CA-CB	6.44	1.64	1.53
4	E	92	THR	CB-CG2	6.44	1.73	1.52
5	F	93	ILE	N-CA	-6.44	1.39	1.46
1	A	1014	ALA	C-O	-6.44	1.15	1.24
2	B	311	LEU	CA-C	6.44	1.61	1.52
2	B	368	GLU	C-O	6.44	1.32	1.24
6	H	142	LEU	CB-CG	-6.44	1.40	1.53
4	E	46	TYR	N-CA	-6.44	1.39	1.46
2	B	597	MET	CA-CB	-6.44	1.43	1.53
4	E	83	CYS	CA-C	-6.44	1.44	1.52
4	E	168	TYR	CG-CD1	-6.44	1.25	1.39
1	A	131	SER	N-CA	-6.44	1.37	1.46
1	A	1449	SER	N-CA	6.44	1.53	1.45
2	B	1215	ARG	CD-NE	6.44	1.55	1.46
4	E	200	ARG	N-CA	-6.43	1.37	1.45
1	A	980	ASP	CA-C	-6.43	1.42	1.52
1	A	1046	LEU	C-N	-6.43	1.24	1.33
2	B	711	GLU	C-O	6.43	1.32	1.24
1	A	556	TRP	CG-CD2	-6.43	1.32	1.43
2	B	52	ASN	CA-CB	-6.43	1.43	1.53
3	C	112	ASN	CA-C	-6.43	1.43	1.53
4	E	181	ALA	N-CA	-6.43	1.38	1.46
1	A	425	GLN	CD-OE1	6.43	1.35	1.23
1	A	982	THR	C-O	6.43	1.32	1.23
2	B	465	ASN	CG-ND2	6.43	1.46	1.33
1	A	691	LEU	CA-C	-6.43	1.44	1.52
1	A	23	SER	CA-CB	-6.43	1.43	1.53
1	A	768	GLN	N-CA	-6.43	1.37	1.45
2	B	838	SER	CA-CB	-6.43	1.42	1.53
3	C	8	VAL	CA-C	-6.43	1.45	1.52
5	F	72	LYS	CG-CD	6.43	1.71	1.52
1	A	130	ASP	CA-C	-6.42	1.44	1.52
3	C	187	LYS	CA-CB	-6.42	1.42	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	665	GLU	CG-CD	6.42	1.68	1.52
2	B	786	ASN	C-N	-6.42	1.26	1.33
9	K	47	ARG	CA-C	-6.42	1.44	1.52
1	A	428	TYR	CB-CG	-6.42	1.37	1.51
1	A	935	GLN	CG-CD	-6.42	1.35	1.52
2	B	887	HIS	CA-CB	6.42	1.64	1.53
4	E	144	ILE	CA-C	-6.42	1.43	1.52
1	A	136	ALA	CA-C	-6.42	1.44	1.52
1	A	1102	LYS	CD-CE	6.42	1.71	1.52
2	B	27	ALA	C-O	-6.42	1.16	1.24
2	B	135	ARG	C-O	6.42	1.32	1.23
1	A	165	GLY	N-CA	6.42	1.54	1.45
1	A	479	ASN	C-N	-6.42	1.24	1.33
1	A	988	LEU	C-O	-6.42	1.15	1.24
2	B	994	TYR	CG-CD2	-6.42	1.25	1.39
7	I	61	ASP	C-O	-6.42	1.15	1.24
1	A	492	PRO	C-O	-6.42	1.16	1.23
1	A	797	LYS	CA-CB	-6.42	1.44	1.53
3	C	257	SER	CB-OG	6.42	1.54	1.42
7	I	109	ILE	CG1-CD1	6.42	1.76	1.51
1	A	240	PRO	C-O	6.41	1.32	1.23
1	A	662	PHE	CA-CB	-6.41	1.43	1.53
2	B	112	LEU	N-CA	6.41	1.54	1.46
4	E	112	TYR	CA-C	6.41	1.60	1.52
4	E	180	ARG	CD-NE	6.41	1.55	1.46
2	B	502	ILE	CB-CG2	6.41	1.73	1.52
2	B	889	THR	C-N	-6.41	1.24	1.33
1	A	708	MET	N-CA	-6.41	1.38	1.46
1	A	1224	LEU	CA-CB	-6.41	1.42	1.53
4	E	98	ILE	CG1-CD1	6.41	1.76	1.51
9	K	110	ASN	CA-C	-6.41	1.44	1.52
2	B	255	GLN	CA-CB	-6.41	1.39	1.53
2	B	885	MET	C-O	6.41	1.32	1.24
1	A	13	THR	N-CA	6.41	1.53	1.45
2	B	979	LYS	CA-CB	-6.41	1.43	1.53
2	B	1205	GLN	C-O	-6.41	1.16	1.24
9	K	70	ARG	CG-CD	6.41	1.71	1.52
2	B	327	ARG	CA-CB	-6.40	1.42	1.53
2	B	405	ARG	NE-CZ	-6.40	1.26	1.33
2	B	679	TYR	CA-C	-6.40	1.44	1.52
2	B	404	LYS	CG-CD	6.40	1.71	1.52
1	A	277	GLU	CA-C	6.40	1.61	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	199	MET	CA-C	-6.40	1.43	1.52
2	B	1016	ALA	CA-C	-6.40	1.43	1.52
3	C	159	ALA	CA-C	-6.40	1.44	1.53
9	K	53	ASP	CB-CG	6.40	1.68	1.52
2	B	257	LYS	N-CA	-6.40	1.38	1.46
2	B	737	THR	CA-CB	-6.40	1.44	1.53
4	E	194	GLU	CA-C	-6.40	1.44	1.52
10	L	29	TYR	C-N	-6.40	1.25	1.33
1	A	940	ARG	CD-NE	-6.40	1.37	1.46
2	B	425	THR	CA-CB	6.40	1.63	1.53
2	B	1075	GLY	C-N	-6.39	1.25	1.33
3	C	219	PHE	CA-C	-6.39	1.44	1.52
2	B	174	LEU	CA-C	-6.39	1.44	1.52
2	B	300	HIS	C-N	-6.39	1.26	1.33
7	I	87	GLN	CA-C	-6.39	1.44	1.53
8	J	48	ARG	CZ-NH1	-6.39	1.23	1.32
2	B	851	PHE	CA-C	-6.39	1.42	1.52
1	A	793	SER	C-N	-6.39	1.25	1.33
1	A	922	ASP	CA-CB	-6.39	1.44	1.53
2	B	1108	ARG	CZ-NH1	6.39	1.41	1.32
4	E	63	ASN	C-O	-6.39	1.17	1.24
4	E	67	GLU	C-O	6.39	1.31	1.24
9	K	83	PRO	CA-CB	-6.39	1.43	1.53
6	H	123	MET	N-CA	-6.39	1.37	1.45
1	A	1277	GLU	CA-CB	6.39	1.64	1.53
3	C	43	THR	N-CA	-6.39	1.38	1.46
3	C	225	ALA	C-O	-6.39	1.16	1.24
1	A	751	SER	CA-C	-6.38	1.43	1.52
2	B	1034	VAL	N-CA	-6.38	1.39	1.46
2	B	466	TRP	C-N	6.38	1.42	1.33
2	B	1165	ILE	CB-CG1	6.38	1.66	1.53
1	A	25	GLU	CD-OE2	6.38	1.37	1.25
1	A	701	LEU	CG-CD1	6.38	1.73	1.52
1	A	885	THR	CB-OG1	-6.38	1.33	1.43
2	B	347	LYS	CB-CG	6.38	1.71	1.52
4	E	105	PHE	CA-CB	-6.38	1.44	1.53
2	B	328	GLU	N-CA	6.38	1.54	1.46
1	A	303	TYR	C-O	-6.38	1.16	1.24
1	A	1203	ASN	CB-CG	-6.38	1.36	1.52
1	A	1301	GLU	CD-OE2	6.38	1.37	1.25
2	B	579	ARG	CA-CB	-6.38	1.43	1.53
2	B	734	HIS	CB-CG	6.38	1.59	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	661	LEU	CA-CB	-6.38	1.43	1.53
2	B	885	MET	CG-SD	6.38	1.96	1.80
6	H	115	TYR	N-CA	6.38	1.54	1.46
6	H	41	ASP	CA-CB	6.38	1.61	1.53
1	A	123	ARG	CG-CD	6.37	1.71	1.52
1	A	754	SER	CA-C	6.37	1.60	1.52
4	E	40	GLU	C-O	-6.37	1.16	1.24
3	C	200	GLU	CA-CB	6.37	1.63	1.53
4	E	17	ARG	CA-C	6.37	1.61	1.52
7	I	96	SER	C-O	-6.37	1.15	1.23
1	A	297	GLN	CA-C	-6.37	1.43	1.52
1	A	621	THR	C-N	-6.37	1.26	1.33
1	A	710	LEU	C-N	-6.37	1.25	1.34
2	B	217	ARG	CD-NE	-6.37	1.37	1.46
2	B	486	TYR	C-O	-6.37	1.16	1.24
1	A	1331	SER	N-CA	-6.37	1.38	1.46
5	F	97	ARG	CB-CG	-6.37	1.33	1.52
1	A	400	PRO	CB-CG	-6.37	1.26	1.51
2	B	738	PHE	N-CA	-6.37	1.38	1.46
1	A	904	THR	C-N	-6.36	1.23	1.33
2	B	1178	ASN	C-O	6.36	1.34	1.24
1	A	147	VAL	CB-CG2	6.36	1.73	1.52
2	B	1156	ASP	CG-OD1	6.36	1.37	1.25
9	K	3	ALA	N-CA	6.36	1.56	1.46
10	L	66	GLN	CG-CD	6.36	1.68	1.52
1	A	350	ARG	CA-CB	-6.36	1.43	1.53
2	B	810	GLU	CA-CB	6.36	1.63	1.53
1	A	177	ASP	CA-C	-6.36	1.44	1.52
1	A	536	LEU	N-CA	-6.36	1.37	1.45
1	A	544	ASP	CA-CB	6.36	1.63	1.53
1	A	637	LYS	CE-NZ	6.36	1.68	1.49
1	A	879	GLU	C-O	-6.36	1.16	1.23
1	A	1161	THR	CB-CG2	-6.36	1.31	1.52
1	A	1256	GLU	CG-CD	6.36	1.68	1.52
1	A	1447	GLU	C-N	6.36	1.42	1.33
2	B	245	GLU	CG-CD	6.36	1.68	1.52
2	B	109	THR	CB-OG1	6.36	1.53	1.43
7	I	77	LYS	CG-CD	6.36	1.71	1.52
2	B	61	ASP	CG-OD1	6.35	1.37	1.25
1	A	451	HIS	CA-CB	-6.35	1.43	1.53
2	B	777	ALA	C-O	-6.35	1.15	1.23
1	A	661	GLY	C-O	-6.35	1.15	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	777	PHE	CE2-CZ	-6.35	1.19	1.38
1	A	383	TYR	CA-CB	6.35	1.63	1.53
1	A	420	ARG	C-O	-6.35	1.15	1.24
1	A	933	TYR	CG-CD1	-6.35	1.26	1.39
7	I	118	ARG	CA-CB	6.35	1.63	1.53
1	A	361	LEU	C-N	-6.35	1.24	1.33
2	B	515	HIS	CD2-NE2	-6.34	1.30	1.37
4	E	33	GLU	N-CA	-6.34	1.37	1.46
1	A	213	HIS	CA-CB	6.34	1.63	1.53
4	E	191	LYS	CB-CG	6.34	1.71	1.52
3	C	251	LEU	N-CA	-6.34	1.38	1.46
1	A	174	ILE	CB-CG2	-6.34	1.31	1.52
1	A	979	SER	CB-OG	6.34	1.54	1.42
1	A	1359	ASP	N-CA	6.34	1.54	1.46
1	A	1360	GLY	C-N	6.34	1.42	1.33
2	B	29	ASP	CG-OD1	6.34	1.37	1.25
2	B	847	ASP	C-O	-6.34	1.16	1.24
3	C	190	ASP	CA-CB	-6.34	1.43	1.53
5	F	78	GLN	CD-NE2	6.34	1.46	1.33
8	J	35	ALA	CA-CB	-6.34	1.43	1.53
1	A	465	TYR	CG-CD2	-6.34	1.26	1.39
1	A	1018	PHE	CA-CB	-6.34	1.43	1.53
2	B	435	THR	C-N	6.34	1.42	1.33
1	A	657	LEU	N-CA	-6.34	1.37	1.46
1	A	1125	ALA	C-O	-6.34	1.15	1.24
1	A	1195	LEU	N-CA	6.34	1.53	1.45
1	A	1344	GLY	C-N	-6.34	1.25	1.33
1	A	1169	ILE	CA-CB	6.33	1.62	1.54
2	B	57	TYR	CG-CD1	-6.33	1.26	1.39
4	E	127	ILE	CA-CB	-6.33	1.46	1.54
2	B	594	ALA	C-N	-6.33	1.25	1.33
1	A	36	ARG	CD-NE	6.33	1.55	1.46
1	A	40	THR	CA-C	6.33	1.60	1.52
1	A	908	LEU	N-CA	-6.33	1.38	1.46
3	C	154	LYS	CE-NZ	6.33	1.68	1.49
1	A	1093	LYS	C-O	6.33	1.32	1.24
8	J	8	PHE	CD2-CE2	6.33	1.57	1.38
1	A	757	ASN	C-O	-6.33	1.16	1.24
2	B	273	LEU	N-CA	-6.33	1.37	1.45
2	B	500	THR	CA-CB	-6.33	1.45	1.53
2	B	756	ILE	CA-C	6.33	1.58	1.53
5	F	88	TYR	C-N	-6.33	1.25	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	975	HIS	CB-CG	6.33	1.59	1.50
2	B	745	PRO	CA-CB	-6.33	1.45	1.53
1	A	492	PRO	CA-C	-6.32	1.44	1.52
1	A	1382	THR	N-CA	-6.32	1.38	1.46
2	B	95	ILE	CB-CG2	-6.32	1.31	1.52
2	B	312	GLU	CA-CB	-6.32	1.42	1.53
2	B	1173	ALA	CA-C	6.32	1.61	1.53
4	E	163	GLU	CD-OE1	6.32	1.37	1.25
1	A	830	LYS	CE-NZ	6.32	1.68	1.49
3	C	87	PHE	CD2-CE2	6.32	1.57	1.38
6	H	87	ARG	NE-CZ	6.32	1.40	1.33
1	A	918	GLU	CA-C	-6.32	1.41	1.52
6	H	129	TYR	CE2-CZ	6.32	1.53	1.38
1	A	414	ASP	CB-CG	-6.32	1.36	1.52
1	A	986	ILE	CB-CG1	6.32	1.66	1.53
1	A	1342	GLU	N-CA	6.32	1.53	1.46
2	B	371	GLU	CD-OE2	6.32	1.37	1.25
2	B	604	ARG	N-CA	6.32	1.54	1.46
5	F	91	ALA	C-O	6.32	1.32	1.24
1	A	772	GLY	C-O	-6.31	1.15	1.24
1	A	1157	ASP	CG-OD1	6.31	1.37	1.25
1	A	1172	LEU	N-CA	6.31	1.54	1.46
1	A	730	GLY	C-O	-6.31	1.15	1.23
1	A	1272	THR	C-O	6.31	1.31	1.24
1	A	455	MET	SD-CE	-6.31	1.63	1.79
1	A	623	GLY	CA-C	-6.31	1.44	1.51
2	B	1147	LEU	CA-CB	-6.31	1.43	1.53
10	L	47	ARG	CA-C	6.31	1.56	1.53
1	A	1211	GLN	C-O	-6.31	1.16	1.24
1	A	1442	ASP	CA-CB	-6.31	1.43	1.53
2	B	68	THR	CA-C	6.30	1.60	1.52
2	B	256	VAL	CB-CG1	-6.30	1.31	1.52
2	B	487	THR	C-O	-6.30	1.16	1.23
2	B	513	GLN	CD-NE2	6.30	1.46	1.33
2	B	527	THR	CA-C	-6.30	1.45	1.52
4	E	36	GLU	C-O	-6.30	1.15	1.24
4	E	119	SER	CA-C	6.30	1.60	1.52
1	A	244	PRO	C-N	6.30	1.42	1.34
5	F	97	ARG	CZ-NH2	-6.30	1.25	1.33
1	A	356	ASP	C-O	-6.30	1.16	1.24
1	A	713	SER	C-N	-6.30	1.25	1.33
2	B	518	HIS	CG-ND1	-6.30	1.31	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	131	ASN	C-N	6.30	1.42	1.33
8	J	25	LEU	CA-C	6.30	1.61	1.52
1	A	1326	ARG	CG-CD	6.30	1.71	1.52
2	B	654	ARG	CG-CD	-6.30	1.33	1.52
2	B	1170	THR	CB-OG1	-6.30	1.33	1.43
1	A	900	ASP	CB-CG	-6.30	1.36	1.52
2	B	183	GLU	CA-CB	6.30	1.64	1.53
1	A	435	HIS	CG-CD2	-6.30	1.28	1.35
1	A	758	ILE	CA-C	-6.30	1.44	1.52
2	B	586	TRP	N-CA	6.30	1.54	1.46
2	B	1026	LEU	CG-CD1	-6.30	1.31	1.52
6	H	137	GLN	CD-OE1	6.30	1.35	1.23
2	B	736	THR	CA-CB	-6.29	1.43	1.53
3	C	34	ARG	CD-NE	-6.29	1.37	1.46
4	E	148	GLU	C-O	-6.29	1.15	1.24
1	A	514	PRO	C-N	-6.29	1.25	1.33
3	C	252	GLN	CA-CB	6.29	1.63	1.53
5	F	147	SER	CA-CB	6.29	1.63	1.53
6	H	19	ARG	CA-CB	6.29	1.64	1.53
7	I	119	THR	CB-CG2	6.29	1.73	1.52
1	A	28	ARG	N-CA	-6.29	1.38	1.46
1	A	933	TYR	CG-CD2	-6.29	1.26	1.39
2	B	956	THR	C-O	6.29	1.31	1.24
2	B	562	GLY	CA-C	-6.29	1.41	1.51
2	B	643	ASP	CB-CG	6.29	1.67	1.52
4	E	112	TYR	CZ-OH	6.29	1.51	1.38
9	K	29	ASN	CG-ND2	6.29	1.46	1.33
10	L	37	LYS	C-N	-6.29	1.24	1.33
2	B	766	ARG	CZ-NH2	6.29	1.41	1.33
4	E	101	GLN	C-O	6.29	1.31	1.24
2	B	1021	MET	CG-SD	-6.29	1.65	1.80
2	B	1102	LYS	CA-CB	6.29	1.63	1.53
4	E	17	ARG	CZ-NH1	6.29	1.41	1.32
1	A	231	PRO	CA-CB	-6.28	1.44	1.53
2	B	267	ARG	CA-C	6.28	1.61	1.52
2	B	555	ILE	CG1-CD1	-6.28	1.27	1.51
1	A	1027	ALA	C-O	6.28	1.31	1.23
2	B	324	ILE	CG1-CD1	-6.28	1.27	1.51
1	A	53	LEU	CB-CG	6.28	1.66	1.53
2	B	1129	ARG	NE-CZ	6.28	1.40	1.33
3	C	101	LEU	CA-CB	-6.28	1.43	1.53
8	J	64	ASN	CG-ND2	6.28	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	ASN	C-N	-6.28	1.25	1.34
1	A	511	ILE	C-N	-6.28	1.24	1.33
1	A	1133	LEU	C-O	6.28	1.31	1.24
2	B	1189	ILE	C-O	6.28	1.31	1.24
1	A	1291	VAL	CA-C	-6.28	1.45	1.52
4	E	122	LYS	N-CA	6.28	1.54	1.46
7	I	34	TYR	CE1-CZ	-6.28	1.23	1.38
2	B	129	PHE	N-CA	6.27	1.53	1.46
1	A	162	VAL	N-CA	-6.27	1.39	1.46
2	B	809	MET	CG-SD	6.27	1.96	1.80
10	L	50	ASP	C-N	6.27	1.42	1.33
2	B	514	LEU	C-O	6.27	1.31	1.24
3	C	81	GLU	C-N	6.27	1.41	1.33
3	C	107	SER	C-O	-6.27	1.15	1.23
3	C	114	TYR	CE1-CZ	-6.27	1.23	1.38
2	B	1088	GLY	C-O	-6.27	1.15	1.24
1	A	396	PRO	CA-C	-6.26	1.42	1.52
2	B	326	ASP	CA-CB	-6.26	1.42	1.53
3	C	233	GLU	CA-C	-6.26	1.45	1.52
3	C	239	PRO	CG-CD	-6.26	1.29	1.50
8	J	4	PRO	N-CD	-6.26	1.39	1.47
8	J	62	ARG	C-O	-6.26	1.08	1.24
1	A	590	ARG	CA-CB	-6.26	1.43	1.53
2	B	1022	THR	CA-CB	-6.26	1.43	1.53
2	B	1041	GLU	CA-CB	6.26	1.63	1.53
4	E	56	LYS	N-CA	-6.26	1.38	1.46
5	F	109	VAL	CB-CG2	-6.26	1.31	1.52
6	H	128	ASN	CG-ND2	6.26	1.46	1.33
2	B	184	ALA	CA-C	-6.26	1.45	1.52
1	A	99	ILE	CA-C	6.26	1.60	1.52
1	A	937	VAL	C-O	6.26	1.31	1.24
2	B	784	ASN	CG-ND2	6.26	1.46	1.33
2	B	882	THR	CB-CG2	6.26	1.73	1.52
2	B	916	THR	N-CA	6.26	1.58	1.46
6	H	46	LEU	N-CA	-6.25	1.37	1.46
2	B	397	ASP	CA-C	6.25	1.60	1.52
2	B	1020	ARG	CG-CD	-6.25	1.33	1.52
1	A	556	TRP	CZ2-CH2	-6.25	1.25	1.37
1	A	870	GLU	CA-CB	6.25	1.62	1.54
1	A	1369	ALA	C-O	6.25	1.31	1.24
2	B	533	CYS	CA-C	-6.25	1.44	1.52
1	A	405	VAL	CA-C	-6.25	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	459	TYR	CE2-CZ	6.25	1.53	1.38
3	C	184	ASN	C-N	-6.25	1.25	1.33
3	C	186	LEU	N-CA	-6.25	1.37	1.46
9	K	78	THR	CA-CB	-6.25	1.43	1.53
10	L	66	GLN	C-O	-6.25	1.15	1.23
1	A	379	VAL	C-N	6.24	1.41	1.33
1	A	776	ALA	CA-CB	-6.24	1.44	1.53
2	B	816	GLU	N-CA	-6.24	1.38	1.46
3	C	57	VAL	C-O	-6.24	1.16	1.24
3	C	93	ASP	N-CA	-6.24	1.37	1.46
3	C	218	PRO	CG-CD	6.24	1.72	1.50
3	C	260	LEU	CG-CD1	6.24	1.73	1.52
1	A	438	ASP	CG-OD2	6.24	1.37	1.25
2	B	875	GLU	CD-OE2	6.24	1.37	1.25
4	E	175	LEU	C-O	-6.24	1.17	1.23
1	A	1096	SER	CA-CB	6.24	1.65	1.53
3	C	208	GLU	CD-OE2	6.24	1.37	1.25
1	A	449	SER	C-N	-6.24	1.24	1.33
2	B	1147	LEU	CG-CD2	-6.24	1.31	1.52
2	B	437	GLU	N-CA	6.24	1.58	1.46
2	B	485	ARG	NE-CZ	-6.24	1.26	1.33
1	A	528	LEU	CG-CD1	-6.23	1.31	1.52
1	A	984	LYS	C-O	6.23	1.32	1.24
3	C	267	GLN	CB-CG	6.23	1.71	1.52
4	E	71	LYS	CG-CD	6.23	1.71	1.52
8	J	60	PHE	CE1-CZ	-6.23	1.20	1.38
2	B	411	PRO	CA-C	6.23	1.62	1.52
3	C	115	SER	CA-CB	-6.23	1.43	1.53
10	L	47	ARG	N-CA	-6.23	1.41	1.46
1	A	393	ARG	CZ-NH2	6.23	1.41	1.33
1	A	616	VAL	C-O	6.23	1.32	1.24
1	A	1322	ILE	CB-CG2	-6.23	1.31	1.52
3	C	210	GLU	CA-C	6.23	1.60	1.52
6	H	98	TYR	CA-C	-6.23	1.45	1.52
9	K	82	ASP	C-N	-6.23	1.25	1.34
10	L	30	ILE	CA-C	6.23	1.60	1.52
2	B	304	ASP	CG-OD1	6.23	1.37	1.25
1	A	25	GLU	CG-CD	6.22	1.67	1.52
1	A	1011	GLN	CA-C	6.22	1.60	1.52
1	A	1148	ILE	CG1-CD1	6.22	1.76	1.51
2	B	360	PHE	C-O	6.22	1.31	1.24
6	H	81	PRO	CA-C	6.22	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	35	VAL	CB-CG2	-6.22	1.32	1.52
2	B	218	SER	CB-OG	6.22	1.54	1.42
2	B	667	GLN	CA-CB	6.22	1.60	1.52
9	K	31	VAL	C-N	-6.22	1.25	1.33
1	A	284	ALA	CA-C	-6.22	1.45	1.52
2	B	830	TYR	CE1-CZ	-6.22	1.23	1.38
4	E	178	ILE	C-O	6.22	1.30	1.24
1	A	948	VAL	C-O	-6.22	1.15	1.24
1	A	1359	ASP	C-O	-6.22	1.16	1.24
2	B	325	GLN	CG-CD	6.22	1.67	1.52
2	B	511	PRO	CA-C	-6.22	1.41	1.52
2	B	681	TRP	C-N	-6.22	1.25	1.34
3	C	182	PRO	C-O	6.22	1.32	1.24
1	A	5	GLN	CA-CB	6.22	1.63	1.53
1	A	703	THR	C-O	-6.22	1.16	1.23
9	K	16	GLU	CG-CD	6.22	1.67	1.52
1	A	325	ILE	CA-CB	6.22	1.62	1.54
2	B	231	PRO	CG-CD	6.22	1.71	1.50
2	B	746	SER	CA-C	-6.22	1.42	1.52
6	H	137	GLN	CD-NE2	6.22	1.46	1.33
1	A	811	GLN	CD-OE1	6.21	1.35	1.23
1	A	1016	THR	CA-C	6.21	1.61	1.52
3	C	7	GLN	CB-CG	6.21	1.71	1.52
2	B	735	ALA	C-N	6.21	1.42	1.33
2	B	1186	ASP	CG-OD1	6.21	1.37	1.25
1	A	217	LYS	CB-CG	6.21	1.71	1.52
2	B	392	ARG	CA-CB	-6.21	1.44	1.53
3	C	116	LYS	CE-NZ	6.21	1.68	1.49
1	A	34	LYS	CB-CG	6.21	1.71	1.52
1	A	229	SER	N-CA	-6.21	1.39	1.46
2	B	219	ALA	N-CA	6.21	1.53	1.45
2	B	261	ARG	NE-CZ	6.21	1.39	1.33
2	B	1130	PHE	CE1-CZ	-6.21	1.20	1.38
5	F	90	ARG	N-CA	-6.21	1.38	1.46
7	I	13	MET	CA-CB	-6.21	1.43	1.53
1	A	554	PRO	C-O	6.20	1.32	1.24
2	B	378	LEU	CA-C	-6.20	1.44	1.52
5	F	144	GLU	C-N	6.20	1.42	1.33
1	A	916	GLY	C-O	6.20	1.31	1.23
1	A	1237	ILE	CA-C	-6.20	1.44	1.52
1	A	441	PRO	C-O	-6.20	1.16	1.23
1	A	695	LYS	CE-NZ	6.20	1.68	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1448	GLU	C-O	6.20	1.31	1.24
1	A	1296	GLY	C-N	-6.20	1.25	1.33
2	B	416	LEU	C-O	-6.20	1.17	1.24
9	K	83	PRO	N-CA	-6.20	1.39	1.47
1	A	592	ASP	C-O	-6.20	1.16	1.24
2	B	627	PHE	CB-CG	6.20	1.65	1.50
4	E	28	TYR	N-CA	-6.20	1.38	1.45
1	A	1291	VAL	CB-CG2	6.20	1.73	1.52
6	H	52	GLN	CD-OE1	6.20	1.35	1.23
7	I	5	ARG	N-CA	6.20	1.53	1.45
1	A	1208	THR	CA-CB	6.19	1.63	1.53
5	F	106	PRO	CG-CD	-6.19	1.29	1.50
1	A	518	LYS	C-O	-6.19	1.16	1.24
1	A	945	GLU	N-CA	-6.19	1.38	1.46
1	A	1102	LYS	CB-CG	6.19	1.71	1.52
2	B	55	VAL	CA-CB	-6.19	1.47	1.54
2	B	306	ASN	CG-OD1	6.19	1.35	1.23
3	C	66	ARG	N-CA	-6.19	1.38	1.46
1	A	128	ILE	CB-CG2	-6.19	1.32	1.52
7	I	44	TYR	CD2-CE2	6.19	1.57	1.38
9	K	72	LYS	C-O	-6.19	1.17	1.23
1	A	205	GLU	CD-OE2	6.18	1.37	1.25
1	A	1238	ILE	CA-C	6.18	1.60	1.52
2	B	213	ILE	C-O	-6.18	1.16	1.24
2	B	409	ALA	N-CA	-6.18	1.39	1.46
3	C	156	THR	CA-CB	-6.18	1.39	1.53
4	E	32	GLN	CA-C	-6.18	1.44	1.52
5	F	128	LYS	C-N	-6.18	1.26	1.33
6	H	37	LYS	N-CA	6.18	1.53	1.45
6	H	98	TYR	CD1-CE1	6.18	1.57	1.38
2	B	822	ASN	C-N	-6.18	1.24	1.33
4	E	155	ARG	CD-NE	6.18	1.54	1.46
4	E	180	ARG	CG-CD	6.18	1.71	1.52
8	J	53	HIS	N-CA	6.18	1.53	1.46
1	A	774	ARG	C-O	6.18	1.32	1.23
1	A	893	PHE	CG-CD2	-6.18	1.25	1.38
2	B	1220	ARG	N-CA	6.18	1.54	1.46
4	E	14	ARG	CZ-NH2	-6.18	1.25	1.33
4	E	89	GLY	C-O	6.18	1.32	1.23
7	I	66	PRO	N-CD	-6.18	1.39	1.47
1	A	943	LEU	CA-C	-6.18	1.44	1.52
5	F	90	ARG	NE-CZ	-6.18	1.26	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	478	TYR	CD1-CE1	-6.18	1.20	1.38
2	B	594	ALA	CA-CB	-6.18	1.43	1.53
3	C	243	VAL	CA-CB	-6.18	1.45	1.54
2	B	578	THR	CA-CB	-6.17	1.45	1.53
2	B	303	TYR	CG-CD2	-6.17	1.26	1.39
1	A	1358	SER	C-O	6.17	1.31	1.24
2	B	177	LYS	CG-CD	6.17	1.71	1.52
3	C	192	TRP	CE3-CZ3	-6.17	1.20	1.38
1	A	392	VAL	C-O	-6.17	1.16	1.24
2	B	816	GLU	C-O	-6.17	1.16	1.24
1	A	396	PRO	CA-CB	-6.17	1.43	1.53
1	A	489	LEU	N-CA	-6.17	1.38	1.46
2	B	575	PRO	CB-CG	-6.17	1.18	1.49
2	B	704	ALA	C-N	-6.17	1.24	1.33
3	C	117	ASP	C-O	6.17	1.33	1.24
1	A	146	MET	N-CA	-6.17	1.37	1.46
1	A	1209	MET	CG-SD	-6.17	1.65	1.80
6	H	52	GLN	CB-CG	6.17	1.71	1.52
2	B	608	ASP	N-CA	-6.16	1.38	1.46
2	B	1192	TYR	CB-CG	-6.16	1.38	1.51
1	A	446	ARG	CA-CB	-6.16	1.45	1.53
9	K	66	PRO	CG-CD	-6.16	1.29	1.50
1	A	93	VAL	C-O	6.16	1.31	1.24
1	A	616	VAL	CA-C	-6.16	1.45	1.52
2	B	611	PRO	CA-CB	-6.16	1.44	1.53
4	E	22	MET	CA-C	-6.16	1.44	1.52
10	L	60	ARG	C-O	-6.16	1.16	1.23
1	A	763	ALA	N-CA	-6.16	1.38	1.46
1	A	971	PHE	CE2-CZ	-6.16	1.20	1.38
1	A	1035	TYR	CG-CD1	-6.16	1.26	1.39
2	B	227	LYS	C-O	-6.16	1.15	1.23
2	B	852	ARG	CB-CG	-6.16	1.33	1.52
4	E	170	LEU	CG-CD1	-6.16	1.32	1.52
8	J	14	VAL	C-N	-6.16	1.23	1.33
1	A	902	LEU	CG-CD2	-6.15	1.32	1.52
1	A	954	TRP	CG-CD1	-6.15	1.21	1.36
1	A	1315	GLU	CG-CD	6.15	1.67	1.52
2	B	795	ILE	CA-C	-6.15	1.45	1.52
2	B	846	ILE	N-CA	-6.15	1.39	1.46
2	B	1097	HIS	CB-CG	-6.15	1.41	1.50
2	B	1103	ILE	CB-CG1	-6.15	1.41	1.53
7	I	72	ASP	CA-CB	6.15	1.61	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	469	ARG	CA-C	6.15	1.60	1.52
2	B	62	ILE	CA-CB	6.15	1.62	1.54
2	B	89	GLU	CG-CD	6.15	1.67	1.52
2	B	124	TYR	CE2-CZ	-6.15	1.23	1.38
2	B	582	VAL	CA-CB	6.15	1.62	1.54
7	I	45	ARG	CZ-NH1	6.15	1.41	1.32
1	A	358	ASN	CA-CB	-6.15	1.44	1.53
1	A	1173	HIS	CA-CB	6.15	1.65	1.53
2	B	556	THR	N-CA	-6.15	1.39	1.46
2	B	770	GLN	C-N	-6.15	1.25	1.33
2	B	1193	GLN	CD-NE2	6.15	1.46	1.33
7	I	6	PHE	CB-CG	-6.15	1.36	1.50
1	A	391	LEU	CG-CD2	-6.15	1.32	1.52
1	A	903	ASN	CA-CB	6.15	1.64	1.53
2	B	96	TYR	CB-CG	6.15	1.65	1.51
2	B	691	GLU	CD-OE2	6.14	1.37	1.25
2	B	1064	TYR	CE2-CZ	-6.14	1.23	1.38
3	C	192	TRP	N-CA	-6.14	1.38	1.45
1	A	396	PRO	N-CA	-6.14	1.39	1.47
2	B	1127	GLY	CA-C	6.14	1.63	1.52
3	C	157	CYS	C-O	6.14	1.31	1.23
3	C	164	ALA	C-O	-6.14	1.16	1.24
1	A	1315	GLU	CD-OE1	6.14	1.37	1.25
1	A	81	PHE	CE2-CZ	-6.14	1.20	1.38
1	A	115	LEU	C-O	6.14	1.31	1.23
2	B	817	LEU	C-N	-6.14	1.25	1.33
3	C	265	MET	CA-CB	-6.14	1.45	1.54
10	L	27	LEU	CG-CD1	6.14	1.72	1.52
1	A	589	GLN	CG-CD	6.14	1.67	1.52
1	A	909	ASP	CA-CB	-6.14	1.43	1.53
1	A	931	GLU	CA-CB	-6.14	1.43	1.53
1	A	1450	LEU	CA-C	6.14	1.65	1.52
2	B	275	TYR	CE2-CZ	-6.14	1.23	1.38
2	B	1188	LYS	CE-NZ	6.14	1.67	1.49
3	C	76	ASP	CA-CB	6.13	1.62	1.52
4	E	195	VAL	CB-CG1	-6.13	1.32	1.52
9	K	47	ARG	C-N	-6.13	1.24	1.33
7	I	21	GLU	CG-CD	6.13	1.67	1.52
1	A	716	ASP	CG-OD2	6.13	1.36	1.25
6	H	91	ASP	CG-OD1	6.13	1.36	1.25
3	C	7	GLN	CA-C	-6.13	1.45	1.52
4	E	41	ASP	CA-CB	6.13	1.63	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	35	GLN	CG-CD	6.13	1.67	1.52
1	A	135	PHE	CE2-CZ	-6.13	1.20	1.38
1	A	872	GLY	C-N	-6.13	1.24	1.33
1	A	1209	MET	CA-C	-6.13	1.44	1.52
2	B	52	ASN	N-CA	-6.13	1.39	1.46
5	F	114	GLU	CD-OE1	6.13	1.36	1.25
2	B	273	LEU	CA-C	6.13	1.60	1.52
3	C	16	ASP	C-N	-6.13	1.25	1.33
10	L	29	TYR	CE1-CZ	-6.13	1.23	1.38
2	B	485	ARG	CG-CD	-6.12	1.34	1.52
1	A	619	LYS	C-O	-6.12	1.16	1.24
2	B	484	ASN	N-CA	-6.12	1.38	1.46
1	A	1367	HIS	CE1-NE2	-6.12	1.26	1.32
2	B	789	MET	N-CA	-6.12	1.39	1.46
3	C	217	ASP	CG-OD1	6.12	1.36	1.25
9	K	8	GLU	CA-CB	6.12	1.64	1.53
1	A	714	PHE	CA-CB	-6.12	1.43	1.53
1	A	837	ILE	N-CA	-6.12	1.39	1.46
2	B	1194	ILE	C-O	6.12	1.30	1.23
1	A	682	THR	CA-CB	-6.12	1.43	1.53
1	A	833	GLU	CG-CD	6.12	1.67	1.52
1	A	1141	THR	CB-CG2	-6.12	1.32	1.52
1	A	1207	LEU	N-CA	6.12	1.53	1.46
4	E	101	GLN	CD-NE2	6.12	1.46	1.33
1	A	855	THR	C-N	-6.12	1.24	1.33
1	A	1307	GLU	CD-OE1	6.12	1.36	1.25
2	B	198	ASP	CA-C	-6.12	1.44	1.53
2	B	597	MET	CB-CG	-6.12	1.34	1.52
1	A	1264	GLU	CD-OE1	-6.12	1.13	1.25
2	B	974	PRO	C-O	-6.12	1.16	1.23
1	A	88	LYS	C-O	-6.11	1.17	1.24
1	A	198	GLU	CB-CG	6.11	1.70	1.52
1	A	438	ASP	C-N	-6.11	1.24	1.33
1	A	438	ASP	N-CA	-6.11	1.38	1.46
6	H	34	ASP	CG-OD2	6.11	1.36	1.25
1	A	36	ARG	CG-CD	6.11	1.70	1.52
2	B	1194	ILE	N-CA	-6.11	1.39	1.46
5	F	115	THR	CA-CB	-6.11	1.45	1.54
7	I	23	ASN	N-CA	6.11	1.55	1.46
2	B	370	PHE	CD2-CE2	6.11	1.56	1.38
2	B	268	THR	CB-CG2	-6.11	1.32	1.52
1	A	698	GLN	C-N	-6.11	1.25	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	250	PHE	CG-CD2	6.11	1.51	1.38
4	E	59	SER	CA-C	6.11	1.60	1.52
7	I	25	LEU	CG-CD2	-6.11	1.32	1.52
1	A	245	PRO	CA-C	-6.11	1.43	1.52
1	A	685	GLU	CD-OE2	6.11	1.36	1.25
3	C	29	MET	CB-CG	6.10	1.70	1.52
4	E	131	THR	CA-CB	6.10	1.65	1.53
1	A	1206	ASP	CA-CB	6.10	1.62	1.53
2	B	198	ASP	CB-CG	-6.10	1.36	1.52
2	B	812	LEU	CA-C	-6.10	1.44	1.52
2	B	1073	TYR	C-O	6.10	1.30	1.24
3	C	77	ILE	CB-CG1	-6.10	1.41	1.53
3	C	163	ILE	N-CA	-6.10	1.39	1.46
4	E	32	GLN	CG-CD	6.10	1.67	1.52
1	A	771	GLU	CD-OE1	6.10	1.36	1.25
2	B	951	GLN	CB-CG	6.10	1.70	1.52
4	E	205	SER	CA-CB	-6.10	1.45	1.54
8	J	23	ASN	CG-OD1	6.10	1.35	1.23
1	A	109	HIS	CG-CD2	6.10	1.42	1.35
1	A	1012	ARG	N-CA	-6.10	1.38	1.46
1	A	1059	HIS	CE1-NE2	-6.10	1.26	1.32
2	B	832	GLY	C-N	-6.10	1.25	1.33
2	B	1212	ILE	CG1-CD1	-6.10	1.27	1.51
8	J	33	GLY	C-O	-6.10	1.17	1.24
1	A	636	GLU	CA-C	-6.09	1.44	1.52
3	C	209	TYR	CA-C	-6.09	1.44	1.52
10	L	67	PHE	C-O	-6.09	1.16	1.23
2	B	253	THR	N-CA	-6.09	1.38	1.46
3	C	258	ILE	C-O	6.09	1.31	1.24
8	J	3	VAL	CB-CG2	-6.09	1.32	1.52
8	J	45	CYS	CB-SG	6.09	2.01	1.81
1	A	407	ARG	CZ-NH2	6.09	1.41	1.33
1	A	1256	GLU	CD-OE1	6.09	1.36	1.25
2	B	429	PHE	C-N	-6.09	1.25	1.33
2	B	521	LEU	CA-C	6.09	1.58	1.52
2	B	390	LEU	CB-CG	-6.09	1.41	1.53
2	B	646	LEU	CA-CB	6.09	1.63	1.53
2	B	902	GLY	C-O	6.09	1.33	1.24
2	B	1110	PRO	CA-C	6.09	1.65	1.52
6	H	97	MET	N-CA	6.09	1.53	1.45
1	A	572	TRP	CD2-CE3	-6.09	1.30	1.40
1	A	1339	LEU	CA-C	-6.09	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	399	ASP	C-O	-6.09	1.15	1.24
4	E	65	THR	CB-OG1	6.09	1.53	1.43
1	A	148	CYS	CB-SG	-6.09	1.61	1.81
2	B	878	GLN	C-O	6.09	1.31	1.24
4	E	34	GLU	CD-OE1	6.09	1.36	1.25
4	E	211	TYR	CG-CD1	-6.09	1.26	1.39
1	A	404	TYR	CB-CG	-6.08	1.38	1.51
2	B	1097	HIS	CG-CD2	6.08	1.42	1.35
9	K	51	LEU	CA-C	6.08	1.61	1.52
1	A	25	GLU	C-O	6.08	1.31	1.24
1	A	754	SER	C-O	-6.08	1.16	1.23
2	B	627	PHE	N-CA	-6.08	1.38	1.46
3	C	213	PRO	CA-C	6.08	1.59	1.52
1	A	472	LEU	CG-CD1	-6.08	1.32	1.52
1	A	1421	CYS	CA-C	-6.08	1.44	1.53
4	E	21	GLU	CG-CD	6.08	1.67	1.52
1	A	901	LEU	CA-C	6.08	1.61	1.52
1	A	1018	PHE	CA-C	6.08	1.60	1.52
1	A	10	PRO	CG-CD	6.08	1.71	1.50
2	B	353	LYS	N-CA	6.08	1.53	1.46
2	B	582	VAL	CA-C	-6.08	1.45	1.52
6	H	119	GLY	C-O	6.08	1.32	1.23
1	A	769	SER	N-CA	-6.08	1.38	1.45
1	A	927	VAL	CA-C	6.08	1.60	1.52
10	L	34	CYS	C-O	-6.08	1.15	1.24
1	A	740	LEU	N-CA	-6.07	1.38	1.46
2	B	407	ASP	N-CA	-6.07	1.38	1.46
4	E	50	MET	CA-CB	6.07	1.63	1.53
7	I	43	VAL	N-CA	-6.07	1.38	1.46
5	F	148	VAL	CA-CB	-6.07	1.47	1.54
7	I	77	LYS	CA-C	6.07	1.60	1.53
3	C	109	SER	C-O	-6.07	1.16	1.23
1	A	437	MET	C-O	-6.07	1.16	1.23
3	C	3	GLU	CA-CB	-6.07	1.41	1.53
1	A	548	ASN	CA-C	6.07	1.60	1.52
1	A	789	LYS	CG-CD	-6.07	1.34	1.52
1	A	959	ASN	CG-OD1	-6.07	1.12	1.23
1	A	1030	ARG	CZ-NH2	-6.07	1.25	1.33
1	A	441	PRO	N-CA	-6.07	1.40	1.47
1	A	444	PHE	CD1-CE1	-6.07	1.20	1.38
1	A	643	ALA	N-CA	-6.07	1.38	1.46
1	A	718	VAL	C-O	-6.07	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	956	THR	CA-C	-6.07	1.45	1.52
2	B	322	PHE	N-CA	-6.06	1.38	1.46
3	C	55	THR	C-N	6.06	1.42	1.33
3	C	183	TRP	C-N	-6.06	1.26	1.33
5	F	149	GLU	C-O	6.06	1.31	1.24
1	A	261	ASP	N-CA	6.06	1.57	1.46
1	A	998	LEU	CG-CD2	-6.06	1.32	1.52
1	A	1375	MET	C-O	-6.06	1.15	1.24
2	B	279	ASP	N-CA	6.06	1.53	1.46
2	B	686	ASN	N-CA	-6.06	1.38	1.46
2	B	707	PRO	CB-CG	-6.06	1.19	1.49
3	C	225	ALA	N-CA	-6.06	1.38	1.46
3	C	266	ASP	CG-OD2	6.06	1.36	1.25
4	E	56	LYS	CB-CG	6.06	1.70	1.52
7	I	21	GLU	C-N	-6.06	1.25	1.33
1	A	417	TYR	CA-CB	-6.06	1.43	1.53
1	A	1157	ASP	CB-CG	6.06	1.67	1.52
2	B	602	THR	CB-OG1	6.06	1.53	1.43
2	B	879	ARG	CA-CB	6.06	1.63	1.53
3	C	265	MET	CG-SD	6.06	1.95	1.80
1	A	1149	ALA	CA-C	6.06	1.60	1.52
2	B	200	GLY	CA-C	-6.05	1.42	1.51
2	B	1023	VAL	CB-CG2	-6.05	1.32	1.52
2	B	1168	LEU	C-O	-6.05	1.16	1.23
1	A	1422	ARG	CB-CG	-6.05	1.34	1.52
1	A	151	ASP	CA-C	-6.05	1.44	1.52
1	A	611	GLN	C-O	6.05	1.31	1.23
2	B	459	TYR	CG-CD2	6.05	1.52	1.39
3	C	118	LEU	C-O	6.05	1.31	1.24
7	I	74	GLU	CD-OE1	6.05	1.36	1.25
1	A	603	ASN	CA-CB	-6.05	1.44	1.53
2	B	372	SER	N-CA	-6.05	1.39	1.46
2	B	635	ARG	N-CA	-6.05	1.40	1.46
2	B	857	ARG	CB-CG	-6.05	1.34	1.52
2	B	1007	VAL	CA-C	6.05	1.59	1.52
2	B	266	ALA	N-CA	6.05	1.53	1.46
3	C	236	GLY	N-CA	-6.05	1.36	1.45
1	A	1159	ARG	C-O	-6.04	1.15	1.24
2	B	752	ALA	C-O	-6.04	1.16	1.24
3	C	107	SER	N-CA	-6.04	1.37	1.45
5	F	129	LYS	CA-CB	-6.04	1.45	1.53
6	H	117	SER	CA-C	-6.04	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	461	LYS	CA-C	-6.04	1.45	1.52
1	A	551	TYR	N-CA	6.04	1.54	1.46
1	A	1267	MET	CA-CB	6.04	1.63	1.53
1	A	1332	PHE	CA-CB	-6.04	1.42	1.53
2	B	607	GLY	C-N	-6.04	1.25	1.33
2	B	685	LEU	CA-CB	-6.04	1.43	1.53
1	A	46	THR	CB-CG2	6.04	1.72	1.52
1	A	1300	LYS	CD-CE	6.04	1.70	1.52
2	B	371	GLU	C-N	-6.04	1.25	1.33
1	A	1171	GLN	CA-CB	6.04	1.63	1.53
2	B	515	HIS	ND1-CE1	-6.04	1.26	1.32
4	E	145	THR	CA-CB	-6.04	1.43	1.53
5	F	73	ALA	C-N	-6.04	1.26	1.33
3	C	82	TYR	CG-CD2	-6.04	1.26	1.39
4	E	78	LEU	CA-CB	-6.04	1.43	1.53
1	A	1195	LEU	CB-CG	-6.04	1.41	1.53
4	E	103	LYS	N-CA	6.04	1.53	1.46
2	B	116	GLU	CD-OE1	6.03	1.36	1.25
2	B	326	ASP	CG-OD2	6.03	1.36	1.25
9	K	2	ASN	C-N	6.03	1.44	1.33
1	A	351	THR	CB-CG2	-6.03	1.32	1.52
1	A	639	PRO	CA-C	6.03	1.61	1.52
1	A	845	LEU	C-N	-6.03	1.26	1.33
5	F	152	ILE	CA-C	6.03	1.59	1.52
7	I	73	ARG	CZ-NH1	6.03	1.41	1.32
1	A	1139	GLU	CA-CB	-6.03	1.43	1.53
2	B	297	ILE	CA-CB	6.03	1.62	1.54
2	B	381	MET	C-O	-6.03	1.16	1.24
2	B	733	HIS	CA-CB	6.03	1.63	1.53
2	B	949	VAL	CB-CG1	-6.03	1.32	1.52
1	A	68	GLN	CA-CB	6.03	1.62	1.52
2	B	431	TYR	C-O	6.03	1.33	1.23
6	H	14	GLU	CD-OE2	6.03	1.36	1.25
10	L	62	LYS	CG-CD	6.03	1.70	1.52
1	A	526	ASP	CA-CB	6.03	1.62	1.53
1	A	841	LEU	CA-CB	-6.03	1.44	1.53
1	A	850	VAL	CA-C	6.03	1.59	1.52
2	B	39	ARG	CZ-NH2	6.03	1.41	1.33
2	B	698	GLU	C-O	6.03	1.31	1.24
1	A	721	PHE	CE2-CZ	-6.02	1.20	1.38
1	A	743	VAL	CA-C	-6.02	1.44	1.52
2	B	1067	ARG	CA-CB	-6.02	1.43	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	788	ARG	CB-CG	6.02	1.70	1.52
2	B	819	ALA	N-CA	-6.02	1.35	1.46
2	B	827	ILE	C-O	-6.02	1.17	1.24
6	H	129	TYR	CG-CD2	6.02	1.51	1.39
1	A	304	MET	C-N	6.02	1.41	1.33
2	B	51	PHE	CA-CB	6.02	1.62	1.53
2	B	370	PHE	N-CA	6.02	1.53	1.46
4	E	72	PHE	C-O	6.02	1.30	1.24
7	I	115	LYS	CE-NZ	6.02	1.67	1.49
1	A	603	ASN	CB-CG	-6.01	1.37	1.52
2	B	1033	LYS	CB-CG	-6.01	1.34	1.52
6	H	109	LYS	CA-CB	6.01	1.63	1.53
8	J	15	GLY	N-CA	6.01	1.53	1.45
1	A	1226	VAL	C-O	6.01	1.30	1.23
2	B	98	THR	C-O	6.01	1.31	1.23
2	B	765	PRO	N-CA	-6.01	1.39	1.47
4	E	8	ASN	CB-CG	6.01	1.67	1.52
7	I	84	VAL	CB-CG1	-6.01	1.32	1.52
10	L	60	ARG	NE-CZ	6.01	1.39	1.33
2	B	281	PRO	CB-CG	-6.01	1.19	1.49
6	H	128	ASN	CG-OD1	6.01	1.34	1.23
1	A	768	GLN	CB-CG	-6.01	1.34	1.52
1	A	1020	CYS	C-O	6.01	1.31	1.24
2	B	175	ARG	C-O	-6.01	1.14	1.24
6	H	108	SER	N-CA	6.01	1.53	1.45
1	A	196	GLU	N-CA	6.01	1.54	1.46
2	B	25	ILE	N-CA	6.01	1.54	1.46
2	B	1071	VAL	CA-CB	-6.01	1.47	1.54
9	K	112	GLN	CD-NE2	6.01	1.45	1.33
2	B	598	GLU	CD-OE1	6.00	1.36	1.25
1	A	733	ALA	CA-CB	-6.00	1.44	1.53
1	A	998	LEU	N-CA	-6.00	1.38	1.46
6	H	15	VAL	CA-C	6.00	1.60	1.52
6	H	123	MET	C-O	-6.00	1.16	1.23
2	B	198	ASP	CG-OD2	-6.00	1.14	1.25
2	B	457	LEU	CA-C	-6.00	1.45	1.52
3	C	30	ALA	C-N	-6.00	1.25	1.33
1	A	760	GLN	N-CA	-6.00	1.38	1.46
8	J	37	SER	CA-CB	-6.00	1.42	1.53
1	A	289	ILE	C-O	6.00	1.30	1.24
1	A	826	ASP	C-N	-6.00	1.26	1.33
1	A	1287	TYR	CD1-CE1	6.00	1.56	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	100	PRO	CA-C	6.00	1.58	1.52
2	B	263	GLY	CA-C	6.00	1.60	1.51
2	B	423	LYS	CA-C	-6.00	1.46	1.53
2	B	372	SER	C-N	-6.00	1.26	1.33
1	A	121	LEU	CG-CD2	6.00	1.72	1.52
1	A	652	VAL	CB-CG1	-6.00	1.32	1.52
1	A	1347	ALA	C-N	-5.99	1.26	1.33
2	B	707	PRO	N-CA	-5.99	1.39	1.47
3	C	241	ASP	CG-OD2	5.99	1.36	1.25
6	H	140	ALA	C-O	-5.99	1.17	1.24
1	A	291	GLU	CD-OE2	5.99	1.36	1.25
1	A	1222	ASN	C-O	5.99	1.31	1.24
2	B	634	TYR	C-O	-5.99	1.17	1.23
2	B	1135	ARG	CD-NE	-5.99	1.37	1.46
5	F	122	MET	CA-C	-5.99	1.44	1.52
6	H	81	PRO	CA-CB	5.99	1.62	1.54
7	I	81	ARG	CZ-NH1	5.99	1.41	1.32
1	A	62	ASP	CA-CB	5.99	1.63	1.53
1	A	1033	GLN	N-CA	-5.99	1.38	1.46
1	A	1063	MET	SD-CE	-5.99	1.64	1.79
4	E	67	GLU	CG-CD	5.99	1.67	1.52
1	A	781	ASP	CA-C	-5.99	1.43	1.52
2	B	582	VAL	C-O	-5.99	1.18	1.24
3	C	88	CYS	CA-CB	5.99	1.63	1.53
1	A	209	ASN	CA-CB	5.99	1.62	1.53
2	B	96	TYR	C-O	5.99	1.31	1.23
2	B	265	SER	N-CA	5.99	1.53	1.46
2	B	484	ASN	C-O	-5.99	1.16	1.23
2	B	1069	PHE	CG-CD2	-5.99	1.26	1.38
8	J	38	ARG	NE-CZ	5.99	1.39	1.33
1	A	1092	LYS	CA-C	5.98	1.65	1.52
1	A	580	VAL	N-CA	-5.98	1.37	1.46
1	A	632	VAL	C-O	-5.98	1.17	1.24
2	B	435	THR	CA-CB	5.98	1.68	1.53
8	J	5	VAL	CB-CG1	-5.98	1.32	1.52
1	A	65	LEU	C-N	5.98	1.41	1.33
1	A	476	SER	CA-C	-5.98	1.45	1.52
1	A	595	THR	CA-CB	-5.98	1.43	1.53
2	B	762	ASN	CG-OD1	-5.98	1.12	1.23
2	B	847	ASP	CA-C	-5.98	1.45	1.52
3	C	145	CYS	CA-C	-5.98	1.45	1.52
2	B	573	GLN	CD-NE2	5.98	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	86	THR	CA-C	-5.98	1.45	1.52
7	I	47	GLU	C-O	5.98	1.31	1.24
1	A	1290	LYS	C-N	-5.97	1.28	1.33
1	A	1447	GLU	CG-CD	5.97	1.67	1.52
3	C	143	LEU	CB-CG	-5.97	1.41	1.53
1	A	1225	PHE	CD1-CE1	5.97	1.56	1.38
2	B	995	ARG	CZ-NH1	5.97	1.41	1.32
5	F	145	ASP	CG-OD2	5.97	1.36	1.25
7	I	90	GLN	CA-C	-5.97	1.45	1.53
7	I	98	VAL	CB-CG1	5.97	1.72	1.52
7	I	109	ILE	CA-C	-5.97	1.45	1.52
1	A	510	GLN	C-N	5.97	1.41	1.33
1	A	929	LEU	CA-C	-5.97	1.44	1.52
1	A	49	LYS	C-N	5.97	1.41	1.33
9	K	53	ASP	CA-CB	5.97	1.63	1.53
1	A	676	MET	C-N	-5.97	1.25	1.33
2	B	617	ARG	CD-NE	5.97	1.54	1.46
9	K	85	ASP	CG-OD1	5.97	1.36	1.25
1	A	472	LEU	CA-C	-5.97	1.44	1.52
1	A	775	ILE	CG1-CD1	-5.97	1.28	1.51
2	B	65	GLU	CA-C	5.97	1.61	1.53
1	A	113	LEU	C-O	-5.96	1.16	1.23
1	A	407	ARG	CZ-NH1	5.96	1.41	1.32
3	C	151	GLN	CD-OE1	5.96	1.34	1.23
4	E	121	MET	SD-CE	5.96	1.94	1.79
1	A	654	ASN	CA-C	5.96	1.60	1.52
1	A	758	ILE	CA-CB	-5.96	1.47	1.54
1	A	1287	TYR	C-N	5.96	1.41	1.33
1	A	1326	ARG	CA-C	5.96	1.60	1.52
2	B	24	PRO	CB-CG	-5.96	1.19	1.49
2	B	344	LYS	CA-CB	5.96	1.63	1.53
2	B	796	LEU	CG-CD2	-5.96	1.32	1.52
6	H	45	GLU	CD-OE1	5.96	1.36	1.25
7	I	118	ARG	CB-CG	5.96	1.70	1.52
1	A	811	GLN	CA-C	-5.96	1.45	1.52
4	E	152	LYS	CB-CG	5.96	1.70	1.52
7	I	15	TYR	CD2-CE2	5.96	1.56	1.38
7	I	33	SER	C-O	-5.96	1.16	1.23
1	A	609	ASP	CA-CB	-5.96	1.43	1.53
2	B	1032	SER	C-O	5.96	1.31	1.24
4	E	5	ASN	CA-C	-5.96	1.44	1.52
8	J	6	ARG	CB-CG	5.96	1.70	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	194	GLU	N-CA	5.96	1.53	1.46
9	K	68	PHE	CA-CB	-5.96	1.40	1.53
1	A	1327	ILE	C-N	5.95	1.41	1.33
2	B	551	PRO	CB-CG	-5.95	1.19	1.49
1	A	365	GLY	CA-C	-5.95	1.46	1.52
1	A	416	ARG	CG-CD	5.95	1.70	1.52
1	A	1057	VAL	CB-CG2	-5.95	1.32	1.52
2	B	491	THR	CA-C	-5.95	1.45	1.52
2	B	1128	LEU	CG-CD1	-5.95	1.32	1.52
2	B	1189	ILE	C-N	5.95	1.42	1.33
1	A	973	ILE	C-N	5.95	1.41	1.33
1	A	1045	VAL	CB-CG1	-5.95	1.32	1.52
3	C	106	GLU	CG-CD	5.95	1.67	1.52
1	A	290	GLU	N-CA	5.95	1.53	1.46
7	I	92	ARG	CZ-NH2	5.95	1.41	1.33
1	A	396	PRO	C-O	5.95	1.31	1.24
1	A	691	LEU	N-CA	-5.95	1.38	1.46
1	A	1151	GLU	CD-OE1	5.95	1.36	1.25
2	B	38	PHE	CG-CD2	-5.95	1.26	1.38
10	L	58	LYS	N-CA	-5.95	1.38	1.46
2	B	103	ASN	CG-ND2	5.94	1.45	1.33
2	B	843	GLN	C-O	5.94	1.31	1.24
1	A	624	SER	N-CA	5.94	1.54	1.46
1	A	840	ARG	CB-CG	5.94	1.70	1.52
2	B	622	LYS	CG-CD	5.94	1.70	1.52
2	B	1178	ASN	CA-C	5.94	1.61	1.52
3	C	75	MET	C-O	-5.94	1.17	1.24
3	C	76	ASP	N-CA	5.94	1.53	1.46
6	H	25	ARG	CZ-NH2	-5.94	1.25	1.33
6	H	37	LYS	CG-CD	5.94	1.70	1.52
7	I	102	VAL	CB-CG1	-5.94	1.32	1.52
1	A	999	VAL	CA-CB	-5.94	1.45	1.54
1	A	1228	TRP	CG-CD2	5.94	1.54	1.43
2	B	590	HIS	CA-CB	-5.94	1.42	1.53
6	H	22	LYS	CE-NZ	5.94	1.67	1.49
9	K	7	PHE	CA-CB	-5.94	1.43	1.53
9	K	40	HIS	C-N	-5.94	1.26	1.33
1	A	1286	LYS	CE-NZ	5.94	1.67	1.49
1	A	1299	VAL	CB-CG1	-5.94	1.32	1.52
2	B	514	LEU	C-N	-5.94	1.25	1.33
2	B	621	GLU	N-CA	-5.94	1.38	1.46
2	B	1178	ASN	CB-CG	-5.94	1.37	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1211	ASN	CG-OD1	-5.94	1.12	1.23
2	B	1220	ARG	NE-CZ	5.94	1.39	1.33
4	E	12	LEU	CA-C	5.94	1.60	1.52
7	I	19	ASP	C-O	5.94	1.31	1.23
2	B	249	ARG	C-N	5.94	1.42	1.33
2	B	465	ASN	N-CA	5.94	1.54	1.46
7	I	95	THR	N-CA	5.94	1.53	1.46
2	B	57	TYR	CA-CB	5.93	1.63	1.53
2	B	69	LEU	CA-C	5.93	1.60	1.52
2	B	231	PRO	CB-CG	5.93	1.79	1.49
2	B	337	ARG	CZ-NH1	-5.93	1.24	1.32
2	B	688	GLY	C-N	-5.93	1.25	1.33
2	B	755	ILE	CB-CG2	-5.93	1.32	1.52
3	C	7	GLN	CG-CD	-5.93	1.37	1.52
3	C	104	PHE	CA-CB	-5.93	1.43	1.53
6	H	121	LEU	CA-CB	-5.93	1.44	1.53
2	B	934	LYS	N-CA	5.93	1.53	1.46
1	A	874	ASP	N-CA	-5.93	1.38	1.46
1	A	1043	ASP	CA-CB	-5.93	1.43	1.53
2	B	371	GLU	C-O	-5.93	1.16	1.24
2	B	1038	SER	N-CA	-5.93	1.38	1.46
4	E	201	LYS	CA-C	5.93	1.61	1.53
1	A	77	CYS	CA-CB	5.93	1.62	1.52
2	B	202	TYR	CB-CG	-5.93	1.38	1.51
1	A	1109	LYS	CA-C	5.93	1.60	1.52
1	A	1297	GLU	CA-CB	-5.93	1.43	1.53
7	I	78	CYS	CA-C	5.93	1.60	1.52
4	E	171	LYS	CG-CD	5.92	1.70	1.52
2	B	761	HIS	C-O	-5.92	1.15	1.24
4	E	133	GLU	C-N	5.92	1.41	1.33
2	B	241	ARG	CZ-NH1	5.92	1.41	1.32
2	B	385	LEU	CA-CB	-5.92	1.44	1.53
4	E	149	LEU	CG-CD1	-5.92	1.33	1.52
7	I	10	CYS	N-CA	5.92	1.54	1.46
1	A	624	SER	CA-C	-5.92	1.46	1.53
1	A	711	ARG	C-N	-5.92	1.26	1.33
2	B	1183	LYS	N-CA	5.92	1.53	1.46
8	J	58	GLU	CA-C	-5.92	1.44	1.52
1	A	704	ALA	N-CA	5.92	1.53	1.45
1	A	807	GLY	C-O	-5.92	1.16	1.23
2	B	361	LEU	CB-CG	5.92	1.65	1.53
7	I	3	THR	C-O	5.92	1.30	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1212	VAL	CA-C	5.91	1.59	1.52
2	B	42	GLY	C-O	5.91	1.31	1.23
2	B	136	THR	C-N	5.91	1.42	1.33
2	B	866	TYR	CG-CD1	5.91	1.51	1.39
2	B	1086	PHE	CE2-CZ	-5.91	1.21	1.38
2	B	1095	LEU	CA-C	-5.91	1.45	1.52
9	K	40	HIS	CG-ND1	-5.91	1.31	1.38
1	A	296	LEU	CA-C	5.91	1.61	1.52
1	A	1368	MET	C-N	-5.91	1.25	1.33
6	H	22	LYS	CA-C	-5.91	1.45	1.52
6	H	36	CYS	CA-C	5.91	1.60	1.52
1	A	30	ILE	CA-CB	-5.91	1.46	1.54
1	A	489	LEU	CA-CB	-5.91	1.39	1.53
1	A	804	TYR	CG-CD2	-5.91	1.26	1.39
2	B	116	GLU	N-CA	-5.91	1.38	1.46
2	B	228	LYS	CA-C	-5.91	1.45	1.52
2	B	1081	LEU	CA-C	-5.91	1.45	1.52
4	E	50	MET	N-CA	5.91	1.53	1.46
1	A	203	SER	CA-CB	5.91	1.62	1.53
1	A	346	ASP	CA-C	-5.91	1.40	1.52
2	B	25	ILE	C-O	-5.91	1.16	1.23
4	E	162	ARG	CA-CB	5.91	1.63	1.53
1	A	1235	LYS	CA-C	5.91	1.59	1.52
1	A	1298	TYR	N-CA	-5.91	1.38	1.46
1	A	1316	VAL	CA-C	5.91	1.60	1.52
1	A	794	PRO	N-CA	-5.91	1.39	1.47
1	A	892	ALA	N-CA	-5.91	1.38	1.46
1	A	983	ILE	CB-CG2	-5.91	1.33	1.52
1	A	1262	LYS	CA-C	5.91	1.60	1.52
1	A	1328	TYR	CB-CG	5.91	1.64	1.51
2	B	994	TYR	CD1-CE1	-5.91	1.21	1.38
3	C	95	CYS	CB-SG	5.91	2.00	1.81
4	E	39	LEU	CA-CB	-5.91	1.45	1.53
5	F	112	GLU	CD-OE2	5.91	1.36	1.25
2	B	582	VAL	CB-CG1	-5.90	1.33	1.52
9	K	84	LYS	CG-CD	5.90	1.70	1.52
1	A	565	ILE	CG1-CD1	-5.90	1.28	1.51
1	A	945	GLU	C-O	5.90	1.31	1.24
1	A	1003	LYS	CA-CB	5.90	1.62	1.53
2	B	245	GLU	CA-CB	5.90	1.63	1.53
2	B	308	TRP	CE2-CZ2	-5.90	1.27	1.39
2	B	686	ASN	CA-C	-5.90	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	55	ARG	C-O	-5.90	1.17	1.24
9	K	42	LEU	C-N	-5.90	1.27	1.33
3	C	48	SER	C-O	5.90	1.31	1.23
3	C	179	GLU	C-N	-5.90	1.26	1.33
1	A	1444	MET	C-O	5.90	1.31	1.23
2	B	337	ARG	CA-C	-5.90	1.43	1.52
1	A	685	GLU	CA-C	-5.90	1.44	1.52
1	A	1093	LYS	CD-CE	5.90	1.70	1.52
1	A	1365	TYR	CE2-CZ	-5.90	1.24	1.38
2	B	1106	ARG	C-O	5.90	1.31	1.23
6	H	115	TYR	CG-CD2	-5.90	1.26	1.39
1	A	84	ILE	C-O	-5.90	1.17	1.24
9	K	65	HIS	CG-CD2	-5.90	1.29	1.35
1	A	287	HIS	CA-C	5.89	1.60	1.52
1	A	405	VAL	CA-CB	-5.89	1.47	1.54
2	B	419	THR	CB-OG1	-5.89	1.34	1.43
2	B	591	ARG	CZ-NH1	5.89	1.41	1.32
5	F	106	PRO	CB-CG	5.89	1.79	1.49
6	H	57	VAL	CB-CG2	5.89	1.72	1.52
8	J	3	VAL	CB-CG1	-5.89	1.33	1.52
9	K	84	LYS	CE-NZ	5.89	1.67	1.49
2	B	39	ARG	CD-NE	5.89	1.54	1.46
2	B	325	GLN	CD-NE2	5.89	1.45	1.33
3	C	183	TRP	NE1-CE2	-5.89	1.30	1.37
9	K	112	GLN	CB-CG	5.89	1.70	1.52
1	A	137	ALA	N-CA	-5.89	1.38	1.46
1	A	1078	GLN	CG-CD	5.89	1.66	1.52
2	B	127	GLY	C-N	-5.89	1.25	1.33
9	K	67	PHE	CE2-CZ	-5.89	1.21	1.38
1	A	279	LEU	CA-CB	5.89	1.63	1.53
1	A	458	HIS	C-N	5.89	1.41	1.33
1	A	1047	SER	CB-OG	5.89	1.53	1.42
1	A	1063	MET	CG-SD	-5.89	1.66	1.80
2	B	346	GLU	CA-C	-5.89	1.44	1.52
2	B	544	CYS	CA-C	5.89	1.60	1.52
2	B	999	MET	CG-SD	5.89	1.95	1.80
2	B	1056	SER	N-CA	-5.89	1.39	1.46
5	F	76	LYS	CE-NZ	5.89	1.67	1.49
1	A	693	VAL	CA-C	-5.88	1.43	1.52
1	A	1030	ARG	CB-CG	-5.88	1.34	1.52
2	B	840	ILE	N-CA	-5.88	1.39	1.46
2	B	867	GLY	C-O	5.88	1.31	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	990	ILE	CA-CB	-5.88	1.47	1.54
3	C	148	ARG	NE-CZ	5.88	1.39	1.33
7	I	115	LYS	C-O	5.88	1.33	1.23
1	A	700	ASN	CA-C	-5.88	1.44	1.53
2	B	227	LYS	CE-NZ	5.88	1.67	1.49
2	B	878	GLN	CD-OE1	5.88	1.34	1.23
2	B	975	GLN	CD-OE1	5.88	1.34	1.23
2	B	1200	ALA	C-O	-5.88	1.17	1.24
9	K	68	PHE	CA-C	-5.88	1.45	1.52
1	A	171	GLN	C-O	-5.88	1.16	1.24
1	A	1228	TRP	CG-CD1	-5.88	1.22	1.36
2	B	596	LEU	CA-CB	5.88	1.62	1.53
1	A	379	VAL	CB-CG1	-5.88	1.33	1.52
1	A	1215	ARG	CD-NE	5.88	1.54	1.46
2	B	535	LEU	CG-CD1	-5.88	1.33	1.52
2	B	886	LYS	CE-NZ	5.88	1.67	1.49
10	L	28	LYS	CD-CE	5.88	1.70	1.52
2	B	365	THR	CB-CG2	-5.88	1.33	1.52
2	B	1197	PRO	CG-CD	-5.88	1.30	1.50
2	B	1224	PHE	CE1-CZ	5.88	1.56	1.38
1	A	481	ASP	CA-CB	-5.88	1.45	1.54
2	B	125	SER	CA-CB	5.88	1.65	1.53
9	K	101	LEU	CA-C	5.88	1.60	1.52
1	A	195	ASP	C-N	5.87	1.45	1.33
1	A	1006	ILE	N-CA	-5.87	1.39	1.46
1	A	1255	GLU	CA-CB	5.87	1.63	1.53
1	A	606	LEU	CA-CB	-5.87	1.43	1.53
2	B	558	LEU	N-CA	-5.87	1.39	1.46
3	C	140	ASN	CB-CG	5.87	1.66	1.52
1	A	1030	ARG	N-CA	-5.87	1.39	1.46
1	A	1166	ASP	CG-OD2	5.87	1.36	1.25
2	B	226	PHE	CA-C	-5.87	1.45	1.52
2	B	1095	LEU	CG-CD2	-5.87	1.33	1.52
1	A	368	LYS	C-N	-5.87	1.26	1.34
1	A	425	GLN	CA-CB	5.87	1.61	1.53
1	A	438	ASP	CA-CB	-5.87	1.43	1.53
1	A	854	ASN	C-N	5.87	1.41	1.33
2	B	218	SER	C-O	-5.87	1.16	1.23
1	A	71	GLN	CD-OE1	5.86	1.34	1.23
1	A	291	GLU	CD-OE1	5.86	1.36	1.25
1	A	1428	VAL	C-O	-5.86	1.17	1.24
2	B	827	ILE	CB-CG2	-5.86	1.33	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1132	GLU	CB-CG	5.86	1.70	1.52
3	C	90	ASP	CG-OD1	5.86	1.36	1.25
3	C	160	LYS	CG-CD	5.86	1.70	1.52
4	E	167	ARG	C-O	5.86	1.31	1.24
1	A	913	LEU	CG-CD2	-5.86	1.33	1.52
1	A	197	PRO	N-CA	-5.86	1.40	1.47
1	A	478	TYR	C-O	-5.86	1.16	1.24
1	A	1163	ILE	CA-CB	5.86	1.59	1.54
2	B	708	GLU	CA-CB	-5.86	1.43	1.53
6	H	44	VAL	CB-CG1	5.86	1.71	1.52
1	A	143	LYS	CB-CG	5.86	1.70	1.52
2	B	45	SER	N-CA	5.86	1.53	1.46
3	C	114	TYR	CG-CD2	-5.86	1.27	1.39
1	A	224	PHE	CA-C	5.86	1.61	1.53
1	A	1078	GLN	CB-CG	5.86	1.70	1.52
1	A	1196	GLU	C-O	5.86	1.30	1.24
1	A	1305	VAL	CB-CG1	-5.86	1.33	1.52
1	A	1368	MET	CA-CB	-5.86	1.44	1.53
2	B	595	ARG	CB-CG	5.86	1.70	1.52
2	B	608	ASP	CA-CB	5.86	1.62	1.53
2	B	608	ASP	C-O	-5.86	1.17	1.24
3	C	177	GLU	CD-OE2	5.86	1.36	1.25
1	A	49	LYS	CA-CB	5.86	1.64	1.53
1	A	1383	SER	CB-OG	5.86	1.53	1.42
1	A	1441	PHE	N-CA	-5.86	1.38	1.46
2	B	402	GLY	C-O	5.86	1.31	1.23
6	H	114	VAL	CA-CB	-5.86	1.46	1.54
2	B	269	ILE	C-O	-5.85	1.18	1.24
1	A	527	THR	CA-C	-5.85	1.44	1.52
2	B	35	SER	N-CA	-5.85	1.39	1.46
2	B	479	VAL	N-CA	-5.85	1.38	1.46
2	B	1130	PHE	C-O	-5.85	1.15	1.23
4	E	180	ARG	CA-C	5.85	1.60	1.52
6	H	100	THR	N-CA	-5.85	1.38	1.46
1	A	48	ALA	CA-C	5.85	1.60	1.52
1	A	692	ASP	CG-OD2	5.85	1.36	1.25
4	E	104	ASN	CG-ND2	5.85	1.45	1.33
2	B	47	GLN	CD-OE1	5.85	1.34	1.23
2	B	610	ASN	CA-C	-5.85	1.46	1.53
5	F	78	GLN	N-CA	5.85	1.53	1.46
1	A	783	THR	CA-CB	-5.85	1.43	1.53
1	A	848	ILE	CA-C	-5.85	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	724	ASP	CG-OD2	5.85	1.36	1.25
2	B	1130	PHE	C-N	-5.85	1.27	1.33
2	B	1145	SER	C-O	5.85	1.31	1.24
6	H	141	TYR	C-O	-5.85	1.16	1.23
1	A	123	ARG	C-O	5.85	1.31	1.24
1	A	430	TRP	CD2-CE3	-5.85	1.30	1.40
1	A	933	TYR	CA-CB	-5.84	1.43	1.53
2	B	722	ASP	CA-CB	5.84	1.65	1.53
1	A	1159	ARG	CD-NE	5.84	1.54	1.46
4	E	63	ASN	N-CA	5.84	1.50	1.45
2	B	53	GLN	C-N	-5.84	1.25	1.33
2	B	806	THR	C-N	-5.84	1.25	1.33
2	B	1021	MET	SD-CE	-5.84	1.65	1.79
3	C	188	HIS	N-CA	-5.84	1.38	1.46
8	J	47	ARG	C-O	5.84	1.31	1.24
1	A	123	ARG	CZ-NH1	5.84	1.41	1.32
2	B	1103	ILE	C-O	5.84	1.31	1.24
4	E	103	LYS	CE-NZ	5.84	1.66	1.49
7	I	72	ASP	CA-C	5.84	1.60	1.52
1	A	688	LYS	CE-NZ	5.84	1.66	1.49
4	E	28	TYR	CE1-CZ	-5.84	1.24	1.38
1	A	460	VAL	N-CA	-5.84	1.38	1.46
1	A	463	ILE	CA-CB	-5.84	1.46	1.54
1	A	540	PHE	CA-CB	-5.84	1.40	1.53
1	A	974	ASP	CG-OD1	5.84	1.36	1.25
2	B	785	TYR	CD2-CE2	-5.84	1.21	1.38
3	C	230	MET	CB-CG	5.84	1.70	1.52
6	H	26	ILE	N-CA	-5.84	1.40	1.46
9	K	66	PRO	C-N	-5.84	1.24	1.33
2	B	342	GLY	N-CA	-5.83	1.39	1.45
3	C	146	LYS	CG-CD	5.83	1.70	1.52
1	A	235	ILE	CA-C	5.83	1.59	1.52
1	A	1297	GLU	CG-CD	5.83	1.66	1.52
2	B	934	LYS	CA-CB	5.83	1.63	1.53
2	B	1161	HIS	CA-CB	5.83	1.62	1.53
2	B	170	LEU	C-O	5.83	1.31	1.24
2	B	620	ARG	C-N	-5.83	1.24	1.33
2	B	654	ARG	CZ-NH1	-5.83	1.24	1.32
8	J	50	ILE	N-CA	-5.83	1.38	1.46
2	B	1191	ILE	CB-CG1	-5.83	1.41	1.53
1	A	587	HIS	CB-CG	5.83	1.58	1.50
2	B	229	ALA	CA-CB	-5.83	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	257	LYS	CE-NZ	5.83	1.66	1.49
1	A	373	THR	CA-C	-5.83	1.45	1.52
2	B	101	MET	N-CA	-5.83	1.39	1.46
2	B	291	ILE	C-O	5.83	1.30	1.24
2	B	359	GLU	CD-OE1	5.83	1.36	1.25
5	F	124	GLU	C-O	-5.83	1.17	1.24
1	A	359	LEU	C-O	5.82	1.30	1.23
2	B	41	LYS	CE-NZ	5.82	1.66	1.49
2	B	1030	LEU	CB-CG	-5.82	1.41	1.53
2	B	1092	TYR	CG-CD2	-5.82	1.27	1.39
4	E	186	LEU	CA-CB	-5.82	1.43	1.53
2	B	844	SER	N-CA	-5.82	1.39	1.46
10	L	36	SER	CB-OG	5.82	1.53	1.42
1	A	234	MET	CA-CB	-5.82	1.43	1.53
1	A	972	HIS	CA-CB	5.82	1.62	1.53
1	A	1261	LYS	CE-NZ	5.82	1.66	1.49
2	B	581	PHE	CE2-CZ	-5.82	1.21	1.38
1	A	1384	VAL	N-CA	5.82	1.53	1.46
2	B	649	LYS	CB-CG	-5.82	1.34	1.52
9	K	112	GLN	CG-CD	5.82	1.66	1.52
1	A	696	GLU	CD-OE2	5.82	1.36	1.25
1	A	749	ALA	C-N	-5.82	1.24	1.33
1	A	1228	TRP	CB-CG	5.82	1.68	1.50
2	B	783	THR	CA-CB	-5.82	1.43	1.53
7	I	16	PRO	CA-C	-5.82	1.45	1.52
1	A	597	LEU	C-N	-5.82	1.26	1.33
1	A	1192	LEU	C-O	-5.82	1.17	1.24
3	C	38	ILE	CA-CB	-5.82	1.47	1.54
3	C	208	GLU	C-N	-5.82	1.25	1.33
2	B	650	GLU	CA-CB	-5.81	1.44	1.53
3	C	89	GLU	CD-OE1	5.81	1.36	1.25
1	A	222	LEU	CA-C	5.81	1.60	1.52
2	B	70	ILE	CB-CG2	5.81	1.71	1.52
2	B	830	TYR	CG-CD1	-5.81	1.27	1.39
2	B	960	GLY	C-N	-5.81	1.25	1.33
3	C	129	ILE	C-O	-5.81	1.16	1.23
3	C	134	ILE	CG1-CD1	-5.81	1.29	1.51
3	C	236	GLY	CA-C	-5.81	1.43	1.51
4	E	134	THR	N-CA	5.81	1.53	1.46
2	B	252	SER	N-CA	5.81	1.53	1.46
5	F	84	TYR	CZ-OH	5.81	1.50	1.38
1	A	39	GLU	N-CA	5.81	1.53	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	434	ARG	CA-C	5.81	1.60	1.53
2	B	911	ILE	CA-CB	-5.81	1.46	1.54
9	K	84	LYS	C-O	5.81	1.31	1.24
1	A	184	SER	CA-C	-5.81	1.47	1.53
1	A	192	GLY	C-N	5.81	1.41	1.33
2	B	129	PHE	CD1-CE1	-5.81	1.21	1.38
2	B	1085	ILE	N-CA	-5.81	1.39	1.46
1	A	130	ASP	N-CA	-5.81	1.38	1.46
1	A	289	ILE	N-CA	5.81	1.53	1.46
2	B	729	ILE	N-CA	-5.81	1.39	1.46
1	A	653	VAL	N-CA	-5.80	1.39	1.46
1	A	792	TYR	C-N	-5.80	1.24	1.33
2	B	850	LEU	CG-CD1	-5.80	1.33	1.52
4	E	62	ALA	CA-CB	-5.80	1.44	1.53
7	I	81	ARG	NE-CZ	5.80	1.39	1.33
1	A	526	ASP	C-O	-5.80	1.17	1.24
1	A	346	ASP	CG-OD1	5.80	1.36	1.25
1	A	1051	ALA	N-CA	5.80	1.53	1.46
2	B	422	LYS	C-O	-5.80	1.16	1.24
2	B	943	SER	N-CA	5.80	1.53	1.46
1	A	796	SER	C-O	-5.80	1.16	1.24
2	B	247	GLY	C-O	5.80	1.31	1.23
1	A	1176	LEU	CG-CD1	5.80	1.71	1.52
2	B	50	SER	CA-C	-5.80	1.45	1.52
2	B	831	SER	CB-OG	-5.80	1.30	1.42
2	B	1024	ALA	CA-C	-5.80	1.45	1.52
2	B	1062	HIS	C-O	5.80	1.31	1.24
4	E	11	ARG	C-O	5.80	1.30	1.24
4	E	92	THR	N-CA	5.80	1.53	1.46
1	A	434	ARG	C-O	-5.79	1.16	1.23
1	A	978	PRO	C-O	5.79	1.30	1.23
1	A	34	LYS	CD-CE	5.79	1.69	1.52
2	B	878	GLN	CB-CG	5.79	1.69	1.52
1	A	499	ALA	C-O	-5.79	1.17	1.24
1	A	1326	ARG	CA-CB	-5.79	1.44	1.53
2	B	393	LYS	CA-C	-5.79	1.45	1.52
3	C	6	PRO	N-CA	-5.79	1.40	1.47
3	C	246	ARG	C-N	-5.79	1.26	1.33
1	A	1151	GLU	CA-CB	-5.79	1.43	1.53
1	A	1152	ILE	CB-CG1	-5.79	1.41	1.53
1	A	162	VAL	CA-CB	-5.79	1.45	1.55
2	B	857	ARG	C-N	-5.79	1.25	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	10	ILE	CA-C	5.79	1.60	1.52
9	K	102	LYS	C-O	5.79	1.31	1.24
2	B	1104	HIS	N-CA	-5.79	1.38	1.46
2	B	1171	VAL	N-CA	-5.79	1.38	1.46
6	H	12	VAL	N-CA	5.79	1.52	1.46
8	J	59	LYS	N-CA	-5.79	1.38	1.46
1	A	1333	ILE	N-CA	5.79	1.53	1.46
2	B	749	LEU	N-CA	-5.79	1.38	1.45
3	C	127	ARG	CG-CD	-5.79	1.35	1.52
7	I	27	PHE	C-O	-5.79	1.17	1.24
1	A	591	PHE	CE2-CZ	5.78	1.56	1.38
1	A	593	GLU	CG-CD	5.78	1.66	1.52
2	B	1151	LEU	CG-CD2	-5.78	1.33	1.52
3	C	131	HIS	CA-CB	5.78	1.63	1.53
4	E	188	LEU	CA-CB	-5.78	1.44	1.53
6	H	98	TYR	CA-CB	-5.78	1.44	1.53
1	A	1215	ARG	CA-CB	5.78	1.62	1.53
1	A	1377	THR	CA-C	5.78	1.60	1.52
2	B	665	GLU	C-O	-5.78	1.17	1.24
8	J	53	HIS	C-N	-5.78	1.26	1.33
1	A	584	ASN	C-N	-5.78	1.25	1.32
4	E	200	ARG	CA-C	-5.78	1.45	1.52
6	H	81	PRO	CG-CD	5.78	1.70	1.50
7	I	69	PRO	C-O	5.78	1.30	1.23
4	E	154	ILE	CB-CG2	-5.78	1.33	1.52
1	A	724	GLU	CA-CB	5.78	1.62	1.53
1	A	1156	PRO	CA-C	5.78	1.61	1.52
2	B	663	ALA	N-CA	-5.78	1.38	1.46
4	E	113	GLN	CD-NE2	5.78	1.45	1.33
5	F	94	LEU	CA-CB	-5.78	1.43	1.53
6	H	6	PHE	CG-CD2	-5.78	1.26	1.38
9	K	85	ASP	CG-OD2	5.78	1.36	1.25
2	B	100	PRO	CB-CG	-5.78	1.20	1.49
3	C	128	ASN	CG-OD1	5.78	1.34	1.23
1	A	593	GLU	C-N	5.77	1.42	1.33
2	B	768	THR	CB-CG2	-5.77	1.33	1.52
1	A	969	GLN	CA-C	-5.77	1.45	1.52
2	B	915	THR	C-O	-5.77	1.16	1.23
2	B	1136	ASP	N-CA	-5.77	1.39	1.46
3	C	149	LYS	C-N	5.77	1.41	1.33
3	C	210	GLU	CG-CD	5.77	1.66	1.52
4	E	81	GLU	CA-C	-5.77	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	LEU	N-CA	5.77	1.53	1.45
1	A	238	CYS	C-N	-5.77	1.25	1.33
1	A	300	VAL	C-O	-5.77	1.17	1.24
1	A	973	ILE	N-CA	-5.77	1.39	1.46
4	E	7	ARG	CZ-NH2	5.77	1.41	1.33
1	A	265	LYS	C-N	-5.77	1.25	1.33
1	A	740	LEU	CG-CD1	-5.77	1.33	1.52
1	A	151	ASP	CB-CG	5.76	1.66	1.52
4	E	41	ASP	CG-OD2	5.76	1.36	1.25
4	E	85	GLU	CA-C	5.76	1.60	1.52
5	F	146	TRP	C-O	-5.76	1.17	1.24
9	K	87	LEU	N-CA	-5.76	1.38	1.46
2	B	30	SER	CA-CB	-5.76	1.44	1.53
2	B	272	THR	N-CA	-5.76	1.39	1.46
3	C	204	SER	C-O	5.76	1.31	1.23
6	H	79	TRP	CZ2-CH2	-5.76	1.26	1.37
9	K	21	ILE	CG1-CD1	-5.76	1.29	1.51
1	A	140	THR	C-N	-5.76	1.24	1.33
2	B	518	HIS	ND1-CE1	-5.76	1.26	1.32
4	E	30	ILE	CB-CG2	5.76	1.71	1.52
1	A	811	GLN	CB-CG	-5.76	1.35	1.52
2	B	1069	PHE	CB-CG	-5.76	1.37	1.50
5	F	77	ASP	CB-CG	5.76	1.66	1.52
8	J	32	GLU	CA-CB	-5.76	1.43	1.53
1	A	232	GLU	N-CA	-5.76	1.39	1.46
1	A	985	ASP	CG-OD2	5.76	1.36	1.25
2	B	1199	ALA	CA-C	-5.76	1.45	1.52
3	C	62	PHE	CG-CD2	5.76	1.50	1.38
5	F	100	GLN	CD-OE1	5.76	1.34	1.23
1	A	464	PRO	N-CA	-5.76	1.40	1.47
2	B	29	ASP	N-CA	-5.76	1.38	1.46
4	E	208	TYR	CD2-CE2	-5.75	1.21	1.38
1	A	629	LEU	CA-CB	-5.75	1.44	1.53
1	A	1039	LYS	CE-NZ	5.75	1.66	1.49
1	A	1212	VAL	CB-CG1	-5.75	1.33	1.52
3	C	149	LYS	CD-CE	5.75	1.69	1.52
8	J	53	HIS	CD2-NE2	-5.75	1.31	1.37
1	A	176	LYS	CA-CB	-5.75	1.45	1.53
1	A	742	ASN	CB-CG	-5.75	1.37	1.52
1	A	837	ILE	C-O	-5.75	1.17	1.24
3	C	21	ILE	CG1-CD1	5.75	1.74	1.51
1	A	162	VAL	C-N	5.75	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	967	ALA	CA-C	5.75	1.60	1.52
1	A	1379	GLY	C-O	5.75	1.32	1.24
2	B	192	LEU	CG-CD1	-5.75	1.33	1.52
2	B	528	PRO	CG-CD	-5.75	1.31	1.50
2	B	969	ARG	C-O	-5.75	1.17	1.24
8	J	4	PRO	CG-CD	-5.75	1.31	1.50
2	B	728	ARG	CG-CD	5.75	1.69	1.52
2	B	805	THR	CB-OG1	5.75	1.52	1.43
4	E	9	ILE	CB-CG2	5.75	1.71	1.52
4	E	24	LYS	CE-NZ	5.75	1.66	1.49
4	E	37	LEU	CA-C	-5.75	1.45	1.52
5	F	104	ASN	CG-OD1	5.75	1.34	1.23
9	K	17	SER	CA-C	-5.75	1.45	1.52
1	A	74	MET	CA-CB	5.75	1.63	1.53
5	F	119	ARG	CD-NE	5.75	1.54	1.46
6	H	96	VAL	CB-CG2	-5.75	1.33	1.52
9	K	82	ASP	C-O	-5.75	1.16	1.24
10	L	34	CYS	CA-CB	-5.75	1.43	1.53
1	A	91	PHE	CA-C	-5.74	1.45	1.52
1	A	557	ASP	CA-C	5.74	1.60	1.52
1	A	662	PHE	CG-CD2	-5.74	1.26	1.38
4	E	122	LYS	CE-NZ	5.74	1.66	1.49
1	A	175	ARG	CD-NE	5.74	1.54	1.46
4	E	187	TYR	CG-CD2	-5.74	1.27	1.39
1	A	775	ILE	C-O	-5.74	1.17	1.24
1	A	1418	LEU	C-O	-5.74	1.17	1.24
2	B	868	MET	CB-CG	5.74	1.69	1.52
10	L	33	GLU	C-N	5.74	1.42	1.33
2	B	509	ALA	CA-C	5.74	1.65	1.52
2	B	644	GLU	CA-CB	-5.74	1.43	1.53
3	C	23	SER	CA-C	-5.74	1.45	1.52
3	C	228	PHE	C-N	-5.74	1.26	1.33
1	A	70	CYS	CB-SG	5.74	2.00	1.81
1	A	71	GLN	CB-CG	5.74	1.69	1.52
6	H	145	ARG	C-O	5.74	1.31	1.23
9	K	78	THR	CA-C	-5.74	1.45	1.52
1	A	869	GLY	C-O	-5.74	1.16	1.23
1	A	1450	LEU	CA-CB	5.74	1.65	1.53
3	C	26	ASP	CB-CG	5.74	1.66	1.52
3	C	102	GLN	CG-CD	5.74	1.66	1.52
5	F	104	ASN	CG-ND2	5.74	1.45	1.33
1	A	350	ARG	C-N	-5.73	1.25	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	255	VAL	N-CA	-5.73	1.39	1.46
10	L	49	LYS	CA-CB	5.73	1.63	1.53
1	A	961	ARG	CA-CB	-5.73	1.44	1.53
1	A	1140	HIS	CD2-NE2	5.73	1.44	1.37
3	C	257	SER	C-O	-5.73	1.16	1.24
5	F	137	TYR	C-O	-5.73	1.16	1.23
1	A	1062	GLU	CA-C	5.73	1.60	1.52
1	A	1142	THR	CA-CB	-5.73	1.45	1.53
2	B	667	GLN	CG-CD	5.73	1.66	1.52
1	A	575	LYS	CB-CG	-5.73	1.35	1.52
1	A	1277	GLU	C-N	-5.73	1.25	1.33
2	B	249	ARG	CA-C	5.73	1.60	1.52
2	B	879	ARG	CG-CD	5.73	1.69	1.52
1	A	953	ASN	CA-CB	-5.73	1.45	1.53
2	B	203	PHE	CA-CB	-5.73	1.43	1.53
2	B	821	GLN	N-CA	-5.73	1.38	1.45
1	A	230	ARG	N-CA	-5.72	1.38	1.45
2	B	210	LYS	N-CA	5.72	1.53	1.46
2	B	367	LEU	C-O	-5.72	1.16	1.24
1	A	960	ILE	CA-CB	5.72	1.61	1.54
1	A	1285	MET	C-N	-5.72	1.25	1.33
2	B	916	THR	C-O	5.72	1.34	1.23
3	C	120	ILE	CB-CG1	-5.72	1.42	1.53
3	C	155	LEU	CG-CD2	-5.72	1.33	1.52
2	B	602	THR	CB-CG2	-5.72	1.33	1.52
8	J	27	GLU	C-O	5.72	1.30	1.24
8	J	52	THR	CA-C	-5.72	1.45	1.52
9	K	58	PHE	N-CA	-5.72	1.39	1.46
1	A	1406	VAL	CA-CB	5.72	1.61	1.54
3	C	55	THR	CB-OG1	-5.72	1.34	1.43
2	B	595	ARG	C-N	-5.72	1.26	1.33
2	B	940	PRO	N-CD	-5.72	1.39	1.47
6	H	106	GLU	C-O	5.72	1.31	1.24
5	F	123	LYS	CB-CG	5.71	1.69	1.52
1	A	642	CYS	C-N	-5.71	1.26	1.34
7	I	10	CYS	CA-C	-5.71	1.44	1.52
1	A	376	TYR	CA-C	5.71	1.59	1.52
1	A	542	GLU	CA-CB	5.71	1.61	1.53
1	A	1306	LEU	CG-CD2	-5.71	1.33	1.52
2	B	513	GLN	C-O	-5.71	1.16	1.23
2	B	1063	GLY	C-O	-5.71	1.16	1.24
1	A	124	GLN	CG-CD	5.71	1.66	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1135	ARG	CZ-NH1	5.71	1.40	1.32
1	A	1313	LEU	CG-CD1	-5.71	1.33	1.52
2	B	862	GLN	CG-CD	5.71	1.66	1.52
3	C	135	GLN	CG-CD	5.71	1.66	1.52
4	E	131	THR	C-N	-5.71	1.26	1.33
5	F	79	ARG	CZ-NH2	-5.71	1.26	1.33
5	F	147	SER	N-CA	-5.71	1.38	1.45
1	A	568	PRO	N-CD	-5.71	1.39	1.47
1	A	740	LEU	CA-C	-5.71	1.44	1.52
1	A	1042	PHE	CA-CB	5.71	1.62	1.53
2	B	838	SER	CA-C	-5.71	1.45	1.52
2	B	882	THR	N-CA	5.71	1.53	1.46
2	B	904	ARG	CA-CB	-5.71	1.43	1.53
6	H	109	LYS	CB-CG	5.71	1.69	1.52
9	K	73	LEU	CA-CB	-5.71	1.40	1.53
2	B	994	TYR	CG-CD1	-5.71	1.27	1.39
1	A	420	ARG	CZ-NH2	-5.70	1.26	1.33
1	A	593	GLU	CB-CG	5.70	1.69	1.52
3	C	14	SER	CA-CB	-5.70	1.44	1.53
1	A	290	GLU	CA-CB	-5.70	1.44	1.53
1	A	689	LYS	C-N	-5.70	1.26	1.33
1	A	700	ASN	C-O	-5.70	1.15	1.23
2	B	734	HIS	CA-CB	5.70	1.60	1.53
7	I	65	ASP	C-N	-5.70	1.27	1.34
9	K	27	ALA	CA-C	5.70	1.58	1.52
9	K	92	ASN	N-CA	5.70	1.52	1.46
1	A	647	GLY	CA-C	5.70	1.59	1.51
1	A	959	ASN	CA-CB	-5.70	1.45	1.52
2	B	730	ARG	CZ-NH1	-5.70	1.24	1.32
4	E	128	PRO	C-O	5.70	1.30	1.24
7	I	80	SER	CB-OG	5.70	1.53	1.42
1	A	975	HIS	C-N	5.70	1.42	1.33
3	C	81	GLU	CA-CB	-5.70	1.44	1.53
9	K	16	GLU	CA-C	-5.70	1.45	1.52
9	K	62	LYS	CE-NZ	-5.70	1.32	1.49
10	L	26	THR	N-CA	5.70	1.53	1.46
1	A	559	VAL	CA-C	-5.70	1.45	1.52
1	A	1437	GLY	C-O	-5.70	1.16	1.24
2	B	224	GLN	C-O	-5.70	1.17	1.24
2	B	939	THR	CA-CB	-5.70	1.45	1.53
6	H	135	LEU	C-O	5.70	1.31	1.24
1	A	937	VAL	N-CA	-5.69	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	961	ARG	CG-CD	5.69	1.69	1.52
2	B	874	PHE	CD1-CE1	-5.69	1.21	1.38
1	A	88	LYS	CA-C	-5.69	1.46	1.52
2	B	95	ILE	C-O	-5.69	1.18	1.24
4	E	65	THR	C-O	5.69	1.30	1.23
7	I	79	HIS	CA-CB	5.69	1.63	1.53
2	B	534	GLY	C-N	-5.69	1.25	1.33
2	B	773	MET	C-N	-5.69	1.25	1.33
2	B	1052	VAL	CA-CB	5.69	1.62	1.54
1	A	1026	LEU	C-N	-5.69	1.25	1.33
2	B	712	PRO	CB-CG	5.69	1.78	1.49
6	H	121	LEU	CG-CD1	-5.69	1.33	1.52
1	A	1271	ILE	CA-CB	-5.69	1.47	1.54
1	A	1381	LEU	CG-CD2	-5.69	1.33	1.52
2	B	411	PRO	CB-CG	-5.69	1.21	1.49
2	B	992	ILE	N-CA	-5.69	1.40	1.46
3	C	61	GLU	CA-CB	5.69	1.62	1.53
2	B	934	LYS	C-N	5.69	1.41	1.33
3	C	83	SER	CA-CB	-5.69	1.43	1.53
8	J	9	SER	C-O	-5.69	1.16	1.24
1	A	777	PHE	C-N	-5.68	1.26	1.33
2	B	103	ASN	C-N	5.68	1.41	1.33
2	B	295	GLY	C-O	5.68	1.30	1.23
2	B	562	GLY	C-O	-5.68	1.18	1.24
6	H	37	LYS	C-O	5.68	1.30	1.23
1	A	93	VAL	CA-CB	-5.68	1.47	1.54
1	A	218	ASP	CA-C	5.68	1.60	1.52
7	I	34	TYR	CD1-CE1	-5.68	1.21	1.38
1	A	1060	PRO	N-CD	-5.68	1.39	1.47
2	B	321	GLY	CA-C	5.68	1.59	1.51
2	B	892	LYS	N-CA	5.68	1.53	1.45
3	C	189	THR	C-O	5.68	1.30	1.23
9	K	48	ALA	C-N	5.68	1.41	1.33
1	A	1336	MET	CA-CB	-5.68	1.43	1.53
2	B	482	VAL	N-CA	5.68	1.53	1.46
4	E	87	SER	CA-C	-5.68	1.46	1.52
5	F	131	PRO	CA-C	-5.68	1.48	1.53
6	H	20	TYR	CZ-OH	-5.68	1.26	1.38
1	A	1270	ASN	N-CA	-5.68	1.40	1.46
9	K	16	GLU	C-O	-5.68	1.17	1.23
1	A	104	GLU	CD-OE2	5.67	1.36	1.25
1	A	226	GLU	CA-CB	5.67	1.63	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1357	ALA	CA-CB	-5.67	1.43	1.53
2	B	121	ASN	CA-C	-5.67	1.45	1.53
2	B	314	LEU	CA-CB	-5.67	1.43	1.53
4	E	16	PHE	CG-CD2	-5.67	1.26	1.38
4	E	62	ALA	N-CA	-5.67	1.39	1.46
1	A	1133	LEU	N-CA	-5.67	1.39	1.46
2	B	109	THR	C-O	-5.67	1.16	1.24
2	B	1137	CYS	C-N	-5.67	1.26	1.34
3	C	194	GLU	CD-OE1	5.67	1.36	1.25
1	A	71	GLN	C-O	-5.67	1.16	1.24
1	A	545	GLN	C-N	-5.67	1.26	1.33
1	A	1101	LEU	CA-CB	-5.67	1.43	1.53
1	A	1153	TYR	C-N	5.67	1.41	1.33
2	B	281	PRO	N-CD	-5.67	1.39	1.47
2	B	381	MET	C-N	-5.67	1.27	1.33
3	C	80	LEU	CA-CB	-5.67	1.44	1.53
2	B	1017	ILE	N-CA	-5.67	1.39	1.46
2	B	1073	TYR	CE1-CZ	-5.67	1.24	1.38
3	C	18	VAL	N-CA	-5.67	1.39	1.46
3	C	60	ASP	N-CA	-5.67	1.39	1.46
1	A	182	VAL	C-O	-5.67	1.18	1.24
2	B	580	VAL	N-CA	5.67	1.53	1.46
4	E	46	TYR	CA-CB	-5.67	1.41	1.53
1	A	72	GLU	CD-OE1	5.67	1.36	1.25
1	A	883	LEU	CA-C	5.67	1.59	1.52
2	B	261	ARG	CA-CB	5.67	1.62	1.53
9	K	75	ILE	CG1-CD1	-5.67	1.29	1.51
1	A	478	TYR	CG-CD2	-5.67	1.27	1.39
1	A	656	TRP	NE1-CE2	-5.67	1.31	1.37
8	J	10	CYS	C-O	-5.67	1.16	1.24
10	L	40	LEU	C-O	5.67	1.29	1.24
1	A	726	ARG	CA-CB	-5.66	1.44	1.53
2	B	743	ILE	CA-CB	-5.66	1.47	1.54
2	B	1086	PHE	CE1-CZ	-5.66	1.21	1.38
4	E	61	GLN	C-O	-5.66	1.16	1.23
5	F	124	GLU	CD-OE1	-5.66	1.14	1.25
1	A	1298	TYR	CG-CD1	-5.66	1.27	1.39
2	B	400	HIS	CG-ND1	-5.66	1.32	1.38
4	E	32	GLN	C-N	-5.66	1.25	1.33
2	B	608	ASP	CA-C	-5.66	1.45	1.52
2	B	1082	MET	C-O	-5.66	1.17	1.24
8	J	5	VAL	CA-CB	5.66	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	5	ASP	CB-CG	5.66	1.66	1.52
9	K	63	VAL	CB-CG1	-5.66	1.33	1.52
2	B	833	TYR	CG-CD1	-5.66	1.27	1.39
8	J	57	ILE	CB-CG1	-5.66	1.42	1.53
1	A	264	PHE	C-O	-5.66	1.17	1.24
2	B	1207	LEU	C-O	5.66	1.31	1.24
5	F	127	GLU	C-N	-5.66	1.25	1.33
7	I	105	SER	CA-C	5.66	1.60	1.52
1	A	227	VAL	N-CA	-5.66	1.39	1.45
2	B	317	CYS	C-O	5.66	1.30	1.24
4	E	135	PHE	CE2-CZ	-5.66	1.21	1.38
2	B	1087	PHE	CE1-CZ	-5.65	1.21	1.38
1	A	867	ILE	CB-CG1	-5.65	1.42	1.53
1	A	883	LEU	C-O	5.65	1.30	1.24
2	B	251	ILE	CG1-CD1	5.65	1.73	1.51
2	B	942	ARG	C-O	5.65	1.30	1.23
2	B	999	MET	C-N	-5.65	1.26	1.33
3	C	129	ILE	CB-CG2	5.65	1.71	1.52
3	C	232	VAL	C-O	-5.65	1.17	1.24
7	I	82	GLU	C-O	5.65	1.30	1.24
7	I	115	LYS	N-CA	-5.65	1.38	1.46
2	B	387	LEU	CG-CD1	-5.65	1.33	1.52
7	I	106	CYS	CA-CB	-5.65	1.46	1.54
1	A	7	SER	N-CA	5.65	1.52	1.46
2	B	278	GLN	C-O	5.65	1.31	1.24
2	B	333	PHE	CE1-CZ	-5.65	1.21	1.38
2	B	601	ARG	CA-C	-5.65	1.45	1.52
4	E	58	MET	CG-SD	5.65	1.94	1.80
1	A	417	TYR	N-CA	5.65	1.53	1.46
1	A	938	LYS	CE-NZ	5.65	1.66	1.49
2	B	340	ALA	CA-CB	-5.64	1.44	1.53
2	B	842	ASN	C-N	5.64	1.41	1.33
1	A	27	VAL	CB-CG1	5.64	1.71	1.52
1	A	155	GLU	N-CA	-5.64	1.39	1.46
1	A	1438	THR	C-O	-5.64	1.16	1.24
2	B	252	SER	C-O	-5.64	1.17	1.23
2	B	388	CYS	C-N	-5.64	1.26	1.34
2	B	1172	ILE	CA-CB	-5.64	1.47	1.53
4	E	40	GLU	CA-CB	5.64	1.62	1.53
1	A	655	PHE	CA-C	-5.64	1.44	1.52
2	B	630	ALA	CA-CB	-5.64	1.45	1.53
6	H	112	ILE	CB-CG1	-5.64	1.42	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1289	ARG	N-CA	5.64	1.53	1.46
2	B	666	TYR	CD1-CE1	5.64	1.55	1.38
3	C	170	TRP	CZ2-CH2	-5.64	1.26	1.37
2	B	57	TYR	CE2-CZ	-5.64	1.24	1.38
2	B	685	LEU	C-O	-5.64	1.16	1.24
2	B	1149	GLU	N-CA	-5.64	1.39	1.46
2	B	296	GLU	CD-OE1	5.64	1.36	1.25
2	B	1219	ASP	C-O	5.64	1.30	1.24
3	C	201	TRP	C-N	-5.64	1.26	1.33
4	E	73	PRO	CB-CG	5.64	1.77	1.49
4	E	196	VAL	CB-CG1	-5.64	1.33	1.52
1	A	382	PRO	CA-CB	-5.63	1.43	1.53
1	A	724	GLU	CG-CD	5.63	1.66	1.52
7	I	80	SER	C-O	-5.63	1.17	1.23
1	A	652	VAL	CB-CG2	-5.63	1.33	1.52
1	A	911	SER	CA-C	-5.63	1.44	1.52
1	A	1351	GLU	C-O	-5.63	1.17	1.24
3	C	222	LYS	N-CA	-5.63	1.38	1.46
3	C	245	VAL	C-O	-5.63	1.17	1.24
1	A	122	MET	C-O	5.63	1.31	1.24
1	A	489	LEU	CA-C	5.63	1.59	1.52
2	B	655	LYS	CG-CD	5.63	1.69	1.52
2	B	1155	SER	C-O	5.63	1.31	1.24
8	J	32	GLU	N-CA	5.63	1.53	1.46
1	A	589	GLN	N-CA	-5.63	1.38	1.45
1	A	531	ILE	CA-C	5.63	1.60	1.52
1	A	641	VAL	CA-C	-5.63	1.45	1.52
1	A	995	GLU	C-N	-5.63	1.26	1.33
1	A	1321	GLY	N-CA	5.63	1.52	1.45
2	B	408	LEU	N-CA	-5.63	1.38	1.45
2	B	848	ARG	C-N	-5.63	1.25	1.33
4	E	64	PRO	CA-C	-5.63	1.44	1.52
9	K	79	GLU	CB-CG	5.63	1.69	1.52
9	K	97	LYS	N-CA	-5.63	1.38	1.46
1	A	1131	ALA	CA-C	-5.63	1.45	1.52
2	B	282	ILE	N-CA	-5.63	1.39	1.46
10	L	36	SER	CA-C	-5.62	1.46	1.52
1	A	44	THR	C-O	5.62	1.31	1.24
3	C	9	LYS	CE-NZ	5.62	1.66	1.49
6	H	144	ILE	C-O	5.62	1.29	1.24
1	A	19	PHE	CA-C	-5.62	1.45	1.52
2	B	32	ALA	C-N	-5.62	1.26	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	67	SER	N-CA	5.62	1.53	1.46
6	H	58	THR	N-CA	5.62	1.53	1.46
9	K	104	ASN	C-O	5.62	1.31	1.24
1	A	621	THR	CA-CB	-5.62	1.44	1.53
1	A	1436	ILE	N-CA	5.62	1.52	1.46
6	H	8	ASP	N-CA	5.62	1.53	1.46
1	A	453	MET	CG-SD	-5.62	1.66	1.80
1	A	1372	VAL	C-O	5.62	1.30	1.24
2	B	259	TYR	CA-C	-5.62	1.45	1.52
5	F	111	LEU	C-O	5.62	1.29	1.23
2	B	976	ILE	CA-CB	-5.62	1.46	1.54
3	C	72	LEU	CA-C	5.62	1.59	1.52
9	K	33	ILE	CB-CG2	-5.62	1.34	1.52
1	A	35	ILE	C-N	5.61	1.41	1.33
2	B	123	THR	N-CA	5.61	1.53	1.46
2	B	230	ALA	C-N	5.61	1.40	1.34
1	A	593	GLU	CA-CB	5.61	1.63	1.53
1	A	756	ILE	CG1-CD1	5.61	1.73	1.51
2	B	264	SER	CB-OG	5.61	1.53	1.42
1	A	100	LYS	CB-CG	-5.61	1.35	1.52
1	A	508	PRO	CG-CD	5.61	1.69	1.50
1	A	539	THR	CB-CG2	-5.61	1.34	1.52
1	A	634	THR	CA-CB	5.61	1.62	1.53
1	A	1033	GLN	C-O	-5.61	1.16	1.24
2	B	202	TYR	CG-CD1	-5.61	1.27	1.39
7	I	98	VAL	CB-CG2	-5.61	1.34	1.52
9	K	83	PRO	CA-C	-5.61	1.44	1.52
1	A	1079	MET	N-CA	-5.61	1.39	1.46
2	B	1029	CYS	CA-CB	-5.61	1.44	1.53
2	B	1061	GLU	CB-CG	5.61	1.69	1.52
4	E	192	ARG	CZ-NH2	5.61	1.40	1.33
1	A	608	ILE	CA-C	-5.61	1.45	1.52
1	A	932	GLU	CD-OE1	5.61	1.36	1.25
1	A	971	PHE	CB-CG	-5.61	1.37	1.50
1	A	1221	LYS	CD-CE	5.61	1.69	1.52
1	A	955	PRO	CA-C	-5.60	1.46	1.52
2	B	573	GLN	CB-CG	5.60	1.69	1.52
2	B	759	PRO	C-N	-5.60	1.25	1.33
1	A	799	PHE	C-O	-5.60	1.17	1.24
2	B	1139	ILE	CG1-CD1	5.60	1.73	1.51
1	A	173	THR	CA-CB	5.60	1.61	1.53
3	C	7	GLN	CA-CB	5.60	1.63	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	4	PHE	CE2-CZ	5.60	1.55	1.38
1	A	202	LEU	CA-CB	-5.60	1.45	1.53
1	A	226	GLU	CB-CG	5.60	1.69	1.52
1	A	506	ALA	CA-CB	-5.60	1.44	1.53
2	B	452	THR	N-CA	5.60	1.53	1.46
2	B	787	VAL	CA-C	-5.60	1.43	1.52
1	A	370	ILE	CB-CG2	-5.60	1.34	1.52
1	A	562	THR	CA-CB	5.60	1.61	1.53
1	A	775	ILE	C-N	-5.60	1.24	1.33
1	A	1361	SER	N-CA	5.60	1.52	1.45
2	B	37	PHE	N-CA	-5.60	1.39	1.46
3	C	196	ASP	CA-C	5.60	1.59	1.52
2	B	273	LEU	C-O	5.60	1.31	1.23
2	B	526	GLU	CA-CB	5.60	1.59	1.52
3	C	84	ARG	NE-CZ	5.60	1.39	1.33
4	E	168	TYR	C-N	-5.60	1.26	1.33
1	A	61	ILE	C-N	5.59	1.41	1.33
1	A	430	TRP	CZ3-CH2	-5.59	1.26	1.40
1	A	784	LEU	CG-CD2	-5.59	1.34	1.52
2	B	649	LYS	N-CA	5.59	1.53	1.45
5	F	118	LEU	C-O	-5.59	1.17	1.24
3	C	64	ALA	C-O	-5.59	1.17	1.24
1	A	373	THR	CA-CB	-5.59	1.44	1.53
1	A	527	THR	CA-CB	-5.59	1.43	1.53
2	B	1073	TYR	N-CA	5.59	1.53	1.46
4	E	198	ILE	C-O	-5.59	1.18	1.24
7	I	82	GLU	CB-CG	5.59	1.69	1.52
9	K	42	LEU	N-CA	-5.59	1.39	1.46
1	A	218	ASP	CG-OD1	5.59	1.35	1.25
2	B	97	VAL	CB-CG1	-5.59	1.34	1.52
2	B	224	GLN	CD-OE1	5.59	1.34	1.23
2	B	381	MET	CA-CB	-5.59	1.44	1.53
2	B	780	VAL	C-N	-5.59	1.26	1.33
2	B	1026	LEU	CG-CD2	-5.59	1.34	1.52
2	B	1203	LEU	CG-CD1	-5.59	1.34	1.52
3	C	121	VAL	CB-CG2	-5.59	1.34	1.52
3	C	230	MET	CA-CB	-5.59	1.45	1.53
6	H	4	THR	CA-C	5.59	1.60	1.52
10	L	37	LYS	CD-CE	5.59	1.69	1.52
1	A	38	PRO	N-CD	-5.59	1.40	1.47
1	A	1367	HIS	CA-CB	5.59	1.63	1.54
5	F	97	ARG	CD-NE	5.59	1.54	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	599	SER	CB-OG	-5.59	1.30	1.42
2	B	236	HIS	CG-ND1	-5.59	1.32	1.38
2	B	813	LYS	C-O	-5.59	1.15	1.24
1	A	55	ASP	CG-OD1	5.58	1.35	1.25
1	A	171	GLN	CA-C	5.58	1.59	1.52
1	A	758	ILE	CB-CG2	-5.58	1.34	1.52
2	B	328	GLU	CA-C	-5.58	1.45	1.52
1	A	153	PRO	CA-C	5.58	1.60	1.52
1	A	687	LYS	C-O	5.58	1.31	1.24
1	A	1382	THR	CA-CB	5.58	1.61	1.53
1	A	1441	PHE	CB-CG	-5.58	1.37	1.50
2	B	517	THR	CA-C	-5.58	1.43	1.52
3	C	11	ARG	N-CA	-5.58	1.37	1.45
3	C	97	VAL	N-CA	-5.58	1.39	1.46
4	E	153	HIS	N-CA	-5.58	1.39	1.46
7	I	118	ARG	C-N	5.58	1.40	1.33
8	J	44	TYR	CZ-OH	5.58	1.49	1.38
1	A	106	VAL	N-CA	-5.58	1.38	1.46
2	B	696	GLU	CA-C	-5.58	1.45	1.52
2	B	841	MET	C-O	5.58	1.31	1.23
2	B	933	SER	CA-CB	5.58	1.64	1.53
3	C	190	ASP	CB-CG	-5.58	1.38	1.52
7	I	78	CYS	CB-SG	5.58	1.99	1.81
1	A	574	GLY	C-O	-5.58	1.17	1.23
1	A	877	HIS	CG-CD2	-5.58	1.29	1.35
1	A	1441	PHE	CG-CD1	-5.58	1.27	1.38
9	K	114	LEU	CA-C	5.58	1.64	1.52
1	A	591	PHE	CA-CB	5.58	1.61	1.53
2	B	990	ILE	CG1-CD1	-5.58	1.29	1.51
3	C	227	THR	C-N	-5.58	1.25	1.33
2	B	883	LEU	CA-C	5.58	1.60	1.53
6	H	143	LEU	CG-CD2	-5.58	1.34	1.52
1	A	831	THR	C-O	5.58	1.30	1.24
1	A	887	GLY	N-CA	5.58	1.50	1.44
2	B	738	PHE	CA-C	5.58	1.60	1.52
2	B	1079	LYS	C-N	-5.58	1.25	1.33
3	C	241	ASP	CA-C	-5.58	1.45	1.52
10	L	58	LYS	CG-CD	5.58	1.69	1.52
1	A	480	ALA	CA-C	5.57	1.59	1.52
1	A	550	LEU	N-CA	-5.57	1.39	1.46
1	A	971	PHE	C-N	-5.57	1.26	1.33
2	B	239	GLU	N-CA	-5.57	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	297	ILE	CG1-CD1	-5.57	1.30	1.51
2	B	1178	ASN	N-CA	5.57	1.52	1.46
4	E	108	GLY	CA-C	-5.57	1.44	1.51
10	L	55	ILE	CA-C	5.57	1.60	1.52
1	A	700	ASN	CB-CG	-5.57	1.38	1.52
1	A	1171	GLN	CD-OE1	5.57	1.34	1.23
3	C	31	ASN	CG-OD1	5.57	1.34	1.23
7	I	117	LYS	CA-C	5.57	1.60	1.52
1	A	1323	ASP	CA-CB	-5.57	1.44	1.53
2	B	60	GLN	CA-CB	-5.57	1.43	1.53
7	I	114	GLN	C-O	-5.57	1.16	1.24
8	J	24	LEU	CB-CG	-5.57	1.42	1.53
1	A	787	PHE	CD2-CE2	-5.57	1.22	1.38
2	B	396	ASP	CA-CB	-5.57	1.44	1.53
2	B	554	ILE	N-CA	5.57	1.53	1.46
7	I	84	VAL	C-O	5.57	1.30	1.24
1	A	607	ILE	CA-C	-5.57	1.45	1.52
1	A	1333	ILE	CB-CG2	-5.57	1.34	1.52
2	B	345	LYS	CB-CG	-5.57	1.35	1.52
2	B	561	TRP	CB-CG	-5.57	1.32	1.50
2	B	1018	PRO	N-CD	-5.57	1.40	1.47
8	J	18	TRP	C-O	-5.57	1.17	1.24
1	A	438	ASP	CG-OD1	-5.56	1.14	1.25
1	A	1266	THR	CA-C	5.56	1.60	1.52
10	L	38	LEU	CG-CD2	5.56	1.71	1.52
1	A	504	LEU	CA-CB	-5.56	1.44	1.54
2	B	250	PHE	CA-CB	5.56	1.61	1.53
2	B	661	LEU	N-CA	-5.56	1.39	1.46
2	B	969	ARG	CB-CG	-5.56	1.35	1.52
3	C	153	LEU	C-O	5.56	1.30	1.23
1	A	717	ASN	CB-CG	-5.56	1.38	1.52
2	B	664	THR	CB-CG2	-5.56	1.34	1.52
7	I	98	VAL	CA-C	5.56	1.59	1.53
1	A	1006	ILE	C-N	-5.56	1.27	1.34
2	B	432	MET	SD-CE	5.56	1.93	1.79
2	B	752	ALA	C-N	-5.56	1.25	1.33
4	E	162	ARG	CZ-NH2	5.56	1.40	1.33
7	I	70	ARG	CA-CB	-5.56	1.41	1.53
1	A	75	ASN	CB-CG	5.56	1.66	1.52
2	B	1067	ARG	CD-NE	5.56	1.54	1.46
8	J	54	VAL	CB-CG2	-5.56	1.34	1.52
2	B	368	GLU	CG-CD	5.55	1.66	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	587	HIS	C-O	-5.55	1.16	1.24
2	B	1050	ILE	CA-CB	-5.55	1.47	1.54
3	C	151	GLN	CA-C	-5.55	1.46	1.52
1	A	598	LEU	C-O	-5.55	1.16	1.24
1	A	1035	TYR	CA-CB	5.55	1.62	1.53
1	A	1373	ASP	CG-OD2	5.55	1.35	1.25
7	I	83	ASN	CA-CB	-5.55	1.43	1.53
1	A	694	THR	C-N	-5.55	1.26	1.33
1	A	886	ILE	CA-CB	5.55	1.62	1.54
5	F	78	GLN	C-O	-5.55	1.17	1.24
6	H	90	ALA	CA-C	5.55	1.60	1.52
1	A	225	ASN	CA-C	5.55	1.59	1.52
2	B	911	ILE	C-N	-5.55	1.26	1.33
7	I	47	GLU	CG-CD	5.55	1.66	1.52
2	B	1001	PHE	N-CA	-5.55	1.38	1.45
4	E	188	LEU	C-O	5.55	1.32	1.24
1	A	546	VAL	CB-CG2	-5.55	1.34	1.52
2	B	939	THR	CA-C	-5.55	1.45	1.52
3	C	127	ARG	CA-CB	-5.55	1.45	1.53
4	E	117	THR	CB-OG1	5.55	1.52	1.43
6	H	79	TRP	CB-CG	-5.55	1.33	1.50
1	A	11	LEU	C-N	-5.54	1.26	1.33
1	A	1022	LEU	C-N	-5.54	1.26	1.34
1	A	1448	GLU	CA-CB	5.54	1.62	1.53
2	B	392	ARG	CA-C	-5.54	1.45	1.52
2	B	1015	HIS	ND1-CE1	5.54	1.38	1.32
3	C	183	TRP	CE2-CZ2	-5.54	1.28	1.39
6	H	2	SER	C-N	5.54	1.40	1.33
1	A	90	VAL	CA-CB	-5.54	1.45	1.54
1	A	233	TRP	CD2-CE3	-5.54	1.31	1.40
1	A	424	ILE	CB-CG2	-5.54	1.34	1.52
1	A	632	VAL	C-N	-5.54	1.27	1.34
2	B	33	VAL	C-N	-5.54	1.26	1.33
2	B	488	TYR	CG-CD2	-5.54	1.27	1.39
2	B	904	ARG	C-N	-5.54	1.26	1.33
1	A	1309	ASP	N-CA	-5.54	1.39	1.46
9	K	9	LEU	N-CA	-5.54	1.38	1.46
1	A	134	ARG	CG-CD	5.54	1.69	1.52
1	A	1049	ILE	C-O	-5.54	1.17	1.24
7	I	44	TYR	CG-CD1	-5.54	1.27	1.39
7	I	116	ASN	CG-ND2	5.54	1.44	1.33
1	A	713	SER	CA-CB	-5.54	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	861	GLY	C-N	-5.54	1.26	1.33
1	A	1334	ASP	N-CA	-5.54	1.39	1.46
3	C	93	ASP	CA-CB	5.54	1.63	1.53
4	E	105	PHE	CB-CG	-5.54	1.38	1.50
2	B	302	CYS	CA-CB	-5.54	1.44	1.53
2	B	497	ARG	CZ-NH2	5.54	1.40	1.33
3	C	59	ALA	CA-CB	-5.54	1.44	1.53
1	A	990	VAL	C-O	-5.53	1.17	1.24
1	A	1368	MET	CG-SD	5.53	1.94	1.80
2	B	452	THR	CA-CB	5.53	1.62	1.53
2	B	769	TYR	CE2-CZ	-5.53	1.25	1.38
4	E	84	ASP	CG-OD2	5.53	1.35	1.25
1	A	1372	VAL	N-CA	-5.53	1.39	1.46
2	B	1026	LEU	CA-CB	-5.53	1.44	1.53
1	A	583	PRO	N-CD	-5.53	1.40	1.47
1	A	742	ASN	C-O	-5.53	1.17	1.24
1	A	954	TRP	CD2-CE2	-5.53	1.31	1.41
2	B	323	VAL	CA-C	-5.53	1.46	1.52
2	B	685	LEU	CG-CD2	-5.53	1.34	1.52
1	A	1187	GLN	C-N	5.53	1.41	1.33
1	A	1054	LEU	CB-CG	-5.53	1.42	1.53
2	B	51	PHE	CD1-CE1	-5.53	1.22	1.38
2	B	547	VAL	N-CA	5.53	1.53	1.46
2	B	569	TYR	C-N	-5.53	1.27	1.33
2	B	683	SER	C-N	-5.53	1.26	1.34
2	B	963	PHE	N-CA	5.53	1.52	1.46
2	B	1175	LEU	C-O	5.53	1.30	1.23
4	E	68	SER	CA-CB	-5.53	1.44	1.53
4	E	197	LYS	CA-C	-5.52	1.46	1.52
3	C	50	GLU	CB-CG	5.52	1.69	1.52
4	E	69	ILE	C-N	-5.52	1.26	1.33
4	E	79	TRP	CD2-CE3	5.52	1.49	1.40
9	K	67	PHE	CA-C	-5.52	1.45	1.52
2	B	206	ASN	CA-C	-5.52	1.46	1.53
2	B	573	GLN	C-O	-5.52	1.16	1.24
1	A	1316	VAL	CB-CG2	-5.52	1.34	1.52
2	B	376	PHE	CE2-CZ	-5.52	1.22	1.38
6	H	140	ALA	C-N	5.52	1.41	1.33
2	B	355	ILE	CA-C	-5.52	1.45	1.52
1	A	1110	ASN	CA-CB	5.52	1.61	1.52
1	A	544	ASP	C-O	-5.51	1.17	1.24
1	A	614	PHE	CG-CD1	-5.51	1.27	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1224	PHE	CG-CD1	5.51	1.50	1.38
4	E	64	PRO	N-CA	-5.51	1.40	1.47
9	K	65	HIS	C-O	-5.51	1.18	1.24
2	B	374	LYS	CA-C	-5.51	1.45	1.52
3	C	163	ILE	C-N	5.51	1.41	1.33
4	E	154	ILE	CA-C	5.51	1.59	1.52
4	E	182	ASP	CA-CB	-5.51	1.45	1.53
2	B	413	LEU	CA-CB	-5.51	1.45	1.53
9	K	55	LYS	CB-CG	5.51	1.69	1.52
2	B	564	GLU	C-N	-5.51	1.26	1.33
7	I	72	ASP	N-CA	5.51	1.52	1.46
10	L	44	ASP	C-N	5.51	1.41	1.33
2	B	185	THR	CB-CG2	5.51	1.70	1.52
2	B	554	ILE	CG1-CD1	-5.51	1.30	1.51
2	B	1088	GLY	C-N	-5.51	1.26	1.33
8	J	63	TYR	CE2-CZ	-5.51	1.25	1.38
1	A	560	ILE	CA-C	-5.51	1.47	1.52
1	A	1058	VAL	CB-CG2	-5.51	1.34	1.52
2	B	1132	GLU	CA-C	-5.51	1.45	1.52
3	C	245	VAL	CA-C	-5.51	1.45	1.52
6	H	6	PHE	CB-CG	-5.51	1.38	1.50
6	H	109	LYS	CG-CD	5.51	1.69	1.52
9	K	36	GLU	N-CA	5.51	1.52	1.45
9	K	37	LYS	CA-CB	-5.51	1.44	1.53
1	A	415	LEU	CA-C	-5.50	1.45	1.52
1	A	488	ASN	CG-ND2	-5.50	1.21	1.33
2	B	212	LEU	CA-C	-5.50	1.46	1.52
9	K	75	ILE	CA-C	-5.50	1.46	1.52
1	A	133	LYS	CD-CE	5.50	1.69	1.52
1	A	660	ASN	CG-ND2	-5.50	1.21	1.33
1	A	1007	ILE	C-N	-5.50	1.26	1.33
1	A	1342	GLU	CA-CB	5.50	1.62	1.53
2	B	678	GLU	N-CA	5.50	1.56	1.46
9	K	55	LYS	CE-NZ	5.50	1.65	1.49
1	A	1081	LEU	CB-CG	5.50	1.64	1.53
1	A	1338	VAL	CB-CG2	-5.50	1.34	1.52
2	B	138	GLU	CA-CB	5.50	1.64	1.53
2	B	347	LYS	N-CA	-5.50	1.39	1.46
2	B	1186	ASP	CG-OD2	5.50	1.35	1.25
7	I	79	HIS	N-CA	5.50	1.53	1.46
9	K	89	ASN	CA-CB	-5.50	1.44	1.53
1	A	550	LEU	CB-CG	-5.50	1.42	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	653	VAL	C-O	-5.50	1.17	1.24
1	A	1119	TYR	CG-CD2	-5.50	1.27	1.39
2	B	104	GLU	N-CA	5.50	1.53	1.45
1	A	756	ILE	CA-CB	5.50	1.62	1.54
1	A	1162	VAL	CB-CG2	5.50	1.70	1.52
2	B	327	ARG	CB-CG	-5.50	1.35	1.52
2	B	994	TYR	CE1-CZ	-5.50	1.25	1.38
9	K	70	ARG	CA-C	-5.50	1.45	1.52
2	B	322	PHE	CE1-CZ	-5.50	1.22	1.38
2	B	666	TYR	CZ-OH	5.50	1.49	1.38
2	B	736	THR	CA-C	-5.50	1.44	1.52
2	B	912	ILE	N-CA	-5.50	1.39	1.46
1	A	1352	VAL	CA-C	-5.50	1.44	1.52
2	B	893	LEU	CG-CD2	-5.50	1.34	1.52
3	C	134	ILE	CA-C	-5.50	1.45	1.52
1	A	614	PHE	CE2-CZ	-5.49	1.22	1.38
1	A	711	ARG	CZ-NH2	-5.49	1.26	1.33
1	A	1211	GLN	C-N	-5.49	1.27	1.33
2	B	781	PHE	C-O	5.49	1.31	1.24
6	H	132	LEU	C-O	5.49	1.30	1.24
1	A	517	ASN	CA-CB	-5.49	1.43	1.53
2	B	358	LYS	CD-CE	5.49	1.69	1.52
1	A	230	ARG	CA-C	5.49	1.59	1.52
1	A	551	TYR	CA-C	-5.49	1.45	1.52
1	A	760	GLN	CD-NE2	-5.49	1.21	1.33
4	E	212	ARG	CZ-NH1	-5.49	1.25	1.32
1	A	510	GLN	C-O	5.49	1.31	1.24
1	A	685	GLU	CG-CD	5.49	1.65	1.52
2	B	137	TYR	CE1-CZ	5.49	1.51	1.38
2	B	837	ASP	CG-OD2	5.49	1.35	1.25
1	A	566	ILE	CA-C	-5.49	1.47	1.52
1	A	164	ARG	CB-CG	-5.49	1.35	1.52
1	A	364	VAL	CB-CG2	-5.49	1.34	1.52
1	A	1176	LEU	CA-CB	5.49	1.64	1.53
2	B	1100	ASP	CG-OD2	5.49	1.35	1.25
3	C	95	CYS	CA-C	5.49	1.59	1.52
1	A	43	GLU	C-N	5.48	1.41	1.33
1	A	733	ALA	CA-C	5.48	1.59	1.52
1	A	1228	TRP	CZ3-CH2	-5.48	1.26	1.40
2	B	275	TYR	CG-CD1	-5.48	1.27	1.39
3	C	72	LEU	CB-CG	-5.48	1.42	1.53
4	E	102	GLU	CD-OE1	5.48	1.35	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	298	LEU	CG-CD2	-5.48	1.34	1.52
2	B	776	GLN	CD-OE1	5.48	1.33	1.23
2	B	946	ASN	C-N	5.48	1.38	1.32
4	E	199	ILE	C-N	-5.48	1.25	1.33
4	E	202	SER	CA-CB	-5.48	1.44	1.53
2	B	228	LYS	C-N	5.48	1.41	1.33
2	B	1209	ALA	C-N	-5.48	1.26	1.33
7	I	19	ASP	CG-OD1	5.48	1.35	1.25
7	I	32	CYS	N-CA	5.48	1.53	1.45
1	A	572	TRP	CB-CG	-5.48	1.33	1.50
2	B	983	ARG	CA-CB	5.48	1.60	1.53
2	B	986	GLN	CA-CB	5.48	1.61	1.53
2	B	1108	ARG	CD-NE	5.48	1.53	1.46
4	E	46	TYR	CD1-CE1	5.48	1.55	1.38
6	H	47	PHE	CG-CD2	-5.48	1.27	1.38
9	K	37	LYS	CA-C	-5.48	1.45	1.53
1	A	1426	GLU	C-O	5.48	1.30	1.24
1	A	1235	LYS	N-CA	-5.47	1.39	1.46
2	B	391	ASP	CB-CG	5.47	1.65	1.52
2	B	447	ALA	C-N	5.47	1.41	1.33
1	A	1176	LEU	CB-CG	5.47	1.64	1.53
2	B	621	GLU	CD-OE2	5.47	1.35	1.25
2	B	698	GLU	CD-OE1	5.47	1.35	1.25
9	K	53	ASP	CA-C	5.47	1.60	1.52
1	A	1079	MET	CG-SD	5.47	1.94	1.80
1	A	1303	GLU	N-CA	-5.47	1.39	1.46
2	B	1006	ILE	CB-CG2	-5.47	1.34	1.52
1	A	891	ALA	CA-C	-5.47	1.45	1.52
2	B	616	ILE	CG1-CD1	5.47	1.73	1.51
3	C	202	PRO	N-CA	-5.47	1.40	1.47
2	B	961	LEU	C-N	5.47	1.41	1.33
3	C	183	TRP	CD2-CE3	-5.47	1.31	1.40
6	H	143	LEU	C-O	5.47	1.30	1.23
8	J	6	ARG	CZ-NH1	-5.47	1.25	1.32
9	K	79	GLU	CD-OE2	5.47	1.35	1.25
10	L	47	ARG	CB-CG	5.47	1.68	1.52
1	A	248	PRO	CA-C	5.46	1.64	1.52
1	A	1022	LEU	N-CA	5.46	1.52	1.46
6	H	46	LEU	CA-CB	-5.46	1.44	1.53
9	K	50	LEU	CB-CG	-5.46	1.42	1.53
1	A	757	ASN	CA-C	-5.46	1.46	1.52
1	A	1157	ASP	CA-CB	5.46	1.60	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	44	TYR	CE1-CZ	-5.46	1.25	1.38
1	A	357	PRO	C-N	-5.46	1.26	1.33
1	A	660	ASN	CB-CG	-5.46	1.38	1.52
8	J	26	GLN	C-O	5.46	1.31	1.24
9	K	54	ARG	C-O	-5.46	1.17	1.24
1	A	587	HIS	CG-ND1	5.46	1.44	1.38
2	B	648	HIS	CA-C	-5.46	1.45	1.53
2	B	877	PRO	CA-C	5.46	1.59	1.52
2	B	886	LYS	CD-CE	5.46	1.68	1.52
2	B	1217	TYR	CG-CD1	-5.46	1.27	1.39
2	B	224	GLN	N-CA	-5.46	1.39	1.46
5	F	146	TRP	CD2-CE3	-5.46	1.31	1.40
8	J	55	ASP	CB-CG	-5.46	1.38	1.52
1	A	951	GLU	CA-C	-5.45	1.45	1.52
1	A	976	THR	CA-C	-5.45	1.45	1.52
2	B	936	ASP	CB-CG	5.45	1.65	1.52
3	C	111	THR	CB-CG2	5.45	1.70	1.52
7	I	43	VAL	CB-CG1	-5.45	1.34	1.52
10	L	32	ALA	CA-C	5.45	1.60	1.52
1	A	159	THR	C-O	-5.45	1.17	1.24
1	A	424	ILE	C-N	-5.45	1.25	1.33
1	A	567	LYS	CB-CG	-5.45	1.36	1.52
1	A	1356	ILE	CB-CG1	-5.45	1.42	1.53
2	B	681	TRP	NE1-CE2	-5.45	1.31	1.37
2	B	877	PRO	C-O	5.45	1.30	1.23
4	E	79	TRP	CZ2-CH2	5.45	1.47	1.37
7	I	5	ARG	NE-CZ	-5.45	1.27	1.33
1	A	399	HIS	C-O	5.45	1.31	1.24
1	A	821	ARG	NE-CZ	-5.45	1.27	1.33
3	C	131	HIS	CA-C	-5.45	1.46	1.53
1	A	107	CYS	N-CA	5.45	1.52	1.46
2	B	455	SER	CB-OG	5.45	1.53	1.42
10	L	67	PHE	CE2-CZ	-5.45	1.22	1.38
1	A	295	LEU	C-N	5.45	1.40	1.33
1	A	418	SER	CA-CB	-5.45	1.44	1.53
2	B	96	TYR	CE2-CZ	5.45	1.51	1.38
2	B	135	ARG	C-N	5.45	1.41	1.33
2	B	307	ASP	C-N	-5.45	1.26	1.33
2	B	337	ARG	C-O	5.45	1.31	1.24
2	B	993	THR	CB-OG1	-5.45	1.35	1.43
9	K	44	ASN	N-CA	-5.45	1.39	1.46
9	K	103	THR	CA-CB	5.45	1.60	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	811	GLN	CA-CB	5.44	1.61	1.53
1	A	620	LYS	C-N	-5.44	1.26	1.33
1	A	640	GLN	CA-C	-5.44	1.45	1.52
2	B	37	PHE	CE2-CZ	-5.44	1.22	1.38
2	B	1130	PHE	CG-CD2	-5.44	1.27	1.38
4	E	91	LYS	CA-C	5.44	1.59	1.52
6	H	98	TYR	CB-CG	-5.44	1.39	1.51
1	A	96	ILE	C-N	-5.44	1.25	1.33
2	B	596	LEU	C-O	-5.44	1.17	1.24
2	B	1054	GLY	C-O	5.44	1.30	1.23
4	E	29	PHE	CA-CB	5.44	1.59	1.53
7	I	106	CYS	N-CA	-5.44	1.38	1.45
9	K	34	THR	CB-OG1	5.44	1.52	1.43
1	A	905	ASP	C-N	-5.44	1.26	1.33
2	B	800	GLN	N-CA	-5.44	1.38	1.45
1	A	480	ALA	C-N	5.44	1.38	1.33
1	A	1365	TYR	CE1-CZ	5.44	1.51	1.38
2	B	19	GLU	CG-CD	5.44	1.65	1.52
2	B	255	GLN	CA-C	-5.44	1.46	1.52
2	B	605	ARG	C-O	-5.44	1.17	1.24
9	K	12	LEU	C-O	5.44	1.30	1.23
1	A	827	THR	CA-CB	-5.44	1.45	1.53
1	A	878	ILE	C-O	-5.44	1.18	1.24
1	A	961	ARG	CZ-NH1	5.44	1.40	1.32
2	B	550	ASP	CB-CG	5.44	1.65	1.52
6	H	79	TRP	CA-C	-5.43	1.45	1.52
7	I	20	LYS	CE-NZ	5.43	1.65	1.49
1	A	543	LEU	C-N	-5.43	1.26	1.33
1	A	693	VAL	N-CA	-5.43	1.38	1.46
2	B	189	LEU	CA-CB	-5.43	1.44	1.53
3	C	51	VAL	CA-CB	-5.43	1.47	1.54
3	C	209	TYR	C-O	-5.43	1.17	1.24
1	A	286	HIS	CA-CB	5.43	1.62	1.53
1	A	565	ILE	CA-CB	-5.43	1.48	1.54
2	B	1002	THR	N-CA	-5.43	1.39	1.45
4	E	12	LEU	N-CA	5.43	1.53	1.46
7	I	110	PHE	C-O	-5.43	1.17	1.23
9	K	71	PHE	CE1-CZ	-5.43	1.22	1.38
1	A	1132	LYS	CA-CB	5.43	1.61	1.53
2	B	1165	ILE	CG1-CD1	5.43	1.73	1.51
1	A	526	ASP	CG-OD1	5.43	1.35	1.25
2	B	828	ALA	CA-C	5.43	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	118	LEU	CG-CD2	-5.43	1.34	1.52
1	A	698	GLN	CA-CB	-5.42	1.44	1.53
7	I	17	ARG	CZ-NH1	5.42	1.40	1.32
1	A	1188	GLN	CD-NE2	5.42	1.44	1.33
7	I	108	HIS	CA-CB	5.42	1.61	1.53
9	K	89	ASN	CA-C	-5.42	1.45	1.52
1	A	1205	LYS	N-CA	5.42	1.52	1.46
4	E	60	PHE	CG-CD1	5.42	1.50	1.38
1	A	1003	LYS	CB-CG	5.42	1.68	1.52
2	B	1179	GLN	N-CA	5.42	1.52	1.46
1	A	212	LYS	C-N	-5.42	1.26	1.33
1	A	421	ALA	CA-C	-5.42	1.45	1.52
1	A	471	ASN	CB-CG	5.42	1.65	1.52
2	B	1003	ALA	C-O	-5.42	1.17	1.24
2	B	1058	LEU	C-O	5.42	1.30	1.24
3	C	34	ARG	CZ-NH2	5.42	1.40	1.33
3	C	165	LYS	CG-CD	5.42	1.68	1.52
4	E	187	TYR	N-CA	5.42	1.52	1.46
4	E	57	MET	C-O	5.42	1.31	1.24
1	A	448	PRO	CB-CG	-5.42	1.29	1.51
2	B	394	ASP	C-O	-5.42	1.17	1.23
4	E	146	HIS	C-N	-5.42	1.25	1.33
1	A	1128	GLN	N-CA	5.41	1.53	1.46
2	B	1086	PHE	C-O	-5.41	1.17	1.24
7	I	42	LEU	N-CA	-5.41	1.39	1.46
8	J	24	LEU	CG-CD1	-5.41	1.34	1.52
2	B	818	PRO	CG-CD	-5.41	1.32	1.50
3	C	14	SER	C-O	-5.41	1.18	1.24
1	A	1214	GLU	CB-CG	5.41	1.68	1.52
2	B	857	ARG	CD-NE	-5.41	1.38	1.46
2	B	910	VAL	CB-CG1	5.41	1.70	1.52
3	C	26	ASP	N-CA	5.41	1.52	1.45
1	A	81	PHE	N-CA	-5.41	1.39	1.46
2	B	314	LEU	N-CA	-5.41	1.38	1.46
2	B	400	HIS	N-CA	5.41	1.52	1.46
3	C	182	PRO	N-CD	-5.41	1.40	1.47
4	E	136	ASN	CG-OD1	5.41	1.33	1.23
1	A	769	SER	CA-CB	-5.41	1.44	1.53
1	A	1328	TYR	CD2-CE2	-5.41	1.22	1.38
6	H	95	TYR	C-O	-5.41	1.17	1.23
1	A	406	ILE	CB-CG2	5.41	1.70	1.52
1	A	976	THR	C-N	-5.41	1.26	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	91	SER	C-N	5.41	1.41	1.33
2	B	199	MET	CG-SD	5.41	1.94	1.80
4	E	105	PHE	CA-C	5.41	1.59	1.52
1	A	171	GLN	CD-OE1	5.40	1.33	1.23
1	A	261	ASP	CB-CG	5.40	1.65	1.52
1	A	806	ARG	NE-CZ	-5.40	1.27	1.33
2	B	349	ILE	CA-C	5.40	1.59	1.52
1	A	514	PRO	C-O	-5.40	1.16	1.24
2	B	118	ARG	CG-CD	5.40	1.68	1.52
2	B	181	LEU	CA-C	5.40	1.60	1.52
4	E	122	LYS	CB-CG	5.40	1.68	1.52
1	A	411	ASP	CG-OD2	5.40	1.35	1.25
1	A	1021	LEU	C-N	-5.40	1.27	1.33
1	A	1241	ARG	CZ-NH1	5.40	1.40	1.32
2	B	335	GLY	C-N	-5.40	1.26	1.33
2	B	351	TYR	CE2-CZ	-5.40	1.25	1.38
4	E	59	SER	N-CA	-5.40	1.39	1.46
6	H	35	GLN	C-N	5.40	1.41	1.33
1	A	436	ILE	CG1-CD1	-5.40	1.30	1.51
1	A	1349	TYR	CA-CB	-5.40	1.44	1.53
2	B	348	ARG	CZ-NH1	-5.40	1.25	1.32
2	B	366	GLN	C-O	-5.40	1.16	1.24
6	H	135	LEU	CG-CD1	5.40	1.70	1.52
1	A	849	MET	N-CA	-5.40	1.39	1.45
2	B	126	SER	CA-CB	-5.40	1.44	1.54
1	A	186	LYS	CA-CB	5.39	1.62	1.53
1	A	606	LEU	CA-C	-5.39	1.46	1.52
1	A	971	PHE	CA-C	5.39	1.60	1.52
1	A	1187	GLN	CA-C	5.39	1.64	1.52
2	B	250	PHE	CB-CG	5.39	1.63	1.50
1	A	779	PHE	N-CA	-5.39	1.39	1.45
9	K	68	PHE	CE1-CZ	-5.39	1.22	1.38
1	A	951	GLU	CD-OE1	5.39	1.35	1.25
2	B	797	TYR	CE1-CZ	-5.39	1.25	1.38
1	A	394	ASN	N-CA	5.39	1.53	1.46
2	B	773	MET	C-O	-5.39	1.17	1.24
2	B	893	LEU	CA-CB	-5.39	1.44	1.53
4	E	101	GLN	CA-C	5.39	1.59	1.52
7	I	5	ARG	CG-CD	5.39	1.68	1.52
9	K	56	VAL	N-CA	5.39	1.52	1.46
1	A	1052	GLN	C-O	-5.39	1.17	1.24
2	B	166	PHE	CA-CB	-5.39	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	31	THR	C-O	-5.39	1.17	1.23
4	E	105	PHE	N-CA	5.39	1.53	1.46
4	E	137	GLU	C-O	-5.39	1.18	1.24
8	J	48	ARG	CB-CG	-5.39	1.36	1.52
9	K	112	GLN	CA-CB	5.39	1.61	1.53
1	A	917	SER	C-N	-5.39	1.25	1.33
2	B	38	PHE	CD1-CE1	-5.39	1.22	1.38
7	I	42	LEU	C-N	-5.39	1.27	1.34
1	A	687	LYS	N-CA	-5.38	1.39	1.46
1	A	804	TYR	CA-C	-5.38	1.45	1.52
1	A	1223	ASP	N-CA	5.38	1.57	1.46
2	B	252	SER	CA-C	5.38	1.59	1.52
3	C	60	ASP	CB-CG	5.38	1.65	1.52
1	A	404	TYR	CE2-CZ	-5.38	1.25	1.38
2	B	1110	PRO	CA-CB	5.38	1.64	1.53
2	B	1203	LEU	CA-CB	-5.38	1.45	1.53
1	A	455	MET	CB-CG	-5.38	1.36	1.52
1	A	657	LEU	CG-CD1	-5.38	1.34	1.52
1	A	758	ILE	N-CA	5.38	1.52	1.46
1	A	1140	HIS	CB-CG	-5.38	1.42	1.50
2	B	317	CYS	CA-C	-5.38	1.45	1.52
2	B	984	HIS	CA-CB	5.38	1.60	1.53
3	C	148	ARG	CZ-NH1	5.38	1.40	1.32
2	B	682	SER	N-CA	-5.38	1.39	1.46
2	B	758	PHE	CE2-CZ	-5.38	1.22	1.38
2	B	1006	ILE	CG1-CD1	-5.38	1.30	1.51
7	I	115	LYS	CA-C	5.38	1.58	1.53
10	L	29	TYR	CG-CD1	-5.38	1.28	1.39
1	A	877	HIS	CE1-NE2	5.38	1.38	1.32
2	B	973	ILE	CB-CG1	5.38	1.64	1.53
10	L	40	LEU	CG-CD1	5.38	1.70	1.52
4	E	22	MET	C-O	-5.38	1.17	1.24
2	B	267	ARG	CA-CB	-5.37	1.45	1.53
1	A	854	ASN	N-CA	5.37	1.56	1.46
1	A	1093	LYS	CB-CG	5.37	1.68	1.52
1	A	1122	PRO	CA-CB	5.37	1.61	1.53
1	A	1410	PHE	CD1-CE1	-5.37	1.22	1.38
2	B	89	GLU	N-CA	5.37	1.56	1.46
2	B	121	ASN	CA-CB	5.37	1.61	1.53
2	B	487	THR	N-CA	-5.37	1.39	1.45
2	B	655	LYS	CA-CB	-5.37	1.44	1.53
2	B	853	SER	CA-CB	-5.37	1.43	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1323	ASP	N-CA	-5.37	1.38	1.46
2	B	62	ILE	CA-C	5.37	1.60	1.52
3	C	17	ASN	C-N	-5.37	1.26	1.33
1	A	454	SER	CA-C	-5.37	1.45	1.52
1	A	1127	ASP	CG-OD1	5.37	1.35	1.25
4	E	122	LYS	C-O	5.37	1.31	1.24
1	A	1218	GLN	CD-OE1	5.37	1.33	1.23
1	A	1328	TYR	N-CA	-5.37	1.39	1.45
1	A	1354	ASN	CA-CB	-5.37	1.45	1.53
3	C	147	LEU	CG-CD2	-5.37	1.34	1.52
4	E	17	ARG	C-N	-5.37	1.26	1.33
1	A	49	LYS	CB-CG	5.36	1.68	1.52
1	A	708	MET	CA-C	5.36	1.58	1.52
1	A	906	HIS	CA-C	5.36	1.60	1.52
2	B	357	GLN	CG-CD	-5.36	1.38	1.52
7	I	86	PHE	CA-CB	-5.36	1.44	1.53
2	B	187	SER	CA-CB	-5.36	1.44	1.53
2	B	264	SER	CA-CB	5.36	1.62	1.53
2	B	577	ALA	N-CA	5.36	1.52	1.46
1	A	562	THR	CB-OG1	5.36	1.52	1.43
1	A	748	MET	CB-CG	5.36	1.68	1.52
1	A	976	THR	CA-CB	5.36	1.60	1.53
1	A	1263	ILE	CB-CG2	-5.36	1.34	1.52
1	A	1323	ASP	CB-CG	5.36	1.65	1.52
2	B	812	LEU	C-N	-5.36	1.26	1.33
6	H	138	GLU	CD-OE2	5.36	1.35	1.25
1	A	1345	ARG	C-N	-5.36	1.26	1.33
2	B	680	THR	CA-CB	-5.36	1.44	1.53
4	E	107	THR	C-O	-5.36	1.17	1.23
7	I	63	GLY	C-O	-5.36	1.17	1.24
1	A	493	GLN	CD-OE1	5.36	1.33	1.23
2	B	262	GLU	CG-CD	5.36	1.65	1.52
2	B	1213	THR	CB-OG1	5.36	1.52	1.43
1	A	34	LYS	C-N	-5.35	1.26	1.33
1	A	369	SER	C-N	-5.35	1.26	1.33
1	A	824	LEU	CA-C	-5.35	1.45	1.52
2	B	435	THR	N-CA	5.35	1.54	1.46
2	B	792	MET	C-N	-5.35	1.26	1.33
1	A	1255	GLU	C-N	5.35	1.41	1.33
2	B	125	SER	N-CA	5.35	1.52	1.45
2	B	293	PRO	CA-C	-5.35	1.45	1.52
2	B	563	MET	N-CA	5.35	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	866	TYR	CE2-CZ	5.35	1.51	1.38
3	C	35	ARG	CB-CG	5.35	1.68	1.52
3	C	228	PHE	CG-CD2	-5.35	1.27	1.38
1	A	1057	VAL	CA-CB	5.35	1.60	1.54
2	B	1134	GLU	C-N	-5.35	1.26	1.33
1	A	744	LYS	C-N	-5.35	1.26	1.34
2	B	206	ASN	CG-OD1	5.35	1.33	1.23
2	B	529	GLU	CG-CD	5.35	1.65	1.52
2	B	766	ARG	CB-CG	-5.35	1.36	1.52
3	C	214	ASN	CG-ND2	5.35	1.44	1.33
8	J	17	LYS	CD-CE	5.35	1.68	1.52
1	A	999	VAL	C-O	-5.35	1.17	1.24
2	B	608	ASP	CG-OD2	5.35	1.35	1.25
8	J	48	ARG	CG-CD	-5.35	1.36	1.52
1	A	1282	VAL	N-CA	-5.35	1.40	1.46
2	B	286	PHE	CG-CD2	-5.35	1.27	1.38
2	B	974	PRO	N-CA	-5.35	1.40	1.47
1	A	1412	ALA	N-CA	5.34	1.52	1.46
2	B	619	ILE	CA-C	-5.34	1.44	1.52
3	C	51	VAL	CA-C	-5.34	1.45	1.52
1	A	1410	PHE	CG-CD2	-5.34	1.27	1.38
2	B	95	ILE	N-CA	5.34	1.52	1.46
2	B	746	SER	CB-OG	-5.34	1.31	1.42
2	B	1084	GLN	CA-CB	-5.34	1.45	1.53
3	C	112	ASN	C-O	-5.34	1.17	1.23
7	I	18	GLU	CD-OE2	5.34	1.35	1.25
1	A	525	GLN	C-N	-5.34	1.26	1.33
1	A	621	THR	N-CA	-5.34	1.39	1.46
2	B	809	MET	CA-CB	-5.34	1.43	1.53
5	F	134	ILE	CA-C	-5.34	1.46	1.52
1	A	22	PHE	C-N	5.34	1.41	1.33
1	A	925	LEU	C-N	-5.34	1.26	1.34
6	H	145	ARG	CG-CD	5.34	1.68	1.52
7	I	110	PHE	CA-C	-5.34	1.46	1.52
1	A	973	ILE	C-O	5.34	1.30	1.24
4	E	203	GLU	N-CA	5.34	1.53	1.46
1	A	842	VAL	C-N	-5.34	1.27	1.33
1	A	899	VAL	C-O	-5.34	1.18	1.24
1	A	1042	PHE	CE2-CZ	5.34	1.54	1.38
1	A	1053	PHE	CG-CD2	-5.34	1.27	1.38
2	B	502	ILE	CG1-CD1	5.34	1.72	1.51
4	E	134	THR	CA-C	-5.34	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1234	GLU	CB-CG	5.33	1.68	1.52
2	B	516	ASN	CG-ND2	-5.33	1.22	1.33
3	C	262	LEU	CG-CD1	5.33	1.70	1.52
5	F	72	LYS	CD-CE	5.33	1.68	1.52
1	A	360	GLU	C-N	-5.33	1.27	1.33
1	A	647	GLY	C-O	-5.33	1.17	1.23
2	B	479	VAL	C-N	-5.33	1.25	1.33
2	B	880	THR	C-O	5.33	1.29	1.23
2	B	1224	PHE	CB-CG	5.33	1.62	1.50
1	A	216	VAL	N-CA	5.33	1.52	1.46
1	A	1216	ILE	C-O	5.33	1.30	1.24
2	B	798	TYR	CZ-OH	5.33	1.49	1.38
6	H	31	THR	C-O	5.33	1.30	1.24
2	B	109	THR	CA-C	-5.33	1.45	1.52
1	A	49	LYS	C-O	5.33	1.30	1.23
2	B	888	GLY	N-CA	5.33	1.50	1.44
1	A	420	ARG	N-CA	5.33	1.52	1.46
1	A	585	GLY	N-CA	-5.33	1.36	1.44
2	B	544	CYS	C-N	-5.33	1.26	1.33
2	B	998	ASP	CB-CG	-5.33	1.38	1.52
9	K	89	ASN	C-N	-5.33	1.26	1.33
9	K	108	GLU	C-O	5.33	1.30	1.24
1	A	1348	LEU	C-N	5.32	1.41	1.33
9	K	82	ASP	CB-CG	5.32	1.65	1.52
1	A	738	LYS	CA-C	-5.32	1.45	1.53
1	A	1037	LEU	CG-CD2	-5.32	1.34	1.52
2	B	1204	PHE	C-O	5.32	1.30	1.24
3	C	14	SER	C-N	-5.32	1.25	1.33
3	C	165	LYS	CD-CE	5.32	1.68	1.52
4	E	56	LYS	CA-C	-5.32	1.45	1.52
6	H	142	LEU	N-CA	-5.32	1.39	1.46
1	A	225	ASN	CG-ND2	-5.32	1.22	1.33
2	B	319	GLU	CG-CD	5.32	1.65	1.52
2	B	397	ASP	C-O	5.32	1.30	1.23
1	A	411	ASP	CA-CB	5.32	1.62	1.53
1	A	1360	GLY	C-O	5.32	1.31	1.24
8	J	5	VAL	C-N	-5.32	1.25	1.33
1	A	74	MET	N-CA	5.31	1.53	1.46
1	A	436	ILE	CB-CG2	5.31	1.70	1.52
1	A	243	PRO	C-O	-5.31	1.18	1.24
1	A	1062	GLU	CG-CD	-5.31	1.38	1.52
2	B	965	LYS	N-CA	5.31	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1061	GLU	CG-CD	5.31	1.65	1.52
3	C	19	ASP	C-N	-5.31	1.27	1.33
3	C	86	CYS	CB-SG	5.31	1.98	1.81
5	F	129	LYS	C-O	-5.31	1.17	1.24
7	I	79	HIS	C-O	5.31	1.30	1.24
10	L	61	THR	CA-C	-5.31	1.46	1.53
9	K	28	PRO	CA-CB	-5.31	1.48	1.54
9	K	77	THR	N-CA	-5.31	1.39	1.45
1	A	84	ILE	CB-CG2	-5.31	1.35	1.52
1	A	509	LEU	CB-CG	-5.31	1.42	1.53
2	B	109	THR	CA-CB	5.31	1.62	1.53
10	L	44	ASP	CG-OD1	5.31	1.35	1.25
1	A	1140	HIS	CA-C	-5.31	1.45	1.52
2	B	858	SER	CA-CB	-5.31	1.45	1.53
2	B	1000	PRO	CA-C	5.31	1.58	1.52
2	B	1143	ALA	N-CA	-5.31	1.40	1.46
2	B	1180	PHE	C-O	5.31	1.29	1.24
3	C	124	LEU	C-O	5.31	1.37	1.24
1	A	379	VAL	CB-CG2	5.31	1.70	1.52
1	A	1081	LEU	CA-CB	5.31	1.64	1.53
2	B	727	LYS	N-CA	-5.31	1.39	1.45
4	E	79	TRP	CG-CD1	5.31	1.50	1.36
4	E	159	ASP	CG-OD2	5.31	1.35	1.25
1	A	1339	LEU	CG-CD2	-5.30	1.35	1.52
2	B	811	TYR	N-CA	-5.30	1.39	1.46
2	B	909	ASP	CG-OD1	-5.30	1.15	1.25
4	E	20	LYS	CB-CG	5.30	1.68	1.52
1	A	695	LYS	CG-CD	5.30	1.68	1.52
1	A	779	PHE	C-N	-5.30	1.28	1.33
1	A	933	TYR	CE1-CZ	-5.30	1.25	1.38
2	B	89	GLU	C-O	5.30	1.34	1.23
2	B	952	VAL	CA-C	-5.30	1.46	1.52
1	A	237	THR	CB-CG2	5.30	1.70	1.52
1	A	488	ASN	C-O	-5.30	1.17	1.24
1	A	732	LEU	C-N	-5.30	1.26	1.33
1	A	787	PHE	CE1-CZ	-5.30	1.22	1.38
2	B	59	LEU	CA-C	-5.30	1.47	1.53
4	E	29	PHE	CD2-CE2	-5.30	1.22	1.38
1	A	561	PRO	CB-CG	-5.30	1.23	1.49
1	A	772	GLY	C-N	-5.30	1.26	1.33
1	A	1309	ASP	CG-OD1	5.30	1.35	1.25
2	B	436	VAL	C-N	5.30	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1071	VAL	CB-CG2	-5.30	1.35	1.52
1	A	1384	VAL	CB-CG2	5.30	1.70	1.52
1	A	47	ARG	NE-CZ	5.30	1.38	1.33
1	A	362	ASP	N-CA	-5.30	1.39	1.46
1	A	576	GLN	C-O	-5.30	1.17	1.24
1	A	664	THR	CB-OG1	-5.30	1.35	1.43
2	B	512	ARG	CG-CD	-5.30	1.36	1.52
4	E	64	PRO	N-CD	-5.30	1.40	1.47
8	J	17	LYS	CA-CB	-5.30	1.45	1.53
1	A	9	ALA	C-N	-5.29	1.26	1.33
1	A	386	ASP	CG-OD1	5.29	1.35	1.25
1	A	675	THR	CA-CB	-5.29	1.45	1.53
1	A	853	ASP	C-O	-5.29	1.16	1.24
2	B	257	LYS	CA-C	-5.29	1.46	1.52
1	A	1196	GLU	C-N	5.29	1.40	1.33
1	A	1328	TYR	CE1-CZ	-5.29	1.25	1.38
8	J	48	ARG	N-CA	5.29	1.53	1.46
9	K	114	LEU	N-CA	5.29	1.56	1.46
2	B	248	SER	CA-C	5.29	1.59	1.52
2	B	944	THR	CB-OG1	5.29	1.52	1.43
2	B	1182	CYS	CA-CB	5.29	1.60	1.52
3	C	148	ARG	CA-C	5.29	1.59	1.52
7	I	27	PHE	CG-CD2	-5.29	1.27	1.38
10	L	28	LYS	CG-CD	5.29	1.68	1.52
2	B	619	ILE	N-CA	-5.29	1.39	1.46
7	I	29	CYS	C-N	5.29	1.41	1.33
1	A	1039	LYS	CD-CE	5.29	1.68	1.52
1	A	1228	TRP	C-N	-5.29	1.26	1.33
2	B	54	PHE	CD1-CE1	-5.29	1.22	1.38
2	B	339	THR	C-N	-5.29	1.25	1.33
2	B	853	SER	C-O	-5.29	1.17	1.23
2	B	1220	ARG	CG-CD	5.29	1.68	1.52
1	A	192	GLY	N-CA	5.29	1.52	1.45
1	A	383	TYR	N-CA	5.29	1.53	1.46
2	B	102	VAL	CA-C	5.29	1.59	1.52
2	B	267	ARG	CG-CD	5.29	1.68	1.52
2	B	370	PHE	CE2-CZ	5.29	1.54	1.38
2	B	584	GLY	CA-C	-5.29	1.44	1.51
1	A	390	GLN	CA-C	-5.28	1.46	1.52
1	A	514	PRO	CB-CG	-5.28	1.23	1.49
1	A	839	ARG	CZ-NH1	5.28	1.40	1.32
1	A	1100	ARG	C-N	-5.28	1.26	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1411	GLU	CG-CD	5.28	1.65	1.52
2	B	303	TYR	CZ-OH	5.28	1.49	1.38
2	B	323	VAL	C-O	5.28	1.31	1.24
4	E	132	ILE	CA-CB	-5.28	1.47	1.54
1	A	1435	PRO	CB-CG	-5.28	1.23	1.49
2	B	112	LEU	CA-CB	-5.28	1.45	1.53
1	A	1107	VAL	CA-C	5.28	1.59	1.52
2	B	1079	LYS	N-CA	-5.28	1.39	1.46
4	E	19	VAL	N-CA	5.28	1.53	1.46
2	B	561	TRP	CG-CD1	-5.28	1.23	1.36
2	B	289	LEU	N-CA	-5.28	1.39	1.46
3	C	123	ASN	C-N	-5.28	1.20	1.33
3	C	140	ASN	N-CA	-5.28	1.39	1.46
6	H	38	LEU	CA-CB	-5.28	1.45	1.53
9	K	5	ASP	N-CA	5.28	1.52	1.46
10	L	63	ARG	N-CA	5.28	1.52	1.46
1	A	41	MET	CA-CB	5.28	1.62	1.53
1	A	85	ASP	CG-OD2	5.28	1.35	1.25
1	A	113	LEU	N-CA	5.28	1.52	1.46
1	A	385	ILE	C-N	-5.28	1.27	1.33
1	A	631	HIS	CA-CB	-5.28	1.44	1.53
1	A	993	LEU	CA-C	-5.28	1.45	1.52
2	B	792	MET	CA-CB	-5.28	1.43	1.54
2	B	1065	GLN	CD-OE1	-5.28	1.13	1.23
2	B	1102	LYS	CG-CD	5.28	1.68	1.52
4	E	11	ARG	CB-CG	5.28	1.68	1.52
1	A	434	ARG	CZ-NH2	5.27	1.40	1.33
1	A	442	VAL	C-O	-5.27	1.17	1.23
1	A	608	ILE	CB-CG2	-5.27	1.35	1.52
2	B	291	ILE	CB-CG1	-5.27	1.43	1.53
2	B	565	PRO	N-CA	-5.27	1.41	1.46
2	B	890	TYR	C-N	5.27	1.41	1.33
3	C	94	LYS	CD-CE	5.27	1.68	1.52
3	C	108	GLU	C-O	5.27	1.30	1.24
7	I	33	SER	CB-OG	5.27	1.52	1.42
1	A	1406	VAL	CA-C	-5.27	1.46	1.52
1	A	672	ASP	CA-CB	5.27	1.62	1.53
1	A	749	ALA	CA-C	-5.27	1.45	1.52
10	L	50	ASP	CG-OD1	5.27	1.35	1.25
1	A	248	PRO	N-CD	5.27	1.55	1.47
1	A	600	PRO	CB-CG	5.27	1.75	1.49
8	J	37	SER	CA-C	5.27	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	902	LEU	CA-C	-5.27	1.44	1.52
2	B	308	TRP	CG-CD2	-5.27	1.34	1.43
2	B	895	ASP	C-N	5.27	1.41	1.33
3	C	10	ILE	N-CA	-5.27	1.39	1.46
3	C	170	TRP	CA-C	-5.27	1.45	1.52
1	A	760	GLN	CG-CD	5.26	1.65	1.52
2	B	38	PHE	C-O	-5.26	1.17	1.24
3	C	187	LYS	CB-CG	-5.26	1.36	1.52
8	J	43	ARG	CZ-NH1	-5.26	1.25	1.32
1	A	76	GLU	CA-C	5.26	1.59	1.52
2	B	941	LEU	CA-C	-5.26	1.45	1.52
2	B	1076	HIS	CA-C	5.26	1.60	1.52
2	B	1049	ASP	CG-OD2	-5.26	1.15	1.25
1	A	19	PHE	N-CA	-5.26	1.39	1.46
1	A	862	ASN	C-O	-5.26	1.16	1.23
1	A	909	ASP	CG-OD1	5.26	1.35	1.25
1	A	1008	GLN	N-CA	-5.26	1.39	1.46
1	A	1426	GLU	N-CA	-5.26	1.39	1.46
2	B	488	TYR	C-O	5.26	1.30	1.24
2	B	888	GLY	CA-C	-5.26	1.47	1.52
1	A	916	GLY	C-N	5.25	1.40	1.33
1	A	962	ARG	C-N	-5.25	1.27	1.34
2	B	268	THR	C-O	-5.25	1.16	1.23
5	F	120	ILE	CG1-CD1	-5.25	1.31	1.51
1	A	804	TYR	CD1-CE1	5.25	1.54	1.38
1	A	829	VAL	C-O	-5.25	1.18	1.24
2	B	204	ILE	C-N	-5.25	1.27	1.33
3	C	19	ASP	CA-CB	-5.25	1.45	1.53
5	F	77	ASP	CA-C	-5.25	1.46	1.53
9	K	81	TYR	CA-C	-5.25	1.46	1.52
1	A	1145	SER	C-N	-5.25	1.27	1.33
1	A	1147	THR	C-O	-5.25	1.17	1.24
1	A	1205	LYS	CA-C	-5.25	1.46	1.52
1	A	1373	ASP	CA-CB	-5.25	1.45	1.53
2	B	124	TYR	C-O	-5.25	1.17	1.24
2	B	294	ASP	CG-OD2	5.25	1.35	1.25
3	C	238	ILE	N-CA	-5.25	1.40	1.46
1	A	1339	LEU	CB-CG	-5.25	1.43	1.53
4	E	161	LYS	CB-CG	-5.25	1.36	1.52
1	A	178	GLY	CA-C	-5.25	1.44	1.51
1	A	196	GLU	C-N	-5.25	1.26	1.33
2	B	1201	LYS	C-O	5.25	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	60	ASP	CG-OD1	5.25	1.35	1.25
5	F	110	ASP	CG-OD2	5.25	1.35	1.25
1	A	721	PHE	CG-CD2	-5.25	1.27	1.38
1	A	1124	HIS	CA-CB	5.25	1.61	1.53
2	B	634	TYR	CA-C	-5.25	1.46	1.52
2	B	656	GLY	CA-C	-5.25	1.45	1.51
3	C	167	HIS	N-CA	-5.25	1.39	1.46
7	I	50	THR	C-N	-5.25	1.26	1.33
1	A	780	VAL	C-N	-5.24	1.26	1.33
2	B	683	SER	N-CA	-5.24	1.40	1.46
9	K	20	LYS	CB-CG	5.24	1.68	1.52
1	A	1068	ALA	N-CA	-5.24	1.39	1.46
1	A	1365	TYR	CG-CD1	-5.24	1.28	1.39
1	A	383	TYR	C-N	-5.24	1.26	1.33
1	A	1070	GLN	CB-CG	-5.24	1.36	1.52
3	C	87	PHE	CG-CD2	-5.24	1.27	1.38
4	E	15	ALA	C-O	5.24	1.30	1.24
8	J	29	GLU	C-O	5.24	1.32	1.24
1	A	291	GLU	C-O	-5.24	1.17	1.24
2	B	19	GLU	CA-CB	5.24	1.62	1.53
2	B	310	MET	CG-SD	-5.24	1.67	1.80
2	B	460	ALA	CA-CB	5.24	1.61	1.53
2	B	780	VAL	CB-CG1	-5.24	1.35	1.52
2	B	958	GLN	CD-NE2	5.24	1.44	1.33
3	C	124	LEU	CA-CB	5.24	1.61	1.53
1	A	1092	LYS	CA-CB	5.23	1.64	1.53
2	B	286	PHE	CE1-CZ	-5.23	1.23	1.38
1	A	815	PHE	CE2-CZ	-5.23	1.23	1.38
1	A	1055	ARG	NE-CZ	5.23	1.38	1.33
2	B	1017	ILE	CA-CB	-5.23	1.47	1.54
3	C	99	LEU	CA-C	-5.23	1.46	1.52
4	E	212	ARG	CZ-NH2	5.23	1.40	1.33
1	A	400	PRO	N-CA	-5.23	1.38	1.47
1	A	780	VAL	CA-CB	5.23	1.60	1.53
1	A	921	GLY	C-O	5.23	1.30	1.23
1	A	1100	ARG	CB-CG	5.23	1.68	1.52
2	B	224	GLN	CA-C	-5.23	1.46	1.52
2	B	356	LEU	CA-CB	-5.23	1.44	1.53
2	B	876	LYS	CD-CE	5.23	1.68	1.52
2	B	709	ASP	CA-CB	-5.23	1.44	1.53
2	B	764	SER	CA-C	5.23	1.58	1.52
3	C	62	PHE	CD1-CE1	-5.23	1.23	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	52	ASN	C-O	5.23	1.30	1.24
1	A	407	ARG	CG-CD	5.22	1.68	1.52
1	A	854	ASN	CA-CB	-5.22	1.46	1.53
1	A	1014	ALA	CA-C	5.22	1.60	1.52
1	A	1225	PHE	CE1-CZ	5.22	1.54	1.38
2	B	463	THR	CB-OG1	-5.22	1.35	1.43
2	B	567	GLU	CA-CB	5.22	1.62	1.53
1	A	124	GLN	CD-OE1	5.22	1.33	1.23
1	A	164	ARG	CA-C	-5.22	1.46	1.52
1	A	213	HIS	CG-ND1	5.22	1.44	1.38
1	A	278	THR	CA-CB	5.22	1.62	1.53
1	A	940	ARG	CZ-NH1	-5.22	1.25	1.32
2	B	138	GLU	CA-C	5.22	1.64	1.52
3	C	117	ASP	CG-OD1	5.22	1.35	1.25
3	C	156	THR	N-CA	-5.22	1.39	1.45
3	C	239	PRO	C-O	-5.22	1.17	1.23
4	E	3	GLN	CA-CB	5.22	1.61	1.53
1	A	1212	VAL	CB-CG2	-5.22	1.35	1.52
1	A	1295	THR	N-CA	-5.22	1.39	1.46
3	C	18	VAL	CA-CB	-5.22	1.47	1.54
1	A	448	PRO	N-CA	-5.22	1.38	1.47
1	A	1324	PRO	N-CA	-5.22	1.40	1.47
2	B	553	PRO	C-O	-5.22	1.18	1.24
2	B	814	PHE	CE2-CZ	-5.22	1.23	1.38
2	B	988	GLY	N-CA	5.22	1.52	1.45
3	C	89	GLU	CA-C	-5.22	1.46	1.52
5	F	84	TYR	CD1-CE1	5.22	1.54	1.38
6	H	43	ASN	CA-C	5.22	1.59	1.52
1	A	785	PRO	N-CD	-5.22	1.40	1.47
2	B	167	ILE	CG1-CD1	5.22	1.72	1.51
1	A	968	GLN	CG-CD	5.22	1.65	1.52
1	A	1226	VAL	CB-CG1	-5.22	1.35	1.52
2	B	690	VAL	CA-CB	-5.22	1.46	1.55
4	E	123	LEU	C-O	-5.22	1.16	1.24
5	F	97	ARG	CA-C	-5.22	1.45	1.52
7	I	45	ARG	N-CA	5.22	1.52	1.46
1	A	1096	SER	CB-OG	5.21	1.52	1.42
2	B	103	ASN	CA-C	5.21	1.59	1.52
2	B	262	GLU	CD-OE2	5.21	1.35	1.25
2	B	1147	LEU	C-O	-5.21	1.17	1.24
9	K	21	ILE	C-N	-5.21	1.27	1.33
2	B	711	GLU	CD-OE2	5.21	1.35	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1170	THR	CA-C	-5.21	1.45	1.52
6	H	45	GLU	CA-C	-5.21	1.45	1.52
1	A	135	PHE	CA-C	-5.21	1.46	1.52
2	B	1043	ASP	CA-CB	5.21	1.60	1.53
2	B	1049	ASP	CA-C	-5.21	1.45	1.52
10	L	27	LEU	CG-CD2	5.21	1.69	1.52
1	A	68	GLN	CA-C	5.21	1.59	1.53
1	A	205	GLU	N-CA	-5.21	1.40	1.46
1	A	662	PHE	CA-C	-5.21	1.45	1.52
2	B	768	THR	N-CA	-5.21	1.39	1.46
2	B	1025	HIS	C-O	-5.21	1.18	1.24
3	C	81	GLU	N-CA	-5.21	1.39	1.45
7	I	86	PHE	C-N	-5.21	1.26	1.33
7	I	101	PHE	CD2-CE2	5.21	1.54	1.38
9	K	105	PHE	C-O	5.21	1.30	1.23
1	A	596	THR	CA-CB	-5.21	1.45	1.53
1	A	718	VAL	CB-CG2	-5.21	1.35	1.52
2	B	209	GLU	C-N	-5.21	1.25	1.33
2	B	1129	ARG	CZ-NH2	5.21	1.40	1.33
3	C	4	GLU	N-CA	5.21	1.52	1.46
4	E	99	HIS	CB-CG	5.21	1.57	1.50
7	I	29	CYS	CA-C	5.21	1.59	1.52
1	A	59	GLY	C-N	5.21	1.41	1.33
1	A	1193	LEU	CG-CD1	-5.21	1.35	1.52
5	F	138	LEU	C-N	-5.20	1.27	1.34
4	E	174	GLN	C-O	-5.20	1.17	1.24
6	H	110	ASP	CA-C	5.20	1.60	1.52
1	A	22	PHE	N-CA	-5.20	1.40	1.46
1	A	128	ILE	CA-C	5.20	1.59	1.52
1	A	540	PHE	CG-CD2	-5.20	1.27	1.38
1	A	907	THR	CB-CG2	-5.20	1.35	1.52
2	B	611	PRO	CB-CG	-5.20	1.23	1.49
2	B	728	ARG	CZ-NH2	5.20	1.40	1.33
5	F	106	PRO	C-N	-5.20	1.26	1.33
1	A	213	HIS	N-CA	-5.20	1.39	1.46
2	B	1002	THR	CB-OG1	-5.20	1.35	1.43
1	A	838	GLN	CD-OE1	5.20	1.33	1.23
2	B	663	ALA	C-N	-5.20	1.26	1.33
2	B	1222	ARG	CA-CB	5.19	1.62	1.53
1	A	190	ALA	N-CA	5.19	1.52	1.46
1	A	504	LEU	CA-C	5.19	1.59	1.52
1	A	635	ARG	CZ-NH2	5.19	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	877	HIS	C-O	5.19	1.30	1.24
2	B	108	VAL	CB-CG2	5.19	1.69	1.52
2	B	842	ASN	CA-CB	-5.19	1.46	1.53
2	B	967	ARG	N-CA	-5.19	1.39	1.46
3	C	131	HIS	CB-CG	5.19	1.57	1.50
1	A	218	ASP	C-N	5.19	1.41	1.33
1	A	609	ASP	CG-OD2	5.19	1.35	1.25
1	A	1048	ASN	CA-C	-5.19	1.46	1.52
1	A	1148	ILE	N-CA	-5.19	1.40	1.46
1	A	1260	LEU	CG-CD1	-5.19	1.35	1.52
6	H	35	GLN	CD-OE1	5.19	1.33	1.23
7	I	120	GLN	CD-NE2	5.19	1.44	1.33
1	A	67	CYS	N-CA	-5.19	1.39	1.46
2	B	385	LEU	CG-CD2	5.19	1.69	1.52
2	B	684	LEU	CB-CG	-5.19	1.43	1.53
2	B	806	THR	N-CA	5.19	1.52	1.45
9	K	98	LEU	CA-C	-5.19	1.46	1.53
2	B	744	HIS	N-CA	5.19	1.57	1.45
4	E	187	TYR	C-N	-5.19	1.25	1.33
9	K	88	LYS	CB-CG	5.19	1.68	1.52
1	A	719	VAL	C-O	-5.19	1.17	1.24
2	B	513	GLN	CD-OE1	5.19	1.33	1.23
3	C	220	ASP	CG-OD2	5.19	1.35	1.25
1	A	76	GLU	CD-OE2	5.18	1.35	1.25
1	A	765	VAL	CB-CG1	-5.18	1.35	1.52
1	A	1414	ALA	C-N	-5.18	1.25	1.33
1	A	1434	ALA	C-O	-5.18	1.17	1.23
2	B	249	ARG	CD-NE	5.18	1.53	1.46
4	E	171	LYS	CD-CE	5.18	1.68	1.52
1	A	1042	PHE	CA-C	-5.18	1.46	1.52
2	B	974	PRO	N-CD	-5.18	1.40	1.47
3	C	52	GLU	CA-C	-5.18	1.46	1.52
4	E	73	PRO	N-CD	5.18	1.55	1.47
7	I	4	PHE	CB-CG	-5.18	1.38	1.50
7	I	24	ARG	C-O	5.18	1.30	1.23
9	K	57	LEU	N-CA	-5.18	1.39	1.46
1	A	518	LYS	CE-NZ	-5.18	1.33	1.49
1	A	814	PHE	CD1-CE1	-5.18	1.23	1.38
1	A	1127	ASP	CB-CG	5.18	1.65	1.52
2	B	884	ARG	CB-CG	5.18	1.68	1.52
4	E	7	ARG	C-O	5.18	1.30	1.24
1	A	594	GLY	N-CA	5.18	1.52	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	663	SER	N-CA	5.18	1.52	1.46
1	A	388	LEU	CA-C	5.18	1.59	1.52
1	A	984	LYS	CA-C	-5.18	1.45	1.52
1	A	1032	LEU	N-CA	-5.18	1.39	1.46
2	B	306	ASN	CB-CG	5.18	1.65	1.52
3	C	25	VAL	C-O	5.18	1.30	1.23
1	A	532	ARG	CD-NE	-5.17	1.39	1.46
7	I	85	PHE	CA-CB	-5.17	1.43	1.54
1	A	1164	PRO	CB-CG	5.17	1.75	1.49
2	B	380	TYR	CG-CD1	-5.17	1.28	1.39
2	B	498	THR	C-O	-5.17	1.17	1.23
9	K	96	ASN	CG-ND2	5.17	1.44	1.33
1	A	754	SER	CA-CB	5.17	1.62	1.53
1	A	280	GLU	CD-OE1	5.17	1.35	1.25
1	A	691	LEU	CB-CG	-5.17	1.43	1.53
1	A	757	ASN	N-CA	-5.17	1.40	1.46
1	A	1118	VAL	CA-C	-5.17	1.46	1.52
1	A	1356	ILE	C-N	-5.17	1.26	1.33
2	B	389	ALA	CA-C	-5.17	1.45	1.52
2	B	803	LEU	CG-CD2	-5.17	1.35	1.52
2	B	910	VAL	C-O	-5.17	1.17	1.24
2	B	1182	CYS	C-O	5.17	1.29	1.23
5	F	102	SER	CB-OG	-5.17	1.31	1.42
10	L	58	LYS	C-O	-5.17	1.17	1.24
1	A	1231	ASP	CB-CG	-5.17	1.39	1.52
9	K	51	LEU	CA-CB	-5.17	1.45	1.53
2	B	870	ILE	C-N	5.17	1.40	1.33
2	B	1081	LEU	N-CA	-5.17	1.39	1.46
1	A	4	GLN	C-O	5.16	1.30	1.24
1	A	55	ASP	N-CA	5.16	1.53	1.46
1	A	491	VAL	C-N	-5.16	1.26	1.33
1	A	1352	VAL	N-CA	5.16	1.53	1.46
2	B	227	LYS	N-CA	-5.16	1.38	1.45
2	B	530	GLY	CA-C	5.16	1.59	1.52
2	B	1014	PRO	CA-CB	-5.16	1.46	1.53
1	A	935	GLN	CD-NE2	-5.16	1.22	1.33
1	A	947	PHE	C-O	-5.16	1.17	1.23
1	A	1210	GLY	C-O	5.16	1.30	1.24
2	B	304	ASP	N-CA	5.16	1.52	1.46
2	B	1020	ARG	N-CA	-5.16	1.39	1.46
1	A	881	GLN	C-N	5.16	1.40	1.33
1	A	936	LEU	CA-C	-5.16	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1041	ALA	CA-CB	5.16	1.61	1.53
2	B	241	ARG	C-N	-5.16	1.26	1.33
2	B	693	ILE	CB-CG1	-5.16	1.43	1.53
5	F	131	PRO	CB-CG	-5.16	1.23	1.49
10	L	49	LYS	CD-CE	5.16	1.68	1.52
1	A	1417	GLU	CB-CG	5.16	1.68	1.52
2	B	415	GLN	C-O	-5.16	1.18	1.24
1	A	200	ARG	C-N	-5.16	1.27	1.34
1	A	441	PRO	CB-CG	-5.16	1.23	1.49
1	A	645	LEU	CG-CD2	-5.16	1.35	1.52
1	A	968	GLN	CB-CG	-5.16	1.36	1.52
1	A	1265	ASN	N-CA	5.16	1.52	1.46
2	B	68	THR	CB-CG2	5.16	1.69	1.52
2	B	225	VAL	C-N	-5.16	1.26	1.33
2	B	529	GLU	C-N	-5.16	1.25	1.33
10	L	45	ALA	C-O	5.16	1.30	1.24
1	A	962	ARG	CB-CG	5.15	1.68	1.52
2	B	1004	GLU	CD-OE1	5.15	1.35	1.25
8	J	53	HIS	ND1-CE1	-5.15	1.27	1.32
2	B	245	GLU	CD-OE2	5.15	1.35	1.25
2	B	654	ARG	NE-CZ	-5.15	1.27	1.33
5	F	74	ILE	C-O	-5.15	1.18	1.24
5	F	99	LEU	CG-CD1	-5.15	1.35	1.52
9	K	24	ASP	CA-CB	-5.15	1.45	1.53
2	B	449	ASN	N-CA	5.15	1.53	1.46
2	B	1187	ASN	N-CA	5.15	1.52	1.46
3	C	22	LEU	CG-CD2	-5.15	1.35	1.52
3	C	221	TYR	CA-CB	-5.15	1.44	1.53
3	C	232	VAL	CA-C	-5.15	1.46	1.52
1	A	752	LYS	N-CA	-5.15	1.40	1.46
1	A	993	LEU	N-CA	5.15	1.52	1.46
2	B	36	ALA	CA-CB	5.15	1.61	1.53
4	E	26	ARG	CA-CB	-5.15	1.44	1.53
6	H	106	GLU	CA-CB	5.15	1.62	1.53
1	A	205	GLU	C-N	-5.15	1.26	1.33
1	A	711	ARG	CA-CB	-5.15	1.44	1.53
2	B	457	LEU	CA-CB	5.15	1.61	1.53
4	E	115	ASN	CA-CB	5.15	1.61	1.53
9	K	80	GLY	C-O	5.15	1.29	1.24
1	A	111	GLY	N-CA	5.14	1.52	1.45
1	A	185	TRP	C-O	-5.14	1.17	1.23
1	A	1433	MET	CG-SD	5.14	1.93	1.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	97	VAL	CA-C	-5.14	1.46	1.52
9	K	62	LYS	CA-C	-5.14	1.45	1.52
1	A	138	ILE	CA-CB	5.14	1.61	1.54
1	A	157	ASP	CA-C	5.14	1.59	1.52
2	B	1081	LEU	C-N	-5.14	1.27	1.33
3	C	73	GLN	CA-C	-5.14	1.46	1.52
4	E	18	THR	CA-C	-5.14	1.46	1.52
7	I	35	VAL	CA-C	-5.14	1.46	1.52
1	A	804	TYR	C-O	-5.14	1.18	1.24
10	L	42	ARG	CG-CD	5.14	1.67	1.52
1	A	424	ILE	CA-CB	-5.14	1.48	1.54
1	A	765	VAL	C-O	-5.14	1.17	1.24
1	A	883	LEU	CG-CD2	-5.14	1.35	1.52
2	B	372	SER	C-O	5.14	1.30	1.24
2	B	693	ILE	CG1-CD1	5.14	1.71	1.51
2	B	1066	SER	N-CA	-5.14	1.39	1.46
2	B	206	ASN	N-CA	5.14	1.54	1.46
2	B	662	MET	CA-C	-5.14	1.45	1.52
9	K	64	GLU	CA-C	-5.14	1.45	1.52
1	A	576	GLN	N-CA	-5.14	1.39	1.46
2	B	193	LYS	CA-CB	5.14	1.61	1.53
3	C	203	GLN	CG-CD	-5.14	1.39	1.52
3	C	267	GLN	CD-NE2	5.14	1.44	1.33
4	E	34	GLU	N-CA	5.14	1.52	1.46
8	J	40	GLY	N-CA	5.14	1.53	1.45
1	A	802	ASN	CA-CB	-5.13	1.44	1.53
1	A	1260	LEU	C-N	-5.13	1.26	1.33
1	A	1442	ASP	N-CA	-5.13	1.39	1.45
2	B	228	LYS	CG-CD	5.13	1.67	1.52
2	B	496	ARG	CG-CD	5.13	1.67	1.52
2	B	609	ILE	CB-CG2	-5.13	1.35	1.52
2	B	899	ILE	CG1-CD1	-5.13	1.31	1.51
3	C	214	ASN	CA-CB	5.13	1.60	1.53
6	H	85	GLY	C-N	5.13	1.40	1.33
8	J	60	PHE	N-CA	-5.13	1.39	1.46
1	A	504	LEU	N-CA	5.13	1.52	1.46
1	A	536	LEU	C-O	5.13	1.30	1.23
2	B	105	SER	C-N	5.13	1.40	1.33
2	B	585	VAL	CA-CB	-5.13	1.47	1.54
2	B	1175	LEU	CG-CD1	5.13	1.69	1.52
1	A	513	SER	CB-OG	5.13	1.52	1.42
2	B	547	VAL	C-O	-5.13	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	667	GLN	CB-CG	5.13	1.67	1.52
2	B	1128	LEU	C-O	5.13	1.30	1.24
1	A	154	SER	CB-OG	-5.13	1.31	1.42
1	A	377	PRO	CB-CG	-5.13	1.24	1.49
1	A	771	GLU	C-N	-5.13	1.25	1.33
2	B	417	PHE	CD1-CE1	-5.13	1.23	1.38
2	B	1077	THR	N-CA	-5.13	1.38	1.45
3	C	268	ASP	CB-CG	5.13	1.64	1.52
4	E	81	GLU	CG-CD	-5.13	1.39	1.52
4	E	114	ASN	CB-CG	-5.13	1.39	1.52
1	A	28	ARG	CB-CG	5.13	1.67	1.52
1	A	133	LYS	CB-CG	5.13	1.67	1.52
1	A	476	SER	N-CA	-5.13	1.39	1.46
1	A	548	ASN	CG-OD1	5.13	1.33	1.23
1	A	1100	ARG	CZ-NH1	-5.13	1.25	1.32
1	A	1437	GLY	CA-C	-5.13	1.44	1.52
2	B	403	LYS	N-CA	-5.13	1.40	1.46
4	E	49	SER	N-CA	5.13	1.53	1.46
9	K	68	PHE	CB-CG	-5.13	1.38	1.50
1	A	505	CYS	CA-CB	-5.12	1.44	1.53
1	A	996	ASN	C-O	5.12	1.30	1.24
4	E	129	PRO	CA-C	5.12	1.63	1.52
1	A	200	ARG	CZ-NH1	5.12	1.40	1.32
1	A	595	THR	C-O	-5.12	1.17	1.23
2	B	245	GLU	CB-CG	5.12	1.67	1.52
2	B	492	LEU	CG-CD2	-5.12	1.35	1.52
4	E	172	GLU	C-O	-5.12	1.18	1.24
1	A	182	VAL	N-CA	5.12	1.52	1.46
2	B	289	LEU	CG-CD1	-5.12	1.35	1.52
6	H	128	ASN	C-O	-5.12	1.17	1.24
1	A	374	LEU	C-N	-5.12	1.25	1.33
1	A	1122	PRO	CG-CD	5.12	1.68	1.50
2	B	120	ARG	CZ-NH2	5.12	1.40	1.33
2	B	640	VAL	C-O	-5.12	1.18	1.24
1	A	445	ASN	CG-ND2	-5.12	1.22	1.33
1	A	1123	GLY	CA-C	5.12	1.59	1.51
1	A	1140	HIS	N-CA	5.12	1.52	1.46
1	A	1405	THR	N-CA	5.12	1.55	1.46
2	B	789	MET	CA-C	-5.12	1.47	1.53
1	A	480	ALA	N-CA	5.12	1.52	1.45
2	B	678	GLU	CA-CB	5.12	1.63	1.53
2	B	698	GLU	C-N	-5.12	1.26	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	45	ALA	N-CA	5.12	1.52	1.46
1	A	273	ASN	C-N	5.12	1.40	1.33
2	B	754	SER	N-CA	-5.12	1.39	1.46
4	E	25	ASP	CB-CG	5.12	1.64	1.52
5	F	133	VAL	C-N	5.12	1.40	1.33
7	I	38	ALA	C-N	-5.12	1.26	1.33
8	J	55	ASP	C-N	-5.12	1.26	1.34
1	A	722	LEU	CB-CG	-5.11	1.43	1.53
1	A	978	PRO	CA-CB	-5.11	1.46	1.53
2	B	522	VAL	CB-CG2	-5.11	1.35	1.52
2	B	553	PRO	N-CD	-5.11	1.40	1.47
2	B	741	CYS	N-CA	-5.11	1.39	1.45
7	I	37	GLU	CG-CD	5.11	1.64	1.52
1	A	988	LEU	CA-CB	-5.11	1.44	1.53
1	A	1097	GLY	CA-C	-5.11	1.44	1.51
2	B	387	LEU	CB-CG	-5.11	1.43	1.53
2	B	855	PHE	CE2-CZ	-5.11	1.23	1.38
3	C	254	LYS	CD-CE	-5.11	1.37	1.52
1	A	95	PHE	CD1-CE1	5.11	1.53	1.38
1	A	946	VAL	C-N	-5.11	1.25	1.33
1	A	1067	LEU	C-O	-5.11	1.18	1.24
9	K	72	LYS	N-CA	-5.11	1.39	1.46
1	A	377	PRO	N-CD	-5.11	1.40	1.47
2	B	285	ILE	CB-CG1	-5.11	1.43	1.53
2	B	989	THR	CA-C	5.11	1.59	1.52
2	B	1080	LYS	CE-NZ	5.11	1.64	1.49
2	B	519	TRP	CZ2-CH2	5.11	1.47	1.37
3	C	103	ALA	N-CA	5.11	1.52	1.46
3	C	215	GLU	N-CA	5.11	1.52	1.46
1	A	505	CYS	N-CA	-5.10	1.39	1.46
1	A	1243	VAL	CB-CG2	5.10	1.69	1.52
4	E	2	ASP	CB-CG	5.10	1.64	1.52
1	A	375	THR	C-N	-5.10	1.25	1.33
1	A	973	ILE	CB-CG2	5.10	1.69	1.52
3	C	79	GLN	C-O	-5.10	1.17	1.24
3	C	113	VAL	CA-C	-5.10	1.46	1.52
7	I	67	THR	CB-OG1	-5.10	1.35	1.43
3	C	212	PRO	CA-C	-5.10	1.47	1.52
1	A	8	SER	CA-CB	5.10	1.62	1.53
3	C	218	PRO	C-O	5.10	1.29	1.23
7	I	102	VAL	C-N	5.10	1.40	1.33
8	J	63	TYR	CA-CB	5.10	1.61	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	9	ALA	N-CA	5.10	1.54	1.46
1	A	26	GLU	CA-CB	-5.10	1.46	1.53
1	A	326	ARG	CA-CB	5.10	1.62	1.53
1	A	594	GLY	C-N	-5.10	1.26	1.33
1	A	970	THR	N-CA	-5.10	1.39	1.46
1	A	1056	SER	C-O	-5.10	1.17	1.24
2	B	266	ALA	CA-C	5.10	1.59	1.52
1	A	1039	LYS	C-N	-5.10	1.26	1.33
2	B	1109	GLY	C-N	5.10	1.42	1.34
6	H	93	TYR	CE2-CZ	5.10	1.50	1.38
2	B	516	ASN	N-CA	5.09	1.52	1.46
2	B	816	GLU	C-N	-5.09	1.26	1.33
1	A	54	ASN	CB-CG	5.09	1.64	1.52
2	B	894	ASP	CG-OD1	5.09	1.35	1.25
1	A	1020	CYS	N-CA	5.09	1.52	1.46
3	C	193	TYR	N-CA	-5.09	1.40	1.46
9	K	67	PHE	CG-CD1	-5.09	1.28	1.38
1	A	280	GLU	N-CA	-5.09	1.40	1.46
2	B	751	VAL	CB-CG1	-5.09	1.35	1.52
4	E	184	VAL	N-CA	5.09	1.52	1.46
5	F	97	ARG	CZ-NH1	5.09	1.39	1.32
1	A	86	LEU	CG-CD1	-5.09	1.35	1.52
2	B	589	VAL	CB-CG1	-5.09	1.35	1.52
2	B	612	GLU	N-CA	-5.09	1.39	1.46
3	C	219	PHE	CB-CG	5.09	1.62	1.50
1	A	582	ILE	CA-CB	-5.08	1.47	1.54
1	A	586	ILE	CB-CG2	-5.08	1.35	1.52
2	B	695	ALA	C-N	-5.08	1.26	1.33
2	B	1007	VAL	CB-CG2	-5.08	1.35	1.52
10	L	46	VAL	CA-C	-5.08	1.46	1.52
1	A	229	SER	CA-CB	-5.08	1.45	1.52
1	A	434	ARG	CZ-NH1	5.08	1.39	1.32
1	A	443	LEU	CB-CG	-5.08	1.43	1.53
2	B	422	LYS	CG-CD	5.08	1.67	1.52
2	B	730	ARG	C-O	-5.08	1.17	1.23
4	E	183	PRO	N-CD	-5.08	1.40	1.47
9	K	100	ALA	C-N	-5.08	1.27	1.34
1	A	1265	ASN	CB-CG	5.08	1.64	1.52
1	A	1406	VAL	CB-CG1	5.08	1.69	1.52
2	B	650	GLU	C-N	-5.08	1.26	1.33
1	A	1055	ARG	CZ-NH2	5.08	1.40	1.33
3	C	128	ASN	CA-CB	-5.08	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	14	ARG	C-O	5.08	1.30	1.24
8	J	52	THR	CB-CG2	-5.08	1.35	1.52
8	J	59	LYS	CD-CE	5.08	1.67	1.52
2	B	797	TYR	N-CA	-5.08	1.40	1.46
9	K	88	LYS	N-CA	-5.08	1.40	1.46
1	A	714	PHE	CG-CD1	-5.08	1.28	1.38
1	A	1129	GLU	CB-CG	5.08	1.67	1.52
2	B	430	ARG	N-CA	-5.08	1.40	1.46
1	A	556	TRP	CZ3-CH2	-5.07	1.27	1.40
1	A	780	VAL	C-O	5.07	1.28	1.23
1	A	1023	ARG	CZ-NH2	-5.07	1.26	1.33
2	B	241	ARG	CD-NE	5.07	1.53	1.46
3	C	65	HIS	CB-CG	5.07	1.57	1.50
9	K	78	THR	CB-OG1	-5.07	1.35	1.43
1	A	467	THR	CA-C	-5.07	1.46	1.52
1	A	1420	ASP	N-CA	5.07	1.53	1.46
2	B	322	PHE	CD1-CE1	-5.07	1.23	1.38
1	A	1060	PRO	CB-CG	-5.07	1.24	1.49
2	B	330	ALA	N-CA	-5.07	1.40	1.46
2	B	554	ILE	CA-C	-5.07	1.46	1.52
2	B	852	ARG	C-N	-5.07	1.26	1.33
2	B	1136	ASP	C-N	-5.07	1.27	1.33
1	A	85	ASP	N-CA	5.07	1.52	1.45
2	B	1141	HIS	CG-ND1	-5.07	1.32	1.38
2	B	1174	LYS	C-O	5.07	1.30	1.23
3	C	207	CYS	C-O	-5.07	1.18	1.24
3	C	250	THR	C-N	-5.07	1.27	1.33
9	K	65	HIS	N-CA	-5.07	1.38	1.46
1	A	1003	LYS	N-CA	-5.07	1.40	1.46
2	B	91	SER	CA-C	-5.07	1.46	1.52
10	L	61	THR	C-O	5.07	1.30	1.23
1	A	130	ASP	CA-CB	-5.07	1.45	1.53
1	A	248	PRO	CA-CB	5.07	1.63	1.53
1	A	711	ARG	CB-CG	5.07	1.67	1.52
1	A	777	PHE	CA-CB	5.07	1.61	1.53
1	A	1326	ARG	CB-CG	-5.07	1.37	1.52
3	C	236	GLY	C-O	5.07	1.30	1.23
2	B	711	GLU	CD-OE1	5.06	1.34	1.25
2	B	1031	LEU	CA-C	-5.06	1.45	1.52
1	A	694	THR	CA-CB	-5.06	1.45	1.53
1	A	758	ILE	CG1-CD1	-5.06	1.32	1.51
1	A	1049	ILE	N-CA	-5.06	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1224	LEU	C-O	-5.06	1.17	1.24
2	B	816	GLU	CD-OE2	5.06	1.34	1.25
2	B	1174	LYS	C-N	5.06	1.40	1.33
10	L	59	ALA	C-O	-5.06	1.17	1.24
1	A	567	LYS	CG-CD	5.06	1.67	1.52
1	A	929	LEU	CG-CD2	-5.06	1.35	1.52
1	A	1297	GLU	CD-OE2	5.06	1.34	1.25
2	B	618	ASP	CA-C	-5.06	1.46	1.52
2	B	860	MET	CG-SD	5.06	1.93	1.80
4	E	9	ILE	N-CA	5.06	1.52	1.46
6	H	137	GLN	C-O	-5.06	1.17	1.23
1	A	553	VAL	CB-CG1	-5.06	1.35	1.52
1	A	727	ASP	CA-C	-5.06	1.46	1.52
1	A	779	PHE	CG-CD1	-5.06	1.28	1.38
1	A	1193	LEU	C-N	-5.06	1.27	1.33
4	E	61	GLN	CG-CD	-5.06	1.39	1.52
9	K	89	ASN	CG-OD1	5.06	1.33	1.23
1	A	941	LYS	CA-C	-5.06	1.46	1.52
2	B	262	GLU	N-CA	5.06	1.52	1.46
2	B	268	THR	CA-C	-5.06	1.46	1.52
1	A	161	LEU	CA-CB	5.05	1.61	1.53
1	A	389	THR	N-CA	-5.05	1.40	1.46
1	A	530	GLY	N-CA	-5.05	1.38	1.45
1	A	758	ILE	C-N	-5.05	1.27	1.33
1	A	1195	LEU	CA-C	-5.05	1.46	1.52
2	B	112	LEU	CA-C	-5.05	1.46	1.52
2	B	347	LYS	CA-C	-5.05	1.45	1.52
2	B	811	TYR	C-O	-5.05	1.17	1.24
2	B	914	LYS	CB-CG	-5.05	1.37	1.52
3	C	125	MET	C-N	5.05	1.40	1.33
6	H	50	ALA	CA-CB	5.05	1.63	1.53
8	J	62	ARG	CG-CD	-5.05	1.37	1.52
2	B	217	ARG	CZ-NH1	-5.05	1.25	1.32
1	A	726	ARG	CA-C	-5.05	1.46	1.52
1	A	1028	THR	CA-C	5.05	1.59	1.52
3	C	219	PHE	CD2-CE2	-5.05	1.23	1.38
1	A	189	ARG	C-N	5.05	1.40	1.33
2	B	203	PHE	CG-CD1	-5.05	1.28	1.38
2	B	480	SER	C-N	-5.05	1.26	1.33
2	B	566	LEU	CG-CD2	-5.05	1.35	1.52
2	B	635	ARG	NE-CZ	5.05	1.38	1.33
1	A	108	MET	CA-CB	-5.05	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	557	ASP	C-N	-5.05	1.26	1.33
2	B	994	TYR	CD2-CE2	-5.05	1.23	1.38
4	E	142	VAL	CB-CG1	-5.05	1.35	1.52
7	I	42	LEU	CG-CD2	-5.05	1.35	1.52
1	A	664	THR	CB-CG2	-5.05	1.35	1.52
2	B	943	SER	CA-C	5.05	1.59	1.52
2	B	1146	PHE	CE1-CZ	-5.05	1.23	1.38
3	C	238	ILE	CB-CG1	-5.05	1.43	1.53
4	E	58	MET	CB-CG	-5.05	1.37	1.52
4	E	148	GLU	N-CA	5.05	1.52	1.46
4	E	178	ILE	CB-CG2	5.05	1.69	1.52
1	A	277	GLU	CD-OE2	5.04	1.34	1.25
2	B	378	LEU	C-N	-5.04	1.28	1.33
2	B	684	LEU	CG-CD1	-5.04	1.35	1.52
1	A	290	GLU	CA-C	5.04	1.60	1.52
3	C	169	LYS	CD-CE	5.04	1.67	1.52
4	E	84	ASP	CG-OD1	5.04	1.34	1.25
1	A	363	GLN	CB-CG	-5.04	1.37	1.52
1	A	394	ASN	CA-C	-5.04	1.45	1.52
1	A	433	GLU	C-O	5.04	1.30	1.23
1	A	1075	PRO	C-N	-5.04	1.27	1.34
2	B	351	TYR	CA-C	5.04	1.59	1.52
2	B	446	LEU	C-N	5.04	1.40	1.33
2	B	1149	GLU	CG-CD	5.04	1.64	1.52
6	H	129	TYR	C-O	-5.04	1.17	1.24
1	A	191	THR	C-N	5.04	1.41	1.33
1	A	709	THR	CA-C	-5.04	1.46	1.53
2	B	1150	ARG	CD-NE	-5.04	1.39	1.46
10	L	45	ALA	C-N	5.04	1.40	1.33
1	A	562	THR	CB-CG2	5.04	1.69	1.52
1	A	1226	VAL	CA-C	-5.04	1.46	1.52
2	B	358	LYS	CG-CD	5.04	1.67	1.52
2	B	1107	ALA	CA-CB	-5.04	1.46	1.53
4	E	98	ILE	C-O	-5.04	1.17	1.24
8	J	4	PRO	CA-C	-5.04	1.45	1.52
1	A	451	HIS	CD2-NE2	-5.03	1.32	1.37
1	A	473	SER	C-O	-5.03	1.17	1.24
1	A	577	ILE	CG1-CD1	-5.03	1.32	1.51
1	A	859	SER	CA-CB	-5.03	1.44	1.53
2	B	191	LYS	C-N	-5.03	1.25	1.33
4	E	163	GLU	C-N	-5.03	1.27	1.33
7	I	110	PHE	CD1-CE1	5.03	1.53	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	447	GLN	CG-CD	-5.03	1.39	1.52
7	I	100	PHE	CE2-CZ	-5.03	1.23	1.38
1	A	231	PRO	N-CA	-5.03	1.41	1.47
1	A	384	ASN	CG-OD1	-5.03	1.14	1.23
1	A	572	TRP	CD2-CE2	-5.03	1.32	1.41
1	A	639	PRO	N-CA	-5.03	1.40	1.47
2	B	378	LEU	CG-CD2	-5.03	1.35	1.52
3	C	159	ALA	N-CA	-5.03	1.39	1.45
3	C	178	PHE	N-CA	5.03	1.52	1.46
3	C	206	ASN	CB-CG	-5.03	1.39	1.52
6	H	47	PHE	CD1-CE1	-5.03	1.23	1.38
7	I	28	GLU	CA-CB	-5.03	1.46	1.53
9	K	96	ASN	CA-CB	5.03	1.61	1.53
5	F	101	ILE	CA-CB	-5.03	1.47	1.54
1	A	1444	MET	CB-CG	-5.03	1.37	1.52
4	E	45	LYS	CE-NZ	5.03	1.64	1.49
1	A	698	GLN	N-CA	-5.03	1.39	1.46
1	A	1349	TYR	CE1-CZ	-5.03	1.26	1.38
2	B	212	LEU	N-CA	-5.03	1.40	1.46
2	B	401	PHE	CD1-CE1	-5.03	1.23	1.38
3	C	108	GLU	N-CA	5.03	1.52	1.46
6	H	41	ASP	CG-OD2	-5.03	1.15	1.25
1	A	946	VAL	CA-C	-5.02	1.45	1.52
1	A	898	ARG	CD-NE	5.02	1.53	1.46
2	B	787	VAL	CA-CB	-5.02	1.48	1.54
2	B	1071	VAL	CB-CG1	-5.02	1.35	1.52
2	B	33	VAL	CA-CB	5.02	1.60	1.54
2	B	116	GLU	CD-OE2	5.02	1.34	1.25
1	A	213	HIS	CB-CG	5.02	1.57	1.50
2	B	496	ARG	NE-CZ	5.02	1.38	1.33
5	F	114	GLU	CD-OE2	5.02	1.34	1.25
1	A	412	ARG	CA-C	-5.02	1.46	1.52
1	A	1192	LEU	CA-CB	-5.02	1.45	1.53
2	B	327	ARG	CA-C	-5.02	1.45	1.52
3	C	138	GLU	CD-OE2	5.02	1.34	1.25
3	C	208	GLU	CG-CD	5.02	1.64	1.52
4	E	125	PRO	CG-CD	5.02	1.67	1.50
5	F	96	THR	CA-C	5.02	1.59	1.52
7	I	93	LYS	CA-C	5.02	1.59	1.52
1	A	424	ILE	N-CA	5.02	1.52	1.46
1	A	830	LYS	C-O	5.02	1.29	1.24
2	B	41	LYS	CD-CE	5.01	1.67	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	323	VAL	CB-CG2	5.01	1.69	1.52
2	B	732	SER	N-CA	5.01	1.52	1.45
7	I	32	CYS	CB-SG	-5.01	1.64	1.81
9	K	1	MET	CG-SD	-5.01	1.68	1.80
9	K	96	ASN	CB-CG	5.01	1.64	1.52
2	B	1031	LEU	CG-CD1	-5.01	1.36	1.52
1	A	1141	THR	CA-C	5.01	1.58	1.52
1	A	1201	ALA	N-CA	-5.01	1.40	1.46
2	B	114	PRO	N-CA	-5.01	1.41	1.47
5	F	98	ALA	C-N	-5.01	1.27	1.33
7	I	99	LEU	CG-CD1	-5.01	1.36	1.52
1	A	89	PRO	CA-CB	-5.01	1.47	1.53
1	A	605	MET	N-CA	-5.01	1.40	1.46
1	A	786	HIS	CG-CD2	-5.01	1.30	1.35
2	B	567	GLU	CB-CG	5.01	1.67	1.52
2	B	638	PHE	CE1-CZ	-5.01	1.23	1.38
4	E	25	ASP	CG-OD1	-5.01	1.15	1.25
4	E	167	ARG	CG-CD	5.01	1.67	1.52
5	F	125	LEU	CG-CD1	-5.01	1.36	1.52
1	A	805	LEU	C-O	-5.01	1.18	1.24
2	B	454	THR	C-N	-5.01	1.26	1.33
2	B	591	ARG	CA-CB	-5.01	1.45	1.53
2	B	203	PHE	CD2-CE2	-5.00	1.23	1.38
2	B	429	PHE	CE1-CZ	5.00	1.53	1.38
1	A	1081	LEU	N-CA	5.00	1.55	1.46
2	B	68	THR	C-O	5.00	1.29	1.23
2	B	182	SER	CA-C	-5.00	1.46	1.52
4	E	102	GLU	CB-CG	5.00	1.67	1.52
1	A	655	PHE	C-O	-5.00	1.18	1.24
1	A	756	ILE	CB-CG2	-5.00	1.36	1.52
2	B	625	LYS	CA-CB	5.00	1.62	1.53
2	B	818	PRO	CA-C	5.00	1.58	1.52
2	B	821	GLN	CB-CG	-5.00	1.37	1.52
2	B	1109	GLY	N-CA	5.00	1.51	1.44

All (4861) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1064	VAL	CA-C-O	-60.75	44.85	120.78
1	A	1064	VAL	O-C-N	-42.11	69.93	122.57
1	A	1064	VAL	CB-CA-C	22.66	148.46	111.29
1	A	1064	VAL	N-CA-CB	-21.45	75.83	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	43	VAL	N-CA-CB	-18.76	83.56	112.07
1	A	1064	VAL	CA-C-N	-18.27	85.59	121.41
1	A	1064	VAL	C-N-CA	-18.27	85.59	121.41
5	F	136	ARG	NE-CZ-NH1	-18.26	103.24	121.50
2	B	1165	ILE	N-CA-C	-18.12	97.22	111.90
1	A	1166	ASP	N-CA-C	-17.77	92.46	112.72
5	F	81	THR	N-CA-CB	-17.53	86.36	110.38
1	A	1259	MET	N-CA-C	-17.48	92.22	111.28
1	A	93	VAL	CB-CA-C	-17.38	89.27	112.04
2	B	1075	GLY	N-CA-C	17.12	133.36	112.64
2	B	1196	ILE	N-CA-C	16.72	122.90	109.19
8	J	2	ILE	CG1-CB-CG2	-16.51	61.18	110.70
2	B	1183	LYS	N-CA-C	-16.44	85.63	110.30
1	A	1136	SER	N-CA-C	-16.41	92.88	113.23
9	K	94	ILE	N-CA-C	-16.29	95.92	110.74
3	C	183	TRP	CA-C-N	-16.15	98.57	123.12
3	C	183	TRP	C-N-CA	-16.15	98.57	123.12
1	A	466	SER	N-CA-C	16.10	132.34	113.02
2	B	1042	GLY	CA-C-O	-15.92	107.06	120.91
1	A	1367	HIS	CA-CB-CG	-15.81	97.99	113.80
1	A	1146	VAL	N-CA-CB	-15.62	92.11	112.26
2	B	1077	THR	N-CA-CB	-15.59	90.40	110.98
8	J	43	ARG	NE-CZ-NH2	15.55	133.19	119.20
1	A	725	ALA	N-CA-C	15.31	128.05	111.36
2	B	1150	ARG	NE-CZ-NH1	-15.25	106.25	121.50
1	A	821	ARG	NE-CZ-NH2	-15.18	105.54	119.20
4	E	106	GLN	N-CA-C	-15.14	94.81	113.28
2	B	1185	CYS	N-CA-C	-15.12	94.79	113.38
2	B	501	PRO	CA-C-O	-15.11	103.81	121.03
5	F	125	LEU	N-CA-C	-15.07	93.15	112.90
1	A	469	ARG	NE-CZ-NH2	-15.00	105.70	119.20
3	C	70	ILE	CB-CA-C	-14.96	97.03	110.94
1	A	774	ARG	NE-CZ-NH1	14.82	136.32	121.50
2	B	1097	HIS	CB-CG-ND1	-14.81	100.49	122.70
3	C	252	GLN	N-CA-C	-14.74	95.29	111.36
2	B	807	ARG	NE-CZ-NH2	-14.72	105.95	119.20
1	A	830	LYS	CB-CA-C	-14.57	87.75	110.92
1	A	896	ARG	NE-CZ-NH2	-14.41	106.23	119.20
4	E	147	HIS	CB-CG-CD2	14.37	149.88	131.20
2	B	839	MET	CG-SD-CE	-14.28	69.48	100.90
2	B	1150	ARG	NH1-CZ-NH2	14.25	137.82	119.30
2	B	498	THR	N-CA-CB	-14.21	86.97	111.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1241	ARG	NE-CZ-NH2	-14.13	106.48	119.20
7	I	31	THR	N-CA-CB	-14.13	91.80	110.59
2	B	1005	GLY	N-CA-C	14.12	133.97	115.47
3	C	202	PRO	CA-C-O	-14.03	104.47	121.31
2	B	802	PRO	CA-C-O	-14.02	104.56	120.97
2	B	709	ASP	N-CA-C	-13.94	95.61	113.17
1	A	1137	ALA	CA-C-N	-13.92	109.16	122.66
1	A	1137	ALA	C-N-CA	-13.92	109.16	122.66
8	J	22	LEU	N-CA-CB	-13.92	89.56	110.16
1	A	1318	THR	N-CA-CB	-13.75	90.14	110.49
4	E	5	ASN	N-CA-C	-13.73	96.20	113.23
1	A	1004	ASN	N-CA-C	13.73	128.04	110.33
7	I	98	VAL	CA-C-O	-13.72	106.90	122.13
1	A	982	THR	N-CA-CB	-13.71	89.61	110.45
2	B	642	ASP	N-CA-C	-13.62	84.03	107.99
10	L	57	LEU	N-CA-C	13.56	131.99	107.99
1	A	295	LEU	N-CA-C	-13.54	95.03	111.69
8	J	7	CYS	CA-CB-SG	13.51	145.46	114.40
1	A	9	ALA	N-CA-C	-13.50	92.84	109.72
4	E	176	PRO	CB-CA-C	-13.43	93.79	111.12
1	A	630	ILE	N-CA-C	-13.41	96.38	111.00
4	E	11	ARG	NE-CZ-NH1	-13.39	108.11	121.50
2	B	260	GLY	N-CA-C	-13.39	96.28	112.48
1	A	661	GLY	CA-C-O	-13.37	110.61	122.24
1	A	949	ASP	N-CA-CB	-13.35	88.64	110.40
1	A	538	ASP	CB-CA-C	-13.26	86.14	110.01
1	A	50	ILE	N-CA-C	13.26	126.73	108.17
1	A	1014	ALA	CA-C-O	13.23	135.50	119.49
2	B	995	ARG	NE-CZ-NH2	-13.21	107.31	119.20
1	A	1006	ILE	CG1-CB-CG2	-13.21	71.07	110.70
2	B	453	ILE	N-CA-C	-13.18	98.75	110.74
1	A	607	ILE	CA-C-O	-13.17	106.55	120.64
3	C	230	MET	N-CA-C	13.16	128.51	110.35
2	B	620	ARG	NH1-CZ-NH2	13.12	136.35	119.30
1	A	832	ALA	N-CA-C	13.11	125.09	111.07
2	B	531	GLN	N-CA-C	-13.08	96.67	112.89
8	J	43	ARG	NE-CZ-NH1	-13.02	108.48	121.50
4	E	204	THR	CA-CB-CG2	12.97	132.55	110.50
2	B	680	THR	N-CA-CB	-12.97	90.61	111.62
1	A	170	THR	N-CA-C	-12.94	93.84	110.53
7	I	10	CYS	N-CA-C	12.88	128.86	112.89
1	A	102	VAL	N-CA-C	-12.88	98.43	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	768	THR	CA-CB-OG1	12.86	128.89	109.60
9	K	85	ASP	N-CA-C	-12.86	96.95	112.89
4	E	98	ILE	CB-CA-C	12.71	129.27	112.24
4	E	147	HIS	CG-CD2-NE2	-12.69	94.52	107.20
3	C	77	ILE	N-CA-C	-12.60	99.69	113.43
1	A	704	ALA	CA-C-N	-12.57	103.87	123.23
1	A	704	ALA	C-N-CA	-12.57	103.87	123.23
5	F	82	THR	CB-CA-C	-12.47	89.19	109.27
2	B	419	THR	OG1-CB-CG2	-12.46	84.38	109.30
9	K	47	ARG	NE-CZ-NH2	-12.43	108.01	119.20
2	B	753	ALA	N-CA-C	-12.40	98.18	113.18
2	B	496	ARG	NE-CZ-NH1	12.36	133.86	121.50
2	B	511	PRO	N-CD-CG	-12.36	84.66	103.20
5	F	114	GLU	CA-C-O	-12.36	108.08	121.56
10	L	70	ARG	NE-CZ-NH1	12.29	133.79	121.50
6	H	59	ILE	CB-CA-C	-12.26	97.72	111.45
1	A	1135	ARG	NE-CZ-NH1	-12.22	109.28	121.50
1	A	774	ARG	NE-CZ-NH2	-12.20	108.22	119.20
1	A	1438	THR	N-CA-CB	-12.19	89.06	110.39
3	C	15	LYS	CG-CD-CE	12.15	139.24	111.30
4	E	98	ILE	N-CA-C	-12.14	97.77	111.00
1	A	1310	GLY	CA-C-O	-12.12	113.86	122.23
1	A	1336	MET	CG-SD-CE	12.10	127.52	100.90
8	J	21	TYR	N-CA-C	-12.10	94.61	112.04
8	J	1	MET	CG-SD-CE	-12.07	74.34	100.90
1	A	389	THR	OG1-CB-CG2	-12.06	85.18	109.30
3	C	240	VAL	N-CA-C	12.03	122.87	110.72
1	A	1275	GLY	N-CA-C	-12.03	97.42	111.85
2	B	1139	ILE	O-C-N	-12.02	109.40	121.90
6	H	102	TYR	CA-C-O	12.02	132.51	118.69
2	B	1135	ARG	NE-CZ-NH2	-12.01	108.39	119.20
1	A	566	ILE	CB-CA-C	-11.99	97.76	111.55
2	B	601	ARG	NE-CZ-NH1	-11.99	109.51	121.50
1	A	806	ARG	NE-CZ-NH1	-11.98	109.52	121.50
10	L	68	GLU	CG-CD-OE1	11.89	145.75	118.40
6	H	26	ILE	CB-CA-C	-11.88	97.18	111.08
3	C	253	LYS	N-CA-C	11.86	125.68	111.33
3	C	210	GLU	O-C-N	-11.85	110.21	123.48
2	B	895	ASP	N-CA-C	-11.84	98.80	113.01
1	A	170	THR	OG1-CB-CG2	-11.82	85.65	109.30
2	B	598	GLU	CB-CG-CD	11.81	132.68	112.60
5	F	136	ARG	NE-CZ-NH2	11.77	129.79	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	93	LYS	N-CA-C	-11.75	98.32	112.89
1	A	1062	GLU	CB-CA-C	-11.73	89.59	109.65
2	B	1183	LYS	CB-CA-C	11.73	126.36	110.06
6	H	12	VAL	N-CA-C	11.73	125.69	107.98
3	C	18	VAL	CB-CA-C	-11.72	92.06	111.29
6	H	57	VAL	N-CA-C	11.71	124.68	106.88
1	A	466	SER	CB-CA-C	-11.63	89.67	110.37
4	E	125	PRO	N-CA-C	-11.59	91.21	110.21
2	B	981	ALA	N-CA-C	11.58	127.17	108.99
2	B	963	PHE	CB-CA-C	-11.57	87.26	109.37
3	C	53	THR	OG1-CB-CG2	-11.57	86.16	109.30
1	A	605	MET	CG-SD-CE	-11.57	75.45	100.90
1	A	866	PHE	N-CA-C	-11.55	99.29	113.50
1	A	464	PRO	O-C-N	-11.55	107.05	122.64
2	B	131	ASP	N-CA-C	-11.51	88.01	107.23
4	E	102	GLU	N-CA-C	-11.49	99.39	113.41
7	I	106	CYS	CA-CB-SG	11.48	140.80	114.40
4	E	17	ARG	CA-C-O	11.47	133.17	120.90
2	B	525	ALA	N-CA-C	11.47	127.93	112.68
2	B	962	LYS	N-CA-C	-11.44	90.47	109.46
1	A	980	ASP	N-CA-C	11.39	126.69	113.02
1	A	1284	MET	N-CA-C	-11.38	92.22	110.32
4	E	24	LYS	CD-CE-NZ	-11.37	75.52	111.90
1	A	1154	TYR	CA-C-O	-11.33	107.74	120.43
2	B	206	ASN	N-CA-C	-11.32	96.75	111.92
1	A	1133	LEU	N-CA-C	-11.29	98.72	111.82
1	A	1299	VAL	N-CA-CB	-11.28	95.54	112.35
1	A	1130	GLN	N-CA-C	-11.27	99.55	113.18
3	C	247	GLY	CA-C-O	-11.24	108.74	120.66
1	A	557	ASP	O-C-N	-11.23	109.00	122.81
2	B	911	ILE	N-CA-CB	-11.23	92.70	111.23
1	A	877	HIS	ND1-CE1-NE2	-11.23	97.17	108.40
1	A	1154	TYR	N-CA-C	-11.20	91.15	108.96
1	A	1013	ASP	N-CA-C	-11.19	99.16	111.36
2	B	653	VAL	CB-CA-C	-11.19	96.92	111.13
2	B	982	SER	CA-C-O	-11.19	107.57	121.67
1	A	708	MET	N-CA-CB	-11.18	92.03	110.81
1	A	789	LYS	N-CA-C	11.16	125.05	110.43
1	A	1291	VAL	N-CA-CB	-11.15	99.70	111.64
2	B	268	THR	N-CA-CB	-11.13	94.11	110.70
2	B	416	LEU	CB-CA-C	-11.13	93.69	110.95
2	B	1019	SER	CB-CA-C	-11.12	87.06	110.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	229	TYR	N-CA-C	11.11	127.05	109.39
1	A	1376	THR	N-CA-CB	-11.09	90.59	111.43
2	B	903	VAL	N-CA-C	11.09	123.52	108.89
3	C	241	ASP	N-CA-C	-11.06	98.99	111.71
2	B	942	ARG	CB-CA-C	-11.05	94.35	109.71
8	J	50	ILE	N-CA-C	-11.04	99.87	111.58
2	B	855	PHE	CA-C-O	-11.04	108.54	120.24
2	B	620	ARG	NE-CZ-NH2	-11.02	109.28	119.20
2	B	678	GLU	CB-CG-CD	11.02	131.33	112.60
1	A	50	ILE	CB-CA-C	-11.01	94.43	110.83
4	E	11	ARG	NH1-CZ-NH2	10.99	133.59	119.30
2	B	272	THR	OG1-CB-CG2	-10.99	87.32	109.30
2	B	747	MET	CG-SD-CE	-10.97	76.75	100.90
10	L	40	LEU	CA-C-O	-10.97	109.53	121.05
4	E	14	ARG	CA-C-N	-10.96	103.64	120.31
4	E	14	ARG	C-N-CA	-10.96	103.64	120.31
2	B	365	THR	N-CA-C	-10.96	92.03	108.79
1	A	1129	GLU	N-CA-C	-10.95	99.65	113.23
3	C	49	VAL	CA-C-O	-10.95	108.92	120.64
1	A	1368	MET	N-CA-C	-10.95	99.65	113.23
1	A	646	PHE	CA-C-N	-10.94	106.33	120.22
1	A	646	PHE	C-N-CA	-10.94	106.33	120.22
1	A	876	ALA	N-CA-C	10.90	125.68	112.38
2	B	860	MET	CB-CA-C	-10.90	91.81	109.80
2	B	1203	LEU	CA-C-O	10.89	133.12	120.92
2	B	137	TYR	CA-CB-CG	10.88	133.48	113.90
1	A	469	ARG	NE-CZ-NH1	10.87	132.37	121.50
7	I	110	PHE	CA-C-O	-10.86	109.83	121.45
2	B	212	LEU	CD1-CG-CD2	-10.86	86.92	110.80
2	B	598	GLU	N-CA-CB	10.86	126.22	110.16
3	C	35	ARG	NE-CZ-NH2	-10.85	109.43	119.20
4	E	77	SER	N-CA-C	-10.85	92.73	109.65
1	A	815	PHE	N-CA-C	-10.85	99.44	112.89
7	I	27	PHE	N-CA-C	10.83	126.38	108.73
2	B	1183	LYS	CA-C-N	-10.81	111.84	123.30
2	B	1183	LYS	C-N-CA	-10.81	111.84	123.30
3	C	163	ILE	CA-CB-CG2	10.81	128.88	110.50
2	B	1025	HIS	ND1-CE1-NE2	-10.80	97.60	108.40
10	L	53	HIS	N-CA-C	10.80	126.13	108.96
2	B	452	THR	CA-C-N	10.79	134.04	120.88
2	B	452	THR	C-N-CA	10.79	134.04	120.88
3	C	267	GLN	N-CA-C	10.79	126.31	108.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	99	ILE	N-CA-C	-10.78	98.33	110.62
1	A	218	ASP	N-CA-C	-10.78	98.44	111.69
3	C	124	LEU	N-CA-C	10.76	128.22	113.37
1	A	826	ASP	N-CA-C	-10.76	99.63	111.36
1	A	1018	PHE	CA-CB-CG	-10.76	103.04	113.80
2	B	267	ARG	N-CA-C	10.76	125.40	109.59
2	B	165	VAL	CB-CA-C	-10.75	93.66	111.29
1	A	1042	PHE	N-CA-C	-10.74	99.58	111.07
6	H	107	VAL	N-CA-C	-10.74	87.01	109.34
3	C	66	ARG	NE-CZ-NH1	-10.73	110.77	121.50
1	A	982	THR	N-CA-C	10.73	125.04	110.55
1	A	969	GLN	N-CA-C	-10.72	100.05	113.55
2	B	546	SER	CA-C-O	-10.70	109.89	121.56
1	A	636	GLU	N-CA-C	-10.68	98.91	112.90
2	B	983	ARG	NE-CZ-NH2	-10.68	109.59	119.20
1	A	738	LYS	CA-C-O	-10.67	109.13	121.72
1	A	516	SER	N-CA-CB	-10.66	96.08	111.54
2	B	90	ILE	CB-CA-C	-10.66	93.81	111.29
1	A	790	ASP	CA-C-O	-10.64	109.20	121.54
7	I	13	MET	N-CA-CB	-10.64	95.15	110.36
9	K	83	PRO	N-CD-CG	-10.63	87.26	103.20
1	A	1228	TRP	CB-CA-C	-10.62	90.59	110.56
8	J	43	ARG	N-CA-C	10.61	125.98	110.28
2	B	836	GLU	CA-C-O	-10.60	108.78	122.03
4	E	47	CYS	N-CA-C	10.60	126.67	109.40
4	E	53	PRO	CA-C-N	-10.60	107.46	123.14
4	E	53	PRO	C-N-CA	-10.60	107.46	123.14
8	J	2	ILE	CB-CG1-CD1	-10.59	91.55	113.80
3	C	89	GLU	N-CA-C	-10.59	91.88	109.46
2	B	983	ARG	NE-CZ-NH1	10.59	132.09	121.50
1	A	793	SER	N-CA-C	10.57	125.59	109.41
2	B	1164	GLY	CA-C-O	10.57	128.66	119.04
2	B	293	PRO	CA-C-O	-10.56	108.63	121.31
2	B	1097	HIS	CA-CB-CG	-10.56	103.23	113.80
2	B	639	ILE	CA-CB-CG1	10.54	128.32	110.40
8	J	38	ARG	N-CA-C	-10.53	98.97	112.23
1	A	504	LEU	N-CA-CB	-10.53	95.23	110.81
2	B	869	SER	CA-C-N	10.53	131.54	121.65
2	B	869	SER	C-N-CA	10.53	131.54	121.65
2	B	97	VAL	N-CA-C	-10.52	92.97	108.12
5	F	136	ARG	CA-C-O	-10.50	109.34	120.58
1	A	964	ILE	N-CA-C	-10.50	99.55	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	69	THR	CA-C-N	10.50	135.20	120.29
1	A	69	THR	C-N-CA	10.50	135.20	120.29
1	A	59	GLY	N-CA-C	10.50	138.06	113.18
1	A	93	VAL	N-CA-C	10.46	122.55	110.62
2	B	394	ASP	N-CA-CB	-10.46	94.39	110.29
9	K	6	ARG	NE-CZ-NH2	-10.46	109.78	119.20
3	C	165	LYS	CD-CE-NZ	10.46	145.37	111.90
1	A	535	THR	N-CA-CB	-10.43	95.33	110.56
1	A	396	PRO	CA-C-O	-10.43	104.99	118.86
2	B	833	TYR	CA-C-O	-10.41	107.38	119.56
2	B	848	ARG	NE-CZ-NH1	-10.41	111.08	121.50
2	B	828	ALA	N-CA-C	10.41	125.21	108.76
1	A	907	THR	CB-CA-C	-10.41	90.12	114.16
2	B	416	LEU	N-CA-CB	10.41	125.07	109.98
1	A	288	ALA	CA-C-N	10.40	133.87	120.56
1	A	288	ALA	C-N-CA	10.40	133.87	120.56
7	I	75	CYS	CA-CB-SG	10.39	138.29	114.40
1	A	744	LYS	N-CA-C	-10.39	98.92	111.69
6	H	80	ARG	N-CA-C	-10.38	92.36	108.55
2	B	983	ARG	CA-CB-CG	10.37	134.84	114.10
6	H	82	PRO	N-CA-C	-10.37	91.12	112.47
1	A	419	LYS	N-CA-C	-10.36	99.74	112.38
8	J	49	MET	CG-SD-CE	-10.35	78.14	100.90
4	E	197	LYS	CB-CA-C	-10.34	93.23	110.19
4	E	154	ILE	CB-CA-C	-10.31	96.50	110.42
7	I	75	CYS	CA-C-O	-10.30	111.33	120.60
7	I	53	GLY	N-CA-C	10.28	130.65	115.64
2	B	604	ARG	NE-CZ-NH2	-10.27	109.95	119.20
5	F	150	GLU	N-CA-CB	-10.27	94.92	110.33
4	E	66	GLU	N-CA-C	-10.26	100.17	111.36
1	A	151	ASP	N-CA-C	-10.26	92.97	108.46
2	B	1184	GLY	N-CA-C	-10.26	102.60	113.58
2	B	65	GLU	N-CA-C	-10.26	97.47	110.19
1	A	182	VAL	N-CA-C	10.25	122.47	108.11
1	A	934	LYS	N-CA-C	-10.25	100.11	111.28
1	A	802	ASN	N-CA-C	10.24	124.27	110.35
7	I	81	ARG	CA-C-O	10.23	135.15	120.51
9	K	34	THR	CA-C-O	10.23	131.25	120.30
2	B	628	THR	OG1-CB-CG2	-10.21	88.87	109.30
8	J	3	VAL	CB-CA-C	-10.20	92.80	111.36
1	A	475	THR	N-CA-CB	-10.20	95.07	110.16
6	H	117	SER	CB-CA-C	-10.20	93.83	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	184	SER	N-CA-C	10.19	124.24	107.23
4	E	118	PRO	N-CD-CG	10.18	118.47	103.20
1	A	659	HIS	CB-CG-ND1	-10.17	107.44	122.70
2	B	59	LEU	N-CA-C	-10.16	95.30	111.04
2	B	1054	GLY	O-C-N	10.16	132.02	122.17
1	A	163	SER	N-CA-CB	10.15	126.96	110.41
4	E	212	ARG	CD-NE-CZ	10.15	138.62	124.40
7	I	119	THR	N-CA-C	10.11	122.00	110.97
10	L	68	GLU	CB-CG-CD	10.11	129.78	112.60
4	E	65	THR	CA-C-N	-10.09	105.97	120.29
4	E	65	THR	C-N-CA	-10.09	105.97	120.29
2	B	1200	ALA	N-CA-C	10.08	122.03	111.14
3	C	4	GLU	O-C-N	10.08	135.99	122.59
9	K	110	ASN	N-CA-C	-10.07	98.45	112.45
2	B	559	SER	N-CA-C	-10.07	101.12	113.50
2	B	1099	VAL	CB-CA-C	-10.06	94.78	111.29
1	A	1384	VAL	CA-C-O	-10.06	109.25	120.32
2	B	104	GLU	N-CA-C	10.04	125.35	110.48
1	A	1280	GLU	O-C-N	-10.04	109.23	122.59
4	E	107	THR	N-CA-C	10.04	124.79	109.23
1	A	1239	ARG	N-CA-CB	-10.03	93.46	110.80
1	A	946	VAL	CB-CA-C	-10.02	98.82	112.24
1	A	919	ILE	N-CA-CB	10.01	123.22	112.21
1	A	925	LEU	N-CA-C	-10.01	100.33	111.14
2	B	530	GLY	N-CA-C	10.01	129.27	110.86
2	B	940	PRO	N-CD-CG	-10.01	88.19	103.20
3	C	33	LEU	N-CA-C	-9.98	99.22	111.40
4	E	49	SER	N-CA-C	9.98	126.30	108.24
1	A	11	LEU	CD1-CG-CD2	-9.96	88.88	110.80
1	A	70	CYS	CA-CB-SG	9.96	137.31	114.40
1	A	1100	ARG	NE-CZ-NH1	9.96	131.46	121.50
7	I	115	LYS	N-CA-C	-9.96	95.67	109.71
2	B	956	THR	CB-CA-C	-9.94	91.51	109.71
9	K	13	GLY	N-CA-C	-9.93	96.86	112.85
2	B	1223	ASP	CA-C-N	9.93	139.57	121.70
2	B	1223	ASP	C-N-CA	9.93	139.57	121.70
1	A	27	VAL	N-CA-C	9.91	119.94	110.42
1	A	366	VAL	CA-C-O	9.91	128.50	119.98
9	K	4	PRO	CA-C-O	-9.90	109.60	121.48
1	A	600	PRO	N-CD-CG	-9.89	88.36	103.20
4	E	175	LEU	N-CA-C	-9.89	97.44	110.40
2	B	727	LYS	N-CA-C	-9.88	95.89	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	J	63	TYR	CA-C-O	-9.89	109.13	121.78
2	B	853	SER	CB-CA-C	-9.88	88.34	110.07
1	A	938	LYS	O-C-N	9.88	132.59	122.12
2	B	225	VAL	N-CA-C	9.88	124.28	108.97
1	A	241	VAL	N-CA-C	9.83	116.51	107.56
2	B	888	GLY	CA-C-O	-9.83	110.46	121.77
9	K	35	PHE	CA-C-O	-9.83	109.42	120.43
1	A	728	LYS	N-CA-CB	9.82	124.56	110.12
3	C	86	CYS	CA-CB-SG	9.81	136.97	114.40
2	B	836	GLU	O-C-N	9.80	134.57	122.91
10	L	63	ARG	CA-C-N	-9.79	104.91	122.74
10	L	63	ARG	C-N-CA	-9.79	104.91	122.74
2	B	223	VAL	CB-CA-C	-9.78	98.78	110.91
2	B	228	LYS	CA-C-O	-9.78	109.42	120.66
3	C	20	PHE	N-CA-C	9.78	120.77	108.45
3	C	14	SER	O-C-N	-9.76	112.89	123.04
1	A	291	GLU	N-CA-C	-9.76	100.73	111.36
2	B	880	THR	N-CA-C	9.74	122.89	109.54
9	K	47	ARG	NE-CZ-NH1	9.74	131.24	121.50
4	E	197	LYS	N-CA-C	-9.74	92.64	108.52
3	C	202	PRO	O-C-N	9.73	134.77	123.10
6	H	120	GLY	N-CA-C	9.71	127.54	114.92
1	A	613	ILE	N-CA-C	-9.70	102.36	111.48
2	B	246	LYS	N-CA-C	9.70	125.67	109.76
6	H	91	ASP	CA-C-O	9.70	130.99	120.32
1	A	1161	THR	OG1-CB-CG2	-9.70	89.91	109.30
1	A	111	GLY	CA-C-O	9.70	130.90	119.46
10	L	69	ALA	CB-CA-C	-9.68	97.98	111.73
2	B	63	ILE	O-C-N	-9.68	111.03	122.06
2	B	217	ARG	CG-CD-NE	-9.68	90.72	112.00
2	B	1053	GLU	N-CA-C	-9.66	100.83	111.36
3	C	196	ASP	CB-CA-C	-9.66	96.52	110.62
2	B	429	PHE	N-CA-C	-9.64	101.73	112.72
2	B	496	ARG	NH1-CZ-NH2	-9.64	106.77	119.30
1	A	893	PHE	N-CA-C	-9.64	99.84	111.69
1	A	821	ARG	CG-CD-NE	-9.63	90.81	112.00
2	B	526	GLU	CA-C-O	-9.63	110.91	120.92
2	B	1160	VAL	CB-CA-C	-9.63	95.50	111.29
6	H	11	GLN	CB-CA-C	-9.63	96.08	110.62
2	B	997	GLU	CA-CB-CG	-9.62	94.85	114.10
1	A	724	GLU	N-CA-C	-9.62	100.66	111.82
2	B	285	ILE	CA-C-O	9.61	131.05	121.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	552	MET	CG-SD-CE	9.61	122.05	100.90
1	A	649	ILE	CA-CB-CG1	9.61	126.73	110.40
1	A	90	VAL	N-CA-CB	-9.60	96.31	112.44
1	A	1211	GLN	N-CA-CB	9.60	124.34	110.13
2	B	100	PRO	N-CD-CG	-9.60	88.81	103.20
3	C	50	GLU	CB-CG-CD	9.59	128.91	112.60
1	A	974	ASP	N-CA-CB	9.58	126.04	110.43
2	B	691	GLU	CA-CB-CG	9.57	133.25	114.10
1	A	1143	LEU	N-CA-C	-9.56	100.71	111.71
2	B	644	GLU	CA-C-N	-9.56	103.29	121.54
2	B	644	GLU	C-N-CA	-9.56	103.29	121.54
1	A	346	ASP	CA-CB-CG	9.55	122.15	112.60
6	H	126	GLU	N-CA-C	-9.54	95.15	110.32
1	A	243	PRO	CB-CA-C	-9.54	99.28	110.92
2	B	482	VAL	CB-CA-C	-9.54	98.75	111.15
3	C	100	THR	OG1-CB-CG2	-9.53	90.25	109.30
7	I	4	PHE	N-CA-C	9.53	131.09	110.80
2	B	266	ALA	CA-C-N	-9.53	107.52	121.24
2	B	266	ALA	C-N-CA	-9.53	107.52	121.24
1	A	893	PHE	CA-C-O	-9.52	109.67	120.24
4	E	198	ILE	CA-C-N	-9.51	110.75	123.12
4	E	198	ILE	C-N-CA	-9.51	110.75	123.12
3	C	233	GLU	CA-C-O	-9.51	110.43	120.70
1	A	382	PRO	N-CA-C	-9.50	101.44	114.27
1	A	183	GLY	CA-C-O	-9.50	110.97	121.23
1	A	890	ASP	N-CA-C	-9.49	101.01	111.36
1	A	1027	ALA	N-CA-CB	-9.49	96.50	110.17
1	A	1422	ARG	NE-CZ-NH2	9.49	127.74	119.20
1	A	1001	ARG	CG-CD-NE	-9.49	91.13	112.00
2	B	412	LEU	N-CA-C	-9.48	100.03	111.69
3	C	172	PRO	CB-CA-C	-9.48	95.92	111.56
2	B	626	ILE	N-CA-CB	-9.48	94.39	111.93
1	A	107	CYS	N-CA-C	-9.47	94.22	109.76
1	A	434	ARG	NE-CZ-NH2	-9.47	110.67	119.20
9	K	95	ILE	O-C-N	9.47	131.17	121.89
2	B	813	LYS	N-CA-C	9.47	124.41	112.86
1	A	395	GLY	CA-C-N	9.46	129.20	119.64
1	A	395	GLY	C-N-CA	9.46	129.20	119.64
1	A	410	GLY	N-CA-C	-9.46	102.78	115.36
1	A	957	PRO	N-CA-C	-9.46	97.03	111.13
1	A	1239	ARG	CD-NE-CZ	-9.46	111.16	124.40
2	B	858	SER	CA-CB-OG	-9.45	92.20	111.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1168	LEU	CA-C-N	-9.44	109.09	122.41
2	B	1168	LEU	C-N-CA	-9.44	109.09	122.41
1	A	1062	GLU	CB-CG-CD	9.44	128.64	112.60
1	A	922	ASP	N-CA-C	9.44	123.69	109.25
9	K	12	LEU	N-CA-C	-9.43	94.99	110.17
2	B	184	ALA	CA-C-O	-9.43	111.56	121.55
6	H	55	LEU	N-CA-C	9.43	125.37	108.69
2	B	391	ASP	OD1-CG-OD2	-9.42	100.29	122.90
5	F	107	VAL	CA-C-N	-9.42	107.59	122.29
5	F	107	VAL	C-N-CA	-9.42	107.59	122.29
1	A	912	LEU	N-CA-CB	9.42	124.88	110.28
2	B	974	PRO	CA-C-O	-9.41	110.72	121.36
1	A	801	GLU	OE1-CD-OE2	9.40	145.47	122.90
1	A	107	CYS	CA-CB-SG	9.39	136.01	114.40
6	H	81	PRO	N-CA-C	9.39	122.16	110.70
1	A	621	THR	N-CA-C	9.39	121.59	111.36
3	C	175	ALA	N-CA-CB	-9.39	96.65	110.17
2	B	604	ARG	NE-CZ-NH1	9.39	130.89	121.50
2	B	364	ILE	CA-CB-CG1	-9.38	94.45	110.40
2	B	1185	CYS	CA-CB-SG	9.38	135.99	114.40
3	C	205	LYS	N-CA-CB	9.38	123.62	110.01
9	K	1	MET	CG-SD-CE	9.38	121.54	100.90
1	A	247	ARG	CA-C-O	9.38	125.39	119.29
1	A	1406	VAL	O-C-N	9.37	131.49	121.83
1	A	1241	ARG	NE-CZ-NH1	9.37	130.87	121.50
2	B	982	SER	CA-C-N	-9.37	108.40	122.83
2	B	982	SER	C-N-CA	-9.37	108.40	122.83
7	I	59	VAL	O-C-N	-9.37	112.64	123.04
2	B	552	MET	O-C-N	-9.36	110.55	121.32
1	A	1316	VAL	CB-CA-C	-9.36	97.66	112.16
1	A	93	VAL	CA-C-O	9.35	130.78	121.05
2	B	241	ARG	NE-CZ-NH2	-9.35	110.78	119.20
1	A	162	VAL	CA-C-O	-9.35	111.37	121.28
1	A	850	VAL	CG1-CB-CG2	-9.35	90.24	110.80
2	B	167	ILE	CB-CA-C	-9.34	101.45	110.70
7	I	35	VAL	CB-CA-C	-9.34	93.68	110.48
2	B	1055	ILE	CA-CB-CG1	9.33	126.26	110.40
3	C	155	LEU	CB-CA-C	-9.33	90.40	110.45
1	A	399	HIS	C-N-CD	-9.32	100.09	120.60
1	A	1239	ARG	CB-CA-C	9.32	126.58	109.70
1	A	1370	LEU	CD1-CG-CD2	-9.31	90.31	110.80
4	E	190	LEU	O-C-N	9.31	133.46	122.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	179	GLN	CB-CG-CD	-9.30	96.78	112.60
2	B	478	GLY	N-CA-C	-9.30	102.06	115.64
1	A	852	TYR	CA-C-O	-9.30	106.94	119.12
3	C	108	GLU	N-CA-C	-9.29	100.26	111.69
3	C	123	ASN	O-C-N	-9.29	110.74	122.82
2	B	1086	PHE	N-CA-C	-9.29	94.04	109.46
3	C	240	VAL	CB-CA-C	-9.29	99.41	112.22
10	L	58	LYS	O-C-N	-9.29	110.24	122.59
1	A	1418	LEU	CB-CA-C	-9.27	95.68	110.79
2	B	644	GLU	N-CA-CB	-9.27	94.83	110.49
1	A	842	VAL	O-C-N	-9.26	112.27	121.90
3	C	86	CYS	N-CA-CB	9.26	125.23	110.23
7	I	118	ARG	CA-CB-CG	9.26	132.62	114.10
8	J	7	CYS	CB-CA-C	-9.26	95.95	109.84
1	A	218	ASP	CA-C-O	-9.25	109.97	120.24
3	C	221	TYR	N-CA-C	9.24	123.66	112.38
1	A	153	PRO	CA-C-N	-9.23	103.93	121.66
1	A	153	PRO	C-N-CA	-9.23	103.93	121.66
3	C	92	CYS	N-CA-CB	-9.23	94.88	110.49
1	A	761	MET	CG-SD-CE	9.23	121.21	100.90
1	A	125	ALA	N-CA-C	-9.23	101.79	113.23
4	E	202	SER	CB-CA-C	-9.23	92.06	110.42
1	A	858	ASN	CA-C-O	-9.22	111.33	121.94
2	B	1097	HIS	CB-CG-CD2	9.22	143.19	131.20
2	B	1083	ALA	CA-C-O	-9.21	110.94	120.71
9	K	23	PRO	N-CD-CG	-9.21	89.39	103.20
8	J	18	TRP	N-CA-C	9.21	123.01	111.69
10	L	58	LYS	N-CA-C	9.20	130.40	110.80
2	B	914	LYS	CB-CA-C	-9.20	93.14	111.17
1	A	87	ALA	CA-C-O	9.20	130.48	120.82
1	A	424	ILE	CA-C-N	-9.20	110.53	122.77
1	A	424	ILE	C-N-CA	-9.20	110.53	122.77
1	A	793	SER	N-CA-CB	-9.19	98.47	109.59
2	B	1127	GLY	N-CA-C	9.19	139.94	113.30
6	H	21	ASN	N-CA-C	9.18	124.79	113.50
3	C	23	SER	N-CA-C	-9.18	93.68	108.55
1	A	771	GLU	CG-CD-OE1	-9.17	97.31	118.40
2	B	531	GLN	CA-C-N	-9.17	107.98	122.65
2	B	531	GLN	C-N-CA	-9.17	107.98	122.65
1	A	814	PHE	CG-CD2-CE2	-9.16	105.12	120.70
2	B	1078	GLY	N-CA-C	9.15	134.87	113.18
2	B	974	PRO	CB-CA-C	-9.15	99.94	111.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1148	LYS	CA-C-O	-9.14	109.46	119.97
1	A	857	ARG	NE-CZ-NH2	9.14	127.42	119.20
1	A	299	HIS	N-CA-C	-9.14	101.70	113.12
1	A	174	ILE	N-CA-C	-9.13	95.32	108.11
2	B	360	PHE	CA-C-O	9.13	130.33	120.38
2	B	430	ARG	N-CA-C	-9.13	100.07	112.94
9	K	62	LYS	CB-CA-C	-9.13	95.30	109.99
7	I	106	CYS	CA-C-N	9.12	135.87	122.74
7	I	106	CYS	C-N-CA	9.12	135.87	122.74
1	A	77	CYS	CA-C-O	-9.11	112.58	119.32
3	C	79	GLN	CA-C-O	9.10	130.33	119.59
2	B	768	THR	O-C-N	-9.10	111.57	122.22
1	A	1109	LYS	CB-CA-C	9.09	128.93	110.38
2	B	1153	GLU	N-CA-C	9.09	123.94	110.48
4	E	187	TYR	N-CA-C	9.09	121.19	111.28
3	C	14	SER	N-CA-C	-9.09	95.07	107.88
1	A	230	ARG	N-CA-CB	-9.08	99.21	109.74
2	B	1155	SER	CA-CB-OG	9.08	129.26	111.10
1	A	129	LYS	N-CA-CB	-9.07	98.52	110.59
2	B	962	LYS	CG-CD-CE	9.07	132.17	111.30
1	A	603	ASN	N-CA-CB	-9.07	97.19	110.70
1	A	1385	THR	N-CA-CB	-9.06	96.09	111.50
3	C	93	ASP	N-CA-C	-9.06	102.22	113.28
1	A	878	ILE	N-CA-CB	-9.06	94.45	111.21
5	F	85	MET	CG-SD-CE	-9.06	80.97	100.90
2	B	654	ARG	NE-CZ-NH1	-9.05	112.45	121.50
1	A	596	THR	CB-CA-C	-9.04	89.94	111.65
2	B	118	ARG	N-CA-C	-9.04	100.37	111.40
3	C	239	PRO	CA-C-O	9.04	133.08	121.96
1	A	1148	ILE	N-CA-C	9.04	119.02	110.53
8	J	7	CYS	N-CA-CB	9.03	123.48	109.48
3	C	252	GLN	CA-C-O	-9.03	110.85	120.42
2	B	1050	ILE	CG1-CB-CG2	-9.02	83.64	110.70
2	B	532	ALA	O-C-N	9.02	133.16	122.34
4	E	66	GLU	N-CA-CB	9.01	123.49	110.16
2	B	461	LEU	N-CA-C	9.00	122.06	111.71
5	F	75	PRO	N-CA-C	9.00	125.32	111.19
9	K	114	LEU	CB-CG-CD2	9.00	137.70	110.70
2	B	329	THR	N-CA-C	9.00	122.22	111.33
2	B	120	ARG	N-CA-C	8.99	123.85	113.15
2	B	788	ARG	CA-C-N	-8.98	109.01	122.47
2	B	788	ARG	C-N-CA	-8.98	109.01	122.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	886	ILE	CA-C-O	8.97	130.31	120.71
2	B	652	LYS	CA-C-O	-8.97	110.94	120.63
7	I	30	ARG	N-CA-C	8.96	124.47	113.17
6	H	127	GLY	N-CA-C	8.96	134.42	113.18
2	B	1007	VAL	N-CA-CB	-8.95	98.68	111.21
6	H	139	ASN	CA-C-N	-8.95	110.15	122.86
6	H	139	ASN	C-N-CA	-8.95	110.15	122.86
2	B	316	PRO	N-CD-CG	-8.95	89.78	103.20
1	A	1210	GLY	O-C-N	8.95	132.38	122.54
1	A	588	LEU	N-CA-CB	-8.94	95.75	111.39
1	A	289	ILE	N-CA-C	-8.93	102.13	110.53
1	A	751	SER	N-CA-C	8.93	124.30	113.23
1	A	264	PHE	CA-CB-CG	8.92	122.72	113.80
2	B	1023	VAL	CA-C-O	-8.92	111.39	120.85
2	B	372	SER	CA-C-O	8.92	129.87	120.42
1	A	863	VAL	N-CA-C	8.92	120.66	108.89
1	A	885	THR	OG1-CB-CG2	-8.92	91.47	109.30
1	A	1377	THR	CB-CA-C	-8.92	91.35	109.99
4	E	63	ASN	N-CA-C	8.92	124.61	109.09
4	E	12	LEU	N-CA-C	-8.91	101.48	111.82
1	A	1014	ALA	N-CA-C	8.90	123.24	112.38
1	A	873	MET	N-CA-C	8.89	123.68	110.52
2	B	642	ASP	N-CA-CB	8.89	123.59	110.35
1	A	295	LEU	CA-C-O	-8.88	110.39	120.24
1	A	693	VAL	N-CA-C	-8.87	99.62	112.04
3	C	144	ILE	CB-CA-C	-8.87	101.33	111.80
1	A	497	THR	N-CA-CB	-8.86	96.54	110.28
2	B	102	VAL	N-CA-C	8.87	121.11	108.17
1	A	610	GLY	O-C-N	8.86	132.69	122.33
1	A	1077	THR	O-C-N	-8.86	112.10	122.20
2	B	414	ALA	N-CA-C	-8.86	102.39	113.55
1	A	751	SER	CA-C-O	-8.86	108.91	119.27
2	B	758	PHE	CD1-CE1-CZ	-8.86	104.06	120.00
2	B	408	LEU	N-CA-CB	-8.85	96.26	110.51
1	A	843	LYS	CB-CG-CD	8.85	131.65	111.30
1	A	834	THR	OG1-CB-CG2	-8.84	91.61	109.30
1	A	1012	ARG	CG-CD-NE	-8.84	92.56	112.00
7	I	76	PRO	N-CA-C	8.84	126.62	113.81
7	I	74	GLU	CA-CB-CG	8.83	131.76	114.10
1	A	326	ARG	CA-CB-CG	8.82	131.75	114.10
7	I	98	VAL	N-CA-C	8.82	120.18	110.21
2	B	559	SER	CA-CB-OG	-8.82	93.46	111.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	85	GLY	N-CA-C	8.82	134.08	113.18
5	F	75	PRO	CA-C-O	-8.81	110.73	121.31
3	C	76	ASP	CA-C-N	-8.81	111.06	122.16
3	C	76	ASP	C-N-CA	-8.81	111.06	122.16
4	E	87	SER	N-CA-C	-8.81	95.40	109.59
1	A	1062	GLU	CA-CB-CG	8.81	131.72	114.10
1	A	362	ASP	N-CA-C	8.80	123.58	113.02
1	A	748	MET	CG-SD-CE	8.80	120.27	100.90
1	A	795	GLU	CB-CG-CD	8.80	127.56	112.60
1	A	830	LYS	N-CA-CB	8.80	123.20	109.82
5	F	115	THR	N-CA-C	-8.80	101.89	114.12
1	A	752	LYS	CD-CE-NZ	8.80	140.06	111.90
3	C	252	GLN	CB-CA-C	8.80	125.80	110.85
1	A	793	SER	CA-CB-OG	8.79	128.68	111.10
1	A	302	THR	OG1-CB-CG2	-8.78	91.74	109.30
1	A	791	ASP	N-CA-C	8.78	123.22	108.20
1	A	725	ALA	CB-CA-C	-8.78	95.93	110.85
2	B	764	SER	CA-C-O	8.78	127.33	118.73
4	E	21	GLU	CB-CG-CD	8.78	127.52	112.60
6	H	27	GLU	CA-C-O	8.78	130.52	120.60
2	B	589	VAL	O-C-N	-8.77	113.31	123.05
2	B	1018	PRO	CA-C-O	-8.77	104.64	120.60
4	E	153	HIS	O-C-N	-8.77	112.95	123.29
1	A	649	ILE	N-CA-C	-8.76	101.87	110.72
1	A	895	LYS	N-CA-CB	8.75	123.70	110.22
4	E	172	GLU	N-CA-C	-8.75	101.71	111.07
1	A	913	LEU	O-C-N	-8.75	113.17	123.41
1	A	276	LEU	N-CA-C	-8.75	102.74	113.41
7	I	119	THR	CA-C-N	8.74	132.84	122.44
7	I	119	THR	C-N-CA	8.74	132.84	122.44
3	C	40	GLU	N-CA-C	8.74	123.77	112.41
1	A	474	VAL	O-C-N	-8.73	113.67	122.14
5	F	77	ASP	CA-C-N	-8.73	104.86	121.54
5	F	77	ASP	C-N-CA	-8.73	104.86	121.54
5	F	140	ASP	N-CA-C	8.73	125.42	113.37
1	A	1445	ILE	O-C-N	8.72	132.90	122.95
2	B	497	ARG	NE-CZ-NH2	-8.72	111.35	119.20
4	E	193	GLY	N-CA-C	-8.72	103.87	115.21
2	B	573	GLN	CA-C-N	-8.71	112.44	123.16
2	B	573	GLN	C-N-CA	-8.71	112.44	123.16
2	B	801	LYS	CD-CE-NZ	-8.71	84.02	111.90
2	B	56	ASP	O-C-N	-8.70	111.02	122.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	493	GLN	CB-CG-CD	8.69	127.38	112.60
1	A	915	SER	CA-C-N	-8.69	109.18	120.22
1	A	915	SER	C-N-CA	-8.69	109.18	120.22
1	A	978	PRO	CA-C-O	8.69	132.81	121.95
1	A	1218	GLN	N-CA-C	-8.69	102.22	113.17
2	B	1010	LEU	CB-CG-CD1	-8.69	84.63	110.70
1	A	1037	LEU	N-CA-C	8.69	122.83	110.23
4	E	147	HIS	CB-CG-ND1	-8.69	109.67	122.70
7	I	109	ILE	CB-CG1-CD1	-8.69	95.56	113.80
5	F	120	ILE	N-CA-C	-8.68	101.95	110.72
1	A	264	PHE	N-CA-C	-8.67	100.65	111.75
1	A	557	ASP	CA-C-N	-8.67	104.42	121.41
1	A	557	ASP	C-N-CA	-8.67	104.42	121.41
2	B	739	THR	CB-CA-C	-8.67	94.82	109.38
1	A	864	ILE	O-C-N	8.66	131.08	122.07
1	A	1039	LYS	CA-C-O	8.66	129.93	119.97
2	B	567	GLU	O-C-N	-8.66	111.07	122.59
1	A	1226	VAL	CB-CA-C	-8.66	95.42	110.65
2	B	96	TYR	CA-C-N	-8.65	110.96	122.99
2	B	96	TYR	C-N-CA	-8.65	110.96	122.99
1	A	1164	PRO	N-CD-CG	8.65	116.18	103.20
2	B	773	MET	CA-C-O	8.65	129.72	120.55
1	A	600	PRO	N-CA-C	-8.65	99.77	113.78
1	A	1108	ALA	N-CA-C	8.65	123.94	109.76
2	B	281	PRO	CA-C-O	-8.65	111.59	121.36
4	E	5	ASN	N-CA-CB	8.65	123.93	110.44
4	E	136	ASN	CA-C-O	-8.64	111.48	121.16
2	B	735	ALA	O-C-N	8.64	134.38	123.14
3	C	79	GLN	O-C-N	-8.64	111.97	122.25
1	A	1258	HIS	N-CA-CB	8.63	122.59	110.07
1	A	72	GLU	N-CA-C	8.63	129.18	110.80
4	E	55	ARG	NE-CZ-NH2	8.63	126.97	119.20
1	A	514	PRO	CA-C-O	8.63	130.77	118.86
1	A	718	VAL	N-CA-C	-8.63	100.51	112.50
1	A	1377	THR	N-CA-CB	8.62	124.46	110.40
5	F	148	VAL	CA-C-O	-8.62	112.03	121.17
2	B	106	ASP	CB-CG-OD2	8.62	138.23	118.40
3	C	150	GLY	CA-C-O	8.62	128.54	118.97
9	K	47	ARG	O-C-N	-8.62	113.13	122.09
2	B	883	LEU	CA-CB-CG	8.61	146.44	116.30
2	B	944	THR	N-CA-C	8.61	123.78	113.28
8	J	1	MET	N-CA-CB	-8.61	95.87	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	247	ARG	CB-CA-C	8.60	119.97	110.08
4	E	73	PRO	CA-C-O	-8.60	104.95	120.60
2	B	648	HIS	N-CA-C	8.59	123.68	110.36
1	A	1222	ASN	CA-C-O	-8.59	111.45	120.55
1	A	1284	MET	CA-CB-CG	-8.59	96.93	114.10
1	A	77	CYS	O-C-N	8.58	129.25	121.35
2	B	843	GLN	CA-C-N	-8.58	108.78	120.28
2	B	843	GLN	C-N-CA	-8.58	108.78	120.28
3	C	16	ASP	N-CA-CB	-8.58	99.48	110.90
7	I	32	CYS	N-CA-C	-8.58	97.59	109.95
7	I	24	ARG	NH1-CZ-NH2	8.58	130.46	119.30
1	A	1320	PRO	N-CD-CG	-8.58	90.33	103.20
9	K	51	LEU	N-CA-C	8.57	122.50	112.72
2	B	459	TYR	O-C-N	-8.57	112.25	122.11
1	A	537	ARG	CB-CG-CD	8.57	131.01	111.30
2	B	745	PRO	N-CD-CG	-8.57	90.35	103.20
3	C	24	ASN	CB-CA-C	-8.57	98.89	112.09
1	A	214	ILE	O-C-N	8.56	132.83	122.72
1	A	911	SER	O-C-N	8.56	134.27	122.46
2	B	1198	TYR	N-CA-C	-8.56	101.95	111.28
7	I	84	VAL	N-CA-CB	-8.56	91.61	111.81
2	B	498	THR	CA-C-O	-8.56	111.73	121.40
3	C	84	ARG	NE-CZ-NH2	8.56	126.90	119.20
3	C	66	ARG	CD-NE-CZ	-8.55	112.42	124.40
8	J	34	THR	OG1-CB-CG2	-8.55	92.19	109.30
1	A	1328	TYR	N-CA-C	8.54	122.47	109.23
2	B	429	PHE	O-C-N	-8.54	111.85	122.35
4	E	103	LYS	N-CA-CB	8.54	124.58	110.92
8	J	46	CYS	CA-C-O	-8.54	111.41	120.63
2	B	289	LEU	CA-C-N	-8.53	106.61	122.05
2	B	289	LEU	C-N-CA	-8.53	106.61	122.05
4	E	36	GLU	CB-CG-CD	8.53	127.10	112.60
8	J	26	GLN	CB-CA-C	8.53	124.17	109.24
2	B	852	ARG	NH1-CZ-NH2	-8.53	108.21	119.30
3	C	3	GLU	CA-CB-CG	-8.53	97.04	114.10
1	A	850	VAL	N-CA-C	8.53	120.81	109.21
5	F	97	ARG	NE-CZ-NH2	-8.53	111.53	119.20
10	L	54	ARG	N-CA-C	8.52	128.95	110.80
1	A	720	ARG	NE-CZ-NH2	8.52	126.87	119.20
4	E	100	ILE	CB-CA-C	-8.52	100.88	111.87
6	H	102	TYR	N-CA-CB	-8.51	99.75	110.98
3	C	161	LYS	N-CA-C	-8.51	99.06	110.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	336	ARG	CB-CA-C	-8.50	92.39	110.32
2	B	1213	THR	CB-CA-C	-8.50	100.31	110.08
2	B	979	LYS	CB-CA-C	-8.49	95.15	109.50
1	A	481	ASP	CA-C-O	-8.49	110.18	121.47
1	A	973	ILE	N-CA-CB	-8.48	101.47	110.72
3	C	158	VAL	N-CA-C	8.48	120.09	107.80
2	B	1183	LYS	CA-CB-CG	8.47	131.05	114.10
2	B	1103	ILE	N-CA-CB	8.47	125.21	111.23
1	A	21	LEU	N-CA-C	8.47	123.42	109.95
1	A	353	ILE	CG1-CB-CG2	-8.47	85.29	110.70
1	A	453	MET	N-CA-C	-8.47	102.86	113.02
4	E	61	GLN	N-CA-C	-8.47	96.54	109.41
8	J	14	VAL	CA-C-O	8.47	131.36	120.78
1	A	563	PRO	O-C-N	-8.46	112.47	123.13
1	A	633	VAL	CA-C-N	-8.46	108.93	120.44
1	A	633	VAL	C-N-CA	-8.46	108.93	120.44
2	B	105	SER	CA-CB-OG	8.46	128.02	111.10
2	B	593	PRO	CA-C-N	-8.46	106.33	121.14
2	B	593	PRO	C-N-CA	-8.46	106.33	121.14
8	J	5	VAL	N-CA-C	8.46	118.54	110.42
1	A	1108	ALA	O-C-N	8.45	133.08	123.19
2	B	870	ILE	CB-CG1-CD1	8.45	131.55	113.80
4	E	136	ASN	CA-C-N	8.45	131.43	120.44
4	E	136	ASN	C-N-CA	8.45	131.43	120.44
1	A	96	ILE	CA-CB-CG1	8.45	124.76	110.40
1	A	61	ILE	N-CA-C	-8.44	91.78	109.34
1	A	151	ASP	OD1-CG-OD2	-8.44	102.65	122.90
9	K	16	GLU	CA-C-O	-8.44	111.32	121.28
2	B	798	TYR	CA-C-N	8.44	128.50	119.90
2	B	798	TYR	C-N-CA	8.44	128.50	119.90
10	L	68	GLU	OE1-CD-OE2	-8.44	102.65	122.90
1	A	204	THR	CA-C-N	8.43	131.58	120.28
1	A	204	THR	C-N-CA	8.43	131.58	120.28
1	A	491	VAL	N-CA-C	8.43	115.23	107.56
1	A	806	ARG	N-CA-C	8.43	121.60	111.82
1	A	1234	GLU	CA-CB-CG	8.43	130.96	114.10
1	A	1357	ALA	N-CA-C	8.43	123.38	113.18
2	B	939	THR	N-CA-C	8.43	121.94	110.31
9	K	17	SER	CB-CA-C	-8.42	93.32	109.66
4	E	130	ALA	N-CA-C	-8.42	97.82	110.28
2	B	312	GLU	N-CA-C	-8.42	102.27	112.54
1	A	373	THR	N-CA-C	8.41	122.03	111.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	474	VAL	N-CA-C	-8.40	104.51	112.83
1	A	1134	ILE	CA-CB-CG2	-8.40	96.21	110.50
1	A	407	ARG	NH1-CZ-NH2	8.40	130.22	119.30
1	A	1171	GLN	N-CA-C	-8.39	102.09	111.82
2	B	996	ARG	NH1-CZ-NH2	8.39	130.21	119.30
1	A	1208	THR	CA-CB-OG1	8.38	122.18	109.60
1	A	1411	GLU	CA-C-O	8.38	129.60	119.97
2	B	97	VAL	CB-CA-C	8.37	122.56	110.33
1	A	1432	GLN	N-CA-C	8.37	122.72	109.50
2	B	1201	LYS	CA-C-N	-8.37	109.56	120.44
2	B	1201	LYS	C-N-CA	-8.37	109.56	120.44
1	A	1318	THR	CB-CA-C	8.37	124.06	110.09
8	J	7	CYS	N-CA-C	-8.37	97.94	110.24
2	B	523	CYS	CA-C-N	8.37	129.42	120.47
2	B	523	CYS	C-N-CA	8.37	129.42	120.47
2	B	587	HIS	O-C-N	-8.36	110.48	122.36
1	A	641	VAL	N-CA-C	-8.36	102.28	110.72
3	C	80	LEU	O-C-N	-8.36	113.43	123.29
2	B	1164	GLY	CA-C-N	-8.35	114.56	122.66
2	B	1164	GLY	C-N-CA	-8.35	114.56	122.66
2	B	1183	LYS	CG-CD-CE	8.35	130.51	111.30
1	A	98	LYS	CG-CD-CE	-8.35	92.10	111.30
2	B	501	PRO	O-C-N	8.35	132.45	123.10
1	A	411	ASP	CA-C-O	-8.34	112.02	121.19
1	A	977	LYS	CB-CA-C	8.34	121.54	109.45
1	A	295	LEU	CB-CA-C	-8.34	95.45	110.70
2	B	914	LYS	CA-C-O	-8.33	112.55	121.38
2	B	1161	HIS	CB-CA-C	8.33	123.76	109.51
5	F	119	ARG	O-C-N	8.33	131.97	122.22
4	E	147	HIS	ND1-CG-CD2	-8.33	97.77	106.10
6	H	87	ARG	CA-CB-CG	8.33	130.77	114.10
7	I	80	SER	N-CA-C	8.33	122.31	110.23
1	A	559	VAL	N-CA-CB	-8.33	101.46	111.21
2	B	910	VAL	CA-C-O	-8.33	111.20	121.11
8	J	26	GLN	N-CA-C	-8.33	103.25	113.41
2	B	690	VAL	N-CA-CB	-8.32	96.53	111.93
4	E	117	THR	N-CA-C	8.32	120.56	110.07
1	A	524	VAL	N-CA-C	8.32	120.95	108.80
1	A	626	ASN	N-CA-C	-8.32	97.17	109.15
2	B	1166	CYS	CA-CB-SG	8.32	133.54	114.40
1	A	864	ILE	N-CA-C	-8.32	105.16	111.90
3	C	66	ARG	NE-CZ-NH2	8.32	126.69	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1278	ASN	CA-C-N	-8.31	112.04	122.93
1	A	1278	ASN	C-N-CA	-8.31	112.04	122.93
2	B	423	LYS	N-CA-C	-8.31	98.16	111.04
3	C	79	GLN	N-CA-C	-8.31	102.16	112.88
7	I	74	GLU	CA-C-O	-8.30	111.78	121.16
2	B	342	GLY	CA-C-O	-8.30	112.78	119.83
1	A	1302	PRO	O-C-N	8.30	133.27	123.06
1	A	354	SER	CA-CB-OG	8.29	127.69	111.10
3	C	247	GLY	O-C-N	8.29	130.23	122.19
9	K	47	ARG	CA-C-N	-8.29	106.63	121.14
9	K	47	ARG	C-N-CA	-8.29	106.63	121.14
1	A	590	ARG	CA-C-O	-8.29	110.34	120.54
2	B	729	ILE	N-CA-CB	-8.29	101.50	110.53
6	H	104	PHE	O-C-N	-8.29	111.57	122.59
7	I	57	GLY	CA-C-N	-8.29	112.08	122.93
7	I	57	GLY	C-N-CA	-8.29	112.08	122.93
1	A	1195	LEU	CA-C-O	8.28	130.51	121.16
4	E	201	LYS	CD-CE-NZ	-8.28	85.41	111.90
1	A	235	ILE	N-CA-CB	-8.28	101.06	110.99
10	L	55	ILE	CB-CA-C	-8.28	99.02	110.77
2	B	256	VAL	CG1-CB-CG2	-8.27	92.60	110.80
2	B	31	TRP	O-C-N	-8.27	111.58	122.33
2	B	642	ASP	CB-CA-C	8.27	125.36	111.30
2	B	969	ARG	CD-NE-CZ	-8.27	112.82	124.40
1	A	137	ALA	N-CA-C	8.27	122.33	111.75
2	B	583	ASN	CA-C-N	-8.27	109.53	122.51
2	B	583	ASN	C-N-CA	-8.27	109.53	122.51
6	H	130	ARG	NE-CZ-NH1	-8.27	113.23	121.50
1	A	1269	GLU	N-CA-C	8.26	123.94	112.45
1	A	779	PHE	N-CA-C	-8.25	97.57	110.36
2	B	46	GLN	N-CA-C	-8.25	102.28	111.28
1	A	244	PRO	N-CA-C	8.25	120.77	110.70
2	B	1062	HIS	CB-CA-C	-8.25	96.62	110.56
1	A	396	PRO	CA-C-N	-8.25	109.42	122.29
1	A	396	PRO	C-N-CA	-8.25	109.42	122.29
1	A	1192	LEU	CB-CA-C	-8.25	95.45	109.72
2	B	1037	LEU	N-CA-C	-8.25	101.55	111.69
2	B	1212	ILE	N-CA-CB	-8.25	101.73	110.72
4	E	147	HIS	CA-CB-CG	8.25	122.05	113.80
7	I	55	THR	CA-CB-CG2	8.25	124.52	110.50
1	A	1226	VAL	N-CA-C	8.24	119.56	108.27
4	E	113	GLN	N-CA-CB	8.24	122.54	110.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	115	THR	OG1-CB-CG2	-8.24	92.81	109.30
3	C	202	PRO	CA-C-N	8.24	132.44	120.82
3	C	202	PRO	C-N-CA	8.24	132.44	120.82
2	B	612	GLU	CB-CG-CD	8.24	126.60	112.60
4	E	31	THR	N-CA-C	-8.24	96.91	110.17
1	A	264	PHE	O-C-N	-8.23	112.81	122.20
2	B	797	TYR	N-CA-C	-8.23	102.25	111.14
1	A	990	VAL	N-CA-C	-8.23	100.75	112.35
2	B	646	LEU	CB-CG-CD2	8.23	135.39	110.70
2	B	708	GLU	CB-CG-CD	8.23	126.59	112.60
2	B	952	VAL	N-CA-C	-8.23	96.27	108.45
2	B	355	ILE	CA-CB-CG1	8.22	124.38	110.40
2	B	368	GLU	CA-CB-CG	8.22	130.54	114.10
2	B	518	HIS	CA-CB-CG	8.22	122.02	113.80
2	B	738	PHE	CA-C-O	8.22	130.27	121.55
3	C	84	ARG	N-CA-C	-8.22	103.03	113.23
7	I	35	VAL	CA-CB-CG2	-8.22	96.43	110.40
1	A	1295	THR	CB-CA-C	-8.21	96.68	110.56
1	A	404	TYR	CA-C-O	-8.21	112.12	121.40
1	A	525	GLN	CG-CD-NE2	-8.21	104.08	116.40
1	A	1111	MET	O-C-N	-8.21	113.74	122.94
1	A	635	ARG	N-CA-CB	8.21	122.31	110.16
1	A	354	SER	CA-C-N	-8.20	112.81	122.16
1	A	354	SER	C-N-CA	-8.20	112.81	122.16
1	A	590	ARG	NE-CZ-NH2	-8.20	111.82	119.20
6	H	92	ASP	N-CA-C	-8.20	101.43	112.26
1	A	1038	THR	CA-C-O	-8.20	112.61	121.88
2	B	652	LYS	CD-CE-NZ	8.20	138.15	111.90
3	C	28	ALA	N-CA-C	8.20	120.30	111.36
3	C	248	ILE	CB-CG1-CD1	-8.20	96.58	113.80
7	I	75	CYS	CB-CA-C	-8.20	97.05	108.86
7	I	96	SER	CA-CB-OG	8.20	127.50	111.10
1	A	1267	MET	CA-C-N	-8.20	106.56	120.58
1	A	1267	MET	C-N-CA	-8.20	106.56	120.58
2	B	219	ALA	CA-C-N	-8.20	112.86	122.77
2	B	219	ALA	C-N-CA	-8.20	112.86	122.77
1	A	895	LYS	CA-C-O	8.18	129.35	120.10
1	A	1061	GLY	N-CA-C	8.18	124.43	114.69
2	B	731	VAL	N-CA-C	-8.18	95.81	107.75
1	A	407	ARG	NE-CZ-NH2	-8.17	111.84	119.20
1	A	706	HIS	N-CA-CB	8.17	124.30	110.49
1	A	883	LEU	N-CA-C	-8.17	95.41	108.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	584	ASN	CA-C-N	-8.17	111.36	122.63
1	A	584	ASN	C-N-CA	-8.17	111.36	122.63
1	A	616	VAL	CG1-CB-CG2	-8.17	92.83	110.80
3	C	245	VAL	N-CA-C	-8.16	102.47	110.72
1	A	984	LYS	CA-CB-CG	8.16	130.41	114.10
10	L	70	ARG	N-CA-C	8.16	133.84	111.00
6	H	77	ARG	NE-CZ-NH1	8.15	129.66	121.50
1	A	35	ILE	N-CA-C	8.15	126.29	109.34
2	B	852	ARG	N-CA-CB	-8.15	97.99	109.97
1	A	273	ASN	N-CA-C	-8.14	102.38	111.82
1	A	1242	VAL	N-CA-CB	-8.14	97.80	111.23
2	B	1023	VAL	N-CA-CB	-8.13	98.38	110.58
1	A	1148	ILE	N-CA-CB	-8.13	100.16	110.57
2	B	497	ARG	N-CA-C	8.13	121.53	110.55
2	B	711	GLU	OE1-CD-OE2	-8.13	103.39	122.90
1	A	778	GLY	N-CA-C	8.12	124.26	113.37
2	B	399	ASP	N-CA-C	8.13	123.36	112.88
4	E	193	GLY	CA-C-O	-8.12	110.24	119.10
1	A	1194	ARG	CB-CA-C	-8.12	98.38	110.24
2	B	629	ASP	N-CA-C	8.12	121.95	110.50
2	B	772	ALA	N-CA-C	8.12	119.76	111.07
2	B	1166	CYS	N-CA-CB	-8.12	98.72	111.39
8	J	6	ARG	NE-CZ-NH2	8.12	126.51	119.20
1	A	39	GLU	N-CA-C	8.12	122.71	109.72
1	A	415	LEU	CA-C-N	-8.11	107.58	122.09
1	A	415	LEU	C-N-CA	-8.11	107.58	122.09
1	A	720	ARG	CG-CD-NE	8.11	129.84	112.00
7	I	55	THR	N-CA-CB	-8.10	97.62	110.98
9	K	6	ARG	N-CA-CB	-8.10	97.72	110.28
1	A	1433	MET	N-CA-CB	8.10	122.29	110.06
2	B	642	ASP	CA-CB-CG	8.09	120.69	112.60
2	B	1019	SER	CA-C-N	-8.09	105.80	121.58
2	B	1019	SER	C-N-CA	-8.09	105.80	121.58
1	A	824	LEU	CD1-CG-CD2	-8.09	93.00	110.80
1	A	34	LYS	O-C-N	-8.09	112.02	122.37
1	A	590	ARG	N-CA-C	8.09	122.58	108.75
2	B	90	ILE	N-CA-C	8.09	126.16	109.34
3	C	183	TRP	O-C-N	-8.09	111.47	122.23
6	H	106	GLU	N-CA-C	-8.09	103.31	113.01
2	B	740	HIS	N-CA-C	8.09	121.01	108.96
2	B	960	GLY	N-CA-C	8.09	125.43	114.92
6	H	81	PRO	N-CD-CG	-8.08	91.08	103.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	109	HIS	CA-C-N	8.08	131.76	120.29
1	A	109	HIS	C-N-CA	8.08	131.76	120.29
3	C	212	PRO	CA-C-O	-8.08	108.85	120.56
2	B	1071	VAL	CA-C-N	-8.07	109.44	122.36
2	B	1071	VAL	C-N-CA	-8.07	109.44	122.36
10	L	48	CYS	CA-CB-SG	8.07	132.97	114.40
1	A	14	VAL	CA-C-O	-8.07	111.94	120.57
3	C	55	THR	N-CA-C	-8.06	102.48	112.88
1	A	412	ARG	CD-NE-CZ	-8.06	113.12	124.40
1	A	1146	VAL	N-CA-C	8.06	120.64	112.90
2	B	373	ARG	CB-CG-CD	8.06	129.83	111.30
2	B	646	LEU	N-CA-C	8.06	127.96	110.80
2	B	644	GLU	CB-CG-CD	-8.05	98.91	112.60
1	A	243	PRO	N-CD-CG	-8.05	91.13	103.20
1	A	514	PRO	N-CA-CB	-8.05	95.85	103.41
8	J	17	LYS	CA-C-N	-8.04	106.82	120.58
8	J	17	LYS	C-N-CA	-8.04	106.82	120.58
2	B	346	GLU	CA-C-O	-8.04	111.01	120.10
9	K	69	ALA	CA-C-O	-8.04	112.57	121.58
1	A	853	ASP	N-CA-C	8.04	122.75	113.19
1	A	446	ARG	NH1-CZ-NH2	8.03	129.74	119.30
1	A	576	GLN	CB-CA-C	-8.03	95.25	110.67
2	B	177	LYS	N-CA-C	-8.04	102.11	112.23
1	A	1022	LEU	N-CA-C	8.03	120.82	111.02
7	I	93	LYS	CA-CB-CG	8.03	130.16	114.10
2	B	117	ALA	CA-C-N	-8.03	107.31	120.71
2	B	117	ALA	C-N-CA	-8.03	107.31	120.71
7	I	22	ASN	N-CA-C	-8.03	101.62	112.94
3	C	177	GLU	N-CA-C	-8.02	99.19	110.50
1	A	948	VAL	N-CA-CB	-8.02	94.91	110.78
4	E	128	PRO	N-CD-CG	8.02	115.23	103.20
8	J	43	ARG	CG-CD-NE	-8.02	94.36	112.00
1	A	1316	VAL	N-CA-C	8.01	121.06	111.05
2	B	986	GLN	CA-CB-CG	-8.01	98.08	114.10
1	A	585	GLY	O-C-N	8.00	130.83	122.51
1	A	722	LEU	N-CA-C	-8.00	102.42	112.90
1	A	79	GLY	N-CA-C	-8.00	93.22	110.66
1	A	85	ASP	CB-CG-OD1	-8.00	100.01	118.40
1	A	1285	MET	CG-SD-CE	8.00	118.49	100.90
2	B	605	ARG	N-CA-C	8.00	122.47	112.87
1	A	1094	VAL	N-CA-C	8.00	120.08	109.21
1	A	189	ARG	N-CA-C	7.99	124.12	111.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1165	ILE	CB-CA-C	7.99	118.97	111.30
1	A	914	GLU	CG-CD-OE2	-7.99	100.03	118.40
3	C	195	GLN	N-CA-C	-7.99	101.42	112.12
1	A	694	THR	OG1-CB-CG2	-7.98	93.33	109.30
2	B	215	GLN	O-C-N	-7.98	114.25	123.27
1	A	1296	GLY	CA-C-O	7.98	126.61	119.83
2	B	1156	ASP	N-CA-C	-7.98	100.00	110.53
3	C	10	ILE	CB-CA-C	-7.98	98.21	111.29
1	A	96	ILE	CA-C-O	7.97	129.10	120.57
1	A	498	ARG	N-CA-C	-7.97	102.59	111.28
9	K	78	THR	CB-CA-C	-7.97	95.53	109.64
2	B	1083	ALA	CA-C-N	-7.97	106.96	122.02
2	B	1083	ALA	C-N-CA	-7.97	106.96	122.02
7	I	7	CYS	CA-CB-SG	7.97	132.72	114.40
9	K	87	LEU	CA-C-N	-7.97	109.61	120.28
9	K	87	LEU	C-N-CA	-7.97	109.61	120.28
1	A	53	LEU	CA-CB-CG	7.96	144.18	116.30
1	A	174	ILE	CG1-CB-CG2	-7.96	86.81	110.70
2	B	368	GLU	N-CA-CB	7.96	122.09	110.47
2	B	1015	HIS	CA-CB-CG	-7.96	105.84	113.80
1	A	796	SER	N-CA-C	-7.96	102.59	111.82
1	A	179	LEU	CA-C-O	-7.96	109.85	119.32
1	A	882	SER	CA-CB-OG	-7.96	95.19	111.10
5	F	96	THR	CA-C-O	7.95	129.17	120.82
2	B	24	PRO	N-CD-CG	-7.95	91.28	103.20
1	A	667	GLY	N-CA-C	7.95	123.65	113.24
1	A	702	LEU	CA-C-N	-7.95	110.81	122.65
1	A	702	LEU	C-N-CA	-7.95	110.81	122.65
2	B	1177	HIS	N-CA-CB	7.95	122.09	110.57
1	A	567	LYS	CD-CE-NZ	7.95	137.33	111.90
1	A	274	ILE	N-CA-C	-7.94	102.70	110.72
2	B	1176	ASN	CA-C-O	-7.94	109.15	120.51
6	H	63	LEU	CB-CA-C	7.94	125.19	110.10
1	A	525	GLN	CG-CD-OE1	7.93	136.67	120.80
2	B	589	VAL	N-CA-CB	-7.93	98.44	111.45
1	A	1080	THR	CA-CB-CG2	7.93	123.98	110.50
2	B	875	GLU	CB-CG-CD	7.93	126.08	112.60
4	E	201	LYS	N-CA-CB	-7.93	99.52	110.38
9	K	111	LEU	CD1-CG-CD2	7.93	128.25	110.80
1	A	1059	HIS	N-CA-C	7.93	119.63	109.72
2	B	768	THR	CA-CB-CG2	-7.93	97.02	110.50
3	C	248	ILE	N-CA-C	-7.93	102.53	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	135	ARG	CA-C-O	-7.93	111.88	120.36
3	C	182	PRO	N-CD-CG	-7.93	91.31	103.20
1	A	110	CYS	CA-C-O	7.92	128.82	120.42
1	A	966	ASN	CA-C-O	-7.92	112.48	120.80
2	B	534	GLY	N-CA-C	7.92	124.12	114.69
2	B	999	MET	CG-SD-CE	-7.92	83.48	100.90
1	A	361	LEU	CB-CA-C	-7.92	97.22	110.68
7	I	45	ARG	CB-CA-C	-7.92	93.31	109.38
1	A	468	PHE	N-CA-C	-7.92	97.69	110.20
1	A	878	ILE	CB-CG1-CD1	-7.92	97.17	113.80
2	B	1108	ARG	N-CA-C	7.92	127.66	110.80
1	A	206	GLU	CG-CD-OE1	-7.91	100.21	118.40
2	B	512	ARG	CA-C-O	7.91	129.12	119.31
1	A	444	PHE	N-CA-C	-7.90	96.98	109.23
1	A	860	LEU	N-CA-C	7.90	122.18	112.54
3	C	160	LYS	CD-CE-NZ	7.90	137.19	111.90
5	F	79	ARG	CB-CG-CD	-7.90	93.12	111.30
1	A	123	ARG	N-CA-CB	7.90	121.97	110.20
1	A	856	THR	N-CA-CB	-7.90	97.09	110.83
4	E	122	LYS	N-CA-C	-7.90	103.10	112.89
2	B	1023	VAL	N-CA-C	-7.89	102.75	110.72
1	A	1099	PRO	CB-CA-C	-7.89	100.59	112.11
1	A	1227	ILE	N-CA-C	-7.89	98.90	108.53
2	B	724	ASP	CA-C-O	7.89	130.97	120.16
3	C	94	LYS	CA-CB-CG	7.89	129.88	114.10
1	A	1417	GLU	N-CA-C	-7.88	97.74	110.20
1	A	135	PHE	N-CA-C	-7.88	102.69	111.28
1	A	1019	CYS	CA-C-O	-7.88	110.90	119.97
1	A	1349	TYR	CA-C-O	7.88	128.77	120.42
2	B	110	HIS	O-C-N	-7.88	113.75	123.36
1	A	936	LEU	CD1-CG-CD2	-7.87	93.50	110.80
4	E	21	GLU	CB-CA-C	-7.87	97.73	110.79
3	C	104	PHE	N-CA-C	-7.86	96.64	108.99
1	A	940	ARG	NE-CZ-NH1	7.86	129.36	121.50
1	A	457	ALA	CA-C-O	-7.86	111.81	120.38
1	A	1260	LEU	O-C-N	-7.86	113.97	122.07
2	B	513	GLN	CA-CB-CG	7.86	129.82	114.10
2	B	1017	ILE	CA-CB-CG1	-7.86	97.04	110.40
4	E	102	GLU	CA-C-N	-7.86	110.18	122.67
4	E	102	GLU	C-N-CA	-7.86	110.18	122.67
1	A	560	ILE	CA-C-O	7.85	130.47	119.95
3	C	190	ASP	N-CA-C	7.85	121.75	108.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	110	ASP	CA-C-N	7.85	135.49	122.07
6	H	110	ASP	C-N-CA	7.85	135.49	122.07
2	B	30	SER	N-CA-C	7.84	119.83	111.28
2	B	372	SER	CA-C-N	-7.84	109.64	120.38
2	B	372	SER	C-N-CA	-7.84	109.64	120.38
3	C	110	THR	O-C-N	7.84	132.36	123.19
3	C	163	ILE	CB-CA-C	7.84	122.57	110.50
1	A	491	VAL	O-C-N	-7.84	115.99	121.55
1	A	1136	SER	CA-C-O	-7.84	110.10	119.27
2	B	967	ARG	NE-CZ-NH1	-7.83	113.67	121.50
2	B	1076	HIS	CA-CB-CG	7.83	121.63	113.80
3	C	211	ASP	N-CA-C	-7.83	99.50	110.31
1	A	396	PRO	N-CD-CG	-7.83	91.46	103.20
1	A	621	THR	CA-C-O	7.83	128.72	120.42
3	C	219	PHE	O-C-N	7.83	132.50	122.87
1	A	1290	LYS	CA-C-O	7.83	129.61	120.69
2	B	408	LEU	N-CA-C	7.83	121.98	110.17
4	E	25	ASP	OD1-CG-OD2	-7.83	104.12	122.90
2	B	355	ILE	CB-CA-C	-7.82	101.76	112.24
1	A	382	PRO	CA-C-O	-7.82	109.05	118.90
2	B	27	ALA	O-C-N	-7.82	113.84	122.12
2	B	370	PHE	CB-CA-C	7.82	125.97	110.42
2	B	1109	GLY	N-CA-C	7.81	128.28	112.34
10	L	56	LEU	N-CA-CB	-7.81	96.86	111.00
1	A	1311	VAL	N-CA-CB	-7.81	98.93	111.58
2	B	265	SER	CA-CB-OG	7.81	126.72	111.10
3	C	189	THR	N-CA-C	-7.80	97.14	109.23
1	A	1053	PHE	N-CA-C	-7.80	102.78	111.28
1	A	1434	ALA	N-CA-C	7.80	119.60	109.93
2	B	168	GLY	N-CA-C	7.80	121.46	111.09
2	B	497	ARG	NH1-CZ-NH2	7.80	129.44	119.30
1	A	28	ARG	N-CA-C	-7.80	102.86	111.36
1	A	1214	GLU	O-C-N	7.79	132.78	122.33
2	B	1064	TYR	CA-C-N	-7.79	108.70	120.94
2	B	1064	TYR	C-N-CA	-7.79	108.70	120.94
10	L	65	VAL	CB-CA-C	-7.79	98.50	110.50
2	B	463	THR	N-CA-C	7.79	123.28	112.45
1	A	695	LYS	N-CA-CB	-7.79	98.67	110.12
1	A	850	VAL	O-C-N	-7.79	113.53	122.72
1	A	934	LYS	CA-C-O	-7.79	112.30	120.55
6	H	37	LYS	O-C-N	7.79	133.27	123.15
8	J	6	ARG	CA-C-O	-7.79	112.35	121.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	522	VAL	N-CA-CB	-7.78	95.80	111.91
2	B	884	ARG	CB-CG-CD	7.78	129.20	111.30
7	I	49	ILE	CA-C-N	-7.78	110.59	122.81
7	I	49	ILE	C-N-CA	-7.78	110.59	122.81
1	A	442	VAL	CB-CA-C	-7.78	98.30	110.52
2	B	944	THR	O-C-N	7.78	133.46	122.41
1	A	205	GLU	N-CA-C	-7.78	102.80	111.28
2	B	656	GLY	O-C-N	7.78	130.76	122.28
3	C	75	MET	N-CA-C	-7.77	102.89	111.36
1	A	206	GLU	OE1-CD-OE2	7.77	141.55	122.90
2	B	903	VAL	CB-CA-C	-7.77	101.05	111.15
1	A	1420	ASP	N-CA-C	7.77	122.19	112.87
1	A	377	PRO	CB-CA-C	-7.76	98.75	111.56
7	I	119	THR	O-C-N	7.76	130.10	122.03
9	K	75	ILE	CA-CB-CG1	7.76	123.60	110.40
2	B	1081	LEU	CD1-CG-CD2	-7.76	93.73	110.80
2	B	368	GLU	CA-C-N	-7.76	102.13	121.60
2	B	368	GLU	C-N-CA	-7.76	102.13	121.60
2	B	1139	ILE	CB-CA-C	-7.75	101.86	112.02
4	E	127	ILE	O-C-N	7.75	129.94	121.10
1	A	859	SER	N-CA-C	-7.75	103.09	112.54
6	H	40	LEU	CB-CG-CD2	7.75	133.95	110.70
6	H	53	ASP	CA-C-N	-7.75	109.17	121.87
6	H	53	ASP	C-N-CA	-7.75	109.17	121.87
1	A	15	LYS	N-CA-C	-7.75	103.36	114.12
4	E	167	ARG	NE-CZ-NH1	-7.75	113.75	121.50
2	B	946	ASN	CA-C-O	-7.74	112.94	121.23
2	B	1156	ASP	N-CA-CB	7.74	121.43	110.36
7	I	29	CYS	CA-C-O	-7.74	112.14	121.28
1	A	1271	ILE	CG1-CB-CG2	-7.74	87.48	110.70
2	B	268	THR	CB-CA-C	7.74	124.14	110.36
6	H	38	LEU	CB-CA-C	-7.74	98.22	110.14
1	A	1122	PRO	CA-C-N	-7.74	106.24	121.41
1	A	1122	PRO	C-N-CA	-7.74	106.24	121.41
1	A	553	VAL	O-C-N	-7.74	112.28	121.10
2	B	1218	THR	N-CA-C	-7.74	103.64	113.23
1	A	566	ILE	N-CA-C	7.73	118.46	111.81
1	A	172	PRO	CA-C-O	7.73	131.10	121.67
9	K	26	LYS	N-CA-C	7.73	121.65	111.75
1	A	227	VAL	N-CA-C	7.73	118.16	111.90
2	B	510	LYS	CB-CG-CD	-7.73	93.53	111.30
1	A	999	VAL	CA-C-O	-7.72	113.31	120.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	110	CYS	CA-CB-SG	7.72	132.15	114.40
1	A	208	LEU	N-CA-C	-7.71	102.97	112.38
7	I	24	ARG	NE-CZ-NH1	-7.71	113.79	121.50
1	A	820	GLY	CA-C-N	-7.71	109.34	120.29
1	A	820	GLY	C-N-CA	-7.71	109.34	120.29
6	H	117	SER	O-C-N	7.71	132.29	123.27
7	I	16	PRO	CA-N-CD	-7.71	101.20	112.00
2	B	278	GLN	CA-C-N	-7.71	109.76	120.71
2	B	278	GLN	C-N-CA	-7.71	109.76	120.71
2	B	342	GLY	O-C-N	7.71	128.88	122.71
1	A	1072	ILE	N-CA-C	-7.71	103.41	111.58
3	C	249	ASP	CA-C-O	7.71	128.59	120.42
6	H	63	LEU	CA-C-O	7.71	133.90	120.80
2	B	723	VAL	N-CA-CB	7.70	121.19	110.56
2	B	110	HIS	N-CA-C	7.70	122.32	108.69
7	I	81	ARG	NE-CZ-NH2	-7.70	112.27	119.20
1	A	843	LYS	CB-CA-C	7.70	122.96	110.88
1	A	1385	THR	N-CA-C	7.70	132.55	111.00
10	L	27	LEU	N-CA-C	7.70	127.19	110.80
1	A	1109	LYS	N-CA-C	-7.69	102.54	112.23
1	A	1034	GLU	N-CA-C	-7.69	102.45	112.68
1	A	659	HIS	N-CA-CB	-7.69	98.30	110.98
1	A	885	THR	CA-CB-CG2	7.69	123.57	110.50
1	A	896	ARG	NH1-CZ-NH2	7.69	129.29	119.30
2	B	845	SER	CA-C-N	-7.69	109.93	120.46
2	B	845	SER	C-N-CA	-7.69	109.93	120.46
1	A	240	PRO	CA-C-O	-7.69	113.20	121.27
1	A	351	THR	CA-C-N	7.68	130.80	120.50
1	A	351	THR	C-N-CA	7.68	130.80	120.50
1	A	495	GLU	CA-CB-CG	7.68	129.47	114.10
1	A	541	ILE	CB-CA-C	-7.68	98.67	110.50
4	E	109	ILE	CB-CA-C	-7.68	98.67	110.50
1	A	1417	GLU	CG-CD-OE1	7.68	136.07	118.40
3	C	70	ILE	CA-CB-CG1	7.68	123.46	110.40
8	J	14	VAL	O-C-N	-7.68	112.97	122.57
1	A	688	LYS	N-CA-C	-7.68	102.25	111.69
1	A	416	ARG	NE-CZ-NH2	-7.68	112.29	119.20
4	E	66	GLU	CA-CB-CG	7.68	129.45	114.10
9	K	88	LYS	N-CA-C	-7.68	102.91	111.28
3	C	119	VAL	N-CA-C	7.67	119.19	107.99
1	A	1208	THR	CB-CA-C	-7.67	96.59	109.48
1	A	1267	MET	CG-SD-CE	-7.67	84.02	100.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1118	VAL	N-CA-CB	7.67	122.00	111.41
3	C	12	GLU	CA-C-O	-7.67	112.67	121.10
1	A	561	PRO	CA-C-O	-7.67	111.27	122.31
2	B	406	LEU	O-C-N	-7.67	114.61	123.27
7	I	31	THR	CA-C-N	7.67	137.45	123.27
7	I	31	THR	C-N-CA	7.67	137.45	123.27
1	A	1308	THR	CA-C-O	-7.66	111.97	121.78
5	F	153	VAL	N-CA-C	7.66	118.53	106.88
2	B	791	THR	OG1-CB-CG2	-7.66	93.98	109.30
4	E	139	ALA	CA-C-O	-7.66	109.96	119.38
4	E	172	GLU	CB-CG-CD	7.66	125.61	112.60
1	A	126	LEU	O-C-N	7.65	131.68	122.27
1	A	596	THR	CA-C-O	-7.65	112.91	121.40
1	A	36	ARG	CG-CD-NE	7.65	128.83	112.00
2	B	1097	HIS	CB-CA-C	7.64	125.63	110.42
3	C	3	GLU	CA-C-N	7.64	136.14	121.54
3	C	3	GLU	C-N-CA	7.64	136.14	121.54
7	I	17	ARG	CB-CG-CD	7.64	128.88	111.30
2	B	222	ILE	CA-C-O	-7.64	112.01	120.72
2	B	415	GLN	N-CA-C	-7.64	98.77	111.37
1	A	475	THR	CB-CA-C	7.63	123.83	110.85
1	A	1422	ARG	NH1-CZ-NH2	-7.63	109.38	119.30
3	C	222	LYS	N-CA-C	-7.63	103.56	113.17
4	E	110	PHE	CB-CA-C	-7.63	98.39	110.14
9	K	47	ARG	CG-CD-NE	7.63	128.79	112.00
3	C	177	GLU	CA-C-O	-7.63	113.24	121.56
2	B	883	LEU	N-CA-C	-7.63	101.44	111.74
1	A	1074	GLU	CB-CG-CD	7.62	125.56	112.60
1	A	1297	GLU	N-CA-C	7.62	120.59	110.53
4	E	163	GLU	CG-CD-OE1	7.62	135.93	118.40
1	A	1006	ILE	N-CA-C	-7.62	103.26	110.42
4	E	180	ARG	N-CA-C	-7.62	102.95	111.71
5	F	72	LYS	CA-C-N	7.61	136.08	121.54
5	F	72	LYS	C-N-CA	7.61	136.08	121.54
3	C	81	GLU	N-CA-C	-7.61	98.22	110.32
2	B	465	ASN	N-CA-C	7.61	121.38	107.99
2	B	169	ARG	CA-C-O	7.61	128.30	120.24
5	F	148	VAL	O-C-N	7.60	129.36	121.91
3	C	192	TRP	O-C-N	-7.60	113.89	122.86
1	A	717	ASN	CB-CG-ND2	-7.60	105.00	116.40
9	K	68	PHE	CA-C-N	-7.60	110.19	122.34
9	K	68	PHE	C-N-CA	-7.60	110.19	122.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	272	THR	CA-C-O	-7.59	112.64	120.54
1	A	469	ARG	CA-C-O	-7.59	112.58	121.46
1	A	1056	SER	N-CA-CB	-7.59	98.82	110.44
2	B	434	ARG	CG-CD-NE	7.59	128.70	112.00
2	B	655	LYS	CD-CE-NZ	7.59	136.19	111.90
2	B	996	ARG	N-CA-C	7.59	119.56	111.28
2	B	1194	ILE	CA-C-N	-7.59	111.55	122.94
2	B	1194	ILE	C-N-CA	-7.59	111.55	122.94
7	I	70	ARG	N-CA-C	7.59	121.87	109.72
5	F	97	ARG	N-CA-CB	-7.59	98.52	110.28
7	I	109	ILE	CG1-CB-CG2	-7.59	87.94	110.70
1	A	709	THR	N-CA-CB	-7.59	99.51	110.36
1	A	1445	ILE	CA-C-O	-7.59	112.14	120.71
6	H	42	ILE	N-CA-C	7.59	119.76	108.46
7	I	16	PRO	O-C-N	7.59	132.69	123.13
1	A	174	ILE	O-C-N	-7.58	115.07	123.26
2	B	1131	GLY	N-CA-C	7.58	122.95	112.57
1	A	1204	ASP	CA-C-O	-7.58	109.67	120.51
9	K	14	GLU	CB-CA-C	7.58	123.05	109.64
1	A	283	GLY	N-CA-C	-7.58	95.22	113.18
2	B	1008	PRO	CB-CA-C	-7.57	100.17	110.85
7	I	109	ILE	CA-CB-CG1	7.57	123.28	110.40
6	H	81	PRO	CB-CA-C	7.57	120.16	110.92
1	A	492	PRO	CA-C-O	-7.57	112.78	121.56
1	A	934	LYS	N-CA-CB	7.56	121.24	110.12
3	C	51	VAL	O-C-N	-7.56	114.25	123.10
4	E	46	TYR	CA-C-O	7.56	126.87	119.08
1	A	731	ARG	O-C-N	-7.56	114.11	122.12
2	B	398	ARG	CB-CA-C	-7.55	95.62	110.27
2	B	1085	ILE	O-C-N	-7.55	114.67	123.05
3	C	172	PRO	O-C-N	7.55	132.83	122.64
2	B	589	VAL	CB-CA-C	7.55	123.77	110.71
8	J	42	LYS	CD-CE-NZ	7.55	136.06	111.90
2	B	205	ILE	CA-C-N	7.55	133.37	122.35
2	B	205	ILE	C-N-CA	7.55	133.37	122.35
2	B	433	GLN	N-CA-C	-7.55	104.20	113.41
1	A	92	HIS	CA-C-N	-7.55	109.89	120.53
1	A	92	HIS	C-N-CA	-7.55	109.89	120.53
1	A	161	LEU	CA-C-O	-7.55	112.78	121.68
1	A	1337	GLU	CA-C-O	-7.55	110.89	119.79
1	A	206	GLU	CB-CA-C	-7.54	95.85	110.11
1	A	188	ASP	CB-CG-OD2	7.54	135.74	118.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	337	ARG	CG-CD-NE	-7.54	95.42	112.00
2	B	1034	VAL	N-CA-C	-7.54	102.93	110.62
7	I	40	SER	CA-C-O	-7.54	109.84	120.16
2	B	397	ASP	CA-C-O	7.53	128.75	120.92
1	A	462	VAL	O-C-N	7.53	131.27	122.83
1	A	1012	ARG	CA-CB-CG	7.53	129.16	114.10
2	B	217	ARG	CB-CG-CD	7.53	128.62	111.30
2	B	531	GLN	CB-CG-CD	7.53	125.39	112.60
2	B	457	LEU	N-CA-C	-7.52	101.54	111.24
1	A	927	VAL	CA-CB-CG2	-7.51	97.62	110.40
1	A	1116	LEU	N-CA-C	-7.51	96.66	108.90
3	C	11	ARG	CB-CA-C	-7.51	96.95	109.27
1	A	416	ARG	N-CA-CB	7.51	121.43	110.47
1	A	1299	VAL	CB-CA-C	7.51	122.31	110.52
1	A	383	TYR	CA-C-O	7.50	128.60	119.97
3	C	81	GLU	CB-CA-C	-7.50	96.68	109.51
1	A	413	ILE	CA-C-O	-7.50	111.87	120.65
2	B	353	LYS	N-CA-CB	7.50	121.15	110.12
1	A	687	LYS	N-CA-C	7.50	121.35	111.75
1	A	1218	GLN	O-C-N	7.50	131.72	122.34
2	B	656	GLY	CA-C-O	-7.50	112.05	120.30
1	A	1169	ILE	N-CA-C	-7.50	103.15	110.72
2	B	50	SER	CB-CA-C	-7.50	98.10	110.85
2	B	735	ALA	CA-C-O	-7.50	110.81	120.25
7	I	106	CYS	N-CA-CB	-7.50	100.53	110.88
1	A	419	LYS	CD-CE-NZ	-7.50	87.92	111.90
1	A	629	LEU	CD1-CG-CD2	-7.49	94.33	110.80
2	B	369	GLY	N-CA-C	7.49	124.59	115.31
5	F	79	ARG	CA-CB-CG	7.49	129.07	114.10
3	C	223	ALA	CA-C-O	-7.48	112.98	121.81
2	B	942	ARG	CG-CD-NE	-7.48	95.54	112.00
6	H	84	ALA	CA-C-N	7.48	136.07	121.41
6	H	84	ALA	C-N-CA	7.48	136.07	121.41
1	A	441	PRO	N-CA-CB	-7.48	96.78	103.36
2	B	559	SER	CA-C-O	-7.47	110.92	119.14
2	B	838	SER	N-CA-CB	-7.47	99.52	111.62
9	K	62	LYS	N-CA-C	7.47	119.88	108.52
4	E	66	GLU	CA-C-N	-7.47	110.27	120.28
4	E	66	GLU	C-N-CA	-7.47	110.27	120.28
7	I	16	PRO	CA-C-O	-7.47	112.75	121.86
5	F	143	PHE	N-CA-C	7.47	120.51	109.24
2	B	486	TYR	N-CA-C	7.46	119.06	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	553	PRO	N-CA-C	-7.46	103.80	113.57
2	B	1048	THR	CA-C-O	-7.46	111.02	121.98
1	A	1360	GLY	N-CA-C	7.46	125.24	115.40
1	A	49	LYS	N-CA-C	7.45	120.54	108.32
1	A	277	GLU	CA-CB-CG	7.45	129.01	114.10
1	A	1125	ALA	N-CA-C	7.45	122.20	113.18
2	B	103	ASN	CA-CB-CG	7.45	120.05	112.60
3	C	33	LEU	CB-CA-C	7.45	123.31	110.79
4	E	128	PRO	CB-CA-C	7.45	120.01	110.92
1	A	26	GLU	CA-C-N	-7.45	111.17	120.56
1	A	26	GLU	C-N-CA	-7.45	111.17	120.56
8	J	56	LEU	CD1-CG-CD2	-7.45	94.41	110.80
1	A	292	ALA	O-C-N	7.45	130.64	122.15
1	A	948	VAL	CA-C-N	7.45	134.17	121.14
1	A	948	VAL	C-N-CA	7.45	134.17	121.14
1	A	1063	MET	O-C-N	-7.45	113.40	122.71
1	A	1340	GLY	CA-C-O	-7.45	116.64	122.52
2	B	760	ASP	N-CA-C	7.44	122.05	113.19
1	A	146	MET	N-CA-CB	-7.44	99.44	110.53
1	A	360	GLU	CA-CB-CG	7.44	128.98	114.10
1	A	922	ASP	O-C-N	-7.44	113.87	123.02
9	K	78	THR	N-CA-C	7.44	119.91	110.24
1	A	1202	MET	N-CA-C	-7.44	103.19	111.82
7	I	92	ARG	NE-CZ-NH1	-7.43	114.06	121.50
1	A	938	LYS	CG-CD-CE	-7.43	94.21	111.30
2	B	429	PHE	CA-C-O	7.43	128.62	119.78
2	B	258	LEU	CD1-CG-CD2	-7.43	94.46	110.80
7	I	52	ILE	CA-C-O	7.42	130.06	120.78
1	A	1243	VAL	N-CA-CB	-7.42	98.88	111.50
7	I	54	GLU	OE1-CD-OE2	7.42	140.71	122.90
2	B	916	THR	N-CA-C	7.42	131.78	111.00
1	A	704	ALA	CA-C-O	-7.42	113.06	121.81
1	A	719	VAL	CA-CB-CG1	-7.42	97.79	110.40
2	B	92	PHE	N-CA-CB	7.42	122.24	110.23
1	A	99	ILE	CA-C-O	7.42	128.76	121.05
1	A	203	SER	CA-C-O	-7.41	112.94	121.47
1	A	1412	ALA	O-C-N	7.41	129.97	122.12
8	J	11	GLY	N-CA-C	7.41	125.18	115.40
1	A	177	ASP	N-CA-C	-7.40	95.03	110.80
3	C	57	VAL	N-CA-CB	-7.40	99.02	111.23
2	B	566	LEU	CD1-CG-CD2	-7.40	94.52	110.80
2	B	1028	GLU	CB-CA-C	-7.40	98.27	110.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1203	LEU	O-C-N	-7.40	113.60	122.11
4	E	78	LEU	N-CA-CB	-7.40	97.76	111.52
1	A	916	GLY	CA-C-N	7.39	130.05	120.44
1	A	916	GLY	C-N-CA	7.39	130.05	120.44
1	A	858	ASN	N-CA-C	7.39	120.07	110.53
2	B	106	ASP	CB-CG-OD1	-7.39	101.40	118.40
2	B	362	PRO	CA-C-O	-7.39	107.73	118.89
2	B	955	THR	CB-CA-C	-7.39	96.67	112.78
6	H	27	GLU	N-CA-C	7.39	120.12	108.67
2	B	1011	ILE	CB-CG1-CD1	-7.39	98.29	113.80
2	B	563	MET	CG-SD-CE	7.39	117.15	100.90
2	B	564	GLU	CG-CD-OE2	-7.39	101.41	118.40
2	B	982	SER	O-C-N	7.39	131.42	121.74
3	C	132	PRO	CA-C-O	-7.39	107.16	120.60
2	B	434	ARG	CA-CB-CG	7.38	128.87	114.10
2	B	1191	ILE	O-C-N	7.38	129.39	122.97
1	A	351	THR	CB-CA-C	-7.38	93.93	111.65
5	F	113	GLY	N-CA-C	7.38	123.47	114.69
2	B	1192	TYR	CA-C-O	7.38	129.74	121.40
2	B	654	ARG	NE-CZ-NH2	7.38	125.84	119.20
1	A	962	ARG	O-C-N	-7.38	111.44	122.28
1	A	137	ALA	N-CA-CB	-7.37	98.49	110.14
1	A	917	SER	CA-CB-OG	-7.37	96.36	111.10
1	A	583	PRO	CA-C-N	-7.37	109.37	120.94
1	A	583	PRO	C-N-CA	-7.37	109.37	120.94
2	B	705	MET	CG-SD-CE	-7.37	84.69	100.90
4	E	93	MET	N-CA-C	7.37	118.95	111.07
3	C	51	VAL	N-CA-C	7.37	118.48	107.80
1	A	186	LYS	CB-CG-CD	7.36	128.24	111.30
7	I	17	ARG	N-CA-CB	7.36	124.02	110.99
1	A	811	GLN	N-CA-C	-7.36	103.34	111.36
2	B	646	LEU	CB-CA-C	-7.36	95.77	110.42
6	H	139	ASN	CA-CB-CG	7.36	119.96	112.60
2	B	22	SER	CA-C-O	7.36	128.27	119.59
10	L	25	ALA	CA-C-N	7.36	135.59	121.54
10	L	25	ALA	C-N-CA	7.36	135.59	121.54
1	A	1111	MET	N-CA-CB	-7.36	98.69	110.46
1	A	1146	VAL	O-C-N	-7.36	115.46	122.16
4	E	95	THR	N-CA-C	-7.36	104.11	113.23
2	B	724	ASP	O-C-N	-7.35	112.86	121.32
2	B	954	VAL	CB-CA-C	-7.35	98.66	110.28
1	A	304	MET	N-CA-C	7.35	122.92	113.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1166	ASP	CA-C-N	-7.35	110.94	120.65
1	A	1166	ASP	C-N-CA	-7.35	110.94	120.65
2	B	608	ASP	N-CA-C	-7.35	103.35	111.36
2	B	909	ASP	CB-CG-OD2	7.35	135.31	118.40
2	B	201	GLY	CA-C-O	7.35	128.16	119.19
3	C	58	LEU	N-CA-CB	-7.35	99.30	111.20
2	B	116	GLU	N-CA-C	-7.35	102.24	112.45
2	B	689	LEU	N-CA-C	7.35	121.49	112.23
3	C	171	GLY	N-CA-C	7.35	127.33	112.34
4	E	153	HIS	CA-CB-CG	7.35	121.15	113.80
5	F	149	GLU	N-CA-CB	7.35	121.08	110.06
1	A	833	GLU	CG-CD-OE1	7.34	135.29	118.40
1	A	931	GLU	O-C-N	7.34	130.81	122.22
6	H	91	ASP	N-CA-C	7.34	120.49	108.52
2	B	802	PRO	O-C-N	7.34	131.32	123.03
2	B	1021	MET	N-CA-CB	-7.34	100.76	111.91
1	A	215	SER	CA-C-O	-7.34	112.69	121.05
9	K	45	LEU	N-CA-C	-7.34	102.45	111.40
2	B	452	THR	OG1-CB-CG2	-7.33	94.63	109.30
1	A	907	THR	CA-CB-CG2	7.33	122.96	110.50
1	A	29	ALA	N-CA-C	7.33	126.41	110.80
1	A	978	PRO	CB-CG-CD	-7.33	82.66	106.10
1	A	1021	LEU	CD1-CG-CD2	-7.33	94.68	110.80
3	C	139	GLY	N-CA-C	7.33	125.16	114.10
1	A	894	GLU	CA-C-N	-7.32	109.74	120.28
1	A	894	GLU	C-N-CA	-7.32	109.74	120.28
6	H	107	VAL	CB-CA-C	7.32	123.30	111.29
2	B	284	ILE	CA-CB-CG1	7.32	122.84	110.40
4	E	6	GLU	CB-CG-CD	7.32	125.05	112.60
2	B	1185	CYS	CB-CA-C	7.32	122.38	109.65
1	A	144	THR	CA-CB-CG2	7.32	122.94	110.50
1	A	1024	SER	CA-CB-OG	7.31	125.73	111.10
2	B	228	LYS	CB-CG-CD	7.31	128.11	111.30
1	A	519	PRO	N-CD-CG	7.31	114.16	103.20
2	B	277	LYS	N-CA-CB	-7.30	99.41	110.73
2	B	851	PHE	N-CA-C	7.30	121.53	112.47
9	K	103	THR	CA-C-O	-7.30	113.22	120.89
1	A	912	LEU	O-C-N	-7.30	113.29	122.27
8	J	24	LEU	N-CA-CB	7.30	122.50	110.39
1	A	906	HIS	CA-C-O	7.29	128.56	119.95
2	B	632	ARG	CA-C-N	-7.29	110.90	122.64
2	B	632	ARG	C-N-CA	-7.29	110.90	122.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	50	MET	CG-SD-CE	7.29	116.94	100.90
1	A	1263	ILE	CG1-CB-CG2	-7.29	88.83	110.70
7	I	91	ARG	NE-CZ-NH2	-7.29	112.64	119.20
7	I	93	LYS	CA-C-O	-7.29	110.27	119.31
4	E	212	ARG	NE-CZ-NH2	-7.29	112.64	119.20
1	A	544	ASP	CA-C-N	7.29	129.91	120.44
1	A	544	ASP	C-N-CA	7.29	129.91	120.44
2	B	685	LEU	CD1-CG-CD2	-7.29	94.77	110.80
3	C	181	ASP	CA-C-O	-7.29	110.18	120.16
2	B	1138	MET	N-CA-C	-7.29	103.37	111.82
7	I	70	ARG	CD-NE-CZ	-7.28	114.20	124.40
1	A	856	THR	OG1-CB-CG2	-7.28	94.74	109.30
1	A	1136	SER	CB-CA-C	7.28	124.33	109.55
1	A	1120	LEU	N-CA-C	7.28	121.29	110.52
2	B	732	SER	N-CA-C	7.28	119.97	110.43
10	L	26	THR	CA-C-N	7.28	135.44	121.54
10	L	26	THR	C-N-CA	7.28	135.44	121.54
2	B	599	THR	OG1-CB-CG2	-7.28	94.74	109.30
3	C	248	ILE	CB-CA-C	-7.27	102.32	112.14
1	A	70	CYS	N-CA-CB	7.27	120.92	110.16
2	B	416	LEU	CA-CB-CG	-7.27	90.85	116.30
9	K	4	PRO	N-CA-C	-7.27	98.89	111.32
1	A	861	GLY	O-C-N	-7.27	113.20	122.43
2	B	626	ILE	CA-C-O	-7.27	112.85	121.28
3	C	239	PRO	CA-CB-CG	-7.26	90.70	104.50
5	F	120	ILE	CA-CB-CG1	7.26	122.75	110.40
1	A	1012	ARG	O-C-N	7.26	130.43	122.15
2	B	705	MET	CA-C-O	-7.26	111.10	119.60
1	A	622	VAL	CA-CB-CG1	7.26	122.74	110.40
1	A	696	GLU	CB-CA-C	7.26	122.14	110.96
1	A	970	THR	OG1-CB-CG2	-7.26	94.78	109.30
1	A	1278	ASN	N-CA-C	7.26	126.26	110.80
3	C	156	THR	CA-C-O	-7.26	112.91	121.11
2	B	902	GLY	CA-C-O	-7.25	111.94	119.27
1	A	887	GLY	CA-C-N	-7.25	106.23	122.04
1	A	887	GLY	C-N-CA	-7.25	106.23	122.04
2	B	1193	GLN	O-C-N	-7.25	113.76	123.19
2	B	1043	ASP	CB-CG-OD1	-7.25	101.72	118.40
8	J	28	ASP	O-C-N	7.25	130.88	122.25
5	F	75	PRO	CB-CA-C	-7.25	101.57	111.21
1	A	367	PRO	N-CD-CG	7.25	114.07	103.20
1	A	811	GLN	CG-CD-NE2	-7.25	105.53	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	46	GLN	CA-CB-CG	-7.25	99.61	114.10
2	B	656	GLY	N-CA-C	-7.24	103.67	113.37
1	A	968	GLN	CA-CB-CG	-7.24	99.62	114.10
2	B	286	PHE	CA-C-O	-7.24	113.22	120.82
2	B	877	PRO	CA-C-O	-7.24	112.10	122.31
8	J	24	LEU	CB-CA-C	-7.24	95.18	110.31
1	A	1384	VAL	N-CA-C	7.24	118.03	111.81
2	B	1095	LEU	CB-CA-C	-7.23	97.87	109.80
1	A	771	GLU	OE1-CD-OE2	7.23	140.25	122.90
2	B	519	TRP	CA-C-N	-7.23	111.91	122.46
2	B	519	TRP	C-N-CA	-7.23	111.91	122.46
2	B	622	LYS	CA-CB-CG	7.23	128.56	114.10
2	B	933	SER	CB-CA-C	7.23	123.83	110.10
7	I	95	THR	N-CA-C	7.23	120.71	110.23
9	K	3	ALA	N-CA-C	7.23	120.12	109.50
1	A	93	VAL	N-CA-CB	7.22	119.50	110.47
1	A	209	ASN	N-CA-CB	7.22	121.01	110.47
1	A	179	LEU	O-C-N	7.22	130.97	122.24
2	B	711	GLU	CB-CA-C	-7.22	95.95	110.17
2	B	1043	ASP	O-C-N	-7.21	115.00	123.22
2	B	963	PHE	CA-C-N	-7.21	110.55	122.67
2	B	963	PHE	C-N-CA	-7.21	110.55	122.67
6	H	93	TYR	N-CA-C	7.21	121.13	110.46
2	B	417	PHE	N-CA-C	-7.21	104.48	113.20
2	B	844	SER	N-CA-CB	-7.20	99.53	110.12
2	B	1085	ILE	N-CA-C	7.20	119.11	108.45
4	E	199	ILE	CA-C-N	-7.20	110.71	122.81
4	E	199	ILE	C-N-CA	-7.20	110.71	122.81
5	F	105	ALA	N-CA-C	-7.20	100.35	110.29
1	A	96	ILE	CG1-CB-CG2	-7.20	89.10	110.70
1	A	305	ASP	OD1-CG-OD2	-7.20	105.62	122.90
1	A	1269	GLU	OE1-CD-OE2	7.20	140.18	122.90
2	B	328	GLU	N-CA-CB	7.20	122.66	110.49
2	B	41	LYS	N-CA-C	-7.20	104.65	113.50
2	B	841	MET	CG-SD-CE	7.20	116.73	100.90
2	B	25	ILE	CB-CG1-CD1	-7.19	98.69	113.80
7	I	97	MET	CA-C-N	-7.19	108.97	120.34
7	I	97	MET	C-N-CA	-7.19	108.97	120.34
2	B	271	ALA	CA-C-O	-7.19	112.70	121.11
1	A	1408	ILE	CB-CA-C	-7.19	102.30	112.22
3	C	227	THR	CA-CB-OG1	7.19	120.38	109.60
8	J	19	GLU	N-CA-C	-7.19	103.53	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1049	ASP	OD1-CG-OD2	-7.18	105.66	122.90
1	A	193	ASP	CA-CB-CG	7.18	119.78	112.60
1	A	458	HIS	CA-C-O	-7.18	113.06	121.46
2	B	101	MET	CB-CA-C	-7.18	98.02	110.95
1	A	1135	ARG	NH1-CZ-NH2	7.18	128.63	119.30
4	E	74	ASP	CA-C-O	7.18	130.78	120.51
3	C	143	LEU	CB-CG-CD2	-7.18	89.17	110.70
1	A	418	SER	CA-CB-OG	-7.17	96.75	111.10
1	A	439	ASN	O-C-N	-7.17	112.93	121.97
2	B	329	THR	OG1-CB-CG2	-7.17	94.95	109.30
2	B	118	ARG	CB-CG-CD	7.17	127.79	111.30
1	A	1358	SER	N-CA-C	-7.17	103.40	111.14
2	B	807	ARG	CG-CD-NE	-7.17	96.23	112.00
6	H	115	TYR	N-CA-C	7.17	122.58	113.55
1	A	1079	MET	N-CA-C	-7.17	104.55	112.72
2	B	793	ALA	CA-C-O	-7.17	113.01	120.89
1	A	840	ARG	CD-NE-CZ	7.17	134.43	124.40
2	B	701	ILE	N-CA-C	7.17	124.24	109.34
9	K	51	LEU	N-CA-CB	-7.17	100.02	110.70
4	E	204	THR	N-CA-CB	-7.16	100.01	110.40
2	B	764	SER	N-CA-C	7.16	122.49	112.75
1	A	186	LYS	CG-CD-CE	7.16	127.77	111.30
1	A	40	THR	N-CA-C	-7.16	97.06	108.73
2	B	990	ILE	CB-CA-C	-7.15	100.67	111.33
2	B	1144	ALA	CA-C-N	-7.15	109.44	120.31
2	B	1144	ALA	C-N-CA	-7.15	109.44	120.31
2	B	1212	ILE	N-CA-C	7.15	118.88	108.58
3	C	136	ASP	CB-CG-OD2	7.15	134.84	118.40
10	L	47	ARG	N-CA-C	7.15	115.61	108.75
1	A	465	TYR	O-C-N	-7.15	113.08	122.59
1	A	600	PRO	CA-C-O	-7.15	108.76	120.05
1	A	302	THR	CA-CB-CG2	7.14	122.65	110.50
1	A	399	HIS	CA-C-N	7.14	144.14	127.00
1	A	399	HIS	C-N-CA	7.14	144.14	127.00
3	C	133	ILE	O-C-N	7.14	130.40	122.61
6	H	88	SER	N-CA-C	7.14	126.01	110.80
1	A	788	SER	CA-CB-OG	-7.14	96.82	111.10
2	B	182	SER	N-CA-C	-7.14	102.91	111.69
2	B	244	LEU	N-CA-C	7.13	121.03	109.40
8	J	25	LEU	N-CA-C	7.13	122.08	113.23
2	B	620	ARG	NE-CZ-NH1	-7.13	114.37	121.50
4	E	55	ARG	CA-C-O	7.13	128.11	120.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	K	62	LYS	CA-C-N	-7.13	113.85	123.12
9	K	62	LYS	C-N-CA	-7.13	113.85	123.12
6	H	19	ARG	CG-CD-NE	7.13	127.68	112.00
9	K	48	ALA	O-C-N	7.13	132.30	122.46
2	B	89	GLU	N-CA-C	7.13	130.95	111.00
2	B	1150	ARG	O-C-N	-7.13	114.03	122.15
1	A	155	GLU	CA-CB-CG	7.12	128.35	114.10
1	A	608	ILE	CA-CB-CG1	7.12	122.51	110.40
1	A	1103	GLU	N-CA-CB	-7.12	99.62	110.16
2	B	829	CYS	N-CA-C	-7.12	98.36	109.25
3	C	153	LEU	N-CA-CB	-7.12	99.16	110.77
4	E	20	LYS	CA-CB-CG	7.12	128.34	114.10
7	I	70	ARG	NE-CZ-NH2	-7.12	112.79	119.20
7	I	118	ARG	N-CA-C	7.12	120.98	110.30
1	A	517	ASN	CA-C-O	-7.12	113.70	122.03
3	C	207	CYS	N-CA-C	7.12	118.83	111.14
8	J	30	LEU	CD1-CG-CD2	-7.12	95.14	110.80
1	A	930	ASP	N-CA-C	-7.12	103.60	111.36
4	E	162	ARG	N-CA-C	-7.12	103.56	111.82
6	H	135	LEU	CA-CB-CG	7.11	141.20	116.30
1	A	823	GLY	N-CA-C	7.11	122.90	113.37
4	E	162	ARG	CB-CG-CD	7.11	127.66	111.30
9	K	46	ILE	CA-CB-CG1	7.11	122.49	110.40
9	K	90	ALA	N-CA-C	7.11	122.28	112.04
1	A	1016	THR	N-CA-C	7.11	119.93	111.33
1	A	1188	GLN	CB-CA-C	-7.11	98.67	110.19
3	C	29	MET	CG-SD-CE	7.11	116.54	100.90
3	C	205	LYS	CA-CB-CG	-7.11	99.88	114.10
8	J	13	VAL	CG1-CB-CG2	-7.11	95.17	110.80
6	H	38	LEU	CD1-CG-CD2	-7.10	95.17	110.80
2	B	734	HIS	N-CA-C	-7.10	105.44	112.97
8	J	5	VAL	O-C-N	-7.10	114.95	121.91
2	B	870	ILE	O-C-N	7.10	127.92	121.96
4	E	150	VAL	N-CA-C	-7.10	99.64	107.73
6	H	13	SER	CA-C-O	7.10	127.94	120.42
1	A	962	ARG	N-CA-C	-7.09	102.59	112.45
2	B	711	GLU	N-CA-C	7.09	125.49	109.81
1	A	1129	GLU	CA-CB-CG	7.09	128.28	114.10
2	B	429	PHE	N-CA-CB	-7.09	100.14	110.70
1	A	265	LYS	CA-C-O	7.09	126.94	119.14
1	A	240	PRO	N-CA-C	7.09	122.43	110.95
6	H	41	ASP	OD1-CG-OD2	-7.09	105.89	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	313	MET	N-CA-C	7.08	121.18	112.54
1	A	725	ALA	O-C-N	7.08	130.23	122.15
2	B	689	LEU	N-CA-CB	-7.08	99.39	110.30
1	A	861	GLY	N-CA-C	-7.08	105.55	115.32
2	B	847	ASP	N-CA-C	-7.08	103.56	111.28
2	B	1210	MET	CB-CA-C	-7.08	100.34	111.17
4	E	118	PRO	CB-CG-CD	-7.08	83.44	106.10
2	B	187	SER	CA-C-N	-7.08	109.55	120.31
2	B	187	SER	C-N-CA	-7.08	109.55	120.31
2	B	680	THR	CA-CB-CG2	7.08	122.54	110.50
1	A	979	SER	N-CA-C	-7.08	99.45	110.42
2	B	518	HIS	ND1-CE1-NE2	-7.08	101.33	108.40
2	B	975	GLN	OE1-CD-NE2	7.08	129.68	122.60
4	E	156	LEU	O-C-N	7.08	131.36	123.01
2	B	284	ILE	CG1-CB-CG2	-7.07	89.48	110.70
2	B	621	GLU	N-CA-C	-7.07	104.65	113.28
2	B	1198	TYR	O-C-N	7.07	129.62	122.12
1	A	145	LYS	CB-CA-C	-7.07	98.41	110.22
1	A	1110	ASN	CA-C-O	7.07	132.19	120.81
1	A	670	ILE	CA-CB-CG2	-7.07	98.49	110.50
2	B	258	LEU	N-CA-C	7.07	119.78	108.41
3	C	26	ASP	CA-C-O	7.07	129.84	121.36
6	H	54	SER	N-CA-C	7.06	119.48	108.96
8	J	42	LYS	CA-C-N	-7.06	110.85	120.87
8	J	42	LYS	C-N-CA	-7.06	110.85	120.87
1	A	150	THR	N-CA-C	-7.06	105.20	113.88
2	B	853	SER	CA-CB-OG	7.06	125.21	111.10
1	A	434	ARG	NE-CZ-NH1	7.05	128.56	121.50
2	B	973	ILE	N-CA-CB	-7.05	101.33	111.21
10	L	50	ASP	CA-C-N	7.05	134.18	122.33
10	L	50	ASP	C-N-CA	7.05	134.18	122.33
1	A	390	GLN	CA-C-N	-7.05	110.28	120.29
1	A	390	GLN	C-N-CA	-7.05	110.28	120.29
1	A	1378	GLN	CA-C-N	-7.05	112.56	122.86
1	A	1378	GLN	C-N-CA	-7.05	112.56	122.86
2	B	1154	ALA	N-CA-CB	7.05	120.48	110.12
6	H	139	ASN	N-CA-C	-7.05	95.78	110.80
1	A	546	VAL	CG1-CB-CG2	-7.05	95.30	110.80
1	A	938	LYS	CB-CA-C	-7.05	99.09	110.79
1	A	1316	VAL	CA-C-O	7.05	128.11	120.57
2	B	354	ASP	CA-C-O	-7.05	113.08	120.55
3	C	145	CYS	CA-C-O	-7.05	113.89	121.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	167	ARG	NH1-CZ-NH2	7.04	128.46	119.30
7	I	3	THR	CB-CA-C	-7.04	101.06	111.77
7	I	91	ARG	N-CA-C	-7.04	96.86	108.49
3	C	263	THR	N-CA-CB	-7.04	98.59	110.49
1	A	492	PRO	O-C-N	7.04	131.74	123.01
4	E	69	ILE	CA-C-N	-7.04	110.84	120.28
4	E	69	ILE	C-N-CA	-7.04	110.84	120.28
7	I	81	ARG	NE-CZ-NH1	7.04	128.54	121.50
1	A	1113	THR	N-CA-C	7.04	125.37	109.81
2	B	338	GLY	CA-C-O	-7.04	108.32	120.57
3	C	88	CYS	CA-C-O	-7.04	113.50	121.81
1	A	1138	ILE	N-CA-CB	-7.04	100.07	111.82
1	A	686	ALA	N-CA-CB	7.04	120.74	110.26
2	B	50	SER	N-CA-C	7.04	119.03	111.36
1	A	361	LEU	N-CA-C	7.03	119.84	111.33
2	B	571	PRO	N-CD-CG	-7.03	92.65	103.20
2	B	1042	GLY	O-C-N	7.03	129.03	123.61
1	A	703	THR	N-CA-C	7.03	121.29	109.76
2	B	987	LYS	CB-CA-C	-7.03	97.54	111.60
2	B	1096	ARG	NE-CZ-NH1	-7.03	114.47	121.50
5	F	135	ARG	NE-CZ-NH2	7.03	125.53	119.20
1	A	1008	GLN	N-CA-C	7.03	119.02	111.36
3	C	183	TRP	N-CA-CB	7.03	120.08	110.38
1	A	1103	GLU	CB-CA-C	7.02	122.79	110.85
2	B	605	ARG	NE-CZ-NH2	7.02	125.52	119.20
4	E	98	ILE	CG1-CB-CG2	-7.02	89.63	110.70
2	B	123	THR	CB-CA-C	-7.02	100.36	111.17
9	K	78	THR	N-CA-CB	7.02	121.15	109.92
2	B	399	ASP	N-CA-CB	-7.02	99.85	110.73
2	B	463	THR	OG1-CB-CG2	-7.02	95.27	109.30
10	L	42	ARG	NH1-CZ-NH2	-7.02	110.18	119.30
1	A	1046	LEU	N-CA-C	7.01	119.00	111.36
2	B	1223	ASP	O-C-N	7.01	131.44	122.33
3	C	84	ARG	NH1-CZ-NH2	-7.01	110.19	119.30
6	H	91	ASP	CA-CB-CG	-7.01	105.59	112.60
9	K	114	LEU	N-CA-CB	7.01	122.41	110.50
3	C	180	TYR	CA-C-O	7.00	128.70	120.43
5	F	84	TYR	N-CA-CB	-7.00	99.64	110.29
1	A	1046	LEU	O-C-N	-7.00	114.17	122.15
2	B	981	ALA	N-CA-CB	-7.00	98.49	111.52
1	A	548	ASN	N-CA-C	-7.00	103.08	111.69
2	B	242	SER	CA-CB-OG	7.00	125.10	111.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	941	LEU	CA-C-O	-7.00	112.94	120.92
1	A	267	ALA	CA-C-N	7.00	132.40	120.72
1	A	267	ALA	C-N-CA	7.00	132.40	120.72
1	A	705	LYS	N-CA-C	7.00	123.50	107.48
4	E	181	ALA	N-CA-CB	-7.00	99.69	111.17
2	B	1217	TYR	N-CA-C	7.00	121.71	109.96
1	A	938	LYS	N-CA-CB	6.99	120.40	110.12
1	A	1341	ILE	CA-C-N	-6.99	111.42	120.65
1	A	1341	ILE	C-N-CA	-6.99	111.42	120.65
2	B	267	ARG	N-CA-CB	-6.99	98.94	109.71
2	B	565	PRO	N-CD-CG	6.99	113.68	103.20
3	C	55	THR	CB-CA-C	-6.99	98.91	110.72
6	H	57	VAL	CB-CA-C	-6.99	102.24	111.81
7	I	36	GLU	N-CA-C	6.99	119.80	108.76
2	B	106	ASP	N-CA-C	6.99	125.68	110.80
2	B	186	GLU	CA-C-N	-6.99	110.22	120.28
2	B	186	GLU	C-N-CA	-6.99	110.22	120.28
3	C	219	PHE	CA-C-O	-6.99	113.51	121.19
1	A	1007	ILE	CA-C-N	-6.98	110.38	120.29
1	A	1007	ILE	C-N-CA	-6.98	110.38	120.29
9	K	20	LYS	CB-CG-CD	6.98	127.36	111.30
1	A	547	LEU	N-CA-C	-6.98	104.02	112.54
1	A	1000	LEU	CA-C-N	-6.98	111.27	122.23
1	A	1000	LEU	C-N-CA	-6.98	111.27	122.23
1	A	1310	GLY	O-C-N	6.98	130.73	122.64
2	B	251	ILE	CA-CB-CG2	6.98	122.36	110.50
1	A	367	PRO	CB-CA-C	-6.97	102.31	111.23
1	A	1372	VAL	CA-C-O	6.97	128.24	120.85
2	B	732	SER	CA-C-O	-6.97	114.20	121.87
4	E	194	GLU	CA-C-O	-6.97	113.96	121.56
9	K	32	VAL	CA-CB-CG1	6.97	122.25	110.40
1	A	1197	LEU	CA-C-O	6.97	130.16	121.66
2	B	1049	ASP	CB-CG-OD1	6.97	134.43	118.40
1	A	134	ARG	N-CA-C	-6.97	102.90	111.40
10	L	61	THR	CA-CB-CG2	6.97	122.34	110.50
3	C	6	PRO	N-CA-CB	-6.96	97.73	103.30
1	A	1309	ASP	CB-CA-C	-6.96	98.91	110.19
3	C	210	GLU	CB-CG-CD	6.96	124.43	112.60
9	K	96	ASN	N-CA-CB	6.96	120.57	110.20
2	B	345	LYS	O-C-N	-6.96	114.63	122.08
2	B	878	GLN	N-CA-C	6.96	125.62	110.80
2	B	535	LEU	CD1-CG-CD2	-6.96	95.49	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	182	ASP	CB-CA-C	-6.96	98.53	109.52
1	A	1417	GLU	CA-CB-CG	6.96	128.01	114.10
1	A	618	GLU	OE1-CD-OE2	6.95	139.59	122.90
2	B	490	SER	O-C-N	6.95	130.82	122.27
2	B	853	SER	N-CA-C	6.95	119.74	109.24
3	C	66	ARG	CB-CG-CD	6.95	127.29	111.30
4	E	179	GLN	CG-CD-NE2	-6.95	105.97	116.40
1	A	268	ASP	OD1-CG-OD2	-6.95	106.22	122.90
2	B	268	THR	OG1-CB-CG2	-6.95	95.40	109.30
2	B	553	PRO	N-CD-CG	-6.95	92.78	103.20
9	K	49	GLU	CA-C-O	-6.95	113.54	120.70
1	A	1128	GLN	O-C-N	-6.95	113.35	122.59
1	A	1259	MET	CA-C-N	-6.95	111.41	120.44
1	A	1259	MET	C-N-CA	-6.95	111.41	120.44
2	B	204	ILE	CA-CB-CG2	-6.95	98.69	110.50
4	E	114	ASN	N-CA-CB	6.95	122.23	110.49
1	A	1165	GLU	CA-C-N	-6.95	111.55	122.73
1	A	1165	GLU	C-N-CA	-6.95	111.55	122.73
1	A	1261	LYS	CG-CD-CE	6.94	127.27	111.30
5	F	142	SER	N-CA-C	6.94	119.92	110.55
6	H	101	ALA	CA-C-O	6.94	128.06	120.71
9	K	114	LEU	CA-CB-CG	6.94	140.58	116.30
1	A	982	THR	CA-CB-CG2	6.93	122.29	110.50
3	C	9	LYS	CD-CE-NZ	6.93	134.09	111.90
1	A	373	THR	N-CA-CB	-6.93	99.87	110.20
2	B	297	ILE	N-CA-C	-6.93	103.44	111.00
1	A	1238	ILE	O-C-N	-6.93	115.78	123.26
2	B	770	GLN	OE1-CD-NE2	6.93	129.53	122.60
7	I	27	PHE	CA-C-N	-6.93	110.64	123.05
7	I	27	PHE	C-N-CA	-6.93	110.64	123.05
1	A	1265	ASN	N-CA-C	6.93	119.47	111.02
6	H	52	GLN	CB-CG-CD	6.93	124.37	112.60
1	A	980	ASP	CB-CA-C	-6.92	98.05	110.37
1	A	1070	GLN	N-CA-C	-6.92	103.66	111.14
1	A	1207	LEU	CB-CG-CD1	-6.92	89.93	110.70
9	K	74	ARG	CG-CD-NE	-6.92	96.77	112.00
1	A	7	SER	N-CA-C	6.92	119.69	108.34
7	I	61	ASP	CB-CG-OD2	6.92	134.32	118.40
1	A	394	ASN	CB-CA-C	-6.92	95.85	110.31
1	A	659	HIS	CB-CG-CD2	6.92	140.19	131.20
2	B	273	LEU	CB-CA-C	-6.92	98.37	109.37
2	B	381	MET	CG-SD-CE	-6.92	85.68	100.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	K	29	ASN	N-CA-C	-6.92	101.67	111.56
9	K	74	ARG	CB-CG-CD	6.92	127.21	111.30
2	B	724	ASP	N-CA-C	6.92	125.09	109.81
2	B	768	THR	N-CA-C	-6.92	103.76	111.71
2	B	858	SER	CA-C-O	-6.92	112.84	120.38
3	C	123	ASN	CB-CA-C	6.92	122.32	110.77
9	K	5	ASP	CB-CA-C	-6.92	97.40	109.64
1	A	1290	LYS	CD-CE-NZ	6.92	134.03	111.90
3	C	255	VAL	CA-C-O	-6.92	113.17	120.57
1	A	1356	ILE	CB-CG1-CD1	-6.91	99.28	113.80
3	C	35	ARG	CD-NE-CZ	6.91	134.08	124.40
3	C	180	TYR	O-C-N	-6.91	115.60	123.48
1	A	216	VAL	N-CA-C	-6.91	103.57	110.62
5	F	151	LEU	CA-C-O	-6.91	112.86	120.81
1	A	1138	ILE	O-C-N	6.91	129.25	122.07
4	E	71	LYS	CB-CG-CD	6.91	127.19	111.30
1	A	647	GLY	N-CA-C	6.90	122.62	113.37
1	A	1284	MET	CG-SD-CE	-6.90	85.72	100.90
2	B	1093	GLN	N-CA-CB	-6.90	99.58	110.69
4	E	195	VAL	CA-C-O	-6.90	113.15	120.39
2	B	680	THR	OG1-CB-CG2	-6.90	95.51	109.30
8	J	36	LEU	CA-C-N	-6.90	107.53	121.18
8	J	36	LEU	C-N-CA	-6.90	107.53	121.18
1	A	245	PRO	O-C-N	6.89	130.50	122.23
6	H	23	VAL	CA-C-O	-6.89	112.22	121.32
2	B	1014	PRO	CA-C-O	-6.89	109.32	119.18
4	E	90	VAL	N-CA-CB	-6.89	99.86	111.23
2	B	1106	ARG	N-CA-C	6.89	120.12	107.99
1	A	1227	ILE	N-CA-CB	6.89	120.24	112.32
8	J	25	LEU	CB-CG-CD2	-6.89	90.03	110.70
1	A	1063	MET	N-CA-CB	-6.89	102.13	110.53
4	E	62	ALA	N-CA-CB	-6.89	99.34	111.39
2	B	487	THR	N-CA-CB	-6.88	99.71	111.69
2	B	712	PRO	N-CD-CG	-6.88	92.88	103.20
2	B	550	ASP	CA-C-O	-6.88	113.79	120.19
2	B	845	SER	CA-C-O	6.88	127.84	120.55
2	B	966	VAL	CG1-CB-CG2	-6.88	95.67	110.80
2	B	664	THR	OG1-CB-CG2	-6.88	95.55	109.30
5	F	148	VAL	CA-C-N	-6.88	110.96	120.38
5	F	148	VAL	C-N-CA	-6.88	110.96	120.38
1	A	899	VAL	CG1-CB-CG2	-6.87	95.68	110.80
7	I	47	GLU	O-C-N	-6.87	115.23	123.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	694	ASP	N-CA-C	6.87	121.01	110.36
3	C	239	PRO	O-C-N	-6.87	115.60	123.23
10	L	61	THR	N-CA-CB	6.87	120.09	110.26
2	B	122	LEU	N-CA-C	6.87	119.83	110.35
2	B	267	ARG	O-C-N	-6.87	114.31	122.96
3	C	243	VAL	N-CA-C	-6.87	102.51	111.09
4	E	155	ARG	N-CA-C	-6.87	98.84	109.76
2	B	449	ASN	N-CA-C	6.87	120.04	108.23
2	B	1085	ILE	CA-C-O	6.87	128.31	120.76
1	A	56	PRO	O-C-N	6.86	131.91	122.64
4	E	208	TYR	CG-CD1-CE1	6.86	131.50	121.20
2	B	1130	PHE	CA-C-N	6.86	128.54	122.43
2	B	1130	PHE	C-N-CA	6.86	128.54	122.43
1	A	367	PRO	CA-C-O	6.86	129.52	121.56
2	B	912	ILE	CB-CA-C	-6.86	101.16	110.42
10	L	63	ARG	CB-CA-C	6.86	121.90	109.62
2	B	770	GLN	N-CA-C	-6.86	103.82	111.71
1	A	910	PRO	N-CA-C	-6.86	105.78	114.35
1	A	974	ASP	O-C-N	6.86	131.02	123.27
7	I	5	ARG	CG-CD-NE	6.86	127.08	112.00
1	A	375	THR	CA-C-O	6.85	129.12	121.11
3	C	143	LEU	N-CA-CB	-6.85	98.98	109.94
5	F	81	THR	N-CA-C	6.85	118.83	110.41
9	K	70	ARG	CD-NE-CZ	-6.85	114.81	124.40
2	B	130	VAL	N-CA-C	6.85	123.58	109.34
2	B	633	VAL	O-C-N	-6.85	114.88	122.69
2	B	1151	LEU	O-C-N	-6.85	114.12	122.34
4	E	98	ILE	CA-C-O	-6.85	113.38	120.71
2	B	595	ARG	N-CA-CB	6.85	120.29	110.16
1	A	1046	LEU	CA-C-O	6.84	127.68	120.42
2	B	165	VAL	N-CA-C	6.84	123.58	109.34
2	B	776	GLN	CA-C-O	6.84	128.03	119.95
2	B	888	GLY	O-C-N	6.84	129.24	123.29
5	F	104	ASN	N-CA-C	6.84	120.85	111.54
1	A	544	ASP	N-CA-C	6.84	118.39	111.07
2	B	1160	VAL	CA-C-N	-6.84	110.37	122.07
2	B	1160	VAL	C-N-CA	-6.84	110.37	122.07
1	A	1313	LEU	CA-C-N	-6.84	110.43	120.28
1	A	1313	LEU	C-N-CA	-6.84	110.43	120.28
10	L	27	LEU	CA-CB-CG	6.84	140.23	116.30
1	A	89	PRO	CB-CA-C	-6.84	102.12	111.21
2	B	936	ASP	CA-C-O	-6.83	112.65	120.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	549	MET	CG-SD-CE	6.83	115.93	100.90
1	A	619	LYS	CB-CG-CD	6.83	127.02	111.30
1	A	1141	THR	OG1-CB-CG2	-6.83	95.64	109.30
2	B	606	LYS	N-CA-CB	-6.83	101.82	110.90
5	F	112	GLU	CA-CB-CG	-6.83	100.44	114.10
2	B	294	ASP	CA-C-N	6.83	127.71	119.99
2	B	294	ASP	C-N-CA	6.83	127.71	119.99
2	B	1138	MET	O-C-N	-6.83	113.87	122.27
1	A	1025	ARG	N-CA-CB	6.83	121.09	110.44
2	B	552	MET	CA-CB-CG	6.83	127.75	114.10
3	C	93	ASP	CA-C-N	-6.83	110.45	122.26
3	C	93	ASP	C-N-CA	-6.83	110.45	122.26
1	A	76	GLU	CA-C-N	6.82	131.09	121.61
1	A	76	GLU	C-N-CA	6.82	131.09	121.61
1	A	808	LEU	N-CA-CB	-6.82	99.17	110.23
2	B	297	ILE	CA-CB-CG1	6.82	122.00	110.40
7	I	68	LEU	CA-C-N	-6.82	113.28	120.03
7	I	68	LEU	C-N-CA	-6.82	113.28	120.03
10	L	26	THR	O-C-N	6.82	131.66	122.59
5	F	144	GLU	CA-C-O	-6.82	113.13	121.11
2	B	902	GLY	O-C-N	6.82	129.93	122.56
1	A	1282	VAL	CB-CA-C	-6.82	100.00	110.50
2	B	887	HIS	CA-C-N	6.82	128.54	122.47
2	B	887	HIS	C-N-CA	6.82	128.54	122.47
10	L	34	CYS	CA-CB-SG	-6.82	98.72	114.40
1	A	66	LYS	N-CA-C	6.81	119.46	107.61
1	A	1106	ASN	N-CA-C	6.81	121.44	113.20
2	B	373	ARG	NE-CZ-NH2	-6.81	113.07	119.20
1	A	766	GLY	N-CA-C	6.81	125.09	112.77
1	A	238	CYS	CA-C-N	-6.80	109.23	122.70
1	A	238	CYS	C-N-CA	-6.80	109.23	122.70
4	E	91	LYS	O-C-N	6.80	129.11	122.03
6	H	103	LYS	CA-C-O	-6.80	110.78	120.51
2	B	942	ARG	CA-CB-CG	6.80	127.70	114.10
2	B	750	GLY	N-CA-C	6.80	122.60	112.41
1	A	411	ASP	N-CA-C	6.79	120.08	110.23
2	B	214	ALA	N-CA-CB	-6.79	99.30	109.69
3	C	98	VAL	CA-C-O	-6.79	113.28	120.48
2	B	272	THR	O-C-N	6.79	131.13	123.05
2	B	1150	ARG	N-CA-C	6.79	118.76	111.36
1	A	912	LEU	CA-C-N	-6.78	110.00	121.94
1	A	912	LEU	C-N-CA	-6.78	110.00	121.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1447	GLU	N-CA-CB	6.78	120.31	110.20
2	B	915	THR	CA-CB-OG1	6.78	119.78	109.60
1	A	1337	GLU	O-C-N	6.78	131.42	122.33
2	B	593	PRO	N-CA-C	-6.78	104.50	113.65
2	B	660	LYS	N-CA-C	-6.78	103.12	111.33
2	B	1212	ILE	CA-CB-CG1	-6.78	98.87	110.40
4	E	156	LEU	CD1-CG-CD2	6.78	125.71	110.80
1	A	1217	LYS	CA-C-N	-6.78	111.36	122.54
1	A	1217	LYS	C-N-CA	-6.78	111.36	122.54
2	B	387	LEU	CA-C-O	6.77	127.76	119.97
4	E	140	LEU	N-CA-C	-6.77	104.64	113.17
1	A	411	ASP	N-CA-CB	6.77	120.05	109.83
1	A	205	GLU	CB-CG-CD	6.77	124.10	112.60
2	B	697	GLU	CA-C-O	-6.77	111.06	119.38
2	B	776	GLN	O-C-N	-6.76	113.94	122.26
9	K	79	GLU	CB-CA-C	6.76	120.41	110.26
2	B	914	LYS	O-C-N	6.76	130.36	123.26
2	B	909	ASP	OD1-CG-OD2	-6.76	106.68	122.90
6	H	131	ASN	CA-CB-CG	6.76	119.36	112.60
1	A	446	ARG	NE-CZ-NH2	-6.76	113.12	119.20
8	J	39	LEU	N-CA-C	-6.76	105.36	112.93
1	A	81	PHE	CA-C-O	6.75	127.79	120.43
1	A	812	GLU	N-CA-C	-6.75	103.99	111.82
1	A	999	VAL	N-CA-CB	-6.75	102.65	111.90
1	A	1255	GLU	CB-CG-CD	6.75	124.08	112.60
7	I	30	ARG	NE-CZ-NH1	-6.75	114.75	121.50
7	I	116	ASN	CA-C-O	-6.75	112.58	120.62
2	B	1154	ALA	O-C-N	6.75	129.28	122.12
4	E	81	GLU	OE1-CD-OE2	6.75	139.10	122.90
6	H	103	LYS	CB-CG-CD	6.75	126.82	111.30
3	C	111	THR	CA-CB-OG1	6.75	119.72	109.60
1	A	898	ARG	N-CA-C	6.74	120.01	109.96
1	A	305	ASP	N-CA-C	6.74	129.87	111.00
2	B	1050	ILE	N-CA-C	6.74	123.36	109.34
3	C	207	CYS	CB-CA-C	-6.74	100.25	110.90
5	F	142	SER	CA-C-O	-6.74	113.86	121.81
1	A	731	ARG	NH1-CZ-NH2	6.74	128.06	119.30
2	B	533	CYS	CA-C-N	-6.73	113.03	122.86
2	B	533	CYS	C-N-CA	-6.73	113.03	122.86
10	L	29	TYR	N-CA-C	6.73	120.04	110.14
1	A	1331	SER	N-CA-C	6.73	120.23	108.52
2	B	1043	ASP	CB-CG-OD2	6.73	133.88	118.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	896	ASP	N-CA-C	-6.73	104.89	113.23
2	B	978	ASP	O-C-N	6.73	130.52	122.85
4	E	180	ARG	CA-C-N	-6.73	112.56	122.86
4	E	180	ARG	C-N-CA	-6.73	112.56	122.86
1	A	1113	THR	N-CA-CB	-6.73	98.40	110.37
7	I	34	TYR	O-C-N	6.73	130.56	122.96
1	A	209	ASN	OD1-CG-ND2	6.72	129.32	122.60
1	A	875	ALA	N-CA-C	-6.72	105.04	113.18
1	A	962	ARG	CA-C-O	6.72	128.20	120.00
2	B	484	ASN	N-CA-C	6.72	119.98	110.23
3	C	107	SER	N-CA-C	6.72	119.24	110.43
1	A	613	ILE	CG1-CB-CG2	-6.72	90.53	110.70
2	B	412	LEU	CA-C-O	-6.72	112.78	120.24
2	B	1109	GLY	O-C-N	6.72	128.49	121.77
3	C	127	ARG	NE-CZ-NH1	6.72	128.22	121.50
2	B	164	LYS	CA-C-O	-6.72	109.38	120.80
1	A	77	CYS	N-CA-C	-6.72	99.90	109.24
1	A	938	LYS	CA-C-O	-6.72	113.43	120.55
1	A	227	VAL	O-C-N	6.71	129.05	122.07
1	A	598	LEU	CB-CA-C	-6.71	100.21	111.02
5	F	141	GLY	CA-C-O	-6.71	112.09	119.27
2	B	1204	PHE	CA-C-N	-6.71	111.28	120.28
2	B	1204	PHE	C-N-CA	-6.71	111.28	120.28
3	C	184	ASN	CA-C-N	-6.71	109.64	122.53
3	C	184	ASN	C-N-CA	-6.71	109.64	122.53
1	A	806	ARG	NH1-CZ-NH2	6.71	128.03	119.30
1	A	1210	GLY	CA-C-O	-6.71	111.73	119.65
2	B	253	THR	CB-CA-C	-6.71	99.18	110.19
1	A	127	ALA	O-C-N	6.71	129.23	122.12
2	B	95	ILE	CB-CA-C	-6.71	100.62	110.62
1	A	504	LEU	N-CA-C	6.71	122.36	114.04
2	B	806	THR	N-CA-CB	-6.71	99.88	111.55
1	A	1138	ILE	N-CA-C	6.71	117.33	111.90
1	A	1196	GLU	CG-CD-OE2	-6.71	102.97	118.40
1	A	1275	GLY	CA-C-O	6.71	128.10	122.13
2	B	1165	ILE	CA-CB-CG1	6.71	121.80	110.40
1	A	659	HIS	CA-C-O	6.70	127.39	119.48
4	E	172	GLU	CA-C-O	-6.70	113.78	120.82
7	I	63	GLY	O-C-N	-6.70	112.06	122.18
2	B	55	VAL	CB-CA-C	-6.70	103.10	111.94
2	B	229	ALA	N-CA-C	6.70	120.01	109.96
4	E	87	SER	CA-CB-OG	6.70	124.50	111.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	135	LEU	CB-CG-CD2	6.70	130.80	110.70
9	K	6	ARG	NE-CZ-NH1	6.70	128.20	121.50
2	B	890	TYR	N-CA-C	-6.70	104.73	113.17
1	A	1322	ILE	N-CA-C	-6.69	98.83	109.20
2	B	211	VAL	CA-C-N	-6.69	113.48	122.72
2	B	211	VAL	C-N-CA	-6.69	113.48	122.72
2	B	362	PRO	CB-CA-C	-6.69	101.85	111.62
6	H	20	TYR	N-CA-C	6.69	119.94	110.50
7	I	33	SER	N-CA-C	-6.69	103.43	112.26
2	B	651	LEU	CA-C-N	6.68	129.54	120.38
2	B	651	LEU	C-N-CA	6.68	129.54	120.38
3	C	34	ARG	NE-CZ-NH2	-6.68	113.19	119.20
3	C	155	LEU	CA-C-N	-6.68	112.32	122.81
3	C	155	LEU	C-N-CA	-6.68	112.32	122.81
2	B	799	PRO	CB-CA-C	-6.68	103.08	111.56
2	B	346	GLU	CB-CG-CD	6.68	123.95	112.60
1	A	391	LEU	N-CA-CB	6.68	120.04	110.16
1	A	527	THR	CA-CB-OG1	6.67	119.61	109.60
2	B	789	MET	CB-CA-C	-6.67	101.75	111.23
2	B	1129	ARG	NE-CZ-NH2	-6.67	113.19	119.20
1	A	1161	THR	N-CA-C	6.67	119.30	108.76
1	A	475	THR	CA-CB-CG2	6.67	121.84	110.50
1	A	1219	THR	CA-CB-OG1	6.67	119.61	109.60
3	C	69	LEU	N-CA-C	6.67	121.25	113.18
7	I	45	ARG	NE-CZ-NH1	-6.67	114.83	121.50
1	A	1191	TRP	N-CA-C	-6.67	98.39	109.46
1	A	1384	VAL	CB-CA-C	-6.67	103.88	111.55
2	B	120	ARG	NE-CZ-NH1	-6.67	114.83	121.50
4	E	97	VAL	CA-C-N	-6.67	109.88	120.55
4	E	97	VAL	C-N-CA	-6.67	109.88	120.55
4	E	148	GLU	CB-CG-CD	6.67	123.94	112.60
1	A	186	LYS	CA-C-N	6.67	132.28	122.08
1	A	186	LYS	C-N-CA	6.67	132.28	122.08
2	B	123	THR	N-CA-C	6.67	121.63	107.70
1	A	682	THR	O-C-N	6.67	130.02	122.22
1	A	923	LEU	O-C-N	6.67	131.26	122.33
2	B	1015	HIS	ND1-CE1-NE2	-6.66	101.74	108.40
1	A	566	ILE	O-C-N	6.66	132.68	122.16
1	A	616	VAL	N-CA-CB	-6.66	98.83	110.49
8	J	2	ILE	CB-CA-C	-6.66	99.20	111.18
1	A	570	PRO	N-CD-CG	-6.66	93.21	103.20
8	J	34	THR	N-CA-C	-6.66	103.50	111.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	K	56	VAL	N-CA-CB	6.66	118.59	111.00
9	K	67	PHE	CA-C-N	-6.65	112.36	122.81
9	K	67	PHE	C-N-CA	-6.65	112.36	122.81
2	B	328	GLU	CA-C-N	-6.65	111.27	120.38
2	B	328	GLU	C-N-CA	-6.65	111.27	120.38
1	A	1062	GLU	N-CA-CB	6.65	119.74	109.97
1	A	620	LYS	CD-CE-NZ	6.65	133.17	111.90
2	B	915	THR	OG1-CB-CG2	-6.65	96.00	109.30
3	C	248	ILE	CA-C-O	6.65	127.86	120.95
3	C	201	TRP	N-CA-C	6.65	118.03	109.72
9	K	31	VAL	CA-C-O	6.65	128.10	121.45
1	A	121	LEU	O-C-N	-6.64	113.75	122.59
2	B	665	GLU	CA-CB-CG	6.64	127.39	114.10
1	A	482	PHE	CA-C-O	6.64	129.18	121.34
2	B	24	PRO	CA-C-O	-6.64	113.76	121.86
2	B	35	SER	CB-CA-C	-6.64	99.39	110.68
4	E	208	TYR	CA-C-N	-6.64	113.30	122.93
4	E	208	TYR	C-N-CA	-6.64	113.30	122.93
2	B	957	ASN	N-CA-CB	-6.64	99.27	110.49
4	E	192	ARG	CD-NE-CZ	6.64	133.69	124.40
2	B	710	LEU	CD1-CG-CD2	-6.64	96.20	110.80
5	F	135	ARG	CA-C-N	6.64	131.25	122.42
5	F	135	ARG	C-N-CA	6.64	131.25	122.42
2	B	935	ARG	CD-NE-CZ	6.63	133.69	124.40
1	A	188	ASP	OD1-CG-OD2	-6.63	106.98	122.90
2	B	1000	PRO	CA-C-O	-6.63	113.77	121.86
7	I	75	CYS	N-CA-CB	6.63	118.05	110.03
6	H	110	ASP	O-C-N	6.63	129.13	122.30
1	A	458	HIS	CA-CB-CG	-6.63	107.17	113.80
2	B	764	SER	N-CA-CB	-6.63	100.42	110.30
2	B	239	GLU	CB-CA-C	6.63	122.80	109.68
3	C	29	MET	CA-CB-CG	6.63	127.35	114.10
4	E	139	ALA	N-CA-C	-6.63	104.45	112.54
1	A	996	ASN	N-CA-C	6.62	121.07	112.92
1	A	1021	LEU	N-CA-C	-6.62	103.32	111.40
4	E	25	ASP	CB-CG-OD2	6.62	133.63	118.40
10	L	55	ILE	N-CA-C	6.62	117.42	107.75
1	A	127	ALA	N-CA-C	6.62	118.50	111.28
1	A	229	SER	N-CA-C	6.62	120.22	107.44
1	A	1230	GLU	N-CA-CB	6.62	119.91	110.44
2	B	567	GLU	CB-CA-C	6.62	123.59	110.42
2	B	616	ILE	CB-CA-C	-6.62	102.85	110.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	104	GLU	CA-C-O	6.62	129.08	121.47
2	B	711	GLU	CA-CB-CG	6.62	127.33	114.10
1	A	708	MET	CB-CA-C	6.62	121.23	109.65
1	A	1124	HIS	N-CA-C	-6.62	105.60	113.21
1	A	1274	ARG	CA-CB-CG	-6.62	100.87	114.10
1	A	674	PRO	CA-C-O	6.61	129.33	119.74
1	A	1033	GLN	N-CA-C	-6.61	103.90	112.23
5	F	97	ARG	CB-CG-CD	6.61	126.50	111.30
1	A	870	GLU	CG-CD-OE1	-6.61	103.20	118.40
2	B	1194	ILE	CB-CA-C	-6.61	99.13	110.30
4	E	136	ASN	N-CA-C	-6.61	100.50	110.28
10	L	25	ALA	N-CA-CB	6.61	120.31	110.40
1	A	789	LYS	N-CA-CB	-6.61	100.81	110.26
2	B	532	ALA	N-CA-CB	6.61	120.20	110.56
2	B	1162	ILE	CA-C-O	-6.61	113.23	120.43
9	K	42	LEU	CA-C-N	-6.61	112.74	119.94
9	K	42	LEU	C-N-CA	-6.61	112.74	119.94
2	B	319	GLU	N-CA-C	6.60	119.30	111.71
2	B	958	GLN	CA-C-O	6.60	127.56	119.97
2	B	329	THR	N-CA-CB	-6.60	100.16	110.06
4	E	121	MET	CB-CG-SD	6.60	132.49	112.70
1	A	129	LYS	CB-CG-CD	6.60	126.47	111.30
1	A	1062	GLU	CG-CD-OE1	-6.59	103.23	118.40
1	A	1348	LEU	N-CA-C	-6.59	104.09	111.28
10	L	66	GLN	CA-C-O	-6.59	113.74	121.46
4	E	93	MET	CG-SD-CE	-6.59	86.39	100.90
1	A	523	ILE	N-CA-CB	-6.59	103.35	110.53
6	H	113	ALA	CA-C-N	-6.59	112.79	122.68
6	H	113	ALA	C-N-CA	-6.59	112.79	122.68
9	K	101	LEU	N-CA-C	6.59	120.19	111.75
1	A	420	ARG	NE-CZ-NH1	6.59	128.09	121.50
1	A	1318	THR	CA-CB-CG2	6.59	121.70	110.50
2	B	952	VAL	O-C-N	6.59	130.36	123.05
1	A	966	ASN	N-CA-C	-6.58	102.75	111.24
3	C	11	ARG	CA-C-N	-6.58	108.54	121.91
3	C	11	ARG	C-N-CA	-6.58	108.54	121.91
2	B	429	PHE	CA-C-N	-6.58	112.23	122.37
2	B	429	PHE	C-N-CA	-6.58	112.23	122.37
2	B	608	ASP	N-CA-CB	6.58	119.91	110.16
5	F	139	PRO	CB-CA-C	-6.58	102.50	112.11
1	A	46	THR	CA-C-O	-6.58	114.69	122.13
1	A	411	ASP	CA-CB-CG	-6.58	106.02	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	664	THR	CB-CA-C	-6.58	95.93	109.94
2	B	218	SER	O-C-N	-6.58	114.56	122.65
3	C	39	ALA	CA-C-O	6.58	126.67	119.24
4	E	209	ALA	CA-C-O	-6.58	113.74	120.71
9	K	79	GLU	CA-CB-CG	6.58	127.26	114.10
1	A	37	PHE	O-C-N	-6.58	114.30	121.53
1	A	1138	ILE	CB-CG1-CD1	-6.58	99.99	113.80
1	A	366	VAL	O-C-N	-6.58	112.70	120.66
1	A	1326	ARG	NE-CZ-NH2	6.58	125.12	119.20
1	A	1219	THR	OG1-CB-CG2	-6.57	96.15	109.30
2	B	751	VAL	N-CA-C	6.57	117.32	110.62
1	A	24	PRO	N-CA-C	-6.57	104.96	113.57
1	A	156	ASP	N-CA-C	6.57	124.80	110.80
1	A	740	LEU	CB-CA-C	-6.57	99.12	110.09
2	B	611	PRO	N-CA-C	6.57	122.45	113.98
2	B	1193	GLN	N-CA-CB	-6.57	99.85	111.08
4	E	38	PRO	O-C-N	6.57	131.51	122.64
2	B	330	ALA	N-CA-C	-6.57	104.20	111.36
2	B	633	VAL	CB-CA-C	-6.57	101.39	111.31
1	A	973	ILE	CB-CG1-CD1	-6.57	100.01	113.80
2	B	879	ARG	CG-CD-NE	6.57	126.44	112.00
6	H	135	LEU	CA-C-O	6.57	129.90	120.51
2	B	620	ARG	CG-CD-NE	-6.56	97.56	112.00
7	I	92	ARG	CA-C-O	6.56	129.67	121.66
2	B	463	THR	CB-CA-C	-6.56	97.71	110.11
6	H	104	PHE	N-CA-C	6.56	124.77	110.80
9	K	67	PHE	N-CA-C	-6.56	105.28	113.28
1	A	1232	ASN	CB-CG-ND2	-6.56	106.56	116.40
1	A	438	ASP	N-CA-CB	-6.55	99.66	109.69
1	A	1139	GLU	CB-CA-C	-6.55	99.40	109.89
2	B	619	ILE	CG1-CB-CG2	-6.55	91.03	110.70
10	L	40	LEU	CB-CA-C	6.55	127.07	112.78
6	H	121	LEU	N-CA-CB	-6.55	99.62	109.71
1	A	383	TYR	N-CA-C	6.55	119.42	111.82
1	A	748	MET	CA-C-N	-6.55	109.68	121.14
1	A	748	MET	C-N-CA	-6.55	109.68	121.14
2	B	666	TYR	CE1-CZ-OH	6.55	139.56	119.90
1	A	226	GLU	N-CA-CB	6.55	121.56	110.49
1	A	4	GLN	CB-CA-C	6.55	123.67	109.99
1	A	1159	ARG	N-CA-C	6.55	121.33	112.88
2	B	1095	LEU	CD1-CG-CD2	-6.55	96.39	110.80
2	B	1163	CYS	O-C-N	-6.55	114.90	122.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	73	ALA	N-CA-C	6.55	124.75	110.80
1	A	13	THR	CA-C-O	-6.54	113.58	121.89
1	A	764	CYS	O-C-N	-6.54	116.02	123.48
7	I	85	PHE	O-C-N	-6.54	114.64	123.15
1	A	921	GLY	CA-C-N	-6.54	112.24	121.72
1	A	921	GLY	C-N-CA	-6.54	112.24	121.72
2	B	1171	VAL	N-CA-C	6.54	117.76	108.93
8	J	17	LYS	CD-CE-NZ	-6.54	90.97	111.90
7	I	54	GLU	N-CA-C	-6.54	104.19	111.71
1	A	203	SER	N-CA-CB	6.54	120.23	110.29
1	A	887	GLY	N-CA-C	6.54	122.91	112.58
1	A	1198	ASP	CB-CA-C	-6.54	98.96	109.75
2	B	818	PRO	CB-CA-C	-6.54	101.08	110.75
3	C	214	ASN	N-CA-C	6.54	119.39	108.73
1	A	901	LEU	N-CA-C	6.54	120.85	113.01
1	A	1167	GLU	CB-CA-C	6.54	121.03	110.96
7	I	113	ASP	OD1-CG-OD2	-6.54	107.22	122.90
9	K	110	ASN	CB-CA-C	6.54	122.46	110.11
4	E	113	GLN	CA-C-O	-6.53	112.03	120.00
1	A	1241	ARG	CD-NE-CZ	6.53	133.54	124.40
1	A	1256	GLU	CB-CG-CD	6.53	123.70	112.60
2	B	477	ALA	O-C-N	-6.53	112.55	123.00
1	A	583	PRO	CA-C-O	-6.53	113.53	122.15
2	B	702	LEU	CD1-CG-CD2	-6.53	96.44	110.80
3	C	185	LYS	CD-CE-NZ	-6.53	91.01	111.90
2	B	291	ILE	N-CA-C	-6.53	97.71	107.37
1	A	941	LYS	CB-CA-C	-6.52	100.84	110.95
2	B	111	ALA	CB-CA-C	-6.52	100.64	109.71
2	B	828	ALA	N-CA-CB	-6.52	99.97	111.39
1	A	81	PHE	N-CA-C	6.52	119.87	109.24
2	B	57	TYR	O-C-N	-6.52	113.92	122.59
9	K	92	ASN	CB-CA-C	6.52	121.66	110.84
2	B	30	SER	O-C-N	-6.51	115.22	122.12
2	B	769	TYR	N-CA-C	-6.51	103.68	111.69
1	A	412	ARG	N-CA-C	6.51	119.34	108.20
1	A	1350	LYS	N-CA-CB	-6.51	100.19	110.28
3	C	5	GLY	N-CA-C	6.51	125.62	112.34
4	E	78	LEU	CD1-CG-CD2	-6.51	96.48	110.80
2	B	230	ALA	N-CA-C	6.51	124.19	109.81
2	B	667	GLN	N-CA-C	6.51	119.74	109.39
1	A	782	ARG	N-CA-C	6.51	119.04	108.76
1	A	961	ARG	CA-C-O	6.51	127.45	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	57	GLY	N-CA-C	6.51	124.37	115.00
3	C	124	LEU	CB-CA-C	-6.50	98.01	110.57
1	A	36	ARG	CA-C-O	-6.50	111.21	120.51
1	A	917	SER	CB-CA-C	-6.50	100.67	110.88
9	K	114	LEU	CD1-CG-CD2	-6.50	96.50	110.80
2	B	1158	PHE	N-CA-C	6.50	124.64	110.80
1	A	431	LYS	CA-C-O	-6.50	113.30	120.38
9	K	60	ALA	N-CA-C	6.49	119.02	108.76
6	H	41	ASP	CB-CG-OD1	6.49	133.33	118.40
6	H	56	THR	N-CA-C	-6.49	95.67	107.75
1	A	595	THR	CB-CA-C	-6.49	98.00	109.62
6	H	136	LYS	CA-CB-CG	6.49	127.08	114.10
1	A	1367	HIS	ND1-CG-CD2	-6.49	99.61	106.10
2	B	64	CYS	N-CA-C	-6.49	105.10	114.12
2	B	1011	ILE	CA-CB-CG1	6.49	121.43	110.40
2	B	682	SER	CA-C-N	-6.49	112.01	120.44
2	B	682	SER	C-N-CA	-6.49	112.01	120.44
1	A	619	LYS	CA-CB-CG	6.49	127.07	114.10
2	B	598	GLU	N-CA-C	-6.49	104.29	111.36
3	C	142	VAL	CB-CA-C	-6.49	102.13	111.34
7	I	4	PHE	CA-C-O	-6.49	111.23	120.51
1	A	463	ILE	CB-CG1-CD1	-6.48	100.18	113.80
1	A	844	ALA	N-CA-C	6.48	120.05	111.75
8	J	49	MET	CB-CA-C	6.48	121.14	110.90
1	A	1167	GLU	CB-CG-CD	6.48	123.61	112.60
2	B	616	ILE	CA-C-N	-6.48	113.78	122.72
2	B	616	ILE	C-N-CA	-6.48	113.78	122.72
1	A	569	LYS	O-C-N	-6.48	116.79	121.84
2	B	490	SER	CA-C-O	-6.48	112.52	119.97
5	F	107	VAL	O-C-N	-6.48	116.02	122.76
7	I	3	THR	CA-C-N	6.48	133.91	121.54
7	I	3	THR	C-N-CA	6.48	133.91	121.54
9	K	24	ASP	CB-CG-OD2	6.48	133.30	118.40
9	K	73	LEU	CB-CG-CD1	-6.48	91.27	110.70
1	A	626	ASN	CB-CA-C	6.48	120.51	110.67
2	B	336	ARG	N-CA-C	6.47	120.28	112.38
4	E	1	MET	CG-SD-CE	6.47	115.14	100.90
1	A	685	GLU	N-CA-CB	-6.47	100.33	110.30
1	A	15	LYS	O-C-N	-6.47	114.77	122.27
1	A	1264	GLU	CA-C-N	-6.47	111.80	120.79
1	A	1264	GLU	C-N-CA	-6.47	111.80	120.79
3	C	263	THR	CA-CB-CG2	6.47	121.50	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	503	GLN	O-C-N	-6.47	113.83	122.49
1	A	512	VAL	N-CA-CB	-6.47	103.23	110.99
1	A	1445	ILE	CA-C-N	6.47	131.86	122.16
1	A	1445	ILE	C-N-CA	6.47	131.86	122.16
1	A	826	ASP	CA-C-N	-6.46	112.04	120.44
1	A	826	ASP	C-N-CA	-6.46	112.04	120.44
1	A	1023	ARG	NE-CZ-NH2	6.46	125.02	119.20
2	B	365	THR	OG1-CB-CG2	-6.46	96.37	109.30
2	B	974	PRO	CB-CG-CD	-6.46	85.41	106.10
10	L	25	ALA	O-C-N	6.46	133.34	123.00
1	A	32	VAL	CG1-CB-CG2	-6.46	96.59	110.80
1	A	244	PRO	N-CD-CG	-6.46	93.51	103.20
1	A	940	ARG	NH1-CZ-NH2	-6.46	110.90	119.30
2	B	1099	VAL	CA-C-O	-6.46	112.71	120.78
3	C	16	ASP	O-C-N	-6.46	115.24	122.34
7	I	98	VAL	O-C-N	6.46	129.19	122.54
4	E	208	TYR	CD1-CG-CD2	-6.46	108.42	118.10
6	H	140	ALA	N-CA-C	6.46	119.51	108.02
7	I	41	PRO	CA-CB-CG	-6.46	92.23	104.50
9	K	10	PHE	CA-C-N	6.46	132.68	122.74
9	K	10	PHE	C-N-CA	6.46	132.68	122.74
2	B	20	ASP	CA-C-O	-6.45	113.69	121.05
2	B	227	LYS	CG-CD-CE	-6.45	96.46	111.30
2	B	311	LEU	CD1-CG-CD2	-6.45	96.61	110.80
1	A	1152	ILE	CA-C-O	-6.45	113.64	120.48
2	B	216	GLU	N-CA-C	6.45	119.12	109.25
5	F	87	LYS	O-C-N	6.45	129.55	122.20
2	B	639	ILE	CB-CA-C	-6.45	102.07	111.68
2	B	706	GLN	CB-CG-CD	6.45	123.56	112.60
8	J	10	CYS	N-CA-C	-6.45	105.16	114.12
2	B	391	ASP	N-CA-CB	6.45	121.39	110.49
1	A	761	MET	CB-CA-C	-6.45	99.89	110.85
1	A	1327	ILE	O-C-N	6.44	129.64	122.75
2	B	742	GLU	CA-C-O	-6.44	114.72	121.55
7	I	111	THR	CB-CA-C	-6.44	98.13	110.24
2	B	259	TYR	N-CA-CB	6.44	120.08	110.29
7	I	45	ARG	N-CA-C	6.44	120.01	109.06
2	B	284	ILE	N-CA-C	-6.44	104.24	110.42
2	B	628	THR	N-CA-C	-6.44	103.95	113.61
2	B	903	VAL	CA-C-N	-6.44	110.83	120.94
2	B	903	VAL	C-N-CA	-6.44	110.83	120.94
5	F	119	ARG	CA-C-O	-6.44	112.82	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	405	VAL	CA-C-O	-6.44	113.14	120.67
2	B	877	PRO	CA-C-N	-6.44	109.24	121.54
2	B	877	PRO	C-N-CA	-6.44	109.24	121.54
2	B	1096	ARG	NH1-CZ-NH2	6.44	127.67	119.30
2	B	600	LEU	CA-C-N	-6.43	112.08	120.44
2	B	600	LEU	C-N-CA	-6.43	112.08	120.44
8	J	28	ASP	N-CA-CB	6.43	120.70	110.73
2	B	18	PHE	CB-CA-C	6.43	122.31	110.10
1	A	195	ASP	O-C-N	6.42	130.26	123.06
2	B	98	THR	CB-CA-C	-6.42	99.05	109.72
2	B	497	ARG	CG-CD-NE	-6.42	97.86	112.00
2	B	892	LYS	N-CA-C	-6.42	105.37	113.72
1	A	1081	LEU	CB-CG-CD2	6.42	129.97	110.70
2	B	871	THR	CB-CA-C	6.42	121.56	110.45
4	E	32	GLN	CA-C-N	-6.42	109.06	121.58
4	E	32	GLN	C-N-CA	-6.42	109.06	121.58
4	E	208	TYR	N-CA-C	6.42	119.97	109.06
1	A	1293	SER	O-C-N	6.42	127.09	120.99
1	A	23	SER	CA-CB-OG	-6.42	98.27	111.10
3	C	172	PRO	CA-C-O	-6.42	108.92	120.60
7	I	6	PHE	CA-C-O	-6.42	113.60	121.11
4	E	14	ARG	NE-CZ-NH2	-6.42	113.43	119.20
5	F	94	LEU	CA-C-O	6.42	127.38	120.20
7	I	75	CYS	N-CA-C	6.42	119.14	110.29
2	B	360	PHE	N-CA-CB	-6.41	100.50	110.57
7	I	106	CYS	CB-CA-C	-6.41	98.61	109.38
1	A	601	LYS	CG-CD-CE	6.41	126.05	111.30
1	A	728	LYS	CD-CE-NZ	6.41	132.42	111.90
3	C	44	LEU	CA-C-O	-6.41	113.92	121.16
1	A	638	GLY	CA-C-N	6.41	126.62	119.32
1	A	638	GLY	C-N-CA	6.41	126.62	119.32
1	A	926	GLN	O-C-N	6.41	129.72	122.22
7	I	4	PHE	CA-CB-CG	-6.41	107.39	113.80
1	A	753	GLY	CA-C-O	-6.40	115.93	122.59
2	B	773	MET	O-C-N	-6.40	115.33	122.12
2	B	832	GLY	O-C-N	-6.40	114.94	122.50
1	A	512	VAL	CA-CB-CG1	6.40	121.28	110.40
6	H	85	GLY	CA-C-N	6.40	133.77	121.54
6	H	85	GLY	C-N-CA	6.40	133.77	121.54
1	A	44	THR	CA-CB-CG2	6.40	121.38	110.50
1	A	621	THR	N-CA-CB	-6.40	100.69	110.16
1	A	1267	MET	CB-CA-C	6.40	121.09	110.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	469	ARG	CG-CD-NE	-6.40	97.93	112.00
2	B	1055	ILE	CB-CG1-CD1	-6.40	100.37	113.80
9	K	52	ASN	CA-C-N	6.40	133.76	121.54
9	K	52	ASN	C-N-CA	6.40	133.76	121.54
1	A	1047	SER	N-CA-C	-6.39	104.17	112.23
2	B	728	ARG	N-CA-C	6.39	118.81	110.43
7	I	23	ASN	CA-CB-CG	-6.39	106.21	112.60
9	K	85	ASP	CA-CB-CG	6.39	118.99	112.60
2	B	43	LEU	N-CA-C	6.39	121.08	113.16
3	C	59	ALA	N-CA-C	6.39	119.98	110.52
4	E	125	PRO	N-CA-CB	6.39	107.51	103.23
3	C	70	ILE	CA-CB-CG2	-6.39	99.64	110.50
7	I	83	ASN	CB-CA-C	-6.39	97.27	109.66
2	B	1002	THR	O-C-N	-6.38	115.79	122.94
10	L	48	CYS	N-CA-CB	-6.38	99.70	110.49
3	C	195	GLN	N-CA-CB	6.38	123.01	110.63
4	E	198	ILE	O-C-N	-6.38	115.63	123.10
1	A	1258	HIS	CA-CB-CG	-6.38	107.42	113.80
7	I	37	GLU	CB-CA-C	-6.38	97.07	109.76
7	I	97	MET	CA-C-O	6.38	127.47	119.95
1	A	1271	ILE	CA-CB-CG2	-6.37	99.67	110.50
3	C	39	ALA	N-CA-C	6.37	121.72	113.88
2	B	485	ARG	NE-CZ-NH2	-6.37	113.47	119.20
7	I	40	SER	CA-CB-OG	6.37	123.84	111.10
1	A	591	PHE	CB-CA-C	6.37	120.74	109.72
9	K	49	GLU	N-CA-CB	6.37	119.31	110.07
10	L	33	GLU	N-CA-C	6.37	124.37	110.80
1	A	159	THR	N-CA-CB	6.37	120.20	110.14
1	A	740	LEU	N-CA-C	-6.37	105.15	113.17
1	A	1135	ARG	CG-CD-NE	-6.37	97.99	112.00
7	I	67	THR	N-CA-CB	6.37	120.46	110.46
1	A	158	PRO	CA-C-N	-6.36	111.09	120.38
1	A	158	PRO	C-N-CA	-6.36	111.09	120.38
1	A	363	GLN	CB-CG-CD	6.36	123.42	112.60
2	B	1067	ARG	CB-CG-CD	6.36	125.93	111.30
1	A	896	ARG	CD-NE-CZ	-6.36	115.50	124.40
2	B	31	TRP	CA-C-O	6.36	127.11	119.61
2	B	168	GLY	O-C-N	6.36	131.03	123.46
6	H	106	GLU	CB-CA-C	6.36	123.14	110.17
1	A	731	ARG	N-CA-CB	-6.36	100.77	110.12
2	B	95	ILE	CG1-CB-CG2	-6.36	91.63	110.70
3	C	147	LEU	CD1-CG-CD2	-6.36	96.81	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	183	TRP	CA-C-O	-6.36	114.70	121.88
2	B	166	PHE	N-CA-CB	-6.36	100.63	109.97
5	F	102	SER	O-C-N	6.36	130.09	122.27
1	A	205	GLU	CB-CA-C	6.35	121.33	110.79
1	A	1447	GLU	N-CA-C	-6.35	103.88	111.69
4	E	98	ILE	CA-CB-CG2	6.35	121.30	110.50
1	A	553	VAL	CA-C-O	6.35	128.46	119.95
1	A	1442	ASP	CB-CG-OD1	-6.35	103.80	118.40
2	B	1002	THR	OG1-CB-CG2	-6.35	96.60	109.30
4	E	66	GLU	CB-CG-CD	6.35	123.39	112.60
2	B	249	ARG	NE-CZ-NH1	6.35	127.85	121.50
10	L	56	LEU	N-CA-C	6.35	119.84	109.24
1	A	141	LEU	N-CA-CB	-6.35	100.54	110.44
2	B	276	ILE	CA-CB-CG2	-6.35	99.71	110.50
6	H	77	ARG	CD-NE-CZ	6.35	133.28	124.40
1	A	753	GLY	N-CA-C	6.34	122.76	112.61
3	C	107	SER	CA-C-O	-6.34	114.89	121.87
1	A	557	ASP	CA-C-O	6.34	128.27	121.55
4	E	163	GLU	N-CA-CB	6.34	119.55	110.16
1	A	99	ILE	CA-CB-CG2	-6.34	99.73	110.50
9	K	72	LYS	N-CA-C	-6.34	97.47	108.69
3	C	69	LEU	CD1-CG-CD2	-6.33	96.87	110.80
4	E	215	MET	N-CA-C	6.33	128.73	111.00
1	A	846	GLU	N-CA-CB	-6.33	100.56	110.06
2	B	26	THR	CB-CA-C	-6.33	98.33	110.24
2	B	967	ARG	N-CA-CB	-6.33	100.11	110.43
1	A	1046	LEU	CB-CA-C	-6.33	100.09	110.85
9	K	17	SER	CA-C-N	-6.33	111.83	120.44
9	K	17	SER	C-N-CA	-6.33	111.83	120.44
1	A	424	ILE	N-CA-CB	-6.33	103.40	110.99
1	A	559	VAL	CA-CB-CG2	-6.33	99.64	110.40
2	B	958	GLN	CB-CG-CD	6.33	123.35	112.60
2	B	1193	GLN	CA-C-N	-6.33	113.71	122.69
2	B	1193	GLN	C-N-CA	-6.33	113.71	122.69
3	C	35	ARG	NE-CZ-NH1	6.33	127.83	121.50
1	A	138	ILE	CA-CB-CG2	6.32	121.25	110.50
1	A	812	GLU	OE1-CD-OE2	-6.32	107.73	122.90
2	B	1021	MET	CA-C-N	-6.32	113.28	122.06
2	B	1021	MET	C-N-CA	-6.32	113.28	122.06
2	B	1178	ASN	OD1-CG-ND2	6.32	128.92	122.60
1	A	989	GLY	CA-C-O	-6.32	114.24	120.75
1	A	1239	ARG	CB-CG-CD	6.32	125.83	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1243	VAL	N-CA-C	-6.32	93.31	111.00
8	J	61	LEU	O-C-N	-6.32	114.17	122.39
2	B	455	SER	N-CA-C	-6.32	104.62	112.90
2	B	1094	ARG	CB-CG-CD	6.32	125.83	111.30
9	K	79	GLU	N-CA-C	-6.32	100.30	109.59
1	A	88	LYS	CA-C-N	6.32	126.08	119.76
1	A	88	LYS	C-N-CA	6.32	126.08	119.76
2	B	1083	ALA	N-CA-CB	-6.32	100.52	110.69
7	I	77	LYS	CA-C-N	6.32	132.19	121.14
7	I	77	LYS	C-N-CA	6.32	132.19	121.14
1	A	550	LEU	N-CA-C	-6.31	104.48	111.36
1	A	1382	THR	N-CA-CB	-6.31	100.14	110.43
2	B	106	ASP	N-CA-CB	-6.31	99.83	110.49
2	B	1144	ALA	N-CA-C	6.31	119.14	111.82
2	B	601	ARG	NH1-CZ-NH2	6.31	127.50	119.30
1	A	820	GLY	N-CA-C	6.31	121.50	113.24
1	A	1032	LEU	CB-CG-CD1	-6.31	91.78	110.70
1	A	1291	VAL	CA-C-O	-6.31	114.27	121.59
2	B	184	ALA	N-CA-C	6.31	118.93	110.35
3	C	125	MET	CB-CG-SD	6.31	131.62	112.70
2	B	499	ASN	CB-CA-C	-6.30	96.52	109.94
2	B	787	VAL	CB-CA-C	-6.30	103.39	111.20
1	A	572	TRP	N-CA-C	6.30	120.33	110.32
2	B	21	GLU	N-CA-C	-6.30	105.56	113.18
2	B	327	ARG	N-CA-C	6.30	118.95	111.71
7	I	87	GLN	CA-C-N	-6.30	112.04	121.05
7	I	87	GLN	C-N-CA	-6.30	112.04	121.05
10	L	45	ALA	CA-C-N	6.30	133.30	121.97
10	L	45	ALA	C-N-CA	6.30	133.30	121.97
3	C	38	ILE	CA-C-N	-6.29	111.53	122.36
3	C	38	ILE	C-N-CA	-6.29	111.53	122.36
1	A	470	LEU	CB-CA-C	-6.29	96.53	109.94
1	A	706	HIS	N-CA-C	-6.29	97.39	110.80
2	B	852	ARG	CB-CA-C	6.29	120.41	109.65
3	C	103	ALA	N-CA-C	6.29	119.51	108.75
1	A	889	SER	CA-C-O	-6.29	114.70	121.94
2	B	745	PRO	CA-C-O	-6.29	110.19	119.18
1	A	947	PHE	CE1-CZ-CE2	-6.29	108.69	120.00
7	I	107	SER	CA-C-O	6.29	128.11	120.57
1	A	1011	GLN	CA-C-O	6.28	127.21	120.55
2	B	945	GLU	CG-CD-OE2	-6.28	103.95	118.40
1	A	1376	THR	CA-CB-OG1	6.28	119.02	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	325	GLN	CB-CA-C	-6.28	99.56	110.17
2	B	750	GLY	CA-C-O	-6.28	116.00	122.28
2	B	1085	ILE	N-CA-CB	-6.28	101.15	111.45
4	E	152	LYS	CG-CD-CE	6.28	125.75	111.30
7	I	87	GLN	N-CA-C	6.28	119.03	110.55
1	A	1295	THR	OG1-CB-CG2	-6.28	96.74	109.30
2	B	870	ILE	N-CA-CB	6.28	118.56	112.28
2	B	712	PRO	N-CA-C	6.28	127.79	112.10
2	B	19	GLU	CB-CG-CD	6.27	123.27	112.60
2	B	763	GLN	CB-CA-C	-6.27	99.60	109.70
2	B	563	MET	O-C-N	-6.27	115.61	123.01
1	A	114	LEU	CD1-CG-CD2	-6.27	97.01	110.80
1	A	615	GLY	O-C-N	-6.27	116.54	122.75
2	B	209	GLU	O-C-N	-6.27	115.06	122.96
3	C	34	ARG	CA-C-N	-6.27	110.03	120.68
3	C	34	ARG	C-N-CA	-6.27	110.03	120.68
2	B	642	ASP	CA-C-N	-6.26	110.43	121.70
2	B	642	ASP	C-N-CA	-6.26	110.43	121.70
2	B	832	GLY	CA-C-O	6.26	125.96	119.01
3	C	31	ASN	CA-C-N	-6.26	111.24	120.38
3	C	31	ASN	C-N-CA	-6.26	111.24	120.38
1	A	483	ASP	CB-CA-C	-6.26	101.36	111.06
1	A	1146	VAL	CA-C-O	6.26	125.92	119.35
2	B	564	GLU	N-CA-C	-6.26	100.87	110.32
2	B	939	THR	CB-CA-C	-6.26	99.98	108.68
5	F	121	ALA	CA-C-O	6.26	127.17	119.97
2	B	1048	THR	CB-CA-C	-6.26	98.84	114.11
1	A	302	THR	N-CA-C	-6.26	104.52	111.71
2	B	734	HIS	CA-C-N	6.26	131.51	122.44
2	B	734	HIS	C-N-CA	6.26	131.51	122.44
4	E	132	ILE	N-CA-CB	-6.26	102.39	111.52
1	A	600	PRO	O-C-N	6.25	128.94	122.18
1	A	1129	GLU	CB-CA-C	6.25	122.25	109.55
1	A	1311	VAL	CA-C-O	-6.25	113.61	120.43
4	E	16	PHE	CA-C-O	6.25	127.16	119.97
3	C	46	ILE	CB-CG1-CD1	-6.25	100.67	113.80
1	A	1280	GLU	CB-CG-CD	6.25	123.23	112.60
2	B	871	THR	N-CA-C	-6.25	101.21	110.46
3	C	97	VAL	CB-CA-C	-6.25	102.65	111.21
8	J	6	ARG	CG-CD-NE	-6.25	98.25	112.00
2	B	802	PRO	CB-CA-C	-6.25	103.80	111.11
1	A	1381	LEU	CB-CA-C	-6.25	100.50	110.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	245	GLU	CA-CB-CG	6.25	126.59	114.10
1	A	188	ASP	CB-CA-C	6.24	122.84	110.42
2	B	558	LEU	CA-C-O	6.24	127.16	120.10
3	C	86	CYS	O-C-N	6.24	130.40	123.16
4	E	106	GLN	CB-CG-CD	6.24	123.21	112.60
1	A	922	ASP	CB-CA-C	-6.24	100.05	110.29
2	B	1071	VAL	N-CA-C	-6.24	101.53	109.58
1	A	1280	GLU	CG-CD-OE2	6.24	132.74	118.40
1	A	1345	ARG	CB-CA-C	-6.24	100.08	110.68
2	B	522	VAL	O-C-N	-6.24	116.48	123.03
8	J	62	ARG	NE-CZ-NH1	6.24	127.74	121.50
2	B	788	ARG	CA-CB-CG	6.23	126.57	114.10
2	B	938	SER	CB-CA-C	6.23	120.78	109.37
2	B	1094	ARG	NE-CZ-NH2	6.23	124.81	119.20
1	A	434	ARG	CG-CD-NE	-6.23	98.29	112.00
1	A	1435	PRO	CB-CA-C	-6.23	104.72	112.89
8	J	47	ARG	N-CA-CB	6.23	119.82	110.22
1	A	1104	ILE	CB-CA-C	-6.23	103.83	111.87
2	B	733	HIS	CA-C-O	6.23	129.42	120.51
5	F	96	THR	N-CA-CB	-6.23	100.98	110.01
4	E	141	VAL	CA-C-N	-6.23	114.46	123.06
4	E	141	VAL	C-N-CA	-6.23	114.46	123.06
4	E	148	GLU	N-CA-CB	6.23	120.73	110.39
2	B	413	LEU	CB-CA-C	-6.23	99.70	110.72
8	J	2	ILE	CA-C-O	-6.23	114.78	121.19
2	B	42	GLY	N-CA-C	6.23	127.94	113.18
3	C	265	MET	CG-SD-CE	-6.23	87.20	100.90
1	A	949	ASP	CA-C-O	6.22	127.03	119.31
1	A	175	ARG	N-CA-CB	-6.22	101.27	110.85
1	A	997	LEU	CD1-CG-CD2	-6.22	97.11	110.80
3	C	183	TRP	N-CA-C	-6.22	101.76	110.35
5	F	116	ASP	O-C-N	-6.22	114.45	121.36
6	H	114	VAL	CG1-CB-CG2	-6.22	97.11	110.80
1	A	153	PRO	N-CD-CG	6.22	112.53	103.20
1	A	784	LEU	O-C-N	-6.22	117.11	121.65
1	A	1110	ASN	CA-CB-CG	6.22	118.82	112.60
3	C	178	PHE	N-CA-CB	-6.22	100.39	110.71
4	E	207	ARG	CG-CD-NE	-6.22	98.32	112.00
6	H	15	VAL	CA-C-O	6.22	125.75	120.22
2	B	311	LEU	O-C-N	-6.22	114.62	122.27
9	K	36	GLU	N-CA-C	6.22	120.18	110.17
2	B	1051	THR	N-CA-CB	-6.21	100.88	111.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	123	ASN	CA-C-O	6.21	127.62	120.60
4	E	48	ASP	CA-C-N	-6.21	113.65	122.41
4	E	48	ASP	C-N-CA	-6.21	113.65	122.41
7	I	66	PRO	N-CA-C	6.21	121.67	114.03
2	B	242	SER	O-C-N	-6.21	115.68	123.01
2	B	1051	THR	O-C-N	-6.21	115.66	123.17
2	B	1106	ARG	CD-NE-CZ	6.21	133.09	124.40
5	F	153	VAL	CB-CA-C	-6.21	103.30	111.81
1	A	1194	ARG	NE-CZ-NH2	6.21	124.79	119.20
1	A	1355	VAL	CA-C-O	-6.21	114.59	121.05
2	B	1083	ALA	CB-CA-C	-6.21	98.20	109.38
2	B	650	GLU	CA-C-O	6.21	127.72	120.89
3	C	92	CYS	O-C-N	-6.21	114.33	122.59
6	H	130	ARG	NH1-CZ-NH2	6.20	127.36	119.30
1	A	724	GLU	CB-CA-C	6.20	122.58	110.67
1	A	884	ASP	CA-C-O	-6.20	112.56	120.31
2	B	978	ASP	CA-C-O	-6.20	114.50	121.81
10	L	45	ALA	O-C-N	6.20	130.83	122.59
1	A	219	PHE	CA-C-N	6.20	128.87	120.44
1	A	219	PHE	C-N-CA	6.20	128.87	120.44
2	B	602	THR	CA-CB-CG2	-6.20	99.96	110.50
3	C	119	VAL	CA-CB-CG1	-6.20	99.86	110.40
9	K	10	PHE	O-C-N	6.19	128.57	122.19
2	B	744	HIS	CB-CA-C	-6.19	100.47	109.45
1	A	470	LEU	CA-C-O	6.19	127.92	120.99
1	A	1301	GLU	N-CA-CB	6.19	121.39	110.37
3	C	36	VAL	CG1-CB-CG2	-6.19	97.19	110.80
6	H	86	ASP	CB-CA-C	6.19	122.73	110.42
9	K	32	VAL	CG1-CB-CG2	-6.19	97.19	110.80
6	H	78	SER	CA-CB-OG	-6.18	98.74	111.10
1	A	21	LEU	N-CA-CB	-6.18	100.96	110.85
1	A	985	ASP	CA-C-O	6.18	127.31	120.82
6	H	116	TYR	N-CA-C	6.18	123.97	110.80
1	A	398	GLU	N-CA-C	-6.18	99.12	109.07
1	A	666	ILE	CG1-CB-CG2	6.18	129.24	110.70
1	A	1040	GLN	N-CA-C	-6.18	104.09	111.69
2	B	609	ILE	CA-C-N	-6.18	111.15	120.60
2	B	609	ILE	C-N-CA	-6.18	111.15	120.60
2	B	877	PRO	N-CA-C	6.18	119.87	111.22
9	K	12	LEU	N-CA-CB	6.18	120.70	110.63
2	B	237	VAL	CA-C-N	-6.18	112.98	122.62
2	B	237	VAL	C-N-CA	-6.18	112.98	122.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	89	GLU	CA-C-O	-6.18	113.56	120.54
1	A	564	ALA	N-CA-C	-6.18	105.57	113.23
3	C	10	ILE	N-CA-C	6.18	122.19	109.34
3	C	12	GLU	CB-CG-CD	-6.18	102.10	112.60
2	B	740	HIS	CA-C-N	-6.17	112.10	122.29
2	B	740	HIS	C-N-CA	-6.17	112.10	122.29
1	A	175	ARG	N-CA-C	6.17	119.71	110.14
1	A	229	SER	O-C-N	-6.17	115.24	123.14
10	L	47	ARG	O-C-N	-6.17	116.53	121.65
1	A	1298	TYR	N-CA-C	-6.17	99.59	109.96
1	A	1349	TYR	CE1-CZ-CE2	-6.17	107.96	120.30
7	I	66	PRO	CA-C-O	6.17	127.37	118.86
1	A	673	GLY	CA-C-O	-6.17	115.52	119.65
1	A	779	PHE	O-C-N	-6.17	114.55	122.20
1	A	829	VAL	CA-C-N	6.17	129.36	120.79
1	A	829	VAL	C-N-CA	6.17	129.36	120.79
3	C	16	ASP	CB-CG-OD1	-6.17	104.22	118.40
1	A	170	THR	CA-C-O	6.17	129.03	121.94
2	B	273	LEU	N-CA-C	6.17	118.62	110.36
1	A	1411	GLU	N-CA-C	-6.17	104.67	111.82
2	B	357	GLN	CB-CA-C	-6.17	97.80	110.38
2	B	635	ARG	NH1-CZ-NH2	-6.17	111.29	119.30
1	A	1018	PHE	CA-C-O	6.16	127.08	120.55
2	B	620	ARG	CA-C-O	6.16	126.18	119.15
2	B	1179	GLN	CA-C-O	6.16	127.33	120.43
6	H	27	GLU	CB-CA-C	6.16	121.06	110.77
6	H	3	ASN	CA-C-N	6.16	132.45	122.53
6	H	3	ASN	C-N-CA	6.16	132.45	122.53
1	A	244	PRO	CA-C-O	-6.16	111.63	120.56
1	A	1268	LEU	N-CA-C	-6.16	104.11	111.69
2	B	549	THR	N-CA-C	-6.16	99.36	108.79
1	A	180	LYS	N-CA-C	-6.16	99.15	109.07
4	E	91	LYS	CA-CB-CG	6.16	126.42	114.10
3	C	241	ASP	CB-CA-C	-6.16	99.24	110.63
1	A	1205	LYS	CA-C-O	6.16	126.92	119.78
2	B	1017	ILE	O-C-N	-6.16	114.08	121.10
2	B	339	THR	CA-C-N	-6.15	109.67	122.03
2	B	339	THR	C-N-CA	-6.15	109.67	122.03
1	A	1067	LEU	CD1-CG-CD2	-6.15	97.27	110.80
3	C	94	LYS	CB-CG-CD	6.15	125.45	111.30
7	I	72	ASP	O-C-N	-6.15	114.69	122.26
1	A	690	VAL	CA-C-O	-6.15	114.65	121.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	995	GLU	CA-CB-CG	6.15	126.39	114.10
2	B	198	ASP	CB-CG-OD1	6.15	132.53	118.40
1	A	808	LEU	N-CA-C	6.14	120.28	109.96
1	A	149	GLU	O-C-N	6.14	129.94	122.75
1	A	1134	ILE	CB-CA-C	6.14	120.07	112.02
1	A	1289	ARG	NE-CZ-NH1	-6.14	115.36	121.50
2	B	542	MET	CG-SD-CE	-6.14	87.39	100.90
2	B	561	TRP	CA-C-N	-6.14	112.53	122.30
2	B	561	TRP	C-N-CA	-6.14	112.53	122.30
3	C	76	ASP	CB-CG-OD2	-6.14	104.27	118.40
1	A	325	ILE	CG1-CB-CG2	-6.14	92.28	110.70
2	B	1222	ARG	CA-C-N	6.14	130.52	120.63
2	B	1222	ARG	C-N-CA	6.14	130.52	120.63
2	B	326	ASP	CB-CG-OD2	6.14	132.52	118.40
4	E	206	GLY	O-C-N	6.14	130.68	122.70
1	A	406	ILE	CA-C-O	-6.14	113.86	120.36
1	A	519	PRO	CA-C-O	-6.14	114.34	121.34
1	A	110	CYS	CB-CA-C	-6.13	100.42	110.85
1	A	418	SER	N-CA-C	6.13	123.87	110.80
2	B	355	ILE	CB-CG1-CD1	-6.13	100.92	113.80
2	B	501	PRO	CB-CA-C	-6.13	104.04	111.46
2	B	912	ILE	N-CA-C	6.13	116.85	107.77
4	E	204	THR	CA-CB-OG1	6.13	118.80	109.60
5	F	87	LYS	CG-CD-CE	6.13	125.41	111.30
2	B	760	ASP	CB-CG-OD2	6.13	132.51	118.40
2	B	167	ILE	CA-C-O	6.13	124.24	119.46
3	C	18	VAL	CA-C-O	-6.13	113.12	120.78
6	H	36	CYS	CA-C-O	6.13	127.42	120.80
1	A	181	LEU	N-CA-C	-6.13	99.72	109.59
1	A	1442	ASP	O-C-N	6.13	131.01	123.10
1	A	782	ARG	NE-CZ-NH2	-6.13	113.69	119.20
2	B	737	THR	CA-CB-CG2	-6.13	100.08	110.50
7	I	19	ASP	O-C-N	6.13	130.40	122.43
2	B	116	GLU	CB-CG-CD	6.13	123.02	112.60
2	B	288	ALA	O-C-N	6.13	130.91	122.46
1	A	8	SER	CA-CB-OG	6.12	123.35	111.10
1	A	832	ALA	O-C-N	6.12	128.38	122.07
1	A	900	ASP	CB-CA-C	-6.12	101.74	111.17
1	A	916	GLY	O-C-N	6.12	128.95	122.28
5	F	96	THR	O-C-N	-6.12	115.76	122.07
2	B	1196	ILE	O-C-N	-6.12	117.83	121.69
10	L	42	ARG	NE-CZ-NH2	6.12	124.71	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	392	ARG	CD-NE-CZ	-6.12	115.83	124.40
1	A	293	GLU	CA-C-N	-6.12	110.50	120.72
1	A	293	GLU	C-N-CA	-6.12	110.50	120.72
1	A	736	ASN	CA-C-N	-6.12	109.77	122.07
1	A	736	ASN	C-N-CA	-6.12	109.77	122.07
3	C	84	ARG	CA-C-O	-6.12	112.11	119.27
5	F	111	LEU	N-CA-C	6.12	119.71	108.58
8	J	8	PHE	CA-C-N	-6.12	111.14	122.09
8	J	8	PHE	C-N-CA	-6.12	111.14	122.09
2	B	1082	MET	N-CA-C	-6.12	104.61	111.28
10	L	63	ARG	N-CA-C	-6.12	102.03	110.35
1	A	48	ALA	CA-C-O	-6.12	111.77	120.51
1	A	748	MET	N-CA-C	6.12	119.21	111.69
1	A	669	THR	CB-CA-C	-6.11	99.88	110.09
2	B	969	ARG	NE-CZ-NH2	6.11	124.70	119.20
6	H	126	GLU	CG-CD-OE1	6.11	132.46	118.40
3	C	63	ILE	CB-CG1-CD1	-6.11	100.97	113.80
9	K	55	LYS	CA-C-O	6.11	126.67	119.28
3	C	143	LEU	CA-C-N	6.11	129.90	122.63
3	C	143	LEU	C-N-CA	6.11	129.90	122.63
1	A	603	ASN	CB-CA-C	-6.11	99.49	110.36
1	A	697	ALA	O-C-N	6.11	129.37	122.22
1	A	1271	ILE	N-CA-CB	6.11	120.44	111.52
1	A	793	SER	CB-CA-C	-6.10	97.55	111.89
1	A	1216	ILE	N-CA-C	-6.10	104.79	110.53
1	A	879	GLU	CB-CG-CD	6.10	122.97	112.60
2	B	106	ASP	CA-CB-CG	6.10	118.70	112.60
2	B	1175	LEU	CD1-CG-CD2	6.10	124.22	110.80
3	C	63	ILE	CA-CB-CG2	-6.10	100.13	110.50
2	B	1079	LYS	CB-CA-C	-6.10	99.60	109.72
2	B	51	PHE	O-C-N	6.10	129.10	122.15
2	B	66	ASP	CA-C-N	6.09	128.45	120.28
2	B	66	ASP	C-N-CA	6.09	128.45	120.28
2	B	309	GLN	CA-C-O	-6.09	113.96	120.42
2	B	848	ARG	CA-C-O	6.09	126.80	119.43
1	A	893	PHE	CD1-CG-CD2	-6.09	109.46	118.60
7	I	93	LYS	N-CA-CB	6.09	120.33	110.40
1	A	412	ARG	CB-CG-CD	6.09	125.31	111.30
1	A	1104	ILE	CA-C-O	-6.09	114.11	121.18
3	C	79	GLN	CA-CB-CG	6.09	126.28	114.10
1	A	25	GLU	CB-CG-CD	6.09	122.95	112.60
1	A	159	THR	N-CA-C	-6.09	103.95	111.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	654	ASN	CA-CB-CG	6.09	118.69	112.60
8	J	62	ARG	NE-CZ-NH2	-6.09	113.72	119.20
9	K	102	LYS	CA-C-O	6.09	126.97	119.97
4	E	215	MET	CB-CA-C	-6.09	98.54	110.10
1	A	478	TYR	N-CA-C	-6.08	105.86	113.28
1	A	1053	PHE	O-C-N	-6.08	115.67	122.12
2	B	334	ILE	CA-C-N	-6.08	112.53	120.14
2	B	334	ILE	C-N-CA	-6.08	112.53	120.14
1	A	649	ILE	CA-C-O	6.08	127.30	120.85
1	A	898	ARG	CB-CA-C	-6.08	101.40	110.16
2	B	1006	ILE	CG1-CB-CG2	-6.08	92.45	110.70
5	F	117	PRO	CA-N-CD	-6.08	103.49	112.00
1	A	961	ARG	O-C-N	-6.08	115.11	122.22
2	B	579	ARG	NE-CZ-NH1	-6.08	115.42	121.50
3	C	95	CYS	CA-CB-SG	6.08	128.38	114.40
10	L	70	ARG	N-CA-CB	-6.08	100.17	110.50
1	A	288	ALA	O-C-N	6.08	129.75	122.27
4	E	4	GLU	CB-CG-CD	6.08	122.93	112.60
1	A	902	LEU	N-CA-C	-6.07	106.13	112.93
2	B	239	GLU	N-CA-C	-6.07	98.36	108.75
2	B	252	SER	N-CA-C	6.07	119.15	110.10
2	B	375	ALA	O-C-N	6.07	128.33	122.07
2	B	1140	ALA	N-CA-C	6.07	123.73	110.80
2	B	664	THR	CA-C-N	6.07	128.69	120.44
2	B	664	THR	C-N-CA	6.07	128.69	120.44
2	B	1041	GLU	N-CA-CB	6.07	118.63	109.34
1	A	669	THR	N-CA-C	6.07	120.82	113.17
2	B	212	LEU	N-CA-C	6.07	119.13	109.24
1	A	874	ASP	N-CA-C	6.07	119.13	109.24
1	A	907	THR	N-CA-CB	6.07	118.68	109.94
2	B	628	THR	CA-C-O	-6.07	112.02	119.18
9	K	34	THR	CA-CB-OG1	6.07	118.70	109.60
1	A	387	ARG	NE-CZ-NH1	6.07	127.57	121.50
1	A	1102	LYS	N-CA-CB	-6.07	100.96	110.06
1	A	1427	ASN	N-CA-C	6.07	118.69	111.71
1	A	884	ASP	CA-CB-CG	-6.06	106.54	112.60
1	A	1264	GLU	OE1-CD-OE2	-6.06	108.35	122.90
2	B	332	ASP	N-CA-C	6.06	117.56	111.07
2	B	809	MET	CG-SD-CE	-6.06	87.56	100.90
7	I	120	GLN	N-CA-C	6.06	120.23	111.02
8	J	38	ARG	NE-CZ-NH1	6.06	127.56	121.50
1	A	474	VAL	N-CA-CB	-6.06	101.90	112.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1374	VAL	N-CA-C	-6.06	104.44	110.62
1	A	636	GLU	CA-C-N	-6.06	112.71	121.98
1	A	636	GLU	C-N-CA	-6.06	112.71	121.98
1	A	914	GLU	O-C-N	6.06	128.31	122.07
1	A	918	GLU	CA-C-N	-6.06	114.53	122.16
1	A	918	GLU	C-N-CA	-6.06	114.53	122.16
2	B	1002	THR	CB-CA-C	6.06	120.43	109.83
2	B	1020	ARG	CA-CB-CG	6.06	126.21	114.10
7	I	79	HIS	CA-C-N	6.06	129.31	120.71
7	I	79	HIS	C-N-CA	6.06	129.31	120.71
1	A	701	LEU	CA-C-N	-6.06	113.13	122.09
1	A	701	LEU	C-N-CA	-6.06	113.13	122.09
1	A	358	ASN	N-CA-CB	6.05	120.61	110.92
1	A	821	ARG	NH1-CZ-NH2	6.05	127.17	119.30
2	B	511	PRO	CB-CG-CD	6.05	125.47	106.10
1	A	962	ARG	NE-CZ-NH2	-6.05	113.75	119.20
1	A	1450	LEU	CB-CG-CD2	6.05	128.85	110.70
2	B	49	ASP	O-C-N	-6.05	115.70	122.12
2	B	657	HIS	O-C-N	-6.05	115.25	122.15
2	B	904	ARG	O-C-N	-6.05	115.72	122.86
2	B	1199	ALA	N-CA-C	6.05	118.84	111.82
4	E	39	LEU	CA-C-N	-6.05	112.09	120.38
4	E	39	LEU	C-N-CA	-6.05	112.09	120.38
2	B	1207	LEU	N-CA-C	6.05	118.84	111.82
1	A	847	ASP	N-CA-C	6.05	120.52	113.20
2	B	19	GLU	O-C-N	-6.05	114.55	122.59
7	I	22	ASN	CB-CA-C	-6.05	100.24	110.64
2	B	787	VAL	CA-C-N	-6.04	111.94	122.64
2	B	787	VAL	C-N-CA	-6.04	111.94	122.64
3	C	253	LYS	O-C-N	6.04	128.53	122.12
5	F	89	GLU	N-CA-C	-6.04	104.32	111.03
2	B	596	LEU	N-CA-C	6.04	117.54	111.07
2	B	839	MET	N-CA-C	6.04	119.33	109.06
2	B	975	GLN	CB-CA-C	-6.04	97.46	110.45
2	B	1129	ARG	CG-CD-NE	-6.04	98.71	112.00
4	E	168	TYR	CA-C-O	6.04	126.51	119.32
1	A	555	ASP	OD1-CG-OD2	-6.04	108.41	122.90
1	A	563	PRO	CB-CA-C	-6.04	101.99	110.63
2	B	635	ARG	N-CA-C	6.04	113.44	108.07
2	B	908	GLU	CG-CD-OE1	-6.04	104.51	118.40
10	L	63	ARG	CG-CD-NE	6.04	125.28	112.00
1	A	461	LYS	CB-CA-C	-6.04	100.48	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	483	ASP	N-CA-C	6.04	119.39	112.57
7	I	59	VAL	N-CA-CB	-6.04	102.30	112.44
1	A	241	VAL	CB-CA-C	-6.04	103.95	110.95
1	A	503	GLN	CA-C-O	6.04	125.78	119.14
2	B	1091	TYR	CA-C-O	-6.03	113.85	120.43
5	F	135	ARG	CG-CD-NE	-6.03	98.73	112.00
1	A	986	ILE	N-CA-CB	-6.03	103.83	110.65
7	I	30	ARG	CB-CA-C	-6.03	100.02	110.09
1	A	26	GLU	N-CA-C	-6.03	106.06	113.41
1	A	751	SER	N-CA-CB	-6.03	101.04	110.44
2	B	171	PRO	CA-C-N	-6.03	114.74	123.06
2	B	171	PRO	C-N-CA	-6.03	114.74	123.06
3	C	128	ASN	N-CA-C	-6.03	97.86	108.23
1	A	102	VAL	O-C-N	6.03	128.17	121.90
1	A	931	GLU	N-CA-C	6.02	118.64	111.71
1	A	861	GLY	CA-C-N	-6.02	110.02	120.97
1	A	861	GLY	C-N-CA	-6.02	110.02	120.97
7	I	24	ARG	CB-CA-C	-6.02	96.83	110.07
1	A	601	LYS	CD-CE-NZ	-6.02	92.64	111.90
1	A	702	LEU	N-CA-CB	-6.02	100.48	110.23
1	A	1383	SER	CA-CB-OG	-6.02	99.06	111.10
6	H	10	PHE	N-CA-C	6.02	118.33	109.24
1	A	489	LEU	CA-C-N	6.01	131.25	122.77
1	A	489	LEU	C-N-CA	6.01	131.25	122.77
2	B	512	ARG	CA-CB-CG	6.01	126.13	114.10
2	B	620	ARG	N-CA-CB	-6.01	101.57	110.53
2	B	807	ARG	NE-CZ-NH1	6.01	127.52	121.50
1	A	1097	GLY	CA-C-O	-6.01	110.11	120.57
1	A	143	LYS	CA-C-N	6.01	129.16	120.38
1	A	143	LYS	C-N-CA	6.01	129.16	120.38
1	A	393	ARG	NE-CZ-NH1	-6.01	115.49	121.50
1	A	568	PRO	N-CA-C	-6.01	105.53	113.65
1	A	1237	ILE	CA-C-N	-6.01	115.27	123.14
1	A	1237	ILE	C-N-CA	-6.01	115.27	123.14
2	B	131	ASP	N-CA-CB	6.01	120.59	110.79
1	A	240	PRO	O-C-N	6.01	129.53	122.98
1	A	433	GLU	N-CA-CB	-6.01	101.53	110.24
1	A	1202	MET	CA-C-N	-6.01	110.46	121.52
1	A	1202	MET	C-N-CA	-6.01	110.46	121.52
3	C	199	LYS	CA-CB-CG	-6.01	102.08	114.10
1	A	411	ASP	O-C-N	6.01	130.26	122.87
8	J	50	ILE	CB-CA-C	6.01	119.51	111.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	829	VAL	CA-C-O	-6.01	114.70	120.95
1	A	932	GLU	CB-CG-CD	6.01	122.81	112.60
10	L	29	TYR	O-C-N	-6.01	114.62	122.97
2	B	1198	TYR	CA-C-O	-6.00	114.19	120.55
1	A	61	ILE	CA-C-N	6.00	133.01	121.54
1	A	61	ILE	C-N-CA	6.00	133.01	121.54
1	A	686	ALA	N-CA-C	-6.00	104.11	112.45
2	B	582	VAL	N-CA-C	-6.00	99.41	108.17
5	F	130	ILE	CA-C-O	-6.00	114.69	119.25
8	J	17	LYS	CB-CG-CD	6.00	125.10	111.30
1	A	98	LYS	O-C-N	6.00	128.57	122.09
1	A	226	GLU	CG-CD-OE2	6.00	132.19	118.40
1	A	497	THR	CA-C-O	-6.00	113.07	119.97
1	A	1238	ILE	CA-CB-CG1	6.00	120.60	110.40
2	B	482	VAL	N-CA-CB	-6.00	103.99	110.53
1	A	1006	ILE	CA-CB-CG1	6.00	120.59	110.40
2	B	995	ARG	NE-CZ-NH1	6.00	127.50	121.50
2	B	1053	GLU	N-CA-CB	6.00	119.03	110.16
3	C	195	GLN	CA-CB-CG	6.00	126.09	114.10
4	E	210	SER	CA-CB-OG	6.00	123.09	111.10
2	B	1026	LEU	CA-C-O	-6.00	114.07	120.42
2	B	1082	MET	CB-CA-C	6.00	120.74	110.79
1	A	300	VAL	N-CA-C	5.99	116.73	110.62
2	B	896	ASP	N-CA-CB	5.99	119.79	110.44
2	B	1040	ASN	CA-CB-CG	-5.99	106.61	112.60
1	A	674	PRO	O-C-N	-5.99	114.74	122.23
4	E	47	CYS	N-CA-CB	-5.99	100.40	110.83
9	K	74	ARG	N-CA-C	-5.99	99.13	108.90
1	A	79	GLY	CA-C-N	-5.99	112.75	122.81
1	A	79	GLY	C-N-CA	-5.99	112.75	122.81
2	B	539	LEU	CB-CG-CD2	5.99	128.67	110.70
1	A	873	MET	CB-CG-SD	5.99	130.66	112.70
2	B	276	ILE	CA-C-N	-5.99	113.26	122.60
2	B	276	ILE	C-N-CA	-5.99	113.26	122.60
3	C	38	ILE	CG1-CB-CG2	-5.99	92.73	110.70
3	C	77	ILE	CA-C-N	-5.99	107.51	121.52
3	C	77	ILE	C-N-CA	-5.99	107.51	121.52
1	A	619	LYS	O-C-N	-5.99	115.22	122.22
3	C	237	SER	CA-CB-OG	-5.99	99.12	111.10
4	E	96	PHE	N-CA-C	-5.99	104.10	111.40
1	A	1302	PRO	CA-C-O	-5.99	114.37	121.67
2	B	792	MET	N-CA-C	5.99	118.51	109.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	20	PHE	CA-C-O	-5.99	114.97	121.14
6	H	126	GLU	O-C-N	5.99	129.76	123.06
2	B	577	ALA	N-CA-C	5.98	119.66	110.20
1	A	1113	THR	O-C-N	-5.98	114.44	121.32
6	H	92	ASP	CA-CB-CG	5.98	118.58	112.60
1	A	703	THR	CA-C-O	-5.98	114.16	120.80
1	A	895	LYS	CB-CG-CD	5.98	125.05	111.30
2	B	814	PHE	N-CA-C	-5.98	104.88	111.82
4	E	116	ILE	CA-C-O	5.98	128.26	120.78
2	B	792	MET	CG-SD-CE	-5.98	87.75	100.90
2	B	812	LEU	N-CA-C	-5.98	105.64	113.17
2	B	975	GLN	N-CA-CB	-5.98	101.68	111.66
1	A	894	GLU	CA-C-O	-5.97	113.10	119.97
1	A	1048	ASN	CA-C-O	-5.97	114.09	120.42
2	B	607	GLY	N-CA-C	-5.97	106.73	115.63
7	I	70	ARG	N-CA-CB	-5.97	100.86	111.08
1	A	640	GLN	CB-CG-CD	-5.97	102.45	112.60
1	A	1284	MET	O-C-N	5.97	129.75	123.06
2	B	25	ILE	CA-C-O	-5.97	114.45	121.80
2	B	728	ARG	NE-CZ-NH1	-5.97	115.53	121.50
6	H	121	LEU	CD1-CG-CD2	-5.97	97.66	110.80
2	B	125	SER	CB-CA-C	5.97	121.24	109.66
1	A	720	ARG	CB-CA-C	5.97	120.25	110.88
2	B	348	ARG	CB-CA-C	-5.97	101.51	110.88
2	B	517	THR	N-CA-CB	5.97	120.92	110.42
2	B	634	TYR	O-C-N	-5.97	116.61	122.99
5	F	141	GLY	O-C-N	5.97	129.39	122.65
6	H	44	VAL	N-CA-CB	-5.97	101.39	111.23
1	A	245	PRO	CA-C-O	-5.96	110.55	119.86
1	A	304	MET	CA-C-N	5.96	132.44	121.70
1	A	304	MET	C-N-CA	5.96	132.44	121.70
1	A	514	PRO	CA-CB-CG	5.96	115.83	104.50
2	B	1018	PRO	CB-CA-C	-5.96	101.72	111.56
1	A	80	HIS	CB-CA-C	5.96	121.23	109.66
1	A	1076	ALA	N-CA-C	5.96	118.57	111.71
1	A	670	ILE	CA-CB-CG1	5.96	120.54	110.40
1	A	1100	ARG	CB-CA-C	-5.96	101.52	110.88
1	A	1259	MET	CG-SD-CE	5.96	114.01	100.90
1	A	1264	GLU	N-CA-CB	5.96	118.71	110.07
1	A	1093	LYS	CB-CG-CD	5.96	125.01	111.30
3	C	25	VAL	CB-CA-C	-5.96	100.07	110.38
1	A	1368	MET	O-C-N	-5.96	114.30	122.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	287	ARG	CA-C-O	5.96	126.83	120.10
2	B	1002	THR	N-CA-CB	-5.96	100.92	110.46
1	A	842	VAL	N-CA-C	-5.96	104.93	110.53
1	A	944	ARG	NH1-CZ-NH2	-5.96	111.56	119.30
2	B	1195	HIS	CA-CB-CG	5.96	119.75	113.80
1	A	652	VAL	CG1-CB-CG2	-5.95	97.70	110.80
1	A	935	GLN	CA-C-O	-5.95	113.12	119.97
2	B	1183	LYS	CB-CG-CD	5.95	124.99	111.30
3	C	161	LYS	CA-CB-CG	5.95	126.00	114.10
8	J	62	ARG	CG-CD-NE	-5.95	98.90	112.00
1	A	850	VAL	CB-CA-C	-5.95	102.89	111.34
2	B	778	MET	N-CA-C	-5.95	99.70	109.40
2	B	706	GLN	O-C-N	-5.95	117.68	121.85
2	B	908	GLU	CA-C-N	5.95	130.18	121.31
2	B	908	GLU	C-N-CA	5.95	130.18	121.31
6	H	146	ARG	CD-NE-CZ	5.95	132.73	124.40
9	K	48	ALA	CA-C-O	-5.95	111.93	119.31
1	A	565	ILE	CG1-CB-CG2	-5.95	92.85	110.70
1	A	758	ILE	O-C-N	5.95	127.72	121.89
2	B	950	ASP	CA-C-N	-5.95	111.32	121.85
2	B	950	ASP	C-N-CA	-5.95	111.32	121.85
2	B	981	ALA	CA-C-O	-5.95	114.33	120.99
2	B	824	ILE	CB-CA-C	5.94	118.88	111.15
2	B	592	ASN	O-C-N	-5.94	114.49	121.32
3	C	106	GLU	O-C-N	5.94	129.97	122.19
6	H	19	ARG	NH1-CZ-NH2	5.94	127.03	119.30
1	A	246	VAL	N-CA-C	5.94	116.68	110.62
1	A	931	GLU	CA-C-O	-5.94	113.39	120.10
2	B	1097	HIS	O-C-N	-5.94	114.69	122.59
7	I	28	GLU	CA-C-O	-5.94	114.17	121.78
8	J	54	VAL	N-CA-CB	-5.94	103.74	111.82
1	A	49	LYS	CB-CG-CD	5.94	124.96	111.30
1	A	562	THR	CA-C-N	5.94	126.44	120.14
1	A	562	THR	C-N-CA	5.94	126.44	120.14
2	B	558	LEU	CA-C-N	-5.94	111.65	121.92
2	B	558	LEU	C-N-CA	-5.94	111.65	121.92
1	A	728	LYS	CA-C-N	-5.94	110.81	120.72
1	A	728	LYS	C-N-CA	-5.94	110.81	120.72
2	B	167	ILE	N-CA-C	5.94	118.90	113.20
3	C	24	ASN	N-CA-C	5.94	119.43	111.24
6	H	25	ARG	CG-CD-NE	-5.94	98.94	112.00
1	A	926	GLN	CA-C-O	-5.94	113.39	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	207	ARG	CB-CG-CD	5.93	124.95	111.30
7	I	72	ASP	CB-CA-C	5.93	120.58	111.02
1	A	4	GLN	CA-C-N	5.93	130.90	120.87
1	A	4	GLN	C-N-CA	5.93	130.90	120.87
2	B	606	LYS	CB-CG-CD	5.93	124.94	111.30
2	B	698	GLU	N-CA-C	-5.93	105.14	112.38
6	H	126	GLU	CA-CB-CG	5.93	125.97	114.10
1	A	1262	LYS	CA-CB-CG	5.93	125.96	114.10
1	A	10	PRO	CB-CA-C	-5.93	103.81	111.39
1	A	363	GLN	N-CA-C	-5.93	101.69	110.46
1	A	413	ILE	CG1-CB-CG2	-5.93	92.92	110.70
2	B	509	ALA	CB-CA-C	5.93	119.39	110.50
4	E	112	TYR	OH-CZ-CE2	5.93	137.68	119.90
1	A	1119	TYR	CD1-CE1-CZ	5.92	130.26	119.60
3	C	196	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	500	GLU	CB-CA-C	-5.92	100.96	110.79
1	A	1003	LYS	CB-CG-CD	5.92	124.92	111.30
4	E	47	CYS	CB-CA-C	5.92	120.68	109.37
1	A	1215	ARG	N-CA-CB	5.92	118.66	110.07
2	B	1177	HIS	CA-CB-CG	-5.92	107.88	113.80
1	A	696	GLU	CG-CD-OE2	5.92	132.01	118.40
6	H	60	ALA	CA-C-O	-5.92	114.63	121.26
2	B	346	GLU	N-CA-C	-5.92	104.91	111.71
2	B	385	LEU	CA-C-O	-5.92	114.28	120.55
2	B	787	VAL	N-CA-CB	-5.92	104.63	112.26
6	H	16	ASP	CB-CA-C	-5.92	100.26	109.08
1	A	1021	LEU	CA-C-O	5.92	126.88	120.55
1	A	1066	VAL	CA-CB-CG2	-5.92	100.34	110.40
2	B	355	ILE	N-CA-C	-5.91	104.55	111.00
2	B	689	LEU	CA-C-O	5.91	126.77	119.79
3	C	65	HIS	ND1-CE1-NE2	5.91	114.31	108.40
1	A	826	ASP	CB-CG-OD2	5.91	132.00	118.40
1	A	1154	TYR	CE1-CZ-OH	-5.91	102.16	119.90
1	A	1233	ASP	N-CA-CB	5.91	120.00	110.42
2	B	198	ASP	N-CA-C	-5.91	102.73	110.53
2	B	736	THR	OG1-CB-CG2	-5.91	97.48	109.30
1	A	158	PRO	N-CA-C	5.91	124.64	112.47
1	A	1432	GLN	CA-C-O	-5.91	114.20	121.11
2	B	1037	LEU	CD1-CG-CD2	-5.91	97.80	110.80
3	C	195	GLN	CG-CD-NE2	-5.91	107.53	116.40
4	E	73	PRO	N-CA-C	-5.91	100.30	112.47
10	L	42	ARG	N-CA-CB	5.91	120.21	110.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1001	ARG	NE-CZ-NH1	-5.91	115.59	121.50
2	B	992	ILE	CG1-CB-CG2	-5.91	92.98	110.70
2	B	1050	ILE	O-C-N	-5.91	115.19	122.57
4	E	106	GLN	CB-CA-C	5.91	121.06	109.72
7	I	15	TYR	CA-CB-CG	5.91	124.53	113.90
1	A	792	TYR	O-C-N	-5.91	115.08	122.35
3	C	176	ILE	N-CA-CB	-5.91	104.54	112.10
1	A	1445	ILE	CA-CB-CG2	-5.91	100.46	110.50
2	B	362	PRO	N-CA-C	5.91	121.60	113.98
2	B	547	VAL	N-CA-CB	-5.91	102.16	112.08
2	B	610	ASN	CA-C-N	5.91	125.61	119.82
2	B	610	ASN	C-N-CA	5.91	125.61	119.82
1	A	923	LEU	CB-CG-CD1	-5.90	92.99	110.70
4	E	155	ARG	N-CA-CB	-5.90	100.80	109.95
1	A	662	PHE	CA-C-N	-5.90	112.73	122.11
1	A	662	PHE	C-N-CA	-5.90	112.73	122.11
1	A	976	THR	CB-CA-C	-5.90	101.98	111.18
1	A	590	ARG	NE-CZ-NH1	5.90	127.40	121.50
1	A	1068	ALA	CA-C-N	-5.90	110.65	120.68
1	A	1068	ALA	C-N-CA	-5.90	110.65	120.68
6	H	96	VAL	N-CA-CB	-5.90	102.91	111.52
2	B	662	MET	O-C-N	-5.90	114.32	122.46
2	B	969	ARG	N-CA-C	5.90	118.56	109.07
9	K	113	THR	CA-C-N	5.90	132.31	121.70
9	K	113	THR	C-N-CA	5.90	132.31	121.70
2	B	650	GLU	CG-CD-OE1	-5.89	104.84	118.40
3	C	42	PRO	N-CA-CB	-5.89	98.22	103.35
1	A	375	THR	O-C-N	-5.89	115.99	123.24
1	A	424	ILE	CG1-CB-CG2	-5.89	93.02	110.70
1	A	1221	LYS	N-CA-CB	5.89	120.45	110.49
2	B	1101	ASP	CA-C-O	5.89	126.53	119.10
1	A	1157	ASP	CB-CA-C	-5.89	104.32	110.33
1	A	1276	VAL	CA-CB-CG2	-5.89	100.39	110.40
3	C	163	ILE	CA-C-O	-5.89	114.07	120.67
9	K	11	LEU	CB-CA-C	-5.89	99.04	109.70
1	A	1114	PRO	CA-C-O	-5.89	114.48	121.67
2	B	790	ASP	CB-CA-C	5.89	121.31	110.24
6	H	40	LEU	CD1-CG-CD2	-5.89	97.84	110.80
2	B	181	LEU	CD1-CG-CD2	-5.89	97.85	110.80
2	B	391	ASP	CB-CG-OD2	5.89	131.94	118.40
3	C	34	ARG	NH1-CZ-NH2	5.89	126.95	119.30
2	B	990	ILE	CA-CB-CG1	5.88	120.40	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1209	ALA	O-C-N	5.88	128.88	122.11
3	C	32	SER	N-CA-C	5.88	119.28	111.75
2	B	910	VAL	CG1-CB-CG2	-5.88	97.86	110.80
4	E	7	ARG	CG-CD-NE	5.88	124.94	112.00
1	A	767	GLN	N-CA-C	-5.88	100.91	110.20
3	C	19	ASP	N-CA-CB	-5.88	100.81	110.52
9	K	70	ARG	NE-CZ-NH1	-5.88	115.62	121.50
2	B	813	LYS	CG-CD-CE	-5.88	97.78	111.30
1	A	493	GLN	CA-C-N	-5.88	113.07	122.53
1	A	493	GLN	C-N-CA	-5.88	113.07	122.53
1	A	760	GLN	N-CA-C	-5.88	104.82	112.23
2	B	1167	GLY	N-CA-C	5.88	127.11	113.18
3	C	90	ASP	N-CA-C	5.88	123.32	110.80
7	I	25	LEU	N-CA-C	5.88	118.31	108.96
9	K	52	ASN	N-CA-C	-5.88	105.20	112.90
1	A	981	LEU	N-CA-CB	-5.88	100.70	109.69
1	A	1279	ILE	CA-CB-CG2	5.88	120.49	110.50
1	A	978	PRO	CA-CB-CG	-5.88	93.34	104.50
2	B	493	SER	CA-C-O	5.88	126.78	120.55
2	B	1194	ILE	CA-CB-CG1	5.87	120.39	110.40
2	B	1198	TYR	CA-C-N	-5.87	111.38	120.31
2	B	1198	TYR	C-N-CA	-5.87	111.38	120.31
6	H	126	GLU	CB-CA-C	-5.87	99.47	109.51
1	A	1219	THR	N-CA-CB	5.87	119.38	110.28
2	B	265	SER	N-CA-C	5.87	118.81	109.24
1	A	827	THR	O-C-N	-5.87	116.03	122.07
2	B	1159	ARG	NE-CZ-NH2	-5.87	113.92	119.20
4	E	136	ASN	O-C-N	5.87	130.04	122.89
1	A	183	GLY	O-C-N	5.86	130.25	123.21
2	B	41	LYS	CB-CG-CD	5.86	124.79	111.30
2	B	611	PRO	CA-N-CD	-5.86	103.79	112.00
2	B	767	ASN	CA-C-O	-5.86	114.33	120.55
5	F	110	ASP	CA-C-N	-5.86	112.76	122.32
5	F	110	ASP	C-N-CA	-5.86	112.76	122.32
1	A	94	GLY	CA-C-N	-5.86	113.29	122.49
1	A	94	GLY	C-N-CA	-5.86	113.29	122.49
3	C	10	ILE	CA-CB-CG2	5.86	120.46	110.50
3	C	176	ILE	CA-C-O	-5.86	114.57	120.31
7	I	102	VAL	CG1-CB-CG2	-5.86	97.91	110.80
5	F	102	SER	N-CA-C	5.86	118.62	111.82
1	A	748	MET	CB-CG-SD	-5.86	95.13	112.70
1	A	796	SER	CA-C-O	-5.86	113.23	119.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	816	HIS	N-CA-C	-5.86	105.63	112.89
1	A	1356	ILE	CG1-CB-CG2	-5.86	93.13	110.70
2	B	138	GLU	CG-CD-OE1	5.86	131.87	118.40
1	A	126	LEU	N-CA-C	-5.86	105.03	111.82
1	A	1055	ARG	CG-CD-NE	-5.86	99.12	112.00
1	A	1349	TYR	CZ-CE2-CD2	5.86	130.14	119.60
2	B	175	ARG	N-CA-C	5.86	120.23	113.38
3	C	154	LYS	CD-CE-NZ	5.86	130.64	111.90
1	A	620	LYS	CA-C-N	-5.85	111.98	120.29
1	A	620	LYS	C-N-CA	-5.85	111.98	120.29
3	C	185	LYS	N-CA-C	-5.85	105.80	113.12
2	B	258	LEU	CA-C-N	5.85	131.10	121.39
2	B	258	LEU	C-N-CA	5.85	131.10	121.39
1	A	1450	LEU	CA-C-O	-5.85	110.85	120.80
1	A	840	ARG	CG-CD-NE	-5.85	99.13	112.00
3	C	30	ALA	CA-C-O	5.85	126.96	120.82
1	A	379	VAL	CA-C-O	-5.85	113.59	121.02
7	I	103	CYS	CB-CA-C	-5.85	100.53	109.89
1	A	522	GLY	CA-C-O	-5.85	114.94	121.31
1	A	1274	ARG	NH1-CZ-NH2	5.85	126.90	119.30
5	F	74	ILE	CA-C-N	-5.85	113.91	119.76
5	F	74	ILE	C-N-CA	-5.85	113.91	119.76
1	A	919	ILE	N-CA-C	-5.84	107.06	113.43
2	B	293	PRO	CB-CA-C	-5.84	103.44	111.21
3	C	165	LYS	N-CA-CB	5.84	118.83	110.06
1	A	932	GLU	CB-CA-C	-5.84	101.67	110.90
2	B	986	GLN	CA-C-O	-5.84	114.05	120.30
2	B	1149	GLU	CA-C-O	5.84	126.61	120.42
6	H	40	LEU	CA-C-N	5.84	130.54	122.77
6	H	40	LEU	C-N-CA	5.84	130.54	122.77
1	A	352	VAL	CG1-CB-CG2	-5.84	97.95	110.80
1	A	906	HIS	N-CA-CB	-5.84	101.58	110.92
1	A	1221	LYS	CG-CD-CE	5.84	124.74	111.30
2	B	635	ARG	CA-C-O	-5.84	115.25	120.56
1	A	448	PRO	CA-C-O	-5.84	106.19	120.20
1	A	1109	LYS	CB-CG-CD	5.84	124.73	111.30
1	A	1284	MET	CB-CG-SD	5.84	130.22	112.70
2	B	764	SER	CA-CB-OG	-5.84	99.42	111.10
2	B	878	GLN	CB-CG-CD	5.84	122.53	112.60
4	E	164	LEU	CD1-CG-CD2	-5.84	97.95	110.80
1	A	808	LEU	O-C-N	-5.84	116.39	123.16
2	B	781	PHE	N-CA-C	5.84	119.66	112.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	K	19	LEU	N-CA-CB	-5.84	101.86	110.85
3	C	187	LYS	N-CA-C	-5.84	103.36	111.30
1	A	24	PRO	CB-CA-C	5.83	120.63	112.11
1	A	4	GLN	N-CA-CB	-5.83	100.89	110.40
1	A	883	LEU	CD1-CG-CD2	-5.83	97.97	110.80
2	B	553	PRO	CA-N-CD	5.83	120.16	112.00
4	E	102	GLU	CB-CA-C	5.83	119.44	109.24
9	K	93	SER	N-CA-CB	5.83	120.23	110.32
2	B	365	THR	CA-CB-OG1	5.83	118.34	109.60
2	B	1148	LYS	CA-CB-CG	5.83	125.76	114.10
1	A	962	ARG	NE-CZ-NH1	5.83	127.33	121.50
2	B	979	LYS	CB-CG-CD	5.83	124.71	111.30
9	K	22	ASP	CB-CG-OD1	5.83	131.80	118.40
1	A	640	GLN	CB-CA-C	-5.83	100.95	110.85
4	E	121	MET	N-CA-C	-5.83	105.88	112.87
5	F	115	THR	CA-C-O	-5.83	112.49	118.90
2	B	606	LYS	CG-CD-CE	5.82	124.69	111.30
10	L	69	ALA	O-C-N	5.82	130.21	122.41
1	A	800	VAL	CB-CA-C	-5.82	103.17	111.31
1	A	1172	LEU	CA-C-O	-5.82	112.19	120.51
2	B	611	PRO	CB-CA-C	-5.82	103.13	111.62
2	B	351	TYR	N-CA-C	-5.82	105.02	111.36
3	C	249	ASP	O-C-N	-5.82	115.52	122.15
5	F	75	PRO	O-C-N	5.82	130.08	123.10
8	J	49	MET	N-CA-CB	-5.82	101.64	110.07
1	A	66	LYS	CA-CB-CG	5.81	125.72	114.10
1	A	782	ARG	NE-CZ-NH1	5.81	127.31	121.50
3	C	251	LEU	CB-CA-C	-5.81	101.14	110.79
6	H	120	GLY	O-C-N	5.81	129.52	122.60
1	A	614	PHE	N-CA-C	5.81	118.24	109.23
9	K	45	LEU	CB-CA-C	5.81	120.55	110.79
1	A	446	ARG	CG-CD-NE	5.81	124.78	112.00
1	A	569	LYS	CB-CA-C	-5.81	101.09	109.63
1	A	913	LEU	N-CA-CB	-5.81	100.61	111.13
2	B	659	ALA	O-C-N	5.81	129.42	122.27
2	B	1014	PRO	O-C-N	5.81	130.02	122.24
2	B	1035	ALA	N-CA-CB	5.81	118.66	110.12
2	B	1147	LEU	N-CA-C	-5.81	104.55	111.69
3	C	67	LEU	O-C-N	-5.81	116.05	122.09
2	B	336	ARG	NE-CZ-NH1	-5.81	115.69	121.50
7	I	45	ARG	CA-CB-CG	5.81	125.72	114.10
2	B	345	LYS	CD-CE-NZ	5.81	130.48	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	258	ILE	CA-CB-CG1	-5.81	100.53	110.40
1	A	1430	LEU	CA-C-N	-5.80	111.51	120.91
1	A	1430	LEU	C-N-CA	-5.80	111.51	120.91
2	B	996	ARG	NE-CZ-NH1	-5.80	115.69	121.50
5	F	107	VAL	N-CA-CB	-5.80	101.75	112.43
7	I	50	THR	N-CA-C	5.80	119.01	109.72
8	J	24	LEU	O-C-N	-5.80	114.65	122.43
1	A	5	GLN	N-CA-CB	5.80	118.56	110.26
1	A	560	ILE	O-C-N	-5.80	114.48	121.10
2	B	490	SER	N-CA-C	5.80	118.55	111.82
2	B	414	ALA	CB-CA-C	5.80	118.33	109.34
4	E	91	LYS	CA-C-N	5.80	128.06	120.28
4	E	91	LYS	C-N-CA	5.80	128.06	120.28
2	B	362	PRO	N-CA-CB	-5.80	98.01	103.52
7	I	8	ARG	N-CA-C	-5.80	105.04	111.36
1	A	790	ASP	OD1-CG-OD2	-5.80	108.99	122.90
2	B	645	SER	N-CA-C	5.80	123.15	110.80
4	E	72	PHE	O-C-N	5.80	127.57	121.02
1	A	600	PRO	CA-N-CD	5.80	120.12	112.00
1	A	806	ARG	CD-NE-CZ	-5.80	116.28	124.40
1	A	1430	LEU	CD1-CG-CD2	-5.80	98.05	110.80
6	H	9	ILE	CA-CB-CG1	5.79	120.25	110.40
1	A	199	LEU	CA-CB-CG	5.79	136.58	116.30
2	B	596	LEU	O-C-N	5.79	128.04	122.07
3	C	148	ARG	CB-CG-CD	5.79	124.63	111.30
1	A	590	ARG	N-CA-CB	-5.79	100.65	111.13
1	A	1357	ALA	CB-CA-C	-5.79	98.42	109.95
2	B	418	LYS	N-CA-C	-5.79	103.70	112.04
3	C	253	LYS	CB-CA-C	-5.79	100.83	110.68
9	K	84	LYS	O-C-N	-5.79	114.86	122.39
2	B	1029	CYS	O-C-N	-5.79	115.55	122.15
1	A	58	LEU	CD1-CG-CD2	-5.79	98.06	110.80
1	A	351	THR	N-CA-C	5.79	117.02	108.86
2	B	307	ASP	CA-C-N	-5.79	111.34	120.60
2	B	307	ASP	C-N-CA	-5.79	111.34	120.60
3	C	54	ASN	CA-C-O	5.79	128.79	120.51
2	B	990	ILE	O-C-N	-5.79	116.36	122.67
1	A	1108	ALA	CB-CA-C	-5.79	99.76	109.48
1	A	1270	ASN	CA-C-N	-5.79	114.95	122.99
1	A	1270	ASN	C-N-CA	-5.79	114.95	122.99
2	B	520	GLY	O-C-N	-5.78	115.35	122.46
2	B	1211	ASN	CB-CA-C	-5.78	101.80	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	3	THR	O-C-N	5.78	132.18	122.93
1	A	130	ASP	CB-CG-OD1	5.78	131.70	118.40
2	B	709	ASP	O-C-N	-5.78	115.11	122.34
7	I	7	CYS	CB-CA-C	-5.78	101.17	109.84
1	A	24	PRO	O-C-N	5.78	130.07	122.27
1	A	921	GLY	N-CA-C	5.78	126.88	113.18
1	A	1449	SER	N-CA-C	5.78	118.98	109.85
2	B	903	VAL	CA-CB-CG2	-5.78	100.58	110.40
5	F	112	GLU	N-CA-CB	5.78	120.26	110.49
1	A	298	PHE	CA-C-O	5.78	126.67	120.20
1	A	1025	ARG	NE-CZ-NH1	-5.78	115.72	121.50
2	B	1030	LEU	CB-CA-C	-5.78	102.06	110.96
2	B	565	PRO	CA-C-N	-5.78	112.93	120.44
2	B	565	PRO	C-N-CA	-5.78	112.93	120.44
2	B	897	GLY	CA-C-N	5.78	130.98	121.86
2	B	897	GLY	C-N-CA	5.78	130.98	121.86
4	E	99	HIS	CA-CB-CG	5.78	119.58	113.80
6	H	103	LYS	CB-CA-C	5.78	121.91	110.42
9	K	84	LYS	CA-C-O	5.78	126.48	119.49
2	B	436	VAL	CB-CA-C	5.77	120.76	111.29
4	E	199	ILE	N-CA-CB	-5.77	104.19	111.46
5	F	152	ILE	CA-C-N	-5.77	115.79	122.95
5	F	152	ILE	C-N-CA	-5.77	115.79	122.95
8	J	55	ASP	CA-CB-CG	5.77	118.37	112.60
7	I	92	ARG	CG-CD-NE	-5.77	99.30	112.00
2	B	966	VAL	CA-CB-CG2	-5.77	100.59	110.40
6	H	12	VAL	CB-CA-C	-5.77	105.00	111.23
2	B	524	PRO	N-CA-C	-5.77	104.94	114.75
1	A	393	ARG	NE-CZ-NH2	5.77	124.39	119.20
4	E	17	ARG	NE-CZ-NH2	5.77	124.39	119.20
1	A	235	ILE	CB-CA-C	5.76	118.68	110.84
1	A	563	PRO	N-CA-C	5.76	121.31	111.68
1	A	889	SER	CB-CA-C	-5.76	98.47	110.40
2	B	228	LYS	CG-CD-CE	5.76	124.56	111.30
2	B	1134	GLU	CG-CD-OE1	5.76	131.66	118.40
1	A	616	VAL	CB-CA-C	-5.76	103.68	111.63
1	A	84	ILE	CA-CB-CG1	5.76	120.19	110.40
2	B	56	ASP	N-CA-C	5.76	123.07	110.80
2	B	561	TRP	O-C-N	-5.76	115.26	122.35
2	B	957	ASN	N-CA-C	5.76	123.07	110.80
3	C	35	ARG	CA-C-N	-5.76	110.85	120.30
3	C	35	ARG	C-N-CA	-5.76	110.85	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	208	TYR	CZ-CE2-CD2	5.76	129.97	119.60
1	A	427	GLN	N-CA-CB	-5.76	101.02	110.52
2	B	243	ALA	N-CA-C	5.76	117.01	108.60
4	E	80	VAL	CB-CA-C	-5.76	100.57	110.30
1	A	37	PHE	CA-CB-CG	5.76	119.56	113.80
1	A	894	GLU	N-CA-C	-5.76	105.14	111.82
2	B	91	SER	O-C-N	5.76	130.38	123.36
3	C	193	TYR	N-CA-CB	-5.76	101.90	111.57
9	K	52	ASN	CA-C-O	-5.76	112.86	119.60
1	A	603	ASN	CA-CB-CG	-5.75	106.84	112.60
1	A	1442	ASP	CB-CG-OD2	5.75	131.64	118.40
2	B	166	PHE	CA-C-O	-5.75	114.72	121.16
1	A	374	LEU	CB-CA-C	-5.75	99.82	109.48
2	B	135	ARG	CB-CA-C	5.75	120.21	109.86
2	B	964	VAL	CB-CA-C	5.75	119.68	110.82
1	A	99	ILE	CB-CA-C	5.75	119.57	112.04
4	E	74	ASP	N-CA-C	5.75	123.05	110.80
1	A	1069	ALA	CA-C-N	5.75	128.26	120.44
1	A	1069	ALA	C-N-CA	5.75	128.26	120.44
2	B	165	VAL	N-CA-CB	5.75	120.72	111.23
2	B	1031	LEU	CD1-CG-CD2	-5.75	98.16	110.80
2	B	448	ILE	O-C-N	5.75	129.38	123.18
2	B	555	ILE	CA-CB-CG1	5.75	120.17	110.40
3	C	4	GLU	CA-C-N	5.75	130.89	121.87
3	C	4	GLU	C-N-CA	5.75	130.89	121.87
3	C	21	ILE	CA-C-O	-5.75	114.17	120.43
7	I	6	PHE	CA-C-N	5.75	129.27	121.05
7	I	6	PHE	C-N-CA	5.75	129.27	121.05
8	J	4	PRO	N-CD-CG	-5.75	94.58	103.20
1	A	1266	THR	CB-CA-C	5.74	121.85	110.42
2	B	1103	ILE	CB-CA-C	-5.74	101.87	111.29
4	E	187	TYR	O-C-N	5.74	128.21	122.12
1	A	1212	VAL	O-C-N	-5.74	115.76	121.96
2	B	493	SER	N-CA-C	5.74	117.54	111.28
2	B	1014	PRO	CB-CA-C	-5.74	103.70	111.85
1	A	214	ILE	CA-C-O	-5.74	114.28	121.11
2	B	429	PHE	CB-CA-C	5.74	120.41	110.94
1	A	299	HIS	O-C-N	5.74	130.57	122.20
1	A	918	GLU	CA-CB-CG	5.74	125.57	114.10
1	A	964	ILE	CA-C-O	-5.74	114.57	120.71
2	B	262	GLU	N-CA-CB	5.74	118.69	109.28
2	B	515	HIS	CA-CB-CG	5.74	119.54	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	22	LEU	CB-CA-C	-5.73	99.70	109.51
1	A	591	PHE	N-CA-C	-5.73	99.84	109.07
1	A	910	PRO	N-CA-CB	5.73	109.13	102.88
1	A	1440	ALA	N-CA-C	5.73	119.25	112.72
1	A	84	ILE	CG1-CB-CG2	-5.73	93.51	110.70
1	A	756	ILE	CA-CB-CG2	5.73	120.24	110.50
1	A	833	GLU	CG-CD-OE2	-5.73	105.22	118.40
1	A	685	GLU	N-CA-C	-5.73	105.01	112.23
2	B	968	VAL	N-CA-CB	-5.73	100.61	111.21
2	B	1188	LYS	O-C-N	5.73	128.33	122.09
1	A	359	LEU	CB-CA-C	-5.72	98.89	109.37
1	A	474	VAL	CA-C-O	5.72	126.41	119.54
1	A	482	PHE	O-C-N	-5.72	114.22	121.95
1	A	668	ASP	N-CA-CB	-5.72	101.15	110.42
2	B	663	ALA	N-CA-C	-5.72	105.02	112.23
3	C	254	LYS	CA-C-O	-5.72	114.81	120.82
5	F	116	ASP	CA-C-N	5.72	125.19	119.24
5	F	116	ASP	C-N-CA	5.72	125.19	119.24
1	A	566	ILE	CB-CG1-CD1	-5.72	101.78	113.80
1	A	1436	ILE	CG1-CB-CG2	-5.72	93.53	110.70
2	B	127	GLY	CA-C-N	-5.72	114.92	122.99
2	B	127	GLY	C-N-CA	-5.72	114.92	122.99
2	B	635	ARG	CA-CB-CG	5.72	125.55	114.10
1	A	621	THR	OG1-CB-CG2	-5.72	97.86	109.30
2	B	24	PRO	CA-N-CD	-5.72	103.99	112.00
2	B	233	PRO	N-CD-CG	5.72	111.78	103.20
1	A	878	ILE	O-C-N	-5.72	117.31	123.14
2	B	355	ILE	CA-CB-CG2	-5.72	100.78	110.50
3	C	136	ASP	N-CA-C	5.72	119.56	109.96
3	C	226	ASP	CA-CB-CG	5.72	118.32	112.60
2	B	1141	HIS	CA-CB-CG	5.71	119.51	113.80
4	E	163	GLU	N-CA-C	-5.71	105.13	111.36
8	J	64	ASN	CB-CA-C	5.71	120.96	110.10
7	I	81	ARG	CD-NE-CZ	5.71	132.40	124.40
1	A	851	HIS	CA-C-N	-5.71	110.52	121.94
1	A	851	HIS	C-N-CA	-5.71	110.52	121.94
1	A	1038	THR	CB-CA-C	-5.71	98.97	111.71
1	A	1222	ASN	O-C-N	5.71	128.17	122.12
1	A	1419	ASP	O-C-N	5.71	129.78	122.93
9	K	91	CYS	N-CA-CB	-5.71	100.47	109.78
1	A	1221	LYS	CA-CB-CG	5.71	125.52	114.10
2	B	1052	VAL	CG1-CB-CG2	-5.71	98.24	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	J	12	LYS	CA-C-O	-5.71	115.24	120.95
2	B	660	LYS	CB-CA-C	5.71	120.38	110.68
2	B	1129	ARG	O-C-N	5.71	129.66	123.10
2	B	970	THR	N-CA-CB	-5.71	100.99	111.37
4	E	50	MET	CB-CA-C	5.71	121.77	110.42
1	A	824	LEU	N-CA-CB	5.70	118.50	110.12
2	B	1102	LYS	O-C-N	5.70	128.62	121.95
2	B	1106	ARG	CA-CB-CG	5.70	125.51	114.10
4	E	46	TYR	CA-C-N	-5.70	114.38	122.94
4	E	46	TYR	C-N-CA	-5.70	114.38	122.94
2	B	538	ASN	N-CA-C	5.70	118.40	108.76
1	A	452	LYS	CB-CG-CD	-5.70	98.19	111.30
1	A	1004	ASN	N-CA-CB	-5.70	102.54	110.29
1	A	1071	SER	N-CA-C	5.70	118.26	111.71
1	A	1236	LEU	N-CA-C	5.70	118.02	108.73
3	C	119	VAL	CA-C-O	-5.70	114.38	120.59
3	C	238	ILE	CA-C-O	-5.70	112.31	119.95
4	E	71	LYS	CB-CA-C	-5.70	99.34	110.11
1	A	1232	ASN	CB-CG-OD1	5.70	132.19	120.80
2	B	642	ASP	CA-C-O	5.70	126.84	120.92
3	C	36	VAL	N-CA-C	-5.70	103.97	111.09
2	B	887	HIS	CA-CB-CG	5.69	119.49	113.80
1	A	592	ASP	CA-C-O	-5.69	112.37	120.51
9	K	50	LEU	CA-CB-CG	-5.69	96.38	116.30
1	A	96	ILE	CA-C-N	-5.69	111.01	120.68
1	A	96	ILE	C-N-CA	-5.69	111.01	120.68
2	B	276	ILE	CA-CB-CG1	5.69	120.07	110.40
2	B	477	ALA	N-CA-CB	5.69	118.93	110.40
2	B	945	GLU	N-CA-C	5.69	119.37	110.32
2	B	996	ARG	NE-CZ-NH2	-5.69	114.08	119.20
2	B	1134	GLU	CG-CD-OE2	-5.69	105.31	118.40
3	C	157	CYS	N-CA-C	5.69	118.82	109.72
6	H	30	SER	N-CA-C	5.69	119.52	109.96
1	A	831	THR	CA-C-N	-5.69	113.05	120.44
1	A	831	THR	C-N-CA	-5.69	113.05	120.44
1	A	1107	VAL	CB-CA-C	5.69	120.62	111.29
1	A	1139	GLU	CB-CG-CD	5.69	122.27	112.60
4	E	206	GLY	CA-C-O	-5.69	110.67	120.57
1	A	810	PRO	N-CD-CG	-5.68	94.67	103.20
1	A	824	LEU	N-CA-C	-5.68	105.08	111.28
1	A	1207	LEU	CD1-CG-CD2	5.68	123.31	110.80
1	A	1409	LEU	N-CA-C	-5.68	105.17	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	292	ILE	N-CA-CB	-5.68	103.25	111.21
3	C	169	LYS	N-CA-C	5.68	119.03	111.75
5	F	130	ILE	O-C-N	5.68	124.95	121.37
2	B	290	GLY	N-CA-C	5.68	123.16	115.32
2	B	905	VAL	CA-CB-CG2	5.68	120.06	110.40
1	A	151	ASP	CB-CG-OD2	5.68	131.47	118.40
1	A	756	ILE	CB-CA-C	5.68	120.97	112.16
2	B	698	GLU	CG-CD-OE1	5.68	131.46	118.40
3	C	35	ARG	CG-CD-NE	-5.68	99.50	112.00
1	A	821	ARG	NE-CZ-NH1	5.68	127.18	121.50
4	E	16	PHE	CB-CA-C	5.68	121.57	110.67
2	B	1009	ASP	N-CA-C	-5.68	106.35	113.28
1	A	1295	THR	CA-CB-OG1	5.67	118.11	109.60
1	A	1359	ASP	O-C-N	5.67	130.14	122.59
2	B	453	ILE	O-C-N	5.67	128.86	121.94
2	B	612	GLU	CA-CB-CG	-5.67	102.75	114.10
4	E	28	TYR	N-CA-C	-5.67	100.64	109.72
7	I	1	MET	CA-CB-CG	5.67	125.45	114.10
1	A	609	ASP	CA-C-O	5.67	128.62	120.51
4	E	3	GLN	N-CA-CB	5.67	119.03	109.78
1	A	450	LEU	CB-CG-CD1	-5.67	93.68	110.70
2	B	227	LYS	CD-CE-NZ	5.67	130.05	111.90
2	B	911	ILE	CG1-CB-CG2	-5.67	93.69	110.70
3	C	75	MET	CB-CA-C	5.67	120.49	110.85
1	A	1269	GLU	CG-CD-OE2	-5.67	105.36	118.40
2	B	407	ASP	CA-C-O	5.67	126.56	120.32
2	B	635	ARG	CG-CD-NE	-5.67	99.53	112.00
1	A	278	THR	OG1-CB-CG2	-5.67	97.96	109.30
2	B	745	PRO	N-CA-CB	5.67	109.15	103.48
3	C	204	SER	CA-C-N	-5.67	113.07	120.44
3	C	204	SER	C-N-CA	-5.67	113.07	120.44
6	H	35	GLN	CA-C-N	5.67	130.27	121.26
6	H	35	GLN	C-N-CA	5.67	130.27	121.26
9	K	56	VAL	CA-C-O	5.67	127.28	120.65
1	A	147	VAL	N-CA-C	5.67	116.90	108.46
9	K	70	ARG	O-C-N	-5.67	116.93	123.33
1	A	1001	ARG	N-CA-CB	-5.66	103.06	110.88
2	B	555	ILE	CB-CA-C	-5.66	104.40	112.22
2	B	623	GLU	CB-CG-CD	5.66	122.23	112.60
6	H	84	ALA	O-C-N	5.66	130.12	122.59
1	A	809	THR	N-CA-C	5.66	119.04	109.87
1	A	1233	ASP	N-CA-C	-5.66	106.35	113.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	275	TYR	CA-C-N	-5.66	115.72	123.14
2	B	275	TYR	C-N-CA	-5.66	115.72	123.14
2	B	992	ILE	CB-CA-C	5.66	117.06	111.74
9	K	110	ASN	N-CA-CB	5.66	118.69	110.26
1	A	198	GLU	CA-C-O	-5.66	114.41	120.46
2	B	131	ASP	CA-C-O	5.66	127.29	120.27
2	B	274	PRO	O-C-N	5.66	129.44	123.10
2	B	632	ARG	CA-C-O	5.66	127.14	120.69
2	B	880	THR	CA-C-N	5.66	132.35	121.54
2	B	880	THR	C-N-CA	5.66	132.35	121.54
4	E	123	LEU	CA-CB-CG	-5.66	96.50	116.30
4	E	188	LEU	CD1-CG-CD2	-5.66	98.35	110.80
1	A	576	GLN	CA-C-N	-5.66	110.56	120.29
1	A	576	GLN	C-N-CA	-5.66	110.56	120.29
1	A	671	ALA	CA-C-N	5.66	132.34	121.54
1	A	671	ALA	C-N-CA	5.66	132.34	121.54
1	A	1209	MET	CA-C-N	-5.66	111.01	120.74
1	A	1209	MET	C-N-CA	-5.66	111.01	120.74
1	A	1260	LEU	CD1-CG-CD2	-5.66	98.36	110.80
2	B	794	ASN	N-CA-C	-5.66	99.80	109.24
2	B	1202	LEU	N-CA-C	5.66	117.12	111.07
3	C	19	ASP	N-CA-C	-5.66	100.48	109.76
2	B	502	ILE	CB-CG1-CD1	-5.65	101.93	113.80
1	A	1172	LEU	CB-CA-C	-5.65	99.17	110.42
7	I	95	THR	N-CA-CB	-5.65	101.29	109.83
1	A	639	PRO	CA-C-N	-5.65	112.27	120.29
1	A	639	PRO	C-N-CA	-5.65	112.27	120.29
1	A	884	ASP	CB-CG-OD1	-5.65	105.40	118.40
4	E	147	HIS	CB-CA-C	-5.65	99.94	109.83
7	I	110	PHE	N-CA-C	5.65	117.38	108.96
1	A	1276	VAL	CB-CA-C	-5.65	102.27	110.63
2	B	723	VAL	O-C-N	5.65	129.38	122.83
9	K	78	THR	O-C-N	5.65	130.05	122.82
2	B	953	LEU	CA-C-O	5.65	127.83	120.21
1	A	131	SER	CB-CA-C	5.65	121.19	109.95
2	B	908	GLU	O-C-N	5.65	129.76	122.19
1	A	557	ASP	CB-CG-OD2	5.64	131.38	118.40
1	A	1025	ARG	N-CA-C	-5.64	106.23	113.23
2	B	40	GLU	OE1-CD-OE2	5.64	136.44	122.90
3	C	11	ARG	CA-CB-CG	5.64	125.39	114.10
10	L	57	LEU	CB-CA-C	-5.64	101.59	110.79
10	L	70	ARG	NH1-CZ-NH2	-5.64	111.96	119.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	460	VAL	CG1-CB-CG2	-5.64	98.39	110.80
1	A	58	LEU	N-CA-C	-5.64	98.79	110.80
1	A	225	ASN	O-C-N	5.64	130.24	123.36
1	A	1274	ARG	CA-C-O	-5.64	114.51	121.11
2	B	446	LEU	CB-CA-C	5.64	120.81	110.10
1	A	1151	GLU	CA-C-N	-5.64	116.20	123.19
1	A	1151	GLU	C-N-CA	-5.64	116.20	123.19
1	A	1292	PRO	N-CD-CG	5.64	111.66	103.20
1	A	962	ARG	CG-CD-NE	-5.64	99.60	112.00
1	A	1015	VAL	N-CA-CB	-5.64	104.83	112.16
2	B	643	ASP	CA-CB-CG	5.64	118.24	112.60
2	B	645	SER	O-C-N	-5.64	115.09	122.59
2	B	1181	GLU	CA-CB-CG	5.64	125.37	114.10
6	H	53	ASP	CB-CA-C	-5.64	99.20	110.42
1	A	289	ILE	O-C-N	5.63	127.76	121.90
1	A	1035	TYR	N-CA-C	-5.63	105.52	112.90
3	C	187	LYS	CB-CA-C	5.63	120.40	111.95
9	K	36	GLU	CA-CB-CG	-5.63	102.83	114.10
1	A	227	VAL	CB-CA-C	-5.63	105.89	111.30
2	B	697	GLU	CB-CG-CD	5.63	122.18	112.60
1	A	192	GLY	CA-C-N	5.63	132.30	121.54
1	A	192	GLY	C-N-CA	5.63	132.30	121.54
2	B	703	ILE	N-CA-CB	-5.63	101.59	111.39
2	B	904	ARG	N-CA-C	5.63	118.44	110.50
9	K	26	LYS	CG-CD-CE	5.63	124.25	111.30
10	L	61	THR	N-CA-C	-5.63	103.05	110.43
1	A	196	GLU	CA-CB-CG	5.63	125.36	114.10
1	A	193	ASP	CA-C-N	5.63	132.29	121.54
1	A	193	ASP	C-N-CA	5.63	132.29	121.54
1	A	391	LEU	CB-CG-CD2	-5.63	93.81	110.70
1	A	548	ASN	CA-C-O	5.63	126.49	120.24
2	B	1196	ILE	CA-CB-CG2	-5.63	100.93	110.50
1	A	1217	LYS	N-CA-C	5.63	118.95	111.75
2	B	57	TYR	N-CA-C	-5.63	98.81	110.80
2	B	285	ILE	N-CA-C	5.63	117.03	110.62
2	B	788	ARG	N-CA-CB	-5.63	101.45	110.51
2	B	1209	ALA	CA-C-O	-5.63	114.62	120.92
3	C	96	SER	N-CA-C	5.63	122.78	110.80
3	C	238	ILE	CA-C-N	-5.63	114.77	120.85
3	C	238	ILE	C-N-CA	-5.63	114.77	120.85
7	I	55	THR	CA-CB-OG1	-5.62	101.16	109.60
7	I	109	ILE	CB-CA-C	-5.62	102.26	110.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	563	PRO	CA-C-N	-5.62	111.76	121.66
1	A	563	PRO	C-N-CA	-5.62	111.76	121.66
10	L	58	LYS	CA-C-N	-5.62	110.80	121.54
10	L	58	LYS	C-N-CA	-5.62	110.80	121.54
2	B	743	ILE	CA-CB-CG1	5.62	119.96	110.40
2	B	758	PHE	O-C-N	-5.62	114.86	121.32
9	K	20	LYS	CD-CE-NZ	5.62	129.89	111.90
9	K	91	CYS	CA-C-O	5.62	127.22	120.92
1	A	14	VAL	CB-CA-C	-5.62	103.20	110.84
3	C	36	VAL	CA-C-N	-5.62	112.75	120.28
3	C	36	VAL	C-N-CA	-5.62	112.75	120.28
1	A	941	LYS	N-CA-C	-5.62	104.79	111.03
1	A	1077	THR	CA-CB-CG2	5.62	120.05	110.50
1	A	996	ASN	N-CA-CB	-5.62	102.36	110.56
7	I	61	ASP	CB-CG-OD1	-5.62	105.48	118.40
8	J	47	ARG	CA-CB-CG	-5.62	102.87	114.10
9	K	107	THR	CA-CB-CG2	5.62	120.05	110.50
10	L	48	CYS	CA-C-N	5.62	132.26	121.54
10	L	48	CYS	C-N-CA	5.62	132.26	121.54
1	A	379	VAL	CG1-CB-CG2	-5.61	98.45	110.80
2	B	170	LEU	CB-CA-C	-5.61	102.61	110.13
6	H	25	ARG	CA-C-O	5.61	126.47	120.46
7	I	42	LEU	CB-CA-C	-5.61	101.08	110.29
1	A	759	ALA	N-CA-C	5.61	117.07	111.07
1	A	920	LEU	CD1-CG-CD2	5.61	123.14	110.80
2	B	889	THR	N-CA-CB	5.61	119.32	110.23
1	A	61	ILE	O-C-N	5.61	129.58	122.57
1	A	109	HIS	CB-CA-C	5.61	122.04	112.00
2	B	861	ASP	N-CA-C	5.61	117.62	108.76
2	B	136	THR	N-CA-C	5.61	118.38	109.24
3	C	260	LEU	CA-C-N	-5.61	113.35	122.26
3	C	260	LEU	C-N-CA	-5.61	113.35	122.26
4	E	142	VAL	CG1-CB-CG2	-5.61	98.46	110.80
7	I	46	HIS	CA-C-N	-5.61	114.73	122.30
7	I	46	HIS	C-N-CA	-5.61	114.73	122.30
1	A	479	ASN	CB-CA-C	-5.61	103.93	111.89
4	E	133	GLU	CA-C-N	-5.61	114.80	122.93
4	E	133	GLU	C-N-CA	-5.61	114.80	122.93
1	A	947	PHE	CA-C-O	-5.60	114.22	121.11
1	A	1257	ASP	CA-C-N	-5.60	112.82	120.44
1	A	1257	ASP	C-N-CA	-5.60	112.82	120.44
3	C	228	PHE	N-CA-CB	-5.60	101.10	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1340	GLY	N-CA-C	5.60	119.11	112.33
9	K	94	ILE	CG1-CB-CG2	-5.60	93.89	110.70
1	A	1234	GLU	CA-C-O	-5.60	112.50	120.51
8	J	3	VAL	N-CA-CB	5.60	119.05	111.21
1	A	119	ASN	CA-C-N	-5.60	110.84	121.54
1	A	119	ASN	C-N-CA	-5.60	110.84	121.54
1	A	1377	THR	CA-CB-CG2	5.60	120.02	110.50
6	H	143	LEU	CD1-CG-CD2	-5.60	98.48	110.80
8	J	18	TRP	CA-C-N	5.60	128.24	120.29
8	J	18	TRP	C-N-CA	5.60	128.24	120.29
2	B	1156	ASP	CB-CA-C	5.60	121.15	109.68
2	B	102	VAL	CB-CA-C	-5.60	101.44	110.28
2	B	395	GLN	N-CA-CB	5.60	118.87	109.92
1	A	111	GLY	CA-C-N	-5.59	114.82	122.93
1	A	111	GLY	C-N-CA	-5.59	114.82	122.93
6	H	40	LEU	O-C-N	5.59	129.49	123.56
7	I	89	GLN	N-CA-C	5.59	119.73	113.02
1	A	515	GLN	OE1-CD-NE2	5.59	128.19	122.60
1	A	421	ALA	CA-C-O	-5.59	114.62	120.55
1	A	106	VAL	CA-C-N	-5.59	114.32	122.65
1	A	106	VAL	C-N-CA	-5.59	114.32	122.65
1	A	698	GLN	CA-C-N	-5.59	113.70	122.65
1	A	698	GLN	C-N-CA	-5.59	113.70	122.65
1	A	761	MET	O-C-N	5.59	128.52	122.15
1	A	999	VAL	N-CA-C	-5.59	107.43	112.12
2	B	619	ILE	N-CA-C	-5.59	103.95	111.44
2	B	879	ARG	N-CA-CB	5.59	119.94	110.49
2	B	886	LYS	CD-CE-NZ	5.59	129.79	111.90
2	B	1000	PRO	N-CA-CB	-5.59	97.73	103.15
4	E	141	VAL	N-CA-C	-5.59	104.11	111.09
1	A	1354	ASN	CA-CB-CG	-5.59	107.01	112.60
2	B	728	ARG	CB-CG-CD	5.59	124.15	111.30
6	H	23	VAL	CA-CB-CG2	-5.59	100.90	110.40
2	B	331	LEU	CA-C-N	-5.58	113.18	120.44
2	B	331	LEU	C-N-CA	-5.58	113.18	120.44
1	A	157	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	610	GLY	N-CA-C	5.58	124.25	114.76
2	B	515	HIS	ND1-CE1-NE2	-5.58	102.82	108.40
6	H	112	ILE	CB-CG1-CD1	-5.58	102.07	113.80
6	H	133	ASN	N-CA-C	5.58	122.69	110.80
8	J	32	GLU	O-C-N	-5.58	115.16	122.59
1	A	207	ILE	CA-CB-CG1	5.58	119.89	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	252	SER	CB-CA-C	-5.58	101.19	109.90
2	B	772	ALA	CA-C-N	-5.58	112.80	120.28
2	B	772	ALA	C-N-CA	-5.58	112.80	120.28
4	E	203	GLU	CB-CA-C	-5.58	99.96	110.01
9	K	71	PHE	CA-CB-CG	5.58	119.38	113.80
1	A	161	LEU	O-C-N	5.58	130.92	122.94
2	B	124	TYR	CD1-CG-CD2	-5.58	109.73	118.10
8	J	39	LEU	N-CA-CB	5.58	118.26	110.56
1	A	645	LEU	O-C-N	-5.58	116.21	122.12
2	B	226	PHE	CA-C-N	-5.58	110.58	121.06
2	B	226	PHE	C-N-CA	-5.58	110.58	121.06
7	I	43	VAL	CA-C-O	5.58	125.11	119.20
1	A	546	VAL	CA-C-N	-5.58	111.41	120.72
1	A	546	VAL	C-N-CA	-5.58	111.41	120.72
1	A	1359	ASP	CA-C-O	-5.58	112.54	120.51
2	B	739	THR	N-CA-CB	5.58	118.57	110.88
2	B	1166	CYS	O-C-N	-5.58	114.73	122.20
4	E	159	ASP	N-CA-C	-5.58	104.84	111.03
8	J	52	THR	OG1-CB-CG2	-5.58	98.15	109.30
10	L	26	THR	CA-CB-CG2	5.58	119.98	110.50
1	A	1010	ALA	CA-C-O	5.57	126.33	120.42
3	C	186	LEU	N-CA-CB	-5.57	100.18	110.32
4	E	166	LYS	CB-CA-C	-5.57	102.09	110.90
10	L	44	ASP	O-C-N	5.57	129.96	122.49
2	B	91	SER	CA-C-O	-5.57	113.43	120.28
1	A	242	PRO	CA-C-N	5.57	126.12	120.38
1	A	242	PRO	C-N-CA	5.57	126.12	120.38
2	B	612	GLU	CB-CA-C	5.57	119.34	109.65
1	A	710	LEU	O-C-N	-5.57	116.08	122.09
1	A	894	GLU	OE1-CD-OE2	-5.57	109.53	122.90
1	A	553	VAL	CA-CB-CG2	5.57	119.86	110.40
1	A	268	ASP	N-CA-C	-5.57	105.75	112.54
1	A	1052	GLN	CA-C-O	5.57	126.32	120.42
1	A	1281	ARG	CB-CA-C	-5.57	98.27	109.68
2	B	186	GLU	O-C-N	5.57	128.10	122.09
10	L	40	LEU	CB-CG-CD2	5.57	127.39	110.70
1	A	1256	GLU	N-CA-C	5.56	122.65	110.80
1	A	1367	HIS	CB-CA-C	5.56	118.81	110.08
1	A	1411	GLU	O-C-N	-5.56	115.43	122.27
3	C	62	PHE	CA-CB-CG	5.56	119.36	113.80
2	B	968	VAL	CA-C-O	-5.56	114.38	120.72
2	B	993	THR	N-CA-C	5.56	118.79	109.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	90	GLN	N-CA-C	-5.56	103.15	110.43
1	A	1427	ASN	CA-C-O	5.56	126.38	120.10
2	B	754	SER	O-C-N	-5.56	113.52	122.41
1	A	84	ILE	CB-CG1-CD1	-5.56	102.13	113.80
2	B	827	ILE	N-CA-C	-5.56	99.23	107.51
1	A	1269	GLU	CB-CA-C	-5.55	99.61	110.11
2	B	826	ALA	CA-C-O	-5.55	114.63	120.80
5	F	123	LYS	CB-CG-CD	5.55	124.08	111.30
1	A	675	THR	N-CA-CB	-5.55	101.73	110.06
7	I	18	GLU	OE1-CD-OE2	5.55	136.23	122.90
1	A	416	ARG	CG-CD-NE	-5.55	99.79	112.00
1	A	636	GLU	CG-CD-OE2	5.55	131.17	118.40
1	A	1023	ARG	CB-CG-CD	5.55	124.07	111.30
2	B	94	LYS	CA-C-N	5.55	130.72	123.06
2	B	94	LYS	C-N-CA	5.55	130.72	123.06
2	B	892	LYS	CD-CE-NZ	5.55	129.67	111.90
1	A	88	LYS	CB-CA-C	-5.55	100.78	109.22
1	A	709	THR	CA-C-N	-5.55	112.89	120.44
1	A	709	THR	C-N-CA	-5.55	112.89	120.44
1	A	1033	GLN	CA-C-O	-5.55	113.24	119.79
2	B	980	PHE	CG-CD2-CE2	5.55	130.14	120.70
1	A	491	VAL	CB-CA-C	-5.55	104.51	110.95
1	A	449	SER	CA-C-O	5.55	128.75	122.37
1	A	554	PRO	CA-C-N	-5.55	113.36	123.34
1	A	554	PRO	C-N-CA	-5.55	113.36	123.34
1	A	940	ARG	CG-CD-NE	-5.55	99.80	112.00
2	B	60	GLN	O-C-N	-5.55	115.18	122.39
9	K	107	THR	O-C-N	5.55	128.88	122.17
1	A	239	LEU	CA-C-O	5.54	125.35	119.69
1	A	1275	GLY	O-C-N	5.54	128.62	123.35
5	F	138	LEU	CA-C-N	5.54	125.07	119.19
5	F	138	LEU	C-N-CA	5.54	125.07	119.19
8	J	1	MET	CA-CB-CG	5.54	125.19	114.10
1	A	969	GLN	OE1-CD-NE2	5.54	128.14	122.60
2	B	650	GLU	O-C-N	-5.54	117.27	123.48
2	B	710	LEU	CA-C-O	-5.54	113.38	120.31
2	B	1165	ILE	O-C-N	-5.54	116.31	122.07
10	L	63	ARG	N-CA-CB	5.54	118.19	110.04
1	A	160	GLN	CA-C-N	-5.54	113.11	123.03
1	A	160	GLN	C-N-CA	-5.54	113.11	123.03
1	A	1207	LEU	CB-CA-C	5.54	119.85	109.71
2	B	164	LYS	CG-CD-CE	5.54	124.05	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	936	ASP	OD1-CG-OD2	-5.54	109.60	122.90
4	E	98	ILE	N-CA-CB	5.54	119.81	110.56
1	A	814	PHE	O-C-N	-5.54	115.74	122.22
1	A	962	ARG	CB-CG-CD	5.54	124.04	111.30
2	B	1191	ILE	CB-CG1-CD1	-5.54	102.17	113.80
3	C	68	GLY	N-CA-C	-5.54	107.46	114.16
3	C	157	CYS	N-CA-CB	-5.54	101.61	111.08
1	A	944	ARG	NE-CZ-NH2	5.54	124.18	119.20
1	A	1222	ASN	CB-CA-C	5.54	119.98	110.79
2	B	421	PHE	N-CA-C	-5.54	106.02	112.89
4	E	70	SER	CA-C-O	-5.54	114.68	120.55
4	E	147	HIS	CG-ND1-CE1	-5.54	99.89	109.30
2	B	431	TYR	CB-CA-C	-5.54	103.45	111.14
2	B	1163	CYS	CA-C-N	-5.54	113.89	122.30
2	B	1163	CYS	C-N-CA	-5.54	113.89	122.30
4	E	100	ILE	O-C-N	5.54	127.86	121.94
1	A	80	HIS	ND1-CE1-NE2	5.53	113.93	108.40
1	A	625	SER	CA-CB-OG	5.53	122.17	111.10
1	A	865	GLN	CA-C-N	-5.53	112.35	121.92
1	A	865	GLN	C-N-CA	-5.53	112.35	121.92
2	B	830	TYR	CA-C-O	5.53	126.44	120.63
2	B	974	PRO	N-CA-C	5.53	119.89	111.15
9	K	6	ARG	CG-CD-NE	-5.53	99.83	112.00
1	A	818	MET	CA-C-O	5.53	126.63	120.82
1	A	1440	ALA	N-CA-CB	-5.53	102.46	110.70
7	I	98	VAL	N-CA-CB	-5.53	100.53	111.15
1	A	504	LEU	CA-C-O	-5.53	112.15	119.06
1	A	1005	GLU	CG-CD-OE2	-5.53	105.68	118.40
1	A	1010	ALA	O-C-N	5.53	128.45	122.15
2	B	766	ARG	O-C-N	-5.53	115.84	122.15
1	A	916	GLY	CA-C-O	-5.53	114.22	120.30
4	E	84	ASP	N-CA-C	5.53	118.14	111.40
1	A	1235	LYS	CB-CA-C	5.53	120.29	109.35
2	B	251	ILE	CA-CB-CG1	-5.53	101.00	110.40
2	B	764	SER	O-C-N	-5.53	115.56	120.48
2	B	1061	GLU	CG-CD-OE2	-5.53	105.69	118.40
3	C	93	ASP	CB-CA-C	5.53	120.33	109.72
6	H	7	ASP	N-CA-C	-5.53	99.03	110.80
8	J	45	CYS	O-C-N	-5.53	115.24	122.59
1	A	34	LYS	N-CA-CB	-5.53	102.94	110.56
1	A	222	LEU	CB-CG-CD2	5.53	127.28	110.70
1	A	696	GLU	N-CA-C	-5.53	104.95	110.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	70	ILE	CB-CG1-CD1	-5.53	102.20	113.80
2	B	426	LYS	CD-CE-NZ	5.52	129.58	111.90
1	A	160	GLN	CA-C-O	-5.52	114.71	121.78
1	A	1080	THR	CB-CA-C	5.52	121.41	110.42
5	F	81	THR	O-C-N	-5.52	115.91	122.65
7	I	57	GLY	O-C-N	-5.52	115.87	122.33
1	A	272	ALA	N-CA-CB	5.52	118.84	110.28
1	A	587	HIS	N-CA-C	-5.52	100.02	109.24
1	A	1112	LYS	CD-CE-NZ	5.52	129.57	111.90
2	B	262	GLU	CA-CB-CG	5.52	125.14	114.10
8	J	61	LEU	CB-CG-CD2	5.52	127.26	110.70
1	A	435	HIS	CA-C-O	-5.52	115.70	121.99
1	A	1051	ALA	CA-C-N	-5.52	112.45	120.29
1	A	1051	ALA	C-N-CA	-5.52	112.45	120.29
2	B	1193	GLN	CB-CG-CD	-5.52	103.22	112.60
3	C	197	SER	CA-C-O	-5.52	114.74	120.92
2	B	202	TYR	CA-C-N	5.52	131.75	122.87
2	B	202	TYR	C-N-CA	5.52	131.75	122.87
2	B	353	LYS	CD-CE-NZ	5.52	129.55	111.90
2	B	959	ASP	N-CA-C	-5.52	106.55	113.28
2	B	518	HIS	CB-CA-C	-5.51	100.88	110.09
2	B	740	HIS	N-CA-CB	-5.51	102.85	111.56
2	B	433	GLN	N-CA-CB	5.51	118.52	110.47
1	A	1020	CYS	O-C-N	5.51	128.67	122.22
2	B	116	GLU	CA-C-N	-5.51	110.83	121.58
2	B	116	GLU	C-N-CA	-5.51	110.83	121.58
5	F	78	GLN	O-C-N	-5.51	115.26	122.59
5	F	81	THR	CA-CB-CG2	5.51	119.87	110.50
3	C	56	THR	OG1-CB-CG2	-5.51	98.28	109.30
3	C	121	VAL	CA-CB-CG2	-5.51	101.03	110.40
6	H	140	ALA	CA-C-O	-5.51	114.38	120.33
1	A	970	THR	N-CA-C	5.51	118.21	111.82
2	B	170	LEU	CB-CG-CD1	-5.51	94.17	110.70
1	A	937	VAL	CA-C-N	-5.51	112.90	120.28
1	A	937	VAL	C-N-CA	-5.51	112.90	120.28
1	A	1325	THR	N-CA-CB	-5.51	101.42	110.40
2	B	693	ILE	N-CA-CB	-5.51	103.48	111.52
4	E	85	GLU	CA-CB-CG	5.51	125.11	114.10
10	L	70	ARG	NE-CZ-NH2	-5.51	114.25	119.20
1	A	128	ILE	CA-CB-CG1	5.50	119.76	110.40
1	A	1289	ARG	NE-CZ-NH2	5.50	124.16	119.20
2	B	185	THR	OG1-CB-CG2	-5.50	98.29	109.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	976	ILE	CG1-CB-CG2	-5.50	94.19	110.70
1	A	161	LEU	CA-C-N	-5.50	114.44	122.58
1	A	161	LEU	C-N-CA	-5.50	114.44	122.58
1	A	419	LYS	CG-CD-CE	5.50	123.96	111.30
1	A	779	PHE	CA-C-O	5.50	128.48	121.82
2	B	457	LEU	CD1-CG-CD2	5.50	122.91	110.80
1	A	1028	THR	CA-C-N	-5.50	112.36	120.28
1	A	1028	THR	C-N-CA	-5.50	112.36	120.28
7	I	26	LEU	CA-C-O	-5.50	114.90	121.56
1	A	101	LYS	CA-C-N	-5.50	113.52	120.56
1	A	101	LYS	C-N-CA	-5.50	113.52	120.56
1	A	469	ARG	N-CA-C	5.50	118.54	109.85
2	B	1156	ASP	OD1-CG-OD2	-5.50	109.70	122.90
1	A	349	ALA	CA-C-O	-5.50	115.39	121.33
1	A	687	LYS	CD-CE-NZ	5.50	129.50	111.90
1	A	406	ILE	CB-CG1-CD1	-5.50	102.26	113.80
1	A	1343	ALA	CA-C-N	-5.50	110.64	121.41
1	A	1343	ALA	C-N-CA	-5.50	110.64	121.41
2	B	889	THR	O-C-N	-5.50	116.78	123.16
5	F	109	VAL	CG1-CB-CG2	-5.50	98.71	110.80
9	K	61	TYR	N-CA-CB	-5.50	102.72	111.62
3	C	120	ILE	CB-CG1-CD1	-5.50	102.26	113.80
1	A	723	ASN	OD1-CG-ND2	5.49	128.09	122.60
2	B	625	LYS	CD-CE-NZ	-5.49	94.32	111.90
6	H	61	SER	O-C-N	5.49	129.90	122.59
10	L	41	SER	N-CA-C	5.49	122.50	110.80
1	A	731	ARG	CD-NE-CZ	-5.49	116.71	124.40
2	B	963	PHE	CD1-CG-CD2	5.49	126.84	118.60
4	E	117	THR	CA-C-O	5.49	124.80	120.19
1	A	968	GLN	N-CA-CB	5.49	120.31	110.32
2	B	1136	ASP	N-CA-C	5.49	117.27	111.28
4	E	161	LYS	CA-CB-CG	5.49	125.08	114.10
7	I	5	ARG	O-C-N	5.49	129.99	123.24
1	A	22	PHE	CB-CA-C	-5.49	101.61	110.77
2	B	372	SER	O-C-N	-5.49	115.90	122.15
2	B	556	THR	CA-CB-OG1	5.49	117.83	109.60
2	B	665	GLU	CA-C-N	5.49	128.39	120.38
2	B	665	GLU	C-N-CA	5.49	128.39	120.38
2	B	823	ALA	CA-C-O	-5.49	114.81	121.28
5	F	107	VAL	N-CA-C	5.49	117.70	109.20
1	A	451	HIS	CB-CG-CD2	-5.48	124.07	131.20
2	B	389	ALA	N-CA-C	5.48	118.02	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	31	SER	O-C-N	5.48	129.15	122.96
1	A	106	VAL	O-C-N	-5.48	117.06	122.76
1	A	681	GLU	OE1-CD-OE2	5.48	136.06	122.90
2	B	557	PHE	N-CA-C	-5.48	105.38	111.36
1	A	172	PRO	N-CA-CB	5.48	108.43	103.33
1	A	274	ILE	CA-CB-CG2	5.48	119.82	110.50
1	A	620	LYS	N-CA-C	5.48	117.25	111.28
1	A	794	PRO	CA-N-CD	-5.48	104.33	112.00
3	C	71	PRO	CA-C-O	-5.48	114.73	121.31
3	C	114	TYR	O-C-N	-5.48	114.87	122.76
1	A	476	SER	CA-CB-OG	-5.48	100.14	111.10
1	A	1223	ASP	N-CA-CB	5.48	122.07	110.67
3	C	110	THR	CA-C-O	-5.48	114.72	120.80
9	K	11	LEU	N-CA-C	5.48	118.02	108.76
1	A	932	GLU	CA-CB-CG	5.48	125.06	114.10
1	A	1217	LYS	CB-CG-CD	-5.48	98.70	111.30
2	B	729	ILE	N-CA-C	5.48	116.12	108.89
3	C	87	PHE	CE1-CZ-CE2	-5.48	110.14	120.00
9	K	63	VAL	CA-C-O	5.48	126.39	120.53
1	A	65	LEU	CA-C-N	5.47	130.03	121.76
1	A	65	LEU	C-N-CA	5.47	130.03	121.76
1	A	277	GLU	N-CA-CB	-5.47	102.04	110.20
2	B	959	ASP	CA-C-O	5.47	125.69	119.18
7	I	21	GLU	N-CA-C	-5.47	104.72	111.40
7	I	52	ILE	CB-CA-C	-5.47	102.31	111.29
1	A	589	GLN	CA-C-O	-5.47	114.71	121.06
1	A	904	THR	OG1-CB-CG2	5.47	120.25	109.30
2	B	538	ASN	O-C-N	-5.47	116.91	123.31
2	B	892	LYS	N-CA-CB	5.47	118.69	110.65
2	B	1213	THR	N-CA-C	5.47	118.27	108.47
2	B	621	GLU	CG-CD-OE2	5.47	130.98	118.40
4	E	111	VAL	CG1-CB-CG2	5.47	122.83	110.80
4	E	157	SER	CA-C-O	-5.47	115.75	121.55
5	F	90	ARG	NE-CZ-NH2	-5.47	114.28	119.20
1	A	1170	ILE	O-C-N	5.47	127.98	121.80
1	A	1442	ASP	CA-C-O	-5.47	114.94	121.56
2	B	21	GLU	CB-CA-C	5.47	120.83	109.95
1	A	830	LYS	N-CA-C	5.47	117.69	111.02
2	B	1170	THR	O-C-N	5.47	129.09	122.48
5	F	90	ARG	CA-C-O	-5.47	114.72	120.63
1	A	238	CYS	CA-CB-SG	-5.46	101.83	114.40
2	B	395	GLN	N-CA-C	5.46	117.34	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	640	VAL	O-C-N	-5.46	117.36	123.26
2	B	842	ASN	N-CA-C	-5.46	99.61	108.41
3	C	88	CYS	CA-C-N	-5.46	114.49	122.19
3	C	88	CYS	C-N-CA	-5.46	114.49	122.19
3	C	106	GLU	N-CA-C	-5.46	105.41	112.68
10	L	55	ILE	CA-C-N	-5.46	113.88	122.73
10	L	55	ILE	C-N-CA	-5.46	113.88	122.73
1	A	1038	THR	N-CA-C	5.46	117.89	110.35
7	I	88	SER	CB-CA-C	-5.46	101.65	109.84
1	A	105	CYS	CA-C-O	5.46	124.81	118.97
1	A	148	CYS	CA-CB-SG	5.46	126.96	114.40
1	A	226	GLU	CG-CD-OE1	-5.46	105.84	118.40
1	A	843	LYS	N-CA-CB	-5.46	102.09	110.01
1	A	982	THR	OG1-CB-CG2	-5.46	98.39	109.30
2	B	1154	ALA	CA-C-N	5.46	131.96	121.54
2	B	1154	ALA	C-N-CA	5.46	131.96	121.54
6	H	132	LEU	CA-CB-CG	5.46	135.40	116.30
7	I	115	LYS	CA-C-N	-5.46	113.15	121.66
7	I	115	LYS	C-N-CA	-5.46	113.15	121.66
1	A	553	VAL	N-CA-CB	-5.46	103.57	111.21
2	B	635	ARG	NE-CZ-NH1	5.46	126.95	121.50
6	H	112	ILE	CG1-CB-CG2	-5.46	94.33	110.70
10	L	42	ARG	N-CA-C	-5.46	100.81	109.59
1	A	991	LYS	CA-CB-CG	5.45	125.01	114.10
2	B	783	THR	CA-C-O	-5.45	112.13	119.11
4	E	179	GLN	OE1-CD-NE2	5.45	128.05	122.60
4	E	171	LYS	N-CA-C	5.45	117.91	110.55
1	A	721	PHE	CA-CB-CG	5.45	119.25	113.80
2	B	118	ARG	NE-CZ-NH1	5.45	126.95	121.50
2	B	737	THR	CA-CB-OG1	5.45	117.78	109.60
2	B	1058	LEU	CA-C-O	5.45	126.52	120.63
10	L	48	CYS	CA-C-O	5.45	128.31	120.51
1	A	585	GLY	CA-C-N	-5.45	115.42	122.99
1	A	585	GLY	C-N-CA	-5.45	115.42	122.99
1	A	865	GLN	CG-CD-NE2	5.45	124.57	116.40
1	A	1229	SER	CA-C-O	-5.45	115.20	121.47
2	B	484	ASN	CB-CA-C	-5.45	100.68	109.72
3	C	164	ALA	CA-C-O	-5.45	112.90	119.49
4	E	149	LEU	CA-C-N	-5.45	114.74	123.46
4	E	149	LEU	C-N-CA	-5.45	114.74	123.46
6	H	43	ASN	CB-CG-ND2	5.45	124.57	116.40
1	A	133	LYS	N-CA-CB	-5.45	101.06	110.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	396	PRO	O-C-N	5.45	129.95	122.38
1	A	659	HIS	CG-CD2-NE2	-5.45	101.75	107.20
2	B	477	ALA	CA-C-N	-5.45	113.77	122.10
2	B	477	ALA	C-N-CA	-5.45	113.77	122.10
2	B	642	ASP	O-C-N	5.45	129.60	122.68
2	B	424	LEU	CA-CB-CG	-5.45	97.24	116.30
1	A	44	THR	CA-CB-OG1	5.44	117.76	109.60
2	B	878	GLN	CA-C-O	-5.44	112.73	120.51
9	K	113	THR	O-C-N	5.44	130.02	123.16
1	A	728	LYS	N-CA-C	-5.44	105.35	111.28
1	A	1196	GLU	CB-CA-C	-5.44	101.13	110.16
2	B	253	THR	N-CA-CB	-5.44	102.01	110.55
2	B	294	ASP	CB-CG-OD2	5.44	130.91	118.40
2	B	630	ALA	CB-CA-C	-5.44	99.58	111.71
3	C	147	LEU	N-CA-C	5.44	118.09	109.50
1	A	445	ASN	N-CA-CB	-5.44	101.69	110.71
1	A	855	THR	N-CA-C	-5.44	103.21	110.55
7	I	117	LYS	CA-C-O	5.44	125.96	119.60
2	B	1070	GLU	CB-CG-CD	5.44	121.84	112.60
2	B	31	TRP	CA-C-N	-5.43	111.29	120.58
2	B	31	TRP	C-N-CA	-5.43	111.29	120.58
3	C	41	ILE	N-CA-CB	-5.43	103.60	111.21
1	A	239	LEU	O-C-N	-5.43	116.56	121.39
6	H	112	ILE	N-CA-CB	-5.43	106.15	112.34
1	A	1112	LYS	O-C-N	-5.43	115.60	122.17
2	B	1202	LEU	N-CA-CB	5.43	117.89	110.01
7	I	15	TYR	CA-C-N	5.43	125.90	120.14
7	I	15	TYR	C-N-CA	5.43	125.90	120.14
9	K	95	ILE	CA-C-N	5.43	129.87	120.58
9	K	95	ILE	C-N-CA	5.43	129.87	120.58
1	A	368	LYS	CA-CB-CG	5.43	124.95	114.10
1	A	387	ARG	CA-C-N	-5.43	113.01	120.28
1	A	387	ARG	C-N-CA	-5.43	113.01	120.28
2	B	710	LEU	N-CA-C	5.43	119.86	112.04
1	A	1319	VAL	CA-C-N	5.42	125.19	119.76
1	A	1319	VAL	C-N-CA	5.42	125.19	119.76
2	B	264	SER	CB-CA-C	5.42	121.22	110.42
7	I	32	CYS	N-CA-CB	5.42	118.84	110.60
1	A	509	LEU	CD1-CG-CD2	-5.42	98.87	110.80
2	B	238	ALA	O-C-N	-5.42	116.57	123.24
1	A	800	VAL	N-CA-CB	-5.42	104.64	111.41
1	A	1077	THR	N-CA-CB	-5.42	101.58	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	407	ASP	CA-CB-CG	5.42	118.02	112.60
4	E	190	LEU	CD1-CG-CD2	-5.42	98.88	110.80
7	I	90	GLN	CA-C-O	-5.42	115.91	121.87
1	A	501	LEU	CA-C-N	-5.42	112.12	121.66
1	A	501	LEU	C-N-CA	-5.42	112.12	121.66
2	B	174	LEU	CB-CG-CD2	5.42	126.95	110.70
2	B	292	ILE	N-CA-C	5.42	120.59	108.88
1	A	512	VAL	N-CA-C	5.42	116.10	108.36
1	A	514	PRO	N-CA-C	5.42	120.69	114.03
1	A	1026	LEU	O-C-N	-5.42	114.64	121.95
1	A	1238	ILE	CA-C-O	-5.42	114.70	120.39
2	B	435	THR	CA-C-N	5.42	131.72	121.97
2	B	435	THR	C-N-CA	5.42	131.72	121.97
3	C	67	LEU	CA-C-O	5.42	126.70	120.90
2	B	1012	ILE	CA-C-O	-5.42	115.58	121.92
1	A	656	TRP	O-C-N	5.41	128.55	122.22
2	B	167	ILE	O-C-N	5.41	127.36	121.78
2	B	885	MET	O-C-N	5.41	129.07	122.14
3	C	47	ASP	CB-CG-OD1	-5.41	105.95	118.40
1	A	915	SER	O-C-N	-5.41	115.39	122.59
1	A	1080	THR	N-CA-CB	-5.41	101.34	110.49
2	B	214	ALA	CA-C-N	-5.41	115.25	122.72
2	B	214	ALA	C-N-CA	-5.41	115.25	122.72
2	B	895	ASP	N-CA-CB	5.41	119.86	110.39
6	H	95	TYR	O-C-N	-5.41	116.36	123.28
8	J	55	ASP	CA-C-O	5.41	128.24	122.13
9	K	39	ASP	CB-CA-C	-5.41	102.69	114.10
2	B	226	PHE	N-CA-C	5.41	118.22	108.48
2	B	511	PRO	N-CA-CB	5.41	108.89	103.48
6	H	84	ALA	N-CA-C	-5.41	99.28	110.80
2	B	1192	TYR	N-CA-C	5.41	117.40	109.24
3	C	27	LEU	CA-C-N	-5.41	112.61	120.29
3	C	27	LEU	C-N-CA	-5.41	112.61	120.29
6	H	35	GLN	CA-CB-CG	5.41	124.91	114.10
8	J	48	ARG	CA-CB-CG	5.41	124.91	114.10
1	A	364	VAL	CA-CB-CG2	5.40	119.59	110.40
1	A	217	LYS	N-CA-C	5.40	117.59	111.11
1	A	448	PRO	N-CD-CG	5.40	110.28	103.80
1	A	1408	ILE	CA-C-N	5.40	127.96	120.29
1	A	1408	ILE	C-N-CA	5.40	127.96	120.29
2	B	386	LEU	N-CA-C	5.40	119.13	112.54
2	B	496	ARG	N-CA-C	-5.40	104.95	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	127	ILE	N-CA-CB	-5.40	103.65	111.21
4	E	142	VAL	CB-CA-C	-5.40	102.57	110.62
7	I	104	LEU	N-CA-C	-5.40	106.06	113.30
2	B	580	VAL	CG1-CB-CG2	-5.40	98.92	110.80
1	A	937	VAL	N-CA-C	-5.40	105.27	110.72
1	A	112	LYS	CD-CE-NZ	-5.40	94.63	111.90
4	E	200	ARG	N-CA-CB	5.40	119.94	111.20
6	H	19	ARG	N-CA-CB	5.40	119.61	110.49
1	A	926	GLN	CB-CG-CD	-5.39	103.43	112.60
6	H	107	VAL	CA-CB-CG1	5.39	119.57	110.40
1	A	1239	ARG	CG-CD-NE	-5.39	100.14	112.00
2	B	807	ARG	NH1-CZ-NH2	5.39	126.31	119.30
2	B	1210	MET	CA-C-N	-5.39	114.96	123.91
2	B	1210	MET	C-N-CA	-5.39	114.96	123.91
5	F	94	LEU	CA-C-N	-5.39	110.84	121.41
5	F	94	LEU	C-N-CA	-5.39	110.84	121.41
1	A	7	SER	CA-C-N	-5.39	111.24	121.54
1	A	7	SER	C-N-CA	-5.39	111.24	121.54
2	B	893	LEU	N-CA-C	5.39	117.83	110.55
1	A	586	ILE	O-C-N	5.39	129.02	123.20
3	C	211	ASP	OD1-CG-OD2	5.39	135.83	122.90
2	B	171	PRO	O-C-N	-5.39	116.81	123.01
3	C	4	GLU	CG-CD-OE2	-5.39	106.01	118.40
3	C	151	GLN	CG-CD-NE2	-5.39	108.32	116.40
2	B	1094	ARG	NE-CZ-NH1	-5.38	116.12	121.50
3	C	6	PRO	CA-C-O	5.38	127.22	120.92
7	I	41	PRO	O-C-N	-5.38	115.37	122.64
4	E	16	PHE	CA-C-N	-5.38	113.28	120.54
4	E	16	PHE	C-N-CA	-5.38	113.28	120.54
1	A	130	ASP	CB-CA-C	-5.38	101.07	109.84
3	C	128	ASN	CA-C-N	5.38	129.56	122.51
3	C	128	ASN	C-N-CA	5.38	129.56	122.51
4	E	21	GLU	CA-C-N	-5.38	113.07	120.28
4	E	21	GLU	C-N-CA	-5.38	113.07	120.28
2	B	1162	ILE	CA-CB-CG2	5.38	119.64	110.50
1	A	897	TYR	CZ-CE2-CD2	5.38	129.28	119.60
1	A	1049	ILE	N-CA-C	-5.38	105.14	110.62
2	B	1082	MET	CA-C-N	-5.38	115.14	122.93
2	B	1082	MET	C-N-CA	-5.38	115.14	122.93
3	C	208	GLU	O-C-N	-5.38	115.44	122.59
1	A	293	GLU	O-C-N	-5.38	116.33	122.08
1	A	106	VAL	N-CA-CB	-5.37	102.55	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	186	LYS	CD-CE-NZ	5.37	129.09	111.90
2	B	101	MET	N-CA-CB	-5.37	102.54	111.57
2	B	758	PHE	CG-CD1-CE1	5.37	129.83	120.70
7	I	82	GLU	CG-CD-OE1	5.37	130.76	118.40
9	K	84	LYS	CA-CB-CG	5.37	124.85	114.10
1	A	129	LYS	O-C-N	5.37	129.56	122.36
1	A	375	THR	CA-CB-OG1	5.37	117.66	109.60
1	A	961	ARG	CD-NE-CZ	5.37	131.92	124.40
2	B	198	ASP	CB-CG-OD2	-5.37	106.04	118.40
2	B	256	VAL	CA-C-O	-5.37	114.57	120.48
2	B	213	ILE	CB-CG1-CD1	-5.37	102.52	113.80
2	B	255	GLN	CG-CD-NE2	-5.37	108.34	116.40
4	E	87	SER	CB-CA-C	5.37	119.05	109.38
9	K	8	GLU	CA-C-N	-5.37	111.74	121.14
9	K	8	GLU	C-N-CA	-5.37	111.74	121.14
1	A	1135	ARG	CA-CB-CG	5.37	124.84	114.10
2	B	188	ASP	CB-CG-OD2	5.37	130.75	118.40
2	B	287	ARG	O-C-N	-5.37	115.94	122.22
3	C	44	LEU	CB-CG-CD1	-5.37	94.60	110.70
3	C	113	VAL	CG1-CB-CG2	-5.37	98.99	110.80
1	A	719	VAL	CA-CB-CG2	5.37	119.52	110.40
1	A	891	ALA	N-CA-CB	-5.37	102.23	110.12
1	A	806	ARG	CB-CA-C	-5.37	100.37	110.67
2	B	63	ILE	N-CA-CB	-5.37	100.16	110.78
3	C	139	GLY	O-C-N	5.37	127.67	122.41
4	E	165	LEU	CD1-CG-CD2	-5.37	99.00	110.80
9	K	77	THR	N-CA-CB	-5.37	102.35	111.69
1	A	46	THR	CA-CB-CG2	5.36	119.62	110.50
2	B	591	ARG	NE-CZ-NH2	-5.36	114.37	119.20
4	E	94	LYS	CB-CG-CD	5.36	123.64	111.30
10	L	32	ALA	O-C-N	5.36	128.69	122.20
1	A	494	SER	N-CA-CB	-5.36	102.36	111.31
2	B	974	PRO	CA-C-N	5.36	131.02	121.75
2	B	974	PRO	C-N-CA	5.36	131.02	121.75
1	A	351	THR	N-CA-CB	5.36	120.26	111.31
2	B	846	ILE	CB-CG1-CD1	-5.36	102.55	113.80
1	A	776	ALA	CB-CA-C	-5.36	100.88	111.60
1	A	1448	GLU	N-CA-C	5.36	122.21	110.80
2	B	115	GLN	CG-CD-NE2	5.36	124.44	116.40
2	B	203	PHE	CA-C-N	-5.36	116.16	123.12
2	B	203	PHE	C-N-CA	-5.36	116.16	123.12
2	B	477	ALA	CB-CA-C	5.36	118.54	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	82	PHE	N-CA-C	-5.36	101.39	109.85
7	I	9	ASP	CA-C-O	-5.36	115.18	120.80
1	A	1054	LEU	CA-C-O	5.35	126.13	119.97
2	B	452	THR	CA-CB-CG2	5.35	119.60	110.50
2	B	686	ASN	N-CA-C	5.35	118.03	111.82
1	A	895	LYS	CA-C-N	-5.35	111.43	120.58
1	A	895	LYS	C-N-CA	-5.35	111.43	120.58
2	B	392	ARG	NE-CZ-NH2	-5.35	114.38	119.20
2	B	499	ASN	N-CA-C	5.35	117.39	108.99
2	B	992	ILE	N-CA-CB	-5.35	102.78	109.84
6	H	111	LEU	CB-CA-C	-5.35	100.36	109.51
7	I	17	ARG	CB-CA-C	-5.35	100.23	109.86
1	A	731	ARG	NE-CZ-NH1	-5.35	116.15	121.50
2	B	105	SER	CA-C-N	-5.35	111.32	121.54
2	B	105	SER	C-N-CA	-5.35	111.32	121.54
2	B	746	SER	O-C-N	5.35	130.97	122.41
2	B	804	GLY	N-CA-C	5.35	125.86	113.18
2	B	1071	VAL	CA-C-O	5.35	126.95	121.23
6	H	77	ARG	NH1-CZ-NH2	-5.35	112.35	119.30
9	K	51	LEU	CA-C-O	5.35	126.14	119.78
1	A	920	LEU	CA-C-O	5.35	127.07	121.19
1	A	988	LEU	N-CA-C	5.35	119.06	112.54
1	A	1212	VAL	CA-CB-CG1	-5.35	101.31	110.40
1	A	207	ILE	CB-CA-C	-5.35	104.92	112.14
2	B	568	ASP	OD1-CG-OD2	-5.35	110.07	122.90
2	B	770	GLN	CA-C-O	5.35	126.14	120.10
3	C	42	PRO	CA-N-CD	5.35	119.48	112.00
1	A	1037	LEU	CD1-CG-CD2	-5.34	99.04	110.80
2	B	1017	ILE	N-CA-CB	-5.34	103.73	111.21
3	C	96	SER	CA-CB-OG	5.34	121.79	111.10
3	C	193	TYR	CA-C-N	-5.34	112.55	122.60
3	C	193	TYR	C-N-CA	-5.34	112.55	122.60
3	C	221	TYR	CA-C-N	-5.34	113.72	122.54
3	C	221	TYR	C-N-CA	-5.34	113.72	122.54
2	B	110	HIS	N-CA-CB	-5.34	101.83	110.81
4	E	103	LYS	O-C-N	5.34	128.83	122.26
1	A	839	ARG	N-CA-C	-5.34	105.62	111.82
1	A	877	HIS	CB-CG-ND1	5.34	130.71	122.70
2	B	1188	LYS	CG-CD-CE	5.34	123.59	111.30
1	A	586	ILE	CB-CG1-CD1	-5.34	102.58	113.80
1	A	1165	GLU	CA-C-O	-5.34	113.31	119.61
2	B	58	THR	CA-CB-OG1	-5.34	101.59	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	371	GLU	N-CA-C	-5.34	106.90	113.41
2	B	915	THR	CA-C-O	-5.34	115.37	121.40
3	C	48	SER	CB-CA-C	-5.34	100.25	109.86
3	C	202	PRO	N-CA-C	5.34	119.57	111.19
1	A	886	ILE	N-CA-C	5.34	116.82	111.00
2	B	312	GLU	N-CA-CB	-5.34	101.53	110.39
2	B	535	LEU	N-CA-CB	-5.34	102.68	110.47
1	A	112	LYS	CB-CG-CD	-5.34	99.03	111.30
1	A	863	VAL	CA-C-O	-5.34	114.77	120.85
1	A	1211	GLN	CB-CG-CD	5.34	121.67	112.60
2	B	57	TYR	N-CA-CB	5.34	119.51	110.49
3	C	214	ASN	CA-CB-CG	5.34	117.94	112.60
3	C	230	MET	CA-C-O	-5.34	115.85	121.88
1	A	734	GLU	CA-CB-CG	5.33	124.77	114.10
1	A	1238	ILE	CA-C-N	-5.33	114.52	122.74
1	A	1238	ILE	C-N-CA	-5.33	114.52	122.74
2	B	534	GLY	CA-C-O	5.33	124.98	119.27
2	B	664	THR	CA-C-O	-5.33	114.77	120.42
1	A	646	PHE	CB-CA-C	-5.33	102.51	110.88
1	A	674	PRO	N-CD-CG	5.33	111.20	103.20
1	A	696	GLU	O-C-N	-5.33	116.48	122.03
1	A	833	GLU	CB-CG-CD	5.33	121.66	112.60
1	A	1424	VAL	CB-CA-C	-5.33	103.47	112.16
7	I	78	CYS	N-CA-C	-5.33	106.28	112.89
1	A	663	SER	CA-C-O	-5.33	115.71	121.36
1	A	1214	GLU	N-CA-CB	5.33	118.50	110.30
2	B	136	THR	CA-C-N	5.33	131.72	121.54
2	B	136	THR	C-N-CA	5.33	131.72	121.54
7	I	76	PRO	CA-CB-CG	-5.33	94.37	104.50
1	A	1263	ILE	CA-C-N	5.33	127.68	120.44
1	A	1263	ILE	C-N-CA	5.33	127.68	120.44
1	A	1367	HIS	CG-CD2-NE2	5.33	112.53	107.20
3	C	127	ARG	O-C-N	5.33	129.57	123.02
2	B	327	ARG	NH1-CZ-NH2	5.32	126.22	119.30
2	B	636	PRO	O-C-N	5.32	129.83	122.64
3	C	69	LEU	O-C-N	-5.32	114.66	122.43
3	C	195	GLN	CG-CD-OE1	5.32	131.45	120.80
3	C	266	ASP	CA-C-N	5.32	131.87	122.66
3	C	266	ASP	C-N-CA	5.32	131.87	122.66
4	E	201	LYS	O-C-N	-5.32	116.16	122.65
1	A	164	ARG	CD-NE-CZ	5.32	131.85	124.40
2	B	605	ARG	NE-CZ-NH1	-5.32	116.18	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	894	ASP	N-CA-C	-5.32	102.58	110.46
2	B	1203	LEU	CD1-CG-CD2	-5.32	99.09	110.80
4	E	136	ASN	CB-CA-C	-5.32	100.55	109.65
1	A	949	ASP	CB-CG-OD2	5.32	130.64	118.40
1	A	1433	MET	O-C-N	5.32	129.29	123.01
2	B	1021	MET	CG-SD-CE	-5.32	89.19	100.90
3	C	238	ILE	CA-CB-CG2	5.32	119.55	110.50
4	E	52	ARG	NE-CZ-NH2	-5.32	114.41	119.20
2	B	314	LEU	CA-C-N	-5.32	113.44	120.09
2	B	314	LEU	C-N-CA	-5.32	113.44	120.09
7	I	79	HIS	N-CA-C	5.32	122.13	110.80
8	J	62	ARG	CA-C-N	-5.32	113.53	123.05
8	J	62	ARG	C-N-CA	-5.32	113.53	123.05
9	K	38	GLU	CA-C-O	-5.32	115.39	121.40
1	A	197	PRO	CA-C-O	-5.32	115.13	122.15
3	C	268	ASP	CA-C-O	-5.32	111.76	120.80
1	A	102	VAL	CG1-CB-CG2	-5.31	99.11	110.80
6	H	134	ASN	N-CA-C	-5.31	99.11	108.20
2	B	448	ILE	CA-C-O	-5.31	114.45	120.67
2	B	889	THR	CA-C-O	5.31	127.03	120.92
3	C	55	THR	N-CA-CB	-5.31	102.50	110.73
1	A	232	GLU	N-CA-C	5.31	118.55	111.75
1	A	1413	GLY	CA-C-N	-5.31	111.22	121.58
1	A	1413	GLY	C-N-CA	-5.31	111.22	121.58
2	B	741	CYS	N-CA-C	5.31	117.46	109.23
3	C	130	GLY	O-C-N	-5.31	116.65	122.65
1	A	32	VAL	N-CA-CB	-5.31	102.47	111.23
1	A	664	THR	N-CA-CB	5.31	121.39	111.52
1	A	685	GLU	CA-CB-CG	5.31	124.72	114.10
3	C	111	THR	N-CA-C	5.31	117.17	108.52
3	C	241	ASP	O-C-N	5.31	128.43	122.22
4	E	24	LYS	CA-CB-CG	-5.31	103.49	114.10
4	E	164	LEU	CA-C-N	-5.31	112.64	120.28
4	E	164	LEU	C-N-CA	-5.31	112.64	120.28
1	A	187	LYS	CA-C-N	5.30	131.67	121.54
1	A	187	LYS	C-N-CA	5.30	131.67	121.54
1	A	620	LYS	CB-CG-CD	5.30	123.50	111.30
1	A	678	GLU	CA-CB-CG	5.30	124.71	114.10
2	B	777	ALA	O-C-N	-5.30	116.69	122.84
4	E	53	PRO	N-CD-CG	-5.30	95.24	103.20
6	H	4	THR	O-C-N	-5.30	115.73	122.78
1	A	511	ILE	CB-CA-C	5.30	118.76	111.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1224	LEU	CB-CA-C	-5.30	99.87	110.42
2	B	40	GLU	CG-CD-OE2	-5.30	106.21	118.40
2	B	323	VAL	CA-C-N	-5.30	115.90	123.11
2	B	323	VAL	C-N-CA	-5.30	115.90	123.11
2	B	540	SER	N-CA-CB	-5.30	102.68	110.26
1	A	285	PRO	CA-C-O	-5.30	115.54	121.32
1	A	1059	HIS	CB-CA-C	-5.30	101.18	109.08
2	B	696	GLU	CG-CD-OE1	-5.30	106.21	118.40
3	C	27	LEU	CA-C-O	-5.30	114.91	120.63
4	E	122	LYS	N-CA-CB	5.30	119.04	110.40
6	H	11	GLN	CA-C-N	-5.30	114.48	122.01
6	H	11	GLN	C-N-CA	-5.30	114.48	122.01
1	A	902	LEU	CA-C-N	-5.30	112.62	121.94
1	A	902	LEU	C-N-CA	-5.30	112.62	121.94
2	B	100	PRO	CB-CA-C	5.30	118.53	110.21
1	A	874	ASP	CB-CG-OD1	-5.30	106.22	118.40
1	A	975	HIS	CA-C-N	5.30	132.14	122.50
1	A	975	HIS	C-N-CA	5.30	132.14	122.50
3	C	107	SER	CA-CB-OG	5.30	121.69	111.10
7	I	17	ARG	CA-CB-CG	-5.30	103.50	114.10
1	A	117	GLU	OE1-CD-OE2	5.29	135.61	122.90
2	B	373	ARG	N-CA-C	5.29	117.74	111.33
1	A	1234	GLU	O-C-N	5.29	129.63	122.59
1	A	1319	VAL	O-C-N	5.29	127.14	121.10
1	A	1311	VAL	O-C-N	5.29	128.78	123.07
2	B	172	ILE	CB-CG1-CD1	-5.29	102.69	113.80
2	B	1014	PRO	N-CA-C	5.29	120.72	113.84
5	F	126	ALA	CA-C-N	-5.29	112.80	122.38
5	F	126	ALA	C-N-CA	-5.29	112.80	122.38
5	F	111	LEU	CB-CA-C	-5.29	102.82	111.50
2	B	404	LYS	CB-CG-CD	-5.29	99.14	111.30
2	B	807	ARG	CB-CA-C	-5.29	99.26	110.31
2	B	1069	PHE	N-CA-C	-5.29	103.55	110.53
2	B	1175	LEU	O-C-N	5.29	129.44	122.30
4	E	202	SER	CA-CB-OG	5.29	121.68	111.10
2	B	129	PHE	N-CA-C	5.29	117.03	108.41
1	A	837	ILE	CA-C-O	5.29	126.45	120.95
2	B	398	ARG	N-CA-C	5.29	119.48	113.19
2	B	767	ASN	N-CA-C	-5.29	105.52	111.28
2	B	790	ASP	CB-CG-OD1	5.29	130.56	118.40
2	B	1219	ASP	OD1-CG-OD2	-5.29	110.22	122.90
1	A	49	LYS	CG-CD-CE	5.28	123.45	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	240	ILE	CA-C-O	-5.28	115.68	121.28
1	A	594	GLY	CA-C-O	5.28	129.76	120.57
2	B	250	PHE	CA-C-N	5.28	131.48	121.97
2	B	250	PHE	C-N-CA	5.28	131.48	121.97
1	A	364	VAL	O-C-N	-5.28	117.19	123.05
2	B	855	PHE	CD1-CG-CD2	-5.28	110.68	118.60
2	B	309	GLN	N-CA-C	5.28	117.11	111.36
1	A	55	ASP	O-C-N	5.28	127.39	121.32
1	A	979	SER	CA-C-O	-5.28	115.22	121.66
2	B	499	ASN	CA-C-O	-5.28	115.08	120.99
7	I	93	LYS	O-C-N	5.28	129.74	122.46
10	L	50	ASP	CB-CA-C	5.28	120.92	110.42
1	A	362	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	1149	ALA	CA-C-N	-5.28	113.64	122.92
1	A	1149	ALA	C-N-CA	-5.28	113.64	122.92
1	A	1171	GLN	N-CA-CB	5.28	118.46	110.28
2	B	865	LYS	CA-C-N	5.28	131.62	121.54
2	B	865	LYS	C-N-CA	5.28	131.62	121.54
2	B	1189	ILE	CA-C-O	-5.28	114.19	120.78
5	F	82	THR	N-CA-CB	5.28	117.81	110.11
4	E	148	GLU	CA-C-N	-5.27	112.83	122.38
4	E	148	GLU	C-N-CA	-5.27	112.83	122.38
1	A	191	THR	CA-C-N	5.27	128.50	121.01
1	A	191	THR	C-N-CA	5.27	128.50	121.01
2	B	597	MET	CA-C-O	-5.27	115.26	120.90
2	B	620	ARG	N-CA-C	5.27	119.87	113.38
3	C	133	ILE	CA-C-O	-5.27	115.59	121.23
4	E	71	LYS	N-CA-CB	5.27	118.12	110.26
1	A	743	VAL	N-CA-C	-5.27	104.46	111.05
7	I	94	ASP	CA-C-O	5.27	125.70	119.48
1	A	1140	HIS	ND1-CE1-NE2	-5.27	103.13	108.40
3	C	55	THR	OG1-CB-CG2	-5.27	98.76	109.30
4	E	69	ILE	N-CA-C	5.27	119.48	111.89
7	I	115	LYS	O-C-N	-5.27	115.93	122.83
1	A	690	VAL	N-CA-C	-5.27	105.36	110.42
1	A	1203	ASN	OD1-CG-ND2	5.27	127.87	122.60
1	A	1260	LEU	CA-C-N	-5.27	111.31	121.58
1	A	1260	LEU	C-N-CA	-5.27	111.31	121.58
2	B	114	PRO	N-CD-CG	5.27	111.10	103.20
2	B	449	ASN	N-CA-CB	5.27	117.88	110.24
2	B	810	GLU	CA-C-O	5.27	126.35	120.82
2	B	858	SER	CB-CA-C	-5.27	100.61	109.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	K	17	SER	N-CA-C	5.27	118.17	109.85
1	A	1369	ALA	CA-C-N	-5.26	113.17	120.38
1	A	1369	ALA	C-N-CA	-5.26	113.17	120.38
2	B	566	LEU	N-CA-C	5.26	116.70	111.07
2	B	738	PHE	N-CA-CB	-5.26	102.30	110.04
6	H	36	CYS	N-CA-C	5.26	118.20	110.30
1	A	439	ASN	CB-CG-ND2	-5.26	108.50	116.40
1	A	1012	ARG	N-CA-C	5.26	117.10	111.36
4	E	162	ARG	CB-CA-C	5.26	120.78	110.67
1	A	1405	THR	N-CA-C	5.26	125.73	111.00
2	B	1040	ASN	CB-CG-ND2	5.26	124.29	116.40
3	C	255	VAL	CG1-CB-CG2	-5.26	99.22	110.80
5	F	104	ASN	N-CA-CB	-5.26	104.00	111.84
1	A	1242	VAL	O-C-N	-5.26	116.00	122.57
4	E	41	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	953	ASN	O-C-N	-5.26	117.07	123.27
2	B	341	LEU	N-CA-C	-5.26	101.40	109.76
1	A	50	ILE	CA-C-O	-5.25	114.91	120.48
1	A	84	ILE	CB-CA-C	5.25	119.91	111.29
2	B	616	ILE	CG1-CB-CG2	-5.25	94.94	110.70
3	C	7	GLN	OE1-CD-NE2	5.25	127.85	122.60
4	E	103	LYS	CA-CB-CG	5.25	124.61	114.10
4	E	198	ILE	N-CA-CB	-5.25	104.84	111.46
1	A	233	TRP	CA-C-O	-5.25	112.24	119.12
1	A	490	HIS	CA-C-O	5.25	125.81	120.24
1	A	1315	GLU	CA-C-N	-5.25	112.17	120.47
1	A	1315	GLU	C-N-CA	-5.25	112.17	120.47
4	E	44	ALA	CA-C-O	5.25	128.02	120.51
6	H	45	GLU	OE1-CD-OE2	5.25	135.50	122.90
7	I	71	SER	CB-CA-C	-5.25	100.08	111.11
2	B	217	ARG	CA-CB-CG	5.25	124.60	114.10
9	K	39	ASP	CA-CB-CG	5.25	117.85	112.60
2	B	172	ILE	CA-CB-CG2	5.25	119.42	110.50
3	C	222	LYS	CA-C-N	-5.25	110.30	121.32
3	C	222	LYS	C-N-CA	-5.25	110.30	121.32
1	A	470	LEU	CA-C-N	-5.25	112.68	121.39
1	A	470	LEU	C-N-CA	-5.25	112.68	121.39
1	A	1077	THR	CA-C-O	-5.25	114.32	120.20
1	A	1383	SER	CB-CA-C	-5.25	99.32	109.76
2	B	1200	ALA	CB-CA-C	-5.25	102.61	110.90
4	E	16	PHE	N-CA-C	-5.25	105.73	111.82
6	H	32	THR	OG1-CB-CG2	-5.25	98.81	109.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	212	LYS	CA-CB-CG	5.25	124.59	114.10
1	A	622	VAL	N-CA-C	-5.25	108.01	113.10
2	B	1217	TYR	CA-C-O	-5.25	114.89	120.92
6	H	2	SER	CA-CB-OG	5.25	121.59	111.10
1	A	1327	ILE	CA-CB-CG2	5.24	119.41	110.50
2	B	178	ASN	N-CA-C	5.24	119.30	113.01
3	C	127	ARG	CA-C-O	-5.24	114.41	120.49
4	E	100	ILE	CA-CB-CG2	-5.24	101.59	110.50
1	A	210	ILE	CA-CB-CG1	5.24	119.31	110.40
2	B	242	SER	CB-CA-C	5.24	118.39	109.53
3	C	228	PHE	N-CA-C	5.24	117.62	108.76
1	A	296	LEU	CA-C-N	5.24	128.68	120.82
1	A	296	LEU	C-N-CA	5.24	128.68	120.82
1	A	883	LEU	CA-C-O	5.24	125.97	120.36
1	A	1423	GLY	N-CA-C	5.24	121.28	112.85
2	B	337	ARG	CB-CG-CD	5.24	123.35	111.30
1	A	1028	THR	N-CA-C	5.24	117.41	111.02
2	B	578	THR	CA-C-O	-5.24	114.57	120.43
2	B	1215	ARG	N-CA-C	5.24	117.26	109.25
3	C	69	LEU	CA-C-O	5.24	125.81	119.11
4	E	122	LYS	CB-CA-C	5.24	120.93	109.99
1	A	412	ARG	CG-CD-NE	-5.23	100.48	112.00
1	A	469	ARG	CA-C-N	5.23	131.12	121.85
1	A	469	ARG	C-N-CA	5.23	131.12	121.85
4	E	7	ARG	CA-C-N	-5.23	111.54	121.54
4	E	7	ARG	C-N-CA	-5.23	111.54	121.54
1	A	656	TRP	CD1-NE1-CE2	-5.23	99.48	108.90
1	A	1418	LEU	N-CA-C	5.23	117.25	107.99
2	B	514	LEU	N-CA-CB	-5.23	101.38	110.17
2	B	132	VAL	N-CA-C	5.23	116.72	109.45
2	B	466	TRP	N-CA-CB	-5.23	101.65	110.49
2	B	573	GLN	CB-CA-C	-5.23	100.76	109.55
3	C	113	VAL	O-C-N	-5.23	117.66	123.20
3	C	199	LYS	N-CA-CB	5.23	119.07	110.39
4	E	31	THR	CB-CA-C	-5.23	100.66	109.50
6	H	142	LEU	CA-CB-CG	-5.23	98.00	116.30
8	J	28	ASP	CA-C-O	-5.23	113.42	119.59
1	A	1385	THR	CA-C-O	5.23	129.69	120.80
2	B	272	THR	N-CA-CB	-5.23	101.74	110.37
1	A	909	ASP	CA-C-O	5.23	127.32	120.16
2	B	658	ILE	CB-CA-C	-5.23	103.79	112.26
1	A	498	ARG	CD-NE-CZ	-5.22	117.08	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	798	TYR	CE1-CZ-CE2	-5.22	109.85	120.30
2	B	848	ARG	NH1-CZ-NH2	5.22	126.09	119.30
9	K	1	MET	CB-CG-SD	-5.22	97.03	112.70
1	A	887	GLY	O-C-N	-5.22	116.54	122.91
2	B	935	ARG	N-CA-CB	5.22	118.13	109.88
4	E	205	SER	N-CA-CB	-5.22	103.67	110.88
1	A	46	THR	OG1-CB-CG2	-5.22	98.86	109.30
1	A	537	ARG	O-C-N	5.22	128.11	122.11
1	A	1005	GLU	N-CA-CB	-5.22	102.19	110.28
1	A	1256	GLU	CA-CB-CG	5.22	124.54	114.10
1	A	1376	THR	CA-CB-CG2	5.22	119.37	110.50
3	C	158	VAL	CA-C-O	-5.22	114.94	120.53
1	A	623	GLY	CA-C-O	-5.22	116.03	122.03
2	B	904	ARG	CG-CD-NE	-5.22	100.52	112.00
3	C	190	ASP	N-CA-CB	-5.22	102.41	110.65
1	A	506	ALA	CA-C-N	5.22	124.50	120.33
1	A	506	ALA	C-N-CA	5.22	124.50	120.33
2	B	335	GLY	CA-C-O	5.22	126.03	120.40
1	A	664	THR	N-CA-C	5.21	117.18	108.99
2	B	1057	LYS	N-CA-C	5.21	121.91	110.80
3	C	191	TYR	CD1-CE1-CZ	-5.21	110.22	119.60
3	C	198	ALA	N-CA-C	5.21	118.80	112.23
2	B	340	ALA	N-CA-CB	-5.21	102.50	110.42
3	C	102	GLN	O-C-N	5.21	129.63	123.27
4	E	177	ARG	NE-CZ-NH2	5.21	123.89	119.20
2	B	331	LEU	CD1-CG-CD2	-5.21	99.34	110.80
2	B	1043	ASP	N-CA-C	-5.21	100.24	108.73
3	C	96	SER	N-CA-CB	-5.21	101.69	110.49
4	E	52	ARG	NE-CZ-NH1	5.21	126.71	121.50
6	H	29	ALA	CA-C-O	-5.21	115.26	121.56
1	A	514	PRO	O-C-N	-5.21	115.06	122.35
2	B	217	ARG	CA-C-O	-5.21	115.45	121.49
2	B	1223	ASP	CA-C-O	-5.21	113.47	119.61
3	C	28	ALA	O-C-N	5.21	128.09	122.15
6	H	47	PHE	CA-C-N	-5.21	113.33	119.84
6	H	47	PHE	C-N-CA	-5.21	113.33	119.84
1	A	65	LEU	CB-CA-C	5.21	120.78	110.42
1	A	364	VAL	CG1-CB-CG2	-5.21	99.35	110.80
1	A	1319	VAL	CA-C-O	-5.21	112.98	119.95
6	H	115	TYR	CA-C-N	-5.21	111.60	121.54
6	H	115	TYR	C-N-CA	-5.21	111.60	121.54
1	A	1438	THR	CA-CB-CG2	5.20	119.34	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	661	LEU	N-CA-C	-5.20	105.29	111.69
2	B	827	ILE	CG1-CB-CG2	-5.20	95.09	110.70
2	B	1075	GLY	CA-C-O	5.20	126.41	121.05
3	C	196	ASP	N-CA-C	5.20	116.80	107.80
2	B	751	VAL	CB-CA-C	-5.20	105.12	112.14
1	A	1167	GLU	O-C-N	5.20	127.44	122.03
2	B	22	SER	N-CA-C	-5.20	106.17	112.88
2	B	109	THR	N-CA-C	5.20	121.88	110.80
2	B	236	HIS	CA-C-O	-5.20	115.67	121.23
9	K	82	ASP	N-CA-C	-5.20	103.22	109.83
1	A	90	VAL	O-C-N	-5.20	117.27	123.04
1	A	1059	HIS	CA-C-O	5.20	123.92	119.66
2	B	278	GLN	CA-C-O	5.20	126.31	120.70
2	B	397	ASP	O-C-N	-5.20	116.08	122.68
4	E	32	GLN	N-CA-C	5.20	117.62	111.33
1	A	712	GLU	CA-C-O	-5.20	115.04	120.55
2	B	597	MET	N-CA-C	5.20	117.35	111.11
2	B	1206	GLU	N-CA-C	-5.20	105.61	111.28
9	K	92	ASN	CA-C-N	-5.20	112.28	120.60
9	K	92	ASN	C-N-CA	-5.20	112.28	120.60
3	C	172	PRO	N-CD-CG	5.20	110.99	103.20
4	E	142	VAL	O-C-N	5.20	128.79	123.18
4	E	33	GLU	CA-CB-CG	5.19	124.49	114.10
10	L	63	ARG	NE-CZ-NH2	5.19	123.88	119.20
2	B	297	ILE	CA-C-N	-5.19	111.85	120.68
2	B	297	ILE	C-N-CA	-5.19	111.85	120.68
4	E	69	ILE	CB-CG1-CD1	-5.19	102.89	113.80
6	H	3	ASN	N-CA-C	5.19	115.09	108.24
1	A	648	ASN	N-CA-CB	-5.19	102.22	110.22
2	B	1025	HIS	CB-CG-CD2	5.19	137.95	131.20
3	C	17	ASN	CB-CA-C	-5.19	99.31	111.09
3	C	157	CYS	CA-C-N	-5.19	116.37	123.12
3	C	157	CYS	C-N-CA	-5.19	116.37	123.12
6	H	136	LYS	CD-CE-NZ	5.19	128.51	111.90
1	A	417	TYR	CA-C-O	-5.19	113.09	120.51
2	B	28	GLU	N-CA-CB	-5.19	101.94	110.14
1	A	247	ARG	N-CA-C	5.19	117.75	108.47
1	A	784	LEU	CD1-CG-CD2	-5.19	99.39	110.80
1	A	1241	ARG	O-C-N	-5.19	117.34	123.25
2	B	1033	LYS	N-CA-C	-5.19	105.52	111.07
3	C	140	ASN	CA-C-O	5.19	125.91	119.79
2	B	367	LEU	CB-CG-CD2	5.19	126.26	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	103	MET	N-CA-CB	-5.19	103.11	110.79
1	A	232	GLU	CA-C-O	5.18	126.01	120.20
1	A	1007	ILE	CA-C-O	5.18	126.12	120.57
2	B	939	THR	N-CA-CB	-5.18	101.56	110.11
3	C	75	MET	CB-CG-SD	5.18	128.25	112.70
4	E	23	VAL	CA-C-O	5.18	126.67	121.17
1	A	264	PHE	CB-CA-C	5.18	120.51	110.46
2	B	260	GLY	CA-C-O	-5.18	117.73	122.24
2	B	578	THR	CA-CB-CG2	-5.18	101.69	110.50
8	J	52	THR	CB-CA-C	-5.18	101.72	110.64
10	L	65	VAL	O-C-N	5.18	128.64	123.10
3	C	105	GLY	N-CA-C	-5.18	100.90	113.18
9	K	56	VAL	CG1-CB-CG2	-5.18	99.41	110.80
1	A	455	MET	CG-SD-CE	-5.18	89.51	100.90
2	B	595	ARG	NH1-CZ-NH2	-5.18	112.57	119.30
5	F	152	ILE	CA-CB-CG1	5.18	119.20	110.40
1	A	217	LYS	N-CA-CB	-5.17	102.23	109.94
1	A	685	GLU	CB-CA-C	5.17	120.94	110.38
1	A	1142	THR	CA-CB-OG1	-5.17	101.84	109.60
2	B	435	THR	OG1-CB-CG2	-5.17	98.95	109.30
2	B	666	TYR	OH-CZ-CE2	-5.17	104.38	119.90
1	A	352	VAL	CA-CB-CG1	5.17	119.19	110.40
1	A	695	LYS	CD-CE-NZ	5.17	128.45	111.90
2	B	1026	LEU	N-CA-C	-5.17	105.72	111.36
1	A	420	ARG	N-CA-CB	5.17	119.20	110.92
1	A	787	PHE	CD1-CG-CD2	-5.17	110.84	118.60
3	C	254	LYS	CD-CE-NZ	-5.17	95.35	111.90
1	A	379	VAL	N-CA-C	-5.17	101.01	108.87
2	B	496	ARG	CA-C-O	5.17	125.78	119.78
7	I	31	THR	N-CA-C	5.17	120.24	113.88
1	A	69	THR	CB-CA-C	5.17	120.70	110.42
1	A	418	SER	CA-C-O	5.17	127.90	120.51
2	B	586	TRP	O-C-N	-5.17	115.79	122.77
2	B	964	VAL	CA-CB-CG2	-5.17	101.61	110.40
5	F	92	ARG	CB-CG-CD	5.17	123.19	111.30
1	A	274	ILE	CA-C-O	-5.17	115.38	120.85
1	A	299	HIS	CA-CB-CG	5.17	118.97	113.80
1	A	421	ALA	N-CA-CB	-5.17	102.53	110.12
2	B	302	CYS	N-CA-C	-5.17	97.44	107.62
3	C	110	THR	N-CA-C	-5.17	101.29	109.76
3	C	159	ALA	CA-C-N	5.17	130.69	121.75
3	C	159	ALA	C-N-CA	5.17	130.69	121.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	20	TYR	N-CA-CB	-5.17	102.73	110.17
8	J	45	CYS	CA-CB-SG	5.17	126.28	114.40
4	E	60	PHE	CA-C-N	-5.17	114.14	122.82
4	E	60	PHE	C-N-CA	-5.17	114.14	122.82
7	I	54	GLU	CG-CD-OE2	-5.17	106.52	118.40
1	A	683	ILE	CG1-CB-CG2	-5.16	95.21	110.70
2	B	51	PHE	N-CA-C	-5.16	105.73	111.36
2	B	1049	ASP	N-CA-CB	5.16	118.24	110.65
3	C	194	GLU	O-C-N	5.16	128.96	122.19
3	C	205	LYS	CA-C-O	-5.16	115.40	120.82
4	E	31	THR	CA-C-O	-5.16	115.19	121.28
1	A	893	PHE	CB-CA-C	-5.16	101.25	110.70
4	E	67	GLU	N-CA-C	-5.16	105.65	111.28
9	K	106	GLU	CB-CA-C	5.16	121.74	110.18
1	A	188	ASP	O-C-N	-5.16	115.73	122.59
1	A	491	VAL	CA-C-O	5.16	122.01	119.12
1	A	1443	VAL	CA-C-O	-5.16	114.84	120.72
2	B	1004	GLU	N-CA-C	5.16	121.79	110.80
2	B	1150	ARG	CA-C-O	5.16	125.89	120.42
4	E	86	PRO	CA-C-N	-5.16	115.45	122.93
4	E	86	PRO	C-N-CA	-5.16	115.45	122.93
1	A	94	GLY	N-CA-C	5.16	125.41	113.18
2	B	270	LYS	N-CA-CB	-5.16	103.26	111.62
2	B	282	ILE	CA-C-N	-5.16	111.84	120.30
2	B	282	ILE	C-N-CA	-5.16	111.84	120.30
2	B	304	ASP	N-CA-CB	5.16	119.21	110.49
1	A	862	ASN	CA-C-O	-5.16	115.89	121.87
4	E	146	HIS	CA-CB-CG	5.16	118.96	113.80
6	H	42	ILE	CA-C-O	-5.16	114.90	120.67
1	A	31	SER	N-CA-C	-5.15	102.85	110.48
1	A	346	ASP	N-CA-CB	5.15	119.26	110.50
1	A	833	GLU	O-C-N	5.15	127.38	122.07
1	A	1029	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	A	385	ILE	N-CA-C	-5.15	104.54	111.44
1	A	516	SER	O-C-N	-5.15	115.29	122.19
1	A	572	TRP	N-CA-CB	-5.15	102.02	110.41
1	A	920	LEU	CA-C-N	-5.15	111.32	121.41
1	A	920	LEU	C-N-CA	-5.15	111.32	121.41
2	B	130	VAL	CA-C-N	5.15	129.65	121.72
2	B	130	VAL	C-N-CA	5.15	129.65	121.72
2	B	276	ILE	CB-CG1-CD1	5.15	124.62	113.80
2	B	289	LEU	CD1-CG-CD2	-5.15	99.47	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	328	GLU	CA-CB-CG	-5.15	103.80	114.10
3	C	223	ALA	O-C-N	5.15	128.72	122.85
1	A	390	GLN	CG-CD-NE2	-5.15	108.68	116.40
2	B	297	ILE	CB-CG1-CD1	-5.15	102.99	113.80
2	B	694	ASP	CA-CB-CG	5.15	117.75	112.60
9	K	6	ARG	CD-NE-CZ	5.15	131.61	124.40
1	A	1130	GLN	CB-CA-C	5.15	120.19	109.95
9	K	38	GLU	N-CA-C	5.15	117.01	109.24
1	A	1171	GLN	CB-CG-CD	5.14	121.34	112.60
2	B	1031	LEU	CA-C-O	-5.14	114.29	120.10
9	K	50	LEU	O-C-N	-5.14	115.75	122.59
1	A	589	GLN	CA-CB-CG	5.14	124.38	114.10
1	A	614	PHE	CA-C-O	-5.14	115.09	121.06
1	A	724	GLU	CB-CG-CD	5.14	121.34	112.60
1	A	998	LEU	O-C-N	5.14	129.21	123.19
3	C	78	GLU	CB-CG-CD	5.14	121.34	112.60
1	A	6	TYR	CA-C-O	-5.14	115.35	121.16
1	A	1018	PHE	CB-CG-CD1	5.14	129.44	120.70
1	A	1219	THR	CB-CA-C	-5.14	100.80	110.67
2	B	293	PRO	O-C-N	5.14	129.27	123.10
2	B	662	MET	CA-C-N	-5.14	111.94	120.68
2	B	662	MET	C-N-CA	-5.14	111.94	120.68
3	C	211	ASP	CA-C-O	5.14	124.97	120.19
1	A	74	MET	O-C-N	5.14	129.43	122.59
8	J	6	ARG	O-C-N	5.14	130.00	123.11
1	A	1324	PRO	CB-CG-CD	5.14	122.54	106.10
2	B	1103	ILE	O-C-N	5.14	128.99	122.57
1	A	82	GLY	O-C-N	-5.14	116.64	122.91
1	A	780	VAL	CA-C-O	5.14	127.16	120.69
1	A	941	LYS	CD-CE-NZ	-5.14	95.46	111.90
2	B	172	ILE	N-CA-CB	-5.14	102.45	111.39
2	B	311	LEU	CA-C-O	5.14	125.88	119.97
2	B	658	ILE	CA-C-N	-5.14	112.50	120.31
2	B	658	ILE	C-N-CA	-5.14	112.50	120.31
1	A	201	VAL	CA-C-N	5.13	129.23	122.30
1	A	201	VAL	C-N-CA	5.13	129.23	122.30
1	A	613	ILE	O-C-N	5.13	125.75	121.85
1	A	966	ASN	CA-C-N	-5.13	111.73	121.54
1	A	966	ASN	C-N-CA	-5.13	111.73	121.54
1	A	1242	VAL	CG1-CB-CG2	-5.13	99.50	110.80
2	B	886	LYS	N-CA-C	5.13	117.77	109.40
6	H	52	GLN	CA-C-O	-5.13	113.17	120.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	87	ARG	N-CA-CB	5.13	119.37	110.44
7	I	118	ARG	CA-C-N	5.13	127.43	120.65
7	I	118	ARG	C-N-CA	5.13	127.43	120.65
1	A	640	GLN	N-CA-C	-5.13	105.77	111.36
2	B	299	GLU	N-CA-C	5.13	118.80	112.54
2	B	97	VAL	O-C-N	5.13	128.74	123.20
2	B	178	ASN	CB-CG-ND2	-5.13	108.70	116.40
2	B	332	ASP	CA-C-N	5.13	127.47	120.54
2	B	332	ASP	C-N-CA	5.13	127.47	120.54
6	H	145	ARG	CB-CG-CD	5.13	123.10	111.30
8	J	10	CYS	CB-CA-C	5.13	118.00	109.38
9	K	64	GLU	CG-CD-OE1	5.13	130.20	118.40
1	A	42	ASP	CB-CG-OD2	5.13	130.20	118.40
1	A	832	ALA	CA-C-N	5.13	127.11	120.44
1	A	832	ALA	C-N-CA	5.13	127.11	120.44
2	B	627	PHE	CB-CA-C	-5.13	100.68	109.65
1	A	413	ILE	CB-CA-C	-5.13	104.76	110.96
1	A	770	VAL	CG1-CB-CG2	-5.13	99.52	110.80
1	A	805	LEU	CD1-CG-CD2	-5.13	99.52	110.80
2	B	213	ILE	N-CA-C	-5.13	101.07	108.71
2	B	547	VAL	CG1-CB-CG2	5.13	122.08	110.80
2	B	1153	GLU	CG-CD-OE1	-5.13	106.61	118.40
3	C	37	MET	CA-C-O	5.13	125.98	120.55
8	J	29	GLU	N-CA-C	5.13	119.48	113.23
1	A	1326	ARG	NH1-CZ-NH2	-5.12	112.64	119.30
2	B	905	VAL	CA-C-O	-5.12	116.62	121.64
2	B	966	VAL	N-CA-CB	-5.12	105.00	111.46
1	A	1330	ASN	CA-C-N	-5.12	114.06	122.26
1	A	1330	ASN	C-N-CA	-5.12	114.06	122.26
2	B	57	TYR	CA-CB-CG	5.12	123.12	113.90
2	B	813	LYS	N-CA-CB	-5.12	104.47	112.41
4	E	73	PRO	CB-CA-C	5.12	120.01	111.56
1	A	1191	TRP	CA-C-O	5.12	126.33	120.54
1	A	1277	GLU	N-CA-CB	5.12	117.57	110.04
1	A	1327	ILE	CA-C-O	-5.12	115.29	121.28
2	B	289	LEU	CA-C-O	5.12	125.83	119.12
2	B	327	ARG	N-CA-CB	-5.12	102.33	110.22
3	C	7	GLN	CB-CA-C	-5.12	100.00	109.37
6	H	111	LEU	N-CA-C	5.12	118.46	110.32
7	I	12	ASN	N-CA-C	-5.12	102.20	110.14
1	A	589	GLN	OE1-CD-NE2	5.12	127.72	122.60
2	B	863	GLU	CB-CG-CD	5.12	121.31	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	706	GLN	CB-CA-C	-5.12	101.51	109.55
2	B	837	ASP	CA-C-O	5.12	127.64	121.65
2	B	1222	ARG	N-CA-C	5.12	121.70	110.80
3	C	246	ARG	CA-C-O	5.12	125.86	119.97
2	B	20	ASP	N-CA-CB	5.12	117.79	110.06
4	E	131	THR	CA-CB-CG2	5.12	119.20	110.50
1	A	44	THR	N-CA-CB	5.12	119.14	110.49
1	A	152	VAL	O-C-N	5.12	126.93	121.10
1	A	925	LEU	CB-CG-CD1	-5.12	95.35	110.70
1	A	1124	HIS	CA-C-N	-5.12	111.60	121.58
1	A	1124	HIS	C-N-CA	-5.12	111.60	121.58
1	A	1280	GLU	CG-CD-OE1	-5.12	106.63	118.40
2	B	588	GLY	N-CA-C	-5.12	101.06	113.18
2	B	943	SER	N-CA-C	5.12	121.70	110.80
3	C	255	VAL	CA-C-N	-5.12	111.98	120.68
3	C	255	VAL	C-N-CA	-5.12	111.98	120.68
7	I	11	ASN	CB-CA-C	-5.12	104.47	111.73
1	A	811	GLN	CG-CD-OE1	5.11	131.03	120.80
6	H	40	LEU	N-CA-C	5.11	116.29	108.52
2	B	567	GLU	CB-CG-CD	5.11	121.29	112.60
2	B	1051	THR	CA-CB-CG2	5.11	119.19	110.50
2	B	644	GLU	N-CA-C	5.11	121.68	110.80
2	B	649	LYS	N-CA-C	-5.11	102.92	110.48
9	K	45	LEU	O-C-N	5.11	128.35	122.17
1	A	1135	ARG	CD-NE-CZ	5.11	131.55	124.40
2	B	400	HIS	CA-C-N	-5.11	111.07	121.18
2	B	400	HIS	C-N-CA	-5.11	111.07	121.18
2	B	499	ASN	N-CA-CB	-5.11	102.02	111.52
2	B	1025	HIS	CB-CA-C	-5.11	102.00	110.68
10	L	60	ARG	CA-CB-CG	5.11	124.32	114.10
1	A	1294	PRO	CB-CA-C	5.11	120.18	112.21
3	C	111	THR	CA-CB-CG2	-5.11	101.82	110.50
5	F	89	GLU	CA-C-O	5.11	126.16	120.90
7	I	119	THR	OG1-CB-CG2	5.11	119.51	109.30
1	A	526	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	894	GLU	CA-CB-CG	5.10	124.31	114.10
2	B	389	ALA	N-CA-CB	-5.10	102.36	110.22
1	A	369	SER	N-CA-C	5.10	117.58	111.71
2	B	486	TYR	CB-CA-C	-5.10	102.87	110.88
9	K	23	PRO	CA-C-N	-5.10	115.05	122.65
9	K	23	PRO	C-N-CA	-5.10	115.05	122.65
6	H	58	THR	N-CA-C	5.10	117.02	107.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	161	LEU	N-CA-CB	5.10	118.70	111.05
1	A	456	MET	N-CA-CB	-5.10	103.40	111.05
1	A	1307	GLU	N-CA-C	5.10	117.38	108.76
6	H	43	ASN	O-C-N	-5.10	115.54	122.48
6	H	90	ALA	CA-C-O	5.10	127.80	120.51
1	A	956	LEU	O-C-N	-5.10	117.93	121.65
1	A	988	LEU	CA-C-O	5.10	125.65	119.38
1	A	1109	LYS	CG-CD-CE	5.10	123.02	111.30
1	A	1336	MET	N-CA-C	-5.10	105.91	111.82
3	C	267	GLN	CA-C-O	5.10	127.54	119.13
9	K	84	LYS	N-CA-C	-5.10	106.16	112.38
10	L	61	THR	O-C-N	5.10	128.72	122.75
1	A	920	LEU	N-CA-C	-5.09	102.84	110.23
1	A	53	LEU	CB-CG-CD1	5.09	125.98	110.70
1	A	416	ARG	CA-CB-CG	5.09	124.28	114.10
4	E	33	GLU	N-CA-C	-5.09	107.02	113.18
1	A	516	SER	CA-C-O	5.09	126.53	120.53
1	A	1075	PRO	CA-C-O	-5.09	112.09	118.86
1	A	1192	LEU	CB-CG-CD1	-5.09	95.43	110.70
6	H	82	PRO	CA-C-O	-5.09	111.34	120.60
9	K	94	ILE	N-CA-CB	5.09	116.75	110.64
10	L	65	VAL	N-CA-C	5.09	116.04	108.46
1	A	884	ASP	CB-CG-OD2	5.09	130.10	118.40
1	A	286	HIS	O-C-N	-5.09	115.83	122.59
1	A	465	TYR	CA-C-N	-5.09	113.81	122.56
1	A	465	TYR	C-N-CA	-5.09	113.81	122.56
1	A	881	GLN	CB-CG-CD	5.09	121.25	112.60
3	C	24	ASN	CA-C-N	5.09	130.14	123.17
3	C	24	ASN	C-N-CA	5.09	130.14	123.17
3	C	68	GLY	CA-C-N	-5.08	111.66	121.58
3	C	68	GLY	C-N-CA	-5.08	111.66	121.58
1	A	189	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	A	1202	MET	CG-SD-CE	5.08	112.08	100.90
8	J	25	LEU	CD1-CG-CD2	5.08	121.98	110.80
6	H	51	ALA	O-C-N	5.08	128.69	122.75
6	H	77	ARG	CA-C-N	5.08	131.25	121.54
6	H	77	ARG	C-N-CA	5.08	131.25	121.54
2	B	735	ALA	N-CA-C	5.08	116.59	107.80
2	B	1128	LEU	N-CA-C	5.08	121.61	110.80
7	I	49	ILE	O-C-N	-5.08	115.51	122.62
1	A	449	SER	O-C-N	-5.08	116.42	122.46
1	A	439	ASN	CA-C-O	5.07	128.81	119.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	40	GLU	O-C-N	5.07	128.83	122.23
2	B	165	VAL	CA-C-N	5.07	128.07	120.87
2	B	165	VAL	C-N-CA	5.07	128.07	120.87
2	B	832	GLY	N-CA-C	-5.07	108.12	115.27
4	E	183	PRO	CA-C-N	-5.07	112.96	120.82
4	E	183	PRO	C-N-CA	-5.07	112.96	120.82
4	E	158	SER	CA-C-O	5.07	125.62	119.38
6	H	141	TYR	N-CA-C	5.07	117.40	110.55
1	A	147	VAL	CB-CA-C	-5.07	102.69	110.50
1	A	957	PRO	CA-C-N	5.07	131.10	121.97
1	A	957	PRO	C-N-CA	5.07	131.10	121.97
3	C	88	CYS	CA-CB-SG	5.07	126.06	114.40
3	C	134	ILE	CB-CG1-CD1	5.07	124.45	113.80
4	E	116	ILE	CB-CA-C	5.07	119.61	111.29
6	H	102	TYR	CA-CB-CG	5.07	123.03	113.90
1	A	607	ILE	CB-CA-C	-5.07	101.73	110.65
4	E	54	GLN	CB-CG-CD	5.07	121.22	112.60
4	E	178	ILE	CA-C-N	-5.07	110.67	121.32
4	E	178	ILE	C-N-CA	-5.07	110.67	121.32
1	A	227	VAL	CA-C-O	5.07	125.06	120.30
1	A	946	VAL	CA-CB-CG2	-5.07	101.79	110.40
1	A	1005	GLU	CG-CD-OE1	5.07	130.05	118.40
6	H	77	ARG	CA-CB-CG	5.07	124.23	114.10
10	L	41	SER	N-CA-CB	5.07	119.06	110.49
1	A	394	ASN	N-CA-C	5.07	118.72	112.54
2	B	618	ASP	CA-C-O	-5.07	115.04	120.46
2	B	776	GLN	CA-C-N	-5.07	113.91	122.67
2	B	776	GLN	C-N-CA	-5.07	113.91	122.67
2	B	789	MET	CG-SD-CE	-5.07	89.75	100.90
2	B	264	SER	N-CA-C	-5.06	100.01	110.80
4	E	208	TYR	CE1-CZ-CE2	-5.06	110.17	120.30
1	A	18	GLN	O-C-N	5.06	129.14	123.27
1	A	679	ILE	N-CA-C	-5.06	105.56	110.42
1	A	1235	LYS	CG-CD-CE	5.06	122.94	111.30
3	C	34	ARG	CA-CB-CG	5.06	124.22	114.10
3	C	263	THR	CA-CB-OG1	-5.06	102.01	109.60
1	A	707	GLY	N-CA-C	-5.06	101.19	113.18
2	B	686	ASN	N-CA-CB	-5.06	102.44	110.28
10	L	28	LYS	CD-CE-NZ	5.06	128.09	111.90
1	A	154	SER	CB-CA-C	5.06	122.99	111.71
1	A	392	VAL	CA-CB-CG1	-5.06	101.80	110.40
1	A	633	VAL	N-CA-C	-5.06	104.96	112.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	623	GLU	O-C-N	-5.06	117.02	123.24
5	F	152	ILE	CA-C-O	-5.06	115.27	121.04
7	I	111	THR	CA-C-O	-5.06	115.71	121.68
1	A	724	GLU	CA-C-N	-5.06	113.11	120.29
1	A	724	GLU	C-N-CA	-5.06	113.11	120.29
5	F	112	GLU	CA-C-O	-5.06	113.28	120.51
1	A	77	CYS	CB-CA-C	-5.06	102.10	109.38
4	E	177	ARG	CD-NE-CZ	-5.06	117.32	124.40
1	A	1104	ILE	N-CA-C	-5.05	105.67	110.42
2	B	1052	VAL	CA-C-N	-5.05	113.11	120.29
2	B	1052	VAL	C-N-CA	-5.05	113.11	120.29
1	A	437	MET	CB-CA-C	-5.05	99.62	111.09
6	H	104	PHE	CA-C-O	5.05	127.73	120.51
6	H	128	ASN	N-CA-C	5.05	121.56	110.80
9	K	95	ILE	CA-CB-CG1	-5.05	101.81	110.40
10	L	64	LEU	CB-CG-CD1	5.05	125.86	110.70
4	E	195	VAL	CG1-CB-CG2	-5.05	99.69	110.80
9	K	74	ARG	NE-CZ-NH1	-5.05	116.45	121.50
9	K	110	ASN	CA-C-N	-5.05	111.89	121.54
9	K	110	ASN	C-N-CA	-5.05	111.89	121.54
1	A	801	GLU	CG-CD-OE1	-5.05	106.79	118.40
1	A	1338	VAL	N-CA-C	5.05	116.15	111.81
2	B	625	LYS	CA-C-N	-5.05	114.66	122.69
2	B	625	LYS	C-N-CA	-5.05	114.66	122.69
2	B	754	SER	CA-C-O	5.05	126.99	118.91
2	B	983	ARG	CG-CD-NE	-5.05	100.89	112.00
6	H	42	ILE	N-CA-CB	-5.05	103.16	111.44
7	I	13	MET	CG-SD-CE	-5.05	89.79	100.90
1	A	399	HIS	CA-C-O	-5.05	116.06	120.60
1	A	1006	ILE	CB-CG1-CD1	5.05	124.40	113.80
1	A	1031	VAL	CB-CA-C	-5.05	100.31	111.77
1	A	438	ASP	CA-C-N	5.05	133.80	124.82
1	A	438	ASP	C-N-CA	5.05	133.80	124.82
1	A	443	LEU	N-CA-C	-5.05	101.46	109.59
2	B	385	LEU	CD1-CG-CD2	-5.05	99.70	110.80
2	B	635	ARG	CB-CA-C	-5.04	104.61	110.76
4	E	130	ALA	O-C-N	5.04	129.04	122.89
2	B	316	PRO	CA-CB-CG	-5.04	94.92	104.50
3	C	256	ALA	CA-C-O	-5.04	113.84	119.79
8	J	4	PRO	CB-CA-C	-5.04	104.37	110.98
1	A	41	MET	CB-CG-SD	5.04	127.83	112.70
1	A	641	VAL	N-CA-CB	-5.04	103.02	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	909	ASP	O-C-N	-5.04	115.52	121.32
1	A	1055	ARG	CA-CB-CG	5.04	124.18	114.10
2	B	65	GLU	N-CA-CB	5.04	117.11	110.25
2	B	192	LEU	N-CA-C	5.04	119.15	113.15
5	F	149	GLU	CA-C-O	5.04	126.08	120.63
2	B	816	GLU	N-CA-CB	-5.04	102.77	110.33
2	B	1013	ASN	CB-CA-C	5.04	115.69	108.68
2	B	108	VAL	N-CA-C	5.04	119.82	109.34
2	B	515	HIS	CB-CG-ND1	-5.04	115.14	122.70
2	B	119	LEU	N-CA-CB	-5.04	102.72	110.12
1	A	362	ASP	O-C-N	-5.04	115.89	122.39
1	A	739	ASP	O-C-N	-5.04	115.73	122.43
1	A	865	GLN	O-C-N	-5.04	117.43	123.27
2	B	235	SER	N-CA-CB	5.04	117.67	110.67
3	C	21	ILE	N-CA-C	-5.04	100.82	108.17
7	I	24	ARG	CA-C-N	-5.04	115.50	122.30
7	I	24	ARG	C-N-CA	-5.04	115.50	122.30
9	K	91	CYS	O-C-N	-5.04	116.32	122.11
1	A	527	THR	CA-C-O	5.03	125.57	119.38
3	C	129	ILE	N-CA-C	5.03	116.24	108.44
9	K	89	ASN	N-CA-C	-5.03	105.92	111.71
1	A	948	VAL	CA-C-O	5.03	126.12	120.03
2	B	232	SER	N-CA-C	-5.03	103.69	109.93
2	B	65	GLU	CA-C-O	-5.03	116.73	122.01
2	B	741	CYS	CA-CB-SG	5.03	125.97	114.40
2	B	802	PRO	N-CD-CG	5.03	110.75	103.20
7	I	114	GLN	N-CA-C	5.03	119.05	113.01
1	A	649	ILE	O-C-N	-5.03	116.65	121.83
1	A	1029	ARG	CB-CA-C	-5.03	101.33	110.63
2	B	453	ILE	CA-C-O	-5.03	114.51	121.15
1	A	140	THR	CA-C-O	5.03	125.78	120.10
7	I	118	ARG	CD-NE-CZ	5.03	131.44	124.40
1	A	76	GLU	O-C-N	5.03	128.23	122.25
1	A	152	VAL	CA-CB-CG1	5.03	118.94	110.40
1	A	1207	LEU	CA-C-O	5.03	125.79	120.36
7	I	55	THR	OG1-CB-CG2	5.03	119.35	109.30
10	L	48	CYS	CB-CA-C	5.03	120.42	110.42
3	C	170	TRP	CE2-CD2-CE3	-5.02	113.78	118.80
4	E	211	TYR	CA-C-O	-5.02	114.57	120.60
1	A	90	VAL	N-CA-C	-5.02	100.66	108.95
1	A	434	ARG	CD-NE-CZ	5.02	131.43	124.40
1	A	621	THR	O-C-N	-5.02	116.42	122.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1274	ARG	CB-CA-C	-5.02	98.88	109.38
1	A	1422	ARG	N-CA-C	-5.02	106.57	113.30
2	B	30	SER	CB-CA-C	-5.02	102.45	110.79
2	B	876	LYS	CA-C-O	-5.02	113.28	120.16
2	B	1052	VAL	N-CA-CB	-5.02	101.68	110.77
2	B	1058	LEU	CA-C-N	-5.02	112.14	120.68
2	B	1058	LEU	C-N-CA	-5.02	112.14	120.68
2	B	1106	ARG	CG-CD-NE	5.02	123.05	112.00
2	B	1159	ARG	NE-CZ-NH1	5.02	126.52	121.50
1	A	896	ARG	CA-C-O	-5.02	114.67	120.24
1	A	987	VAL	CA-CB-CG2	-5.02	101.86	110.40
6	H	11	GLN	N-CA-C	-5.02	99.08	108.02
1	A	430	TRP	O-C-N	5.02	128.57	122.85
2	B	62	ILE	CA-C-N	5.02	129.24	120.86
2	B	62	ILE	C-N-CA	5.02	129.24	120.86
2	B	100	PRO	CA-N-CD	-5.02	104.97	112.00
3	C	156	THR	CA-CB-CG2	-5.02	101.97	110.50
3	C	264	GLN	N-CA-C	5.02	119.12	113.15
4	E	184	VAL	N-CA-C	-5.02	105.27	112.35
1	A	496	GLU	N-CA-C	-5.02	105.89	111.36
2	B	788	ARG	NE-CZ-NH1	5.02	126.52	121.50
6	H	82	PRO	CB-CA-C	5.02	119.84	111.56
1	A	52	GLY	CA-C-O	-5.02	111.84	120.57
1	A	168	GLY	N-CA-C	5.02	121.05	115.08
2	B	1100	ASP	N-CA-C	-5.02	105.28	111.40
1	A	203	SER	N-CA-C	-5.01	103.06	110.48
1	A	681	GLU	CB-CG-CD	5.01	121.12	112.60
1	A	770	VAL	CA-CB-CG1	-5.01	101.88	110.40
1	A	1034	GLU	CB-CG-CD	5.01	121.13	112.60
2	B	388	CYS	O-C-N	-5.01	115.24	122.36
2	B	1026	LEU	CB-CA-C	5.01	119.37	110.85
1	A	1343	ALA	N-CA-C	-5.01	105.33	111.75
9	K	85	ASP	CA-C-N	-5.01	112.37	121.14
9	K	85	ASP	C-N-CA	-5.01	112.37	121.14
1	A	123	ARG	CD-NE-CZ	5.01	131.42	124.40
1	A	418	SER	N-CA-CB	5.01	118.96	110.49
1	A	777	PHE	CA-CB-CG	5.01	118.81	113.80
1	A	825	ILE	CB-CA-C	-5.01	105.53	112.24
1	A	965	GLN	OE1-CD-NE2	5.01	127.61	122.60
1	A	1013	ASP	CA-CB-CG	5.01	117.61	112.60
2	B	581	PHE	CA-C-N	-5.01	115.48	122.75
2	B	581	PHE	C-N-CA	-5.01	115.48	122.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1011	ILE	CB-CA-C	-5.01	103.65	110.42
4	E	75	MET	CG-SD-CE	-5.01	89.88	100.90
4	E	166	LYS	O-C-N	5.01	127.50	122.09
4	E	196	VAL	CG1-CB-CG2	-5.01	99.77	110.80
1	A	1425	SER	N-CA-C	5.01	116.43	110.97
1	A	145	LYS	CA-C-O	-5.01	114.82	120.43
1	A	838	GLN	CB-CG-CD	-5.01	104.09	112.60
2	B	1091	TYR	N-CA-C	-5.01	101.08	109.24
3	C	77	ILE	CA-C-O	-5.01	114.20	118.96
7	I	105	SER	CA-C-O	-5.01	113.72	119.78
1	A	242	PRO	CB-CA-C	-5.01	104.81	110.92
2	B	792	MET	N-CA-CB	-5.01	102.22	111.53
6	H	97	MET	CA-C-O	-5.01	115.37	121.78
1	A	174	ILE	N-CA-CB	-5.00	104.50	111.41
1	A	220	THR	O-C-N	5.00	127.49	122.09
1	A	1028	THR	OG1-CB-CG2	-5.00	99.29	109.30
1	A	1297	GLU	N-CA-CB	-5.00	103.20	110.36
1	A	1317	MET	N-CA-C	-5.00	106.28	112.38
5	F	93	ILE	CA-CB-CG1	-5.00	101.89	110.40
6	H	131	ASN	CA-C-N	5.00	131.10	121.54
6	H	131	ASN	C-N-CA	5.00	131.10	121.54
1	A	1201	ALA	N-CA-C	5.00	118.15	111.75
2	B	223	VAL	CA-C-O	-5.00	115.06	120.71
2	B	451	LYS	CA-C-O	-5.00	113.36	120.51
2	B	879	ARG	CB-CA-C	-5.00	100.47	110.42
3	C	138	GLU	CA-C-O	5.00	125.20	119.35
4	E	88	VAL	CB-CA-C	5.00	118.14	111.19

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10606	0	10668	1112	0
2	B	8690	0	8714	954	0
3	C	2095	0	2054	240	0
4	E	1760	0	1788	230	0
5	F	670	0	690	61	0
6	H	1068	0	1040	233	0
7	I	990	0	948	102	0
8	J	525	0	538	63	0
9	K	919	0	929	114	0
10	L	364	0	387	92	0
11	A	2	0	0	0	0
12	A	2	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
14	B	1	0	0	0	0
All	All	27728	0	27765	3057	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 55.

All (3057) 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:CB	2:B:137:TYR:CG	1.77	1.66
9:K:26:LYS:CD	9:K:26:LYS:CE	1.74	1.66
1:A:1225:PHE:CB	1:A:1225:PHE:CG	1.78	1.65
1:A:977:LYS:CG	1:A:977:LYS:CD	1.74	1.64
2:B:884:ARG:CD	2:B:884:ARG:CG	1.75	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:CD2	1:A:860:LEU:CG	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:CG	5:F:135:ARG:CD	1.74	1.63
2:B:228:LYS:CG	2:B:228:LYS:CB	1.75	1.62
2:B:368:GLU:CB	2:B:368:GLU:CA	1.75	1.62
1:A:191:THR:CB	1:A:191:THR:CG2	1.76	1.62
1:A:720:ARG:CG	1:A:720:ARG:CD	1.77	1.62
2:B:423:LYS:CD	2:B:423:LYS:CE	1.76	1.62
2:B:266:ALA:CA	2:B:266:ALA:CB	1.76	1.62
2:B:423:LYS:CD	2:B:423:LYS:CG	1.77	1.62
2:B:1172:ILE:CB	2:B:1172:ILE:CG2	1.76	1.62
4:E:1:MET:CG	4:E:1:MET:CB	1.75	1.62
1:A:132:LYS:CG	1:A:132:LYS:CD	1.77	1.62
1:A:895:LYS:CG	1:A:895:LYS:CD	1.77	1.62
1:A:1238:ILE:CB	1:A:1238:ILE:CG2	1.78	1.62
4:E:45:LYS:CG	4:E:45:LYS:CD	1.75	1.62
1:A:1080:THR:CA	1:A:1080:THR:CB	1.76	1.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:LYS:CD	2:B:227:LYS:CE	1.77	1.61
2:B:426:LYS:CD	2:B:426:LYS:CE	1.78	1.61
6:H:11:GLN:CB	6:H:11:GLN:CG	1.78	1.61
9:K:56:VAL:CA	9:K:56:VAL:CB	1.74	1.61
1:A:1162:VAL:CG1	1:A:1162:VAL:CB	1.77	1.61
2:B:646:LEU:CB	2:B:646:LEU:CG	1.74	1.61
2:B:1058:LEU:CD1	2:B:1058:LEU:CG	1.76	1.61
2:B:1163:CYS:CA	2:B:1163:CYS:CB	1.74	1.61
3:C:94:LYS:CB	3:C:94:LYS:CG	1.74	1.61
1:A:1159:ARG:CB	1:A:1159:ARG:CG	1.74	1.61
2:B:328:GLU:CB	2:B:328:GLU:CG	1.79	1.61
4:E:118:PRO:CG	4:E:118:PRO:CD	1.78	1.61
5:F:80:ALA:CB	5:F:80:ALA:CA	1.77	1.61
10:L:43:THR:CA	10:L:43:THR:CB	1.76	1.61
1:A:393:ARG:CG	1:A:393:ARG:CD	1.76	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:137:LYS:CE	3:C:137:LYS:CD	1.78	1.61
3:C:199:LYS:CD	3:C:199:LYS:CE	1.77	1.61
10:L:65:VAL:CB	10:L:65:VAL:CG2	1.74	1.61
1:A:412:ARG:CD	1:A:412:ARG:CG	1.76	1.60
1:A:1450:LEU:CD1	1:A:1450:LEU:CG	1.76	1.60
2:B:1183:LYS:CG	2:B:1183:LYS:CD	1.79	1.60
3:C:263:THR:CB	3:C:263:THR:CG2	1.79	1.60
4:E:213:ILE:CG1	4:E:213:ILE:CD1	1.80	1.60
2:B:358:LYS:CB	2:B:358:LYS:CG	1.78	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
1:A:1148:ILE:CG1	1:A:1148:ILE:CD1	1.76	1.60
2:B:191:LYS:CG	2:B:191:LYS:CD	1.77	1.60
2:B:367:LEU:CD1	2:B:367:LEU:CG	1.75	1.60
7:I:109:ILE:CG1	7:I:109:ILE:CD1	1.76	1.60
2:B:435:THR:C	2:B:435:THR:CA	1.74	1.60
7:I:117:LYS:CE	7:I:117:LYS:CD	1.75	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:66:LYS:CB	1:A:66:LYS:CG	1.75	1.60
2:B:458:LYS:CD	2:B:458:LYS:CE	1.76	1.60
2:B:620:ARG:CG	2:B:620:ARG:CB	1.77	1.60
2:B:1101:ASP:CA	2:B:1101:ASP:C	1.75	1.60
4:E:44:ALA:CB	4:E:44:ALA:CA	1.77	1.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:8:ARG:CB	7:I:8:ARG:CG	1.76	1.60
1:A:44:THR:CB	1:A:44:THR:CG2	1.79	1.59
1:A:1144:LYS:CD	1:A:1144:LYS:CE	1.79	1.59
2:B:110:HIS:C	2:B:110:HIS:CA	1.75	1.59
1:A:271:LYS:CD	1:A:271:LYS:CG	1.79	1.59
2:B:345:LYS:CD	2:B:345:LYS:CE	1.79	1.59
3:C:156:THR:CB	3:C:156:THR:CG2	1.76	1.59
3:C:205:LYS:CG	3:C:205:LYS:CD	1.78	1.59
2:B:192:LEU:CD2	2:B:192:LEU:CG	1.80	1.59
2:B:446:LEU:CD2	2:B:446:LEU:CG	1.75	1.59
4:E:57:MET:CB	4:E:57:MET:CG	1.76	1.59
4:E:91:LYS:CA	4:E:91:LYS:CB	1.74	1.59
1:A:427:GLN:CB	1:A:427:GLN:CG	1.76	1.59
1:A:1003:LYS:CG	1:A:1003:LYS:CD	1.78	1.59
1:A:1080:THR:CA	1:A:1080:THR:C	1.74	1.59
1:A:1204:ASP:CB	1:A:1204:ASP:CG	1.75	1.59
2:B:1148:LYS:CD	2:B:1148:LYS:CE	1.77	1.59
4:E:66:GLU:CA	4:E:66:GLU:CB	1.75	1.59
4:E:98:ILE:CG1	4:E:98:ILE:CD1	1.76	1.59
9:K:88:LYS:CD	9:K:88:LYS:CE	1.79	1.59
2:B:245:GLU:CA	2:B:245:GLU:C	1.75	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:110:ASN:CB	9:K:110:ASN:CG	1.75	1.59
1:A:176:LYS:CG	1:A:176:LYS:CD	1.80	1.58
1:A:705:LYS:CA	1:A:705:LYS:CB	1.76	1.58
1:A:1112:LYS:CG	1:A:1112:LYS:CD	1.79	1.58
2:B:193:LYS:CD	2:B:193:LYS:CE	1.77	1.58
2:B:958:GLN:CG	2:B:958:GLN:CD	1.74	1.58
3:C:154:LYS:CB	3:C:154:LYS:CG	1.77	1.58
5:F:129:LYS:CG	5:F:129:LYS:CD	1.75	1.58
9:K:26:LYS:CB	9:K:26:LYS:CG	1.75	1.58
10:L:30:ILE:CD1	10:L:30:ILE:CG1	1.81	1.58
1:A:326:ARG:CG	1:A:326:ARG:CD	1.80	1.58
1:A:1109:LYS:CB	1:A:1109:LYS:CG	1.81	1.58
1:A:1144:LYS:CD	1:A:1144:LYS:CG	1.81	1.58
4:E:7:ARG:CG	4:E:7:ARG:CD	1.74	1.58
1:A:596:THR:CB	1:A:596:THR:CG2	1.77	1.58
1:A:705:LYS:CG	1:A:705:LYS:CD	1.76	1.58
1:A:1164:PRO:CB	1:A:1164:PRO:CG	1.75	1.58
1:A:1385:THR:CA	1:A:1385:THR:C	1.75	1.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:PHE:CA	2:B:18:PHE:CB	1.74	1.58
2:B:94:LYS:CB	2:B:94:LYS:CG	1.74	1.58
2:B:1097:HIS:CB	2:B:1097:HIS:CA	1.77	1.58
2:B:1183:LYS:CD	2:B:1183:LYS:CE	1.76	1.58
4:E:7:ARG:CG	4:E:7:ARG:CB	1.81	1.58
6:H:51:ALA:CA	6:H:51:ALA:CB	1.75	1.58
7:I:118:ARG:CG	7:I:118:ARG:CD	1.74	1.58
1:A:291:GLU:CD	1:A:291:GLU:CG	1.76	1.58
1:A:469:ARG:CD	1:A:469:ARG:CG	1.82	1.58
1:A:934:LYS:CG	1:A:934:LYS:CD	1.76	1.58
1:A:1112:LYS:CG	1:A:1112:LYS:CB	1.75	1.58
1:A:1221:LYS:CG	1:A:1221:LYS:CD	1.82	1.58
2:B:99:LYS:CD	2:B:99:LYS:CE	1.75	1.58
2:B:1155:SER:CB	2:B:1155:SER:CA	1.81	1.58
4:E:94:LYS:CD	4:E:94:LYS:CG	1.81	1.58
6:H:32:THR:CA	6:H:32:THR:CB	1.77	1.58
6:H:41:ASP:CB	6:H:41:ASP:CG	1.76	1.58
6:H:87:ARG:CG	6:H:87:ARG:CD	1.79	1.58
6:H:131:ASN:C	6:H:131:ASN:CA	1.74	1.58
1:A:601:LYS:CG	1:A:601:LYS:CD	1.76	1.58
2:B:231:PRO:CB	2:B:231:PRO:CG	1.79	1.58
2:B:249:ARG:CD	2:B:249:ARG:CG	1.79	1.58
9:K:88:LYS:CD	9:K:88:LYS:CG	1.82	1.58
1:A:71:GLN:CG	1:A:71:GLN:CD	1.75	1.57
1:A:838:GLN:CB	1:A:838:GLN:CG	1.76	1.57
1:A:1187:GLN:CB	1:A:1187:GLN:CG	1.80	1.57
2:B:25:ILE:CB	2:B:25:ILE:CG2	1.82	1.57
2:B:1189:ILE:CB	2:B:1189:ILE:CG2	1.79	1.57
7:I:3:THR:CB	7:I:3:THR:CG2	1.77	1.57
1:A:177:ASP:CB	1:A:177:ASP:CG	1.77	1.57
1:A:931:GLU:CG	1:A:931:GLU:CD	1.75	1.57
1:A:1262:LYS:CB	1:A:1262:LYS:CG	1.76	1.57
2:B:227:LYS:CD	2:B:227:LYS:CG	1.82	1.57
9:K:26:LYS:CD	9:K:26:LYS:CG	1.79	1.57
1:A:53:LEU:CD1	1:A:53:LEU:CG	1.78	1.57
1:A:143:LYS:CG	1:A:143:LYS:CD	1.75	1.57
1:A:1092:LYS:CG	1:A:1092:LYS:CD	1.76	1.57
6:H:131:ASN:CA	6:H:131:ASN:CB	1.79	1.57
10:L:26:THR:CB	10:L:26:THR:CG2	1.80	1.57
1:A:46:THR:CA	1:A:46:THR:CB	1.77	1.57
1:A:180:LYS:CB	1:A:180:LYS:CG	1.77	1.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:807:ARG:CB	2:B:807:ARG:CG	1.77	1.57
2:B:1057:LYS:CD	2:B:1057:LYS:CG	1.77	1.57
4:E:20:LYS:CD	4:E:20:LYS:CE	1.76	1.57
4:E:207:ARG:CD	4:E:207:ARG:CG	1.74	1.57
6:H:135:LEU:CD2	6:H:135:LEU:CG	1.76	1.57
1:A:827:THR:CG2	1:A:827:THR:CB	1.76	1.57
1:A:1012:ARG:CG	1:A:1012:ARG:CD	1.83	1.57
1:A:1092:LYS:CG	1:A:1092:LYS:CB	1.78	1.57
7:I:30:ARG:CG	7:I:30:ARG:CD	1.76	1.57
8:J:43:ARG:CG	8:J:43:ARG:CD	1.79	1.57
1:A:633:VAL:CB	1:A:633:VAL:CG2	1.78	1.56
1:A:1081:LEU:CD2	1:A:1081:LEU:CG	1.77	1.56
1:A:1272:THR:CG2	1:A:1272:THR:CB	1.75	1.56
1:A:1445:ILE:CG1	1:A:1445:ILE:CD1	1.83	1.56
2:B:801:LYS:CD	2:B:801:LYS:CG	1.76	1.56
3:C:120:ILE:CG1	3:C:120:ILE:CD1	1.79	1.56
4:E:47:CYS:CA	4:E:47:CYS:C	1.75	1.56
10:L:25:ALA:CA	10:L:25:ALA:CB	1.75	1.56
1:A:187:LYS:CA	1:A:187:LYS:C	1.76	1.56
1:A:1093:LYS:CG	1:A:1093:LYS:CD	1.82	1.56
2:B:164:LYS:CD	2:B:164:LYS:CG	1.77	1.56
2:B:228:LYS:CD	2:B:228:LYS:CE	1.77	1.56
2:B:344:LYS:CD	2:B:344:LYS:CG	1.78	1.56
2:B:958:GLN:CG	2:B:958:GLN:CB	1.83	1.56
2:B:1102:LYS:CB	2:B:1102:LYS:CG	1.78	1.56
10:L:40:LEU:CD2	10:L:40:LEU:CG	1.78	1.56
1:A:217:LYS:CE	1:A:217:LYS:CD	1.83	1.56
1:A:567:LYS:CD	1:A:567:LYS:CE	1.75	1.56
1:A:1206:ASP:CG	1:A:1206:ASP:CB	1.77	1.56
2:B:871:THR:CA	2:B:871:THR:CB	1.77	1.56
2:B:880:THR:CB	2:B:880:THR:CG2	1.77	1.56
2:B:935:ARG:CG	2:B:935:ARG:CD	1.81	1.56
3:C:84:ARG:CG	3:C:84:ARG:CB	1.82	1.56
3:C:260:LEU:CD2	3:C:260:LEU:CG	1.81	1.56
4:E:66:GLU:CD	4:E:66:GLU:CG	1.77	1.56
4:E:71:LYS:CB	4:E:71:LYS:CG	1.74	1.56
7:I:1:MET:CB	7:I:1:MET:CG	1.84	1.56
10:L:40:LEU:CG	10:L:40:LEU:CB	1.77	1.56
1:A:34:LYS:CG	1:A:34:LYS:CD	1.80	1.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASP:CB	1:A:188:ASP:CG	1.78	1.56
1:A:212:LYS:CG	1:A:212:LYS:CD	1.83	1.56
1:A:282:ASN:CB	1:A:282:ASN:CG	1.79	1.56
1:A:368:LYS:CD	1:A:368:LYS:CE	1.78	1.56
1:A:423:ASP:CB	1:A:423:ASP:CG	1.77	1.56
1:A:1385:THR:CB	1:A:1385:THR:CG2	1.79	1.56
2:B:733:HIS:CA	2:B:733:HIS:C	1.77	1.56
4:E:113:GLN:CG	4:E:113:GLN:CB	1.75	1.56
1:A:1359:ASP:CB	1:A:1359:ASP:CG	1.76	1.56
2:B:959:ASP:CB	2:B:959:ASP:CG	1.77	1.56
2:B:1219:ASP:CB	2:B:1219:ASP:CG	1.79	1.56
3:C:199:LYS:CD	3:C:199:LYS:CG	1.84	1.56
6:H:137:GLN:CG	6:H:137:GLN:CD	1.75	1.56
8:J:26:GLN:CG	8:J:26:GLN:CD	1.77	1.56
1:A:186:LYS:CB	1:A:186:LYS:CG	1.81	1.55
1:A:1112:LYS:CD	1:A:1112:LYS:CE	1.84	1.55
3:C:116:LYS:CD	3:C:116:LYS:CE	1.82	1.55
3:C:220:ASP:CB	3:C:220:ASP:CG	1.79	1.55
10:L:50:ASP:CA	10:L:50:ASP:C	1.74	1.55
1:A:268:ASP:CB	1:A:268:ASP:CG	1.79	1.55
1:A:991:LYS:NZ	1:A:991:LYS:CE	1.69	1.55
1:A:1221:LYS:CG	1:A:1221:LYS:CB	1.79	1.55
1:A:1419:ASP:CG	1:A:1419:ASP:CB	1.77	1.55
2:B:70:ILE:CG1	2:B:70:ILE:CD1	1.78	1.55
2:B:191:LYS:CG	2:B:191:LYS:CB	1.83	1.55
2:B:279:ASP:CB	2:B:279:ASP:CG	1.76	1.55
10:L:54:ARG:CG	10:L:54:ARG:CD	1.80	1.55
1:A:40:THR:CB	1:A:40:THR:CA	1.80	1.55
1:A:829:VAL:CB	1:A:829:VAL:CG2	1.77	1.55
1:A:1055:ARG:CG	1:A:1055:ARG:CD	1.80	1.55
2:B:191:LYS:CD	2:B:191:LYS:CE	1.81	1.55
2:B:622:LYS:CB	2:B:622:LYS:CG	1.77	1.55
2:B:706:GLN:CB	2:B:706:GLN:CG	1.83	1.55
2:B:723:VAL:CB	2:B:723:VAL:CG1	1.81	1.55
2:B:1106:ARG:CD	2:B:1106:ARG:CG	1.83	1.55
4:E:115:ASN:CB	4:E:115:ASN:CG	1.75	1.55
4:E:116:ILE:CG1	4:E:116:ILE:CD1	1.77	1.55
6:H:63:LEU:C	6:H:63:LEU:CA	1.79	1.55
6:H:139:ASN:CA	6:H:139:ASN:CB	1.79	1.55
1:A:28:ARG:CD	1:A:28:ARG:CG	1.83	1.55
1:A:302:THR:CG2	1:A:302:THR:CB	1.82	1.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:GLU:CG	1:A:795:GLU:CD	1.80	1.55
1:A:1130:GLN:CG	1:A:1130:GLN:CD	1.79	1.55
2:B:183:GLU:CD	2:B:183:GLU:CG	1.77	1.55
5:F:87:LYS:CE	5:F:87:LYS:CD	1.84	1.55
6:H:136:LYS:C	6:H:136:LYS:CA	1.74	1.55
7:I:1:MET:CB	7:I:1:MET:CA	1.78	1.55
1:A:830:LYS:NZ	1:A:830:LYS:CE	1.68	1.55
2:B:870:ILE:CB	2:B:870:ILE:CG2	1.77	1.55
2:B:916:THR:CB	2:B:916:THR:CG2	1.79	1.55
2:B:961:LEU:CG	2:B:961:LEU:CD1	1.80	1.55
2:B:986:GLN:CB	2:B:986:GLN:CG	1.85	1.55
4:E:41:ASP:CB	4:E:41:ASP:CG	1.77	1.55
10:L:38:LEU:CG	10:L:38:LEU:CD1	1.81	1.55
1:A:186:LYS:CG	1:A:186:LYS:CD	1.80	1.54
1:A:199:LEU:CG	1:A:199:LEU:CD1	1.82	1.54
1:A:271:LYS:CD	1:A:271:LYS:CE	1.78	1.54
1:A:544:ASP:CB	1:A:544:ASP:CG	1.74	1.54
1:A:688:LYS:CD	1:A:688:LYS:CE	1.79	1.54
1:A:840:ARG:CG	1:A:840:ARG:CD	1.80	1.54
1:A:962:ARG:CG	1:A:962:ARG:CD	1.76	1.54
2:B:477:ALA:CA	2:B:477:ALA:CB	1.79	1.54
2:B:620:ARG:CG	2:B:620:ARG:CD	1.81	1.54
2:B:965:LYS:CD	2:B:965:LYS:CE	1.76	1.54
1:A:264:PHE:CB	1:A:264:PHE:CG	1.84	1.54
1:A:1277:GLU:CG	1:A:1277:GLU:CD	1.78	1.54
1:A:1318:THR:CB	1:A:1318:THR:CG2	1.82	1.54
2:B:641:GLU:CG	2:B:641:GLU:CD	1.78	1.54
2:B:1132:GLU:CG	2:B:1132:GLU:CD	1.80	1.54
2:B:1176:ASN:CB	2:B:1176:ASN:CG	1.75	1.54
3:C:199:LYS:CG	3:C:199:LYS:CB	1.82	1.54
9:K:20:LYS:CD	9:K:20:LYS:CE	1.84	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:1129:GLU:CG	1:A:1129:GLU:CD	1.77	1.54
2:B:436:VAL:CA	2:B:436:VAL:CB	1.84	1.54
2:B:1154:ALA:CA	2:B:1154:ALA:CB	1.85	1.54
6:H:27:GLU:CA	6:H:27:GLU:C	1.76	1.54
1:A:133:LYS:NZ	1:A:133:LYS:CE	1.71	1.54
3:C:137:LYS:CD	3:C:137:LYS:CG	1.84	1.54
4:E:31:THR:CB	4:E:31:THR:CG2	1.83	1.54
4:E:103:LYS:CD	4:E:103:LYS:CE	1.80	1.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:20:LYS:CD	9:K:20:LYS:CG	1.86	1.54
1:A:620:LYS:CB	1:A:620:LYS:CG	1.86	1.54
1:A:637:LYS:NZ	1:A:637:LYS:CE	1.68	1.54
1:A:1217:LYS:NZ	1:A:1217:LYS:CE	1.70	1.54
2:B:39:ARG:CB	2:B:39:ARG:CG	1.81	1.54
2:B:1183:LYS:CG	2:B:1183:LYS:CB	1.76	1.54
3:C:154:LYS:NZ	3:C:154:LYS:CE	1.68	1.54
3:C:267:GLN:C	3:C:267:GLN:CA	1.81	1.54
9:K:102:LYS:CD	9:K:102:LYS:CG	1.80	1.54
1:A:744:LYS:CD	1:A:744:LYS:CE	1.86	1.53
1:A:1405:THR:CB	1:A:1405:THR:CA	1.85	1.53
2:B:106:ASP:CG	2:B:106:ASP:CB	1.77	1.53
2:B:1101:ASP:CB	2:B:1101:ASP:CG	1.77	1.53
4:E:43:LYS:CG	4:E:43:LYS:CB	1.83	1.53
4:E:98:ILE:CB	4:E:98:ILE:CG2	1.81	1.53
4:E:129:PRO:CB	4:E:129:PRO:CG	1.82	1.53
5:F:76:LYS:CD	5:F:76:LYS:CG	1.78	1.53
6:H:107:VAL:CG1	6:H:107:VAL:CB	1.80	1.53
2:B:668:ASP:CB	2:B:668:ASP:CG	1.75	1.53
3:C:253:LYS:CD	3:C:253:LYS:CE	1.80	1.53
1:A:49:LYS:NZ	1:A:49:LYS:CE	1.71	1.53
1:A:121:LEU:CG	1:A:121:LEU:CD1	1.84	1.53
1:A:518:LYS:CE	1:A:518:LYS:CD	1.86	1.53
1:A:689:LYS:CD	1:A:689:LYS:CE	1.82	1.53
1:A:1222:ASN:CA	1:A:1222:ASN:CB	1.77	1.53
2:B:134:LYS:CB	2:B:134:LYS:CG	1.78	1.53
2:B:870:ILE:CB	2:B:870:ILE:CA	1.84	1.53
2:B:1150:ARG:NH2	2:B:1150:ARG:CZ	1.69	1.53
4:E:54:GLN:CG	4:E:54:GLN:CB	1.86	1.53
6:H:76:THR:CB	6:H:76:THR:CG2	1.80	1.53
6:H:111:LEU:CD1	6:H:111:LEU:CG	1.86	1.53
10:L:61:THR:CB	10:L:61:THR:CG2	1.80	1.53
1:A:69:THR:C	1:A:69:THR:CA	1.79	1.53
1:A:977:LYS:CG	1:A:977:LYS:CB	1.86	1.53
1:A:1261:LYS:CD	1:A:1261:LYS:CE	1.78	1.53
2:B:358:LYS:NZ	2:B:358:LYS:CE	1.68	1.53
2:B:944:THR:CB	2:B:944:THR:CG2	1.82	1.53
2:B:1186:ASP:CB	2:B:1186:ASP:CG	1.79	1.53
3:C:196:ASP:CB	3:C:196:ASP:CG	1.79	1.53
1:A:191:THR:CB	1:A:191:THR:CA	1.80	1.53
1:A:193:ASP:CG	1:A:193:ASP:CB	1.78	1.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ILE:CB	1:A:274:ILE:CG2	1.82	1.53
1:A:934:LYS:NZ	1:A:934:LYS:CE	1.72	1.53
2:B:595:ARG:CD	2:B:595:ARG:CG	1.81	1.53
4:E:90:VAL:CG1	4:E:90:VAL:CB	1.82	1.53
7:I:20:LYS:CD	7:I:20:LYS:CE	1.84	1.53
1:A:274:ILE:CB	1:A:274:ILE:CA	1.80	1.52
1:A:566:ILE:CB	1:A:566:ILE:CG2	1.85	1.52
1:A:569:LYS:NZ	1:A:569:LYS:CE	1.72	1.52
2:B:343:ILE:CD1	2:B:343:ILE:CG1	1.85	1.52
3:C:9:LYS:CE	3:C:9:LYS:CD	1.85	1.52
3:C:102:GLN:CB	3:C:102:GLN:CG	1.84	1.52
1:A:45:GLN:CA	1:A:45:GLN:C	1.79	1.52
1:A:1120:LEU:CD1	1:A:1120:LEU:CG	1.82	1.52
1:A:1262:LYS:CD	1:A:1262:LYS:CE	1.78	1.52
1:A:1350:LYS:CG	1:A:1350:LYS:CD	1.88	1.52
7:I:82:GLU:CD	7:I:82:GLU:CG	1.74	1.52
1:A:49:LYS:CG	1:A:49:LYS:CD	1.87	1.52
1:A:705:LYS:CE	1:A:705:LYS:NZ	1.69	1.52
1:A:728:LYS:CE	1:A:728:LYS:NZ	1.69	1.52
2:B:239:GLU:CD	2:B:239:GLU:CG	1.78	1.52
2:B:531:GLN:CB	2:B:531:GLN:CG	1.87	1.52
2:B:965:LYS:CE	2:B:965:LYS:NZ	1.72	1.52
3:C:9:LYS:CD	3:C:9:LYS:CG	1.78	1.52
4:E:91:LYS:CB	4:E:91:LYS:CG	1.82	1.52
6:H:77:ARG:CB	6:H:77:ARG:CG	1.85	1.52
1:A:880:LYS:CG	1:A:880:LYS:CD	1.84	1.52
2:B:706:GLN:CG	2:B:706:GLN:CD	1.81	1.52
2:B:775:LYS:CB	2:B:775:LYS:CG	1.84	1.52
2:B:986:GLN:CG	2:B:986:GLN:CD	1.80	1.52
6:H:2:SER:C	6:H:2:SER:CA	1.75	1.52
1:A:1132:LYS:CD	1:A:1132:LYS:CE	1.88	1.52
2:B:120:ARG:CG	2:B:120:ARG:CB	1.82	1.52
2:B:270:LYS:NZ	2:B:270:LYS:CE	1.72	1.52
2:B:418:LYS:CD	2:B:418:LYS:CE	1.84	1.52
2:B:1150:ARG:CZ	2:B:1150:ARG:NH1	1.67	1.52
3:C:127:ARG:N	3:C:127:ARG:CA	1.68	1.52
1:A:157:ASP:CB	1:A:157:ASP:CG	1.79	1.51
1:A:1194:ARG:CB	1:A:1194:ARG:CG	1.83	1.51
2:B:652:LYS:NZ	2:B:652:LYS:CE	1.69	1.51
2:B:915:THR:CA	2:B:915:THR:CB	1.83	1.51
4:E:43:LYS:NZ	4:E:43:LYS:CE	1.70	1.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:43:THR:CB	10:L:43:THR:CG2	1.82	1.51
10:L:47:ARG:CG	10:L:47:ARG:CD	1.84	1.51
1:A:5:GLN:CG	1:A:5:GLN:CB	1.87	1.51
1:A:571:LEU:CD2	1:A:571:LEU:CG	1.88	1.51
4:E:56:LYS:CG	4:E:56:LYS:CD	1.84	1.51
7:I:36:GLU:CG	7:I:36:GLU:CD	1.77	1.51
4:E:37:LEU:CD1	4:E:37:LEU:CG	1.86	1.51
2:B:625:LYS:NZ	2:B:625:LYS:CE	1.74	1.51
3:C:50:GLU:CG	3:C:50:GLU:CD	1.76	1.51
2:B:552:MET:CB	2:B:552:MET:CG	1.86	1.51
2:B:1188:LYS:CD	2:B:1188:LYS:CE	1.88	1.51
4:E:161:LYS:CD	4:E:161:LYS:CE	1.89	1.51
1:A:217:LYS:CD	1:A:217:LYS:CG	1.88	1.50
3:C:205:LYS:CD	3:C:205:LYS:CE	1.84	1.50
1:A:601:LYS:CD	1:A:601:LYS:CE	1.85	1.50
1:A:695:LYS:NZ	1:A:695:LYS:CE	1.67	1.50
1:A:1171:GLN:CG	1:A:1171:GLN:CD	1.85	1.50
2:B:353:LYS:CG	2:B:353:LYS:CD	1.85	1.50
2:B:1188:LYS:CE	2:B:1188:LYS:NZ	1.67	1.50
1:A:188:ASP:C	1:A:188:ASP:CA	1.84	1.50
1:A:941:LYS:CD	1:A:941:LYS:CG	1.84	1.50
2:B:892:LYS:CD	2:B:892:LYS:CE	1.84	1.50
1:A:1235:LYS:CD	1:A:1235:LYS:CE	1.86	1.50
10:L:48:CYS:C	10:L:48:CYS:CA	1.80	1.50
10:L:62:LYS:CD	10:L:62:LYS:CE	1.86	1.50
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:346:GLU:CG	2:B:346:GLU:CD	1.84	1.50
2:B:646:LEU:CG	2:B:646:LEU:CD1	1.90	1.50
2:B:895:ASP:CB	2:B:895:ASP:CG	1.80	1.50
2:B:933:SER:CA	2:B:933:SER:C	1.83	1.50
2:B:1155:SER:CA	2:B:1155:SER:N	1.68	1.50
4:E:52:ARG:CB	4:E:52:ARG:CG	1.84	1.50
5:F:129:LYS:CD	5:F:129:LYS:CE	1.89	1.50
8:J:26:GLN:CG	8:J:26:GLN:CB	1.84	1.50
8:J:42:LYS:CG	8:J:42:LYS:CD	1.90	1.50
1:A:143:LYS:NZ	1:A:143:LYS:CE	1.74	1.49
1:A:705:LYS:CB	1:A:705:LYS:CG	1.86	1.49
2:B:347:LYS:CG	2:B:347:LYS:CD	1.87	1.49
4:E:191:LYS:CD	4:E:191:LYS:CE	1.89	1.49
10:L:64:LEU:CD1	10:L:64:LEU:CG	1.88	1.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LYS:NZ	1:A:101:LYS:CE	1.71	1.49
1:A:186:LYS:CD	1:A:186:LYS:CE	1.86	1.49
1:A:644:LYS:NZ	1:A:644:LYS:CE	1.76	1.49
1:A:1239:ARG:CG	1:A:1239:ARG:CD	1.87	1.49
2:B:736:THR:CB	2:B:736:THR:CG2	1.89	1.49
2:B:962:LYS:CG	2:B:962:LYS:CD	1.83	1.49
1:A:295:LEU:CD2	1:A:295:LEU:CG	1.89	1.49
1:A:1109:LYS:CE	1:A:1109:LYS:CD	1.87	1.49
7:I:45:ARG:CG	7:I:45:ARG:CD	1.87	1.49
1:A:934:LYS:CD	1:A:934:LYS:CE	1.87	1.49
2:B:305:VAL:CG1	2:B:305:VAL:CB	1.88	1.49
2:B:451:LYS:CG	2:B:451:LYS:CD	1.88	1.49
7:I:93:LYS:CG	7:I:93:LYS:CD	1.87	1.49
1:A:895:LYS:CE	1:A:895:LYS:NZ	1.72	1.48
6:H:19:ARG:CB	6:H:19:ARG:CG	1.90	1.48
2:B:251:ILE:CB	2:B:251:ILE:CG2	1.89	1.48
2:B:962:LYS:CD	2:B:962:LYS:CE	1.88	1.48
3:C:116:LYS:CE	3:C:116:LYS:NZ	1.68	1.48
8:J:1:MET:CE	8:J:1:MET:SD	2.02	1.48
2:B:426:LYS:CE	2:B:426:LYS:NZ	1.73	1.48
1:A:687:LYS:NZ	1:A:687:LYS:CE	1.77	1.48
2:B:246:LYS:CA	2:B:246:LYS:C	1.85	1.48
2:B:962:LYS:CE	2:B:962:LYS:NZ	1.74	1.48
4:E:73:PRO:CB	4:E:73:PRO:CG	1.77	1.48
4:E:93:MET:CG	4:E:93:MET:SD	2.02	1.48
2:B:563:MET:CG	2:B:563:MET:SD	2.02	1.48
5:F:87:LYS:CE	5:F:87:LYS:NZ	1.73	1.48
5:F:129:LYS:CE	5:F:129:LYS:NZ	1.75	1.48
2:B:711:GLU:CG	2:B:711:GLU:CD	1.87	1.47
3:C:15:LYS:NZ	3:C:15:LYS:CE	1.72	1.47
2:B:415:GLN:CG	2:B:415:GLN:CB	1.89	1.47
1:A:601:LYS:CE	1:A:601:LYS:NZ	1.73	1.47
1:A:977:LYS:NZ	1:A:977:LYS:CE	1.76	1.47
2:B:951:GLN:CG	2:B:951:GLN:CD	1.87	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
2:B:434:ARG:CG	2:B:434:ARG:CB	1.90	1.47
6:H:9:ILE:CG1	6:H:9:ILE:CD1	1.91	1.47
10:L:26:THR:CB	10:L:26:THR:CA	1.91	1.47
1:A:1408:ILE:CD1	1:A:1408:ILE:CG1	1.93	1.47
1:A:1112:LYS:CE	1:A:1112:LYS:NZ	1.75	1.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:428:ILE:CG1	2:B:428:ILE:CD1	1.91	1.46
2:B:768:THR:C	2:B:768:THR:CA	1.86	1.46
9:K:88:LYS:CE	9:K:88:LYS:NZ	1.77	1.46
1:A:843:LYS:CD	1:A:843:LYS:CE	1.90	1.46
1:A:1223:ASP:CB	1:A:1223:ASP:CG	1.89	1.46
2:B:1188:LYS:CD	2:B:1188:LYS:CG	1.89	1.46
10:L:62:LYS:CE	10:L:62:LYS:NZ	1.77	1.46
1:A:895:LYS:CD	1:A:895:LYS:CE	1.87	1.46
3:C:15:LYS:CG	3:C:15:LYS:CD	1.91	1.46
7:I:93:LYS:CD	7:I:93:LYS:CE	1.90	1.46
1:A:346:ASP:CB	1:A:346:ASP:CG	1.89	1.46
1:A:555:ASP:CB	1:A:555:ASP:CG	1.88	1.46
1:A:368:LYS:CD	1:A:368:LYS:CG	1.90	1.46
2:B:509:ALA:CA	2:B:509:ALA:CB	1.92	1.46
6:H:19:ARG:CG	6:H:19:ARG:CD	1.92	1.46
8:J:38:ARG:CG	8:J:38:ARG:CB	1.92	1.46
10:L:45:ALA:CA	10:L:45:ALA:CB	1.94	1.46
1:A:1232:ASN:CG	1:A:1232:ASN:CB	1.87	1.45
3:C:195:GLN:CG	3:C:195:GLN:CD	1.89	1.45
1:A:427:GLN:CG	1:A:427:GLN:CD	1.87	1.45
2:B:502:ILE:CA	2:B:502:ILE:CB	1.94	1.45
2:B:712:PRO:CB	2:B:712:PRO:CG	1.78	1.45
1:A:1262:LYS:CG	1:A:1262:LYS:CD	1.94	1.45
1:A:1290:LYS:CD	1:A:1290:LYS:CE	1.94	1.45
2:B:622:LYS:NZ	2:B:622:LYS:CE	1.76	1.45
9:K:26:LYS:CE	9:K:26:LYS:NZ	1.76	1.45
2:B:705:MET:SD	2:B:705:MET:CG	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
10:L:50:ASP:CB	10:L:50:ASP:CG	1.87	1.45
1:A:41:MET:CE	1:A:41:MET:SD	2.05	1.44
1:A:1425:SER:CB	1:A:1425:SER:OG	1.64	1.44
2:B:347:LYS:CD	2:B:347:LYS:CE	1.95	1.44
1:A:144:THR:CB	1:A:144:THR:CG2	1.91	1.44
1:A:1080:THR:CB	1:A:1080:THR:CG2	1.93	1.44
1:A:941:LYS:NZ	1:A:941:LYS:CE	1.81	1.44
1:A:1290:LYS:CE	1:A:1290:LYS:NZ	1.81	1.44
4:E:191:LYS:CE	4:E:191:LYS:NZ	1.77	1.44
5:F:123:LYS:NZ	5:F:123:LYS:CE	1.77	1.44
2:B:103:ASN:CB	2:B:103:ASN:CG	1.89	1.44
6:H:131:ASN:CB	6:H:131:ASN:CG	1.88	1.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1156:ASP:CB	2:B:1156:ASP:CG	1.91	1.43
8:J:42:LYS:CD	8:J:42:LYS:CE	1.93	1.43
1:A:123:ARG:CB	1:A:123:ARG:CG	1.95	1.43
1:A:738:LYS:NZ	1:A:738:LYS:CE	1.81	1.43
1:A:1111:MET:SD	1:A:1111:MET:CG	2.06	1.43
1:A:1450:LEU:CG	1:A:1450:LEU:CD2	1.93	1.43
1:A:1110:ASN:CG	1:A:1110:ASN:CB	1.91	1.43
1:A:1235:LYS:CE	1:A:1235:LYS:NZ	1.79	1.43
3:C:197:SER:CB	3:C:197:SER:OG	1.65	1.43
7:I:93:LYS:CE	7:I:93:LYS:NZ	1.77	1.43
6:H:52:GLN:CG	6:H:52:GLN:CD	1.91	1.43
1:A:751:SER:OG	1:A:751:SER:CB	1.64	1.42
2:B:172:ILE:CG1	2:B:172:ILE:CD1	1.98	1.42
4:E:118:PRO:CG	4:E:118:PRO:CB	1.97	1.42
6:H:104:PHE:C	6:H:104:PHE:CA	1.93	1.42
1:A:843:LYS:CD	1:A:843:LYS:CG	1.94	1.42
2:B:598:GLU:CG	2:B:598:GLU:CD	1.93	1.42
2:B:233:PRO:CB	2:B:233:PRO:CG	1.94	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
1:A:1064:VAL:CA	1:A:1064:VAL:O	1.66	1.42
2:B:789:MET:CE	2:B:789:MET:SD	2.06	1.42
2:B:315:LYS:NZ	2:B:315:LYS:CE	1.80	1.42
3:C:125:MET:SD	3:C:125:MET:CG	2.07	1.42
1:A:49:LYS:CE	1:A:49:LYS:CD	1.98	1.41
1:A:1263:ILE:CD1	1:A:1263:ILE:CG1	1.97	1.41
3:C:94:LYS:NZ	3:C:94:LYS:CE	1.82	1.41
1:A:830:LYS:CD	1:A:830:LYS:CG	1.97	1.41
4:E:45:LYS:CD	4:E:45:LYS:CE	1.95	1.41
10:L:28:LYS:NZ	10:L:28:LYS:CE	1.82	1.41
1:A:248:PRO:CB	1:A:248:PRO:CG	1.89	1.41
9:K:12:LEU:CG	9:K:12:LEU:CD1	1.98	1.40
1:A:728:LYS:CG	1:A:728:LYS:CD	1.99	1.40
6:H:139:ASN:CB	6:H:139:ASN:CG	1.95	1.40
2:B:344:LYS:CG	2:B:344:LYS:CB	1.99	1.40
1:A:597:LEU:CD1	1:A:597:LEU:CG	1.99	1.40
1:A:703:THR:CB	1:A:703:THR:CG2	1.99	1.40
7:I:72:ASP:CB	7:I:72:ASP:CG	1.92	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
1:A:1109:LYS:CG	1:A:1109:LYS:CD	1.99	1.39

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1285:MET:CG	1:A:1285:MET:SD	2.10	1.39
1:A:695:LYS:CE	1:A:695:LYS:CD	1.99	1.39
3:C:154:LYS:CG	3:C:154:LYS:CD	1.99	1.39
4:E:57:MET:CG	4:E:57:MET:SD	2.11	1.39
5:F:106:PRO:CG	5:F:106:PRO:CB	1.79	1.39
1:A:304:MET:CG	1:A:304:MET:SD	2.09	1.38
3:C:29:MET:CE	3:C:29:MET:SD	2.09	1.38
4:E:162:ARG:CB	4:E:162:ARG:CG	1.98	1.38
1:A:676:MET:SD	1:A:676:MET:CG	2.12	1.38
7:I:1:MET:CE	7:I:1:MET:SD	2.11	1.38
1:A:1222:ASN:CB	1:A:1222:ASN:CG	1.97	1.38
2:B:164:LYS:CD	2:B:164:LYS:CE	2.00	1.38
7:I:4:PHE:CE1	7:I:13:MET:HE2	1.57	1.37
7:I:120:GLN:CG	7:I:120:GLN:CB	2.00	1.37
4:E:53:PRO:CG	4:E:53:PRO:CB	1.90	1.37
1:A:941:LYS:CD	1:A:941:LYS:CE	2.02	1.37
2:B:531:GLN:CG	2:B:531:GLN:CD	1.97	1.37
4:E:162:ARG:CG	4:E:162:ARG:CD	2.03	1.36
1:A:1102:LYS:CG	1:A:1102:LYS:CD	2.02	1.36
2:B:745:PRO:CD	2:B:745:PRO:CG	1.79	1.36
1:A:600:PRO:CG	1:A:600:PRO:CB	1.76	1.35
1:A:1350:LYS:NZ	1:A:1350:LYS:CE	1.90	1.35
4:E:152:LYS:CD	4:E:152:LYS:CE	2.05	1.35
2:B:1189:ILE:CG1	2:B:1189:ILE:CD1	2.02	1.34
3:C:154:LYS:CE	3:C:154:LYS:CD	2.03	1.34
10:L:68:GLU:CG	10:L:68:GLU:CD	2.00	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
4:E:131:THR:CB	4:E:131:THR:CG2	2.05	1.32
1:A:620:LYS:CD	1:A:620:LYS:CE	2.06	1.32
4:E:1:MET:CG	4:E:1:MET:SD	2.18	1.32
1:A:44:THR:CB	1:A:44:THR:CA	2.07	1.32
9:K:23:PRO:CG	9:K:23:PRO:CB	1.90	1.32
2:B:987:LYS:NZ	2:B:987:LYS:CE	1.93	1.32
1:A:752:LYS:CE	1:A:752:LYS:CD	2.08	1.31
1:A:1135:ARG:CG	1:A:1135:ARG:CD	2.08	1.30

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:938:LYS:CD	1:A:938:LYS:CE	2.09	1.30
1:A:978:PRO:CB	1:A:978:PRO:CG	2.06	1.30
4:E:93:MET:SD	4:E:93:MET:CE	2.20	1.30
2:B:999:MET:CE	2:B:999:MET:SD	1.20	1.30
2:B:646:LEU:CG	2:B:646:LEU:CD2	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
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
2:B:381:MET:CE	2:B:381:MET:SD	1.19	1.28
7:I:55:THR:CB	7:I:55:THR:CG2	2.10	1.28
2:B:955:THR:HG22	10:L:54:ARG:O	1.24	1.26
1:A:1259:MET:SD	1:A:1259:MET:CG	2.23	1.26
4:E:20:LYS:CE	4:E:20:LYS:NZ	1.98	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
2:B:100:PRO:HD2	2:B:180:TYR:CE1	1.74	1.22
2:B:999:MET:CE	2:B:999:MET:CG	2.17	1.22
6:H:138:GLU:O	6:H:139:ASN:C	1.78	1.22
1:A:549:MET:CE	1:A:549:MET:SD	1.10	1.20
1:A:620:LYS:CE	1:A:620:LYS:NZ	2.06	1.19
2:B:999:MET:SD	2:B:999:MET:HE1	1.78	1.19
4:E:1:MET:SD	4:E:1:MET:CE	2.30	1.19
1:A:74:MET:CE	1:A:74:MET:SD	2.31	1.18
1:A:1064:VAL:C	1:A:1066:VAL:N	1.90	1.18
2:B:1097:HIS:ND1	2:B:1097:HIS:HA	1.58	1.18
4:E:12:LEU:HD21	4:E:58:MET:SD	1.84	1.18
1:A:1064:VAL:O	1:A:1064:VAL:C	1.87	1.17
2:B:792:MET:SD	2:B:792:MET:CE	2.33	1.17
1:A:567:LYS:HD3	6:H:95:TYR:CG	1.78	1.16
1:A:752:LYS:CE	1:A:752:LYS:NZ	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
2:B:381:MET:SD	2:B:381:MET:HE3	1.77	1.15
2:B:381:MET:SD	2:B:381:MET:HE1	1.77	1.14
1:A:567:LYS:HD3	6:H:95:TYR:CA	1.78	1.14
6:H:130:ARG:HD2	6:H:130:ARG:C	1.68	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
2:B:999:MET:SD	2:B:999:MET:HE2	1.78	1.12
2:B:104:GLU:OE1	10:L:54:ARG:NE	1.80	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1097:HIS:CA	2:B:1097:HIS:ND1	2.11	1.11
1:A:567:LYS:CD	6:H:95:TYR:HA	1.81	1.11
1:A:708:MET:CE	1:A:708:MET:SD	2.39	1.10
1:A:1064:VAL:CA	1:A:1065:GLY:N	2.14	1.10
2:B:999:MET:SD	2:B:999:MET:HE3	1.78	1.10
9:K:110:ASN:O	9:K:112:GLN:N	1.84	1.10
6:H:138:GLU:O	6:H:140:ALA:N	1.84	1.10
2:B:381:MET:SD	2:B:381:MET:HE2	1.77	1.10
6:H:91:ASP:OD1	6:H:91:ASP:O	1.70	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:CG	2:B:705:MET:CE	2.30	1.08
2:B:885:MET:CE	2:B:885:MET:SD	2.42	1.07
6:H:5:LEU:O	6:H:133:ASN:ND2	1.86	1.07
1:A:535:THR:HG21	1:A:617:VAL:N	1.69	1.07
2:B:134:LYS:O	2:B:135:ARG:HG3	1.54	1.07
1:A:567:LYS:HB3	6:H:96:VAL:H	1.12	1.07
2:B:1128:LEU:HD12	2:B:1128:LEU:C	1.76	1.07
1:A:549:MET:SD	1:A:549:MET:HE2	1.69	1.07
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
1:A:549:MET:SD	1:A:549:MET:HE1	1.69	1.06
5:F:103:MET:CE	5:F:103:MET:SD	2.44	1.06
1:A:549:MET:SD	1:A:549:MET:HE3	1.69	1.05
6:H:130:ARG:HD2	6:H:130:ARG:O	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:SD	1:A:304:MET:CE	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:789:MET:HE3	2:B:965:LYS:HB3	1.40	1.03
2:B:643:ASP:O	2:B:644:GLU:CB	2.02	1.03
4:E:98:ILE:CB	4:E:98:ILE:HA	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:CB	10:L:40:LEU:HG	1.86	1.02
1:A:369:SER:OG	9:K:2:ASN:ND2	1.93	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:VAL:CA	1:A:1064:VAL:C	2.34	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
1:A:535:THR:HG21	1:A:617:VAL:H	0.85	1.00
7:I:109:ILE:CD1	7:I:109:ILE:CB	2.40	1.00
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.01	0.99
6:H:4:THR:C	6:H:5:LEU:HD23	1.87	0.99
1:A:1064:VAL:O	1:A:1065:GLY:N	1.93	0.99
6:H:63:LEU:C	6:H:90:ALA:HB3	1.86	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
6:H:135:LEU:CD2	6:H:135:LEU:HG	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
1:A:752:LYS:HZ3	2:B:1019:SER:H	1.05	0.97
4:E:47:CYS:C	4:E:47:CYS:HA	1.85	0.97
4:E:98:ILE:CG1	4:E:98:ILE:CG2	2.41	0.97
1:A:711:ARG:HE	7:I:95:THR:HG22	1.27	0.96
1:A:535:THR:CG2	1:A:617:VAL:H	1.76	0.96
1:A:588:LEU:HD23	1:A:588:LEU:C	1.89	0.96
2:B:101:MET:HA	2:B:110:HIS:O	1.63	0.96
1:A:567:LYS:CG	1:A:568:PRO:HD3	1.95	0.96
1:A:549:MET:CE	1:A:549:MET:CG	2.42	0.96
8:J:7:CYS:SG	8:J:10:CYS:SG	2.63	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
2:B:101:MET:SD	2:B:101:MET:CE	2.54	0.95
2:B:1097:HIS:CA	2:B:1097:HIS:CG	2.50	0.95
2:B:1156:ASP:CB	2:B:1156:ASP:HA	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
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
10:L:31:CYS:SG	10:L:51:CYS:SG	2.64	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
6:H:103:LYS:HB3	6:H:105:GLU:OE1	1.66	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG2	3:C:156:THR:CA	2.46	0.93
1:A:64:ASN:OD1	1:A:64:ASN:O	1.87	0.92
4:E:66:GLU:CB	4:E:66:GLU:HA	1.99	0.92
2:B:1025:HIS:HE1	2:B:1090:THR:HG21	1.35	0.92
2:B:90:ILE:N	2:B:90:ILE:HD12	1.85	0.92
2:B:1172:ILE:CG2	2:B:1172:ILE:CG1	2.48	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
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:99:LYS:HB3	2:B:100:PRO:HD3	1.52	0.91
1:A:42:ASP:OD2	1:A:46:THR:C	2.13	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
8:J:7:CYS:SG	8:J:46:CYS:SG	2.68	0.90
2:B:18:PHE:CB	2:B:18:PHE:HA	2.00	0.90
5:F:75:PRO:O	5:F:77:ASP:O	1.89	0.90
7:I:4:PHE:CE1	7:I:13:MET:CE	2.52	0.90
1:A:1233:ASP:O	1:A:1234:GLU:HB3	1.68	0.90
1:A:503:GLN:NE2	5:F:90:ARG:NH2	2.19	0.90
2:B:515:HIS:H	2:B:518:HIS:HD2	1.16	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
6:H:2:SER:C	6:H:2:SER:HA	1.96	0.89
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
3:C:120:ILE:CD1	3:C:120:ILE:CB	2.51	0.89
4:E:117:THR:O	4:E:119:SER:N	2.05	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:267:GLN:C	3:C:267:GLN:HA	1.99	0.88
1:A:517:ASN:ND2	1:A:1364:ASN:OD1	2.08	0.87
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
3:C:167:HIS:HD2	3:C:169:LYS:H	1.19	0.87
10:L:34:CYS:HG	12:L:3005:ZN:ZN	0.57	0.87
10:L:58:LYS:O	10:L:59:ALA:HB3	1.74	0.87
1:A:633:VAL:CG2	1:A:633:VAL:CG1	2.53	0.87
6:H:27:GLU:C	6:H:27:GLU:HA	1.98	0.87
8:J:43:ARG:CG	8:J:43:ARG:NE	2.38	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
10:L:38:LEU:O	10:L:39:SER:HB2	1.72	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:752:LYS:HZ3	2:B:1019:SER:N	1.70	0.86
1:A:1385:THR:O	1:A:1385:THR:HG22	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:59:ILE:CG2	6:H:60:ALA:N	2.37	0.86
10:L:47:ARG:HG2	10:L:48:CYS:H	1.40	0.86
2:B:770:GLN:HG2	2:B:983:ARG:O	1.76	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:HB3	1:A:1366:ARG:NH1	1.91	0.85
7:I:4:PHE:HE1	7:I:13:MET:HE2	0.98	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
2:B:129:PHE:CD2	2:B:166:PHE:HA	2.12	0.85
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.75	0.85
1:A:1079:MET:CG	1:A:1359:ASP:OD2	2.24	0.85
1:A:1081:LEU:CD2	1:A:1081:LEU:HG	2.05	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:HG3	2.06	0.85
1:A:1080:THR:C	1:A:1080:THR:HA	2.00	0.84

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:CB	2.55	0.84
9:K:101:LEU:O	9:K:101:LEU:HD13	1.77	0.84
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.57	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
8:J:1:MET:CB	8:J:1:MET:HE3	2.08	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
1:A:73:GLY:C	1:A:75:ASN:N	2.29	0.84
3:C:75:MET:CE	3:C:75:MET:SD	2.65	0.84
2:B:620:ARG:CG	2:B:620:ARG:NE	2.41	0.84
7:I:16:PRO:O	7:I:17:ARG:HD3	1.78	0.84
2:B:428:ILE:HG12	2:B:448:ILE:HD11	1.60	0.84
4:E:91:LYS:CB	4:E:91:LYS:HA	2.08	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
4:E:55:ARG:O	4:E:56:LYS:C	2.19	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
1:A:1385:THR:C	1:A:1385:THR:CB	2.50	0.83
6:H:104:PHE:C	6:H:104:PHE:HA	2.02	0.83
1:A:156:ASP:O	1:A:158:PRO:HD3	1.79	0.83
2:B:1150:ARG:NH1	2:B:1150:ARG:HD2	1.92	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
9:K:101:LEU:HD13	9:K:101:LEU:C	2.04	0.83
2:B:251:ILE:CG2	2:B:251:ILE:HB	2.07	0.82
4:E:117:THR:O	4:E:118:PRO:C	2.18	0.82
6:H:91:ASP:OD1	6:H:91:ASP:C	2.22	0.82
6:H:103:LYS:O	6:H:115:TYR:HD1	1.62	0.82
2:B:246:LYS:C	2:B:246:LYS:HA	2.01	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:HD22	2:B:516:ASN:H	1.25	0.82
1:A:982:THR:HG22	1:A:985:ASP:H	1.44	0.82
1:A:69:THR:C	1:A:69:THR:HA	2.01	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:956:THR:HA	2:B:961:LEU:O	1.80	0.82
1:A:829:VAL:CG2	1:A:829:VAL:CG1	2.58	0.82
7:I:120:GLN:O	7:I:121:PHE:CB	2.27	0.81
1:A:567:LYS:CD	1:A:568:PRO:HD3	2.09	0.81
1:A:1151:GLU:CG	7:I:45:ARG:HD2	2.10	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:NZ	2:B:625:LYS:CD	2.44	0.81
6:H:130:ARG:O	6:H:130:ARG:CD	2.29	0.81
1:A:46:THR:CA	1:A:46:THR:HB	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
8:J:10:CYS:SG	8:J:45:CYS:SG	2.79	0.80
10:L:64:LEU:CD1	10:L:64:LEU:HG	2.09	0.80
1:A:1385:THR:C	1:A:1385:THR:CG2	2.55	0.80
6:H:25:ARG:NH2	6:H:41:ASP:OD2	2.13	0.80
7:I:3:THR:CG2	7:I:3:THR:CA	2.60	0.80
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.63	0.80
2:B:1058:LEU:CD1	2:B:1058:LEU:CD2	2.58	0.80
1:A:858:ASN:C	1:A:858:ASN:HD22	1.87	0.80
1:A:1063:MET:O	1:A:1064:VAL:C	2.23	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
3:C:86:CYS:SG	3:C:88:CYS:SG	2.80	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
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
10:L:34:CYS:HB3	10:L:51:CYS:HB3	1.63	0.79
7:I:45:ARG:CG	7:I:45:ARG:HH11	1.96	0.79
5:F:123:LYS:NZ	5:F:123:LYS:CD	2.45	0.79
6:H:139:ASN:CB	6:H:139:ASN:HA	2.09	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
1:A:122:MET:HE1	1:A:138:ILE:HD13	1.65	0.79
2:B:1222:ARG:HH11	2:B:1222:ARG:HB2	1.47	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:89:LEU:C	6:H:91:ASP:H	1.89	0.79
4:E:28:TYR:CZ	4:E:75:MET:HE2	2.17	0.79
2:B:1220:ARG:O	2:B:1222:ARG:CD	2.31	0.79
6:H:103:LYS:NZ	6:H:105:GLU:CD	2.39	0.79
2:B:680:THR:HG22	2:B:682:SER:H	1.48	0.79
2:B:502:ILE:HA	2:B:502:ILE:HD13	1.63	0.78
2:B:185:THR:HG23	2:B:188:ASP:OD2	1.83	0.78
2:B:915:THR:CA	2:B:915:THR:HB	2.10	0.78
4:E:207:ARG:CG	4:E:207:ARG:NE	2.46	0.78
7:I:16:PRO:HG3	7:I:27:PHE:CE2	2.17	0.78
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.19	0.78
1:A:518:LYS:CD	1:A:518:LYS:NZ	2.46	0.78
4:E:47:CYS:SG	4:E:52:ARG:O	2.40	0.78
1:A:503:GLN:HE22	5:F:90:ARG:NH2	1.81	0.78
1:A:752:LYS:CE	2:B:1019:SER:OG	2.30	0.78
2:B:134:LYS:HE3	2:B:134:LYS:HB2	1.66	0.78
6:H:103:LYS:CG	6:H:105:GLU:OE1	2.32	0.78
2:B:323:VAL:C	2:B:324:ILE:HD12	2.08	0.78
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.64	0.78
3:C:199:LYS:CG	3:C:199:LYS:CA	2.62	0.78
1:A:920:LEU:HD22	1:A:921:GLY:N	1.99	0.78
1:A:1012:ARG:CG	1:A:1012:ARG:NE	2.45	0.78
2:B:129:PHE:CE2	2:B:166:PHE:HA	2.19	0.78
2:B:1222:ARG:HG2	2:B:1222:ARG:NH1	1.98	0.78
10:L:34:CYS:HB3	10:L:51:CYS:CB	2.14	0.78
2:B:561:TRP:O	2:B:590:HIS:HE1	1.66	0.78
2:B:1025:HIS:CE1	2:B:1090:THR:HG21	2.19	0.77
3:C:8:VAL:CG1	3:C:9:LYS:H	1.96	0.77
5:F:135:ARG:CG	5:F:135:ARG:NE	2.47	0.77
1:A:567:LYS:HD2	1:A:568:PRO:HD3	1.63	0.77
3:C:25:VAL:HG11	3:C:29:MET:HG2	1.67	0.77
4:E:116:ILE:CD1	4:E:116:ILE:CB	2.61	0.77
7:I:5:ARG:HD3	7:I:36:GLU:OE2	1.84	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:NZ	2:B:270:LYS:CD	2.48	0.77
2:B:744:HIS:HD2	2:B:746:SER:H	1.32	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
2:B:871:THR:CB	2:B:871:THR:HA	2.09	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:116:ILE:H	4:E:116:ILE:HD12	1.50	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:237:VAL:HG12	2:B:238:ALA:N	1.98	0.77
2:B:986:GLN:CG	2:B:986:GLN:CA	2.62	0.77
2:B:944:THR:CG2	2:B:944:THR:CA	2.63	0.77
2:B:1166:CYS:O	2:B:1168:LEU:HG	1.85	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
2:B:952:VAL:HG22	2:B:966:VAL:HG22	1.66	0.76
1:A:282:ASN:C	1:A:283:GLY:O	2.23	0.76
2:B:367:LEU:CD1	2:B:367:LEU:CB	2.63	0.76
2:B:510:LYS:N	2:B:511:PRO:CD	2.48	0.76
4:E:116:ILE:HD12	4:E:116:ILE:N	2.01	0.76
9:K:11:LEU:CD1	9:K:11:LEU:HG	2.10	0.76
10:L:65:VAL:CG2	10:L:65:VAL:CA	2.59	0.76
1:A:121:LEU:CD1	1:A:121:LEU:HG	2.14	0.76
1:A:547:LEU:HB3	9:K:58:PHE:CE1	2.21	0.76
6:H:13:SER:N	6:H:27:GLU:O	2.19	0.76
6:H:93:TYR:HB3	6:H:144:ILE:O	1.85	0.76
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.18	0.76
6:H:32:THR:CB	6:H:32:THR:HA	2.12	0.76
1:A:55:ASP:C	1:A:57:ARG:H	1.93	0.76
1:A:107:CYS:SG	1:A:148:CYS:SG	2.83	0.75
1:A:413:ILE:HD13	1:A:413:ILE:N	1.99	0.75
1:A:148:CYS:HG	12:A:3006:ZN:ZN	0.43	0.75
2:B:129:PHE:HE2	2:B:166:PHE:HB2	1.50	0.75
2:B:358:LYS:CG	2:B:358:LYS:CA	2.64	0.75
2:B:1101:ASP:C	2:B:1101:ASP:HA	2.08	0.75
2:B:1198:TYR:CZ	2:B:1201:LYS:NZ	2.54	0.75
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.68	0.75
2:B:100:PRO:HD2	2:B:180:TYR:CZ	2.21	0.75
2:B:228:LYS:CG	2:B:228:LYS:CA	2.65	0.75
2:B:999:MET:HB3	2:B:1000:PRO:HD2	1.68	0.75
10:L:34:CYS:SG	10:L:36:SER:OG	2.43	0.75
2:B:933:SER:C	2:B:933:SER:HA	2.09	0.75
1:A:40:THR:CA	1:A:40:THR:HB	2.11	0.74
2:B:654:ARG:H	2:B:657:HIS:HD2	1.35	0.74
2:B:1154:ALA:CB	2:B:1154:ALA:HA	2.13	0.74
1:A:61:ILE:CG2	1:A:61:ILE:HB	2.14	0.74
1:A:886:ILE:HD12	1:A:943:LEU:HB3	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.85	0.74
9:K:102:LYS:O	9:K:106:GLU:HB2	1.87	0.74
1:A:351:THR:CG2	2:B:1103:ILE:CG1	2.65	0.74
1:A:535:THR:CG2	1:A:616:VAL:HA	2.16	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:166:GLY:O	1:A:167:CYS:HB3	1.86	0.74
2:B:846:ILE:CD1	2:B:974:PRO:HB2	2.18	0.74
2:B:955:THR:CG2	10:L:55:ILE:HA	2.18	0.74
2:B:1152:MET:HA	2:B:1152:MET:CE	2.18	0.74
4:E:36:GLU:O	4:E:37:LEU:C	2.29	0.74
5:F:133:VAL:HG22	5:F:147:SER:HA	1.70	0.74
8:J:10:CYS:HG	12:J:3001:ZN:ZN	0.43	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
6:H:63:LEU:C	6:H:90:ALA:CB	2.60	0.74
10:L:48:CYS:C	10:L:48:CYS:HA	2.09	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
1:A:711:ARG:NE	7:I:95:THR:HG22	2.01	0.73
6:H:4:THR:O	6:H:5:LEU:CD2	2.35	0.73
2:B:1152:MET:HA	2:B:1152:MET:HE3	1.69	0.73
1:A:108:MET:H	1:A:171:GLN:HE22	1.36	0.73
1:A:567:LYS:CB	6:H:95:TYR:HA	2.18	0.73
2:B:1222:ARG:NH1	2:B:1222:ARG:CG	2.48	0.73
2:B:1166:CYS:O	2:B:1167:GLY:C	2.24	0.73
4:E:12:LEU:CD2	4:E:58:MET:SD	2.73	0.73
4:E:117:THR:OG1	4:E:120:ALA:HB2	1.88	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
1:A:567:LYS:HE2	6:H:95:TYR:CE2	2.22	0.73
2:B:789:MET:CE	2:B:965:LYS:HB3	2.17	0.73
3:C:8:VAL:CG1	3:C:9:LYS:N	2.51	0.73
4:E:50:MET:CE	4:E:50:MET:SD	2.77	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1385:THR:C	1:A:1385:THR:HA	2.06	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
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:31:SER:CB	1:A:83:HIS:CD2	2.67	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
2:B:1163:CYS:SG	2:B:1166:CYS:SG	2.88	0.72
4:E:63:ASN:O	4:E:64:PRO:O	2.08	0.72
1:A:369:SER:H	9:K:2:ASN:HD21	1.38	0.72
1:A:1080:THR:CG2	1:A:1080:THR:HB	2.13	0.72
2:B:1166:CYS:O	2:B:1168:LEU:N	2.22	0.72
6:H:136:LYS:C	6:H:136:LYS:HA	2.08	0.72
1:A:55:ASP:N	1:A:56:PRO:HD3	2.04	0.72
2:B:624:LEU:C	2:B:624:LEU:HD12	2.14	0.72
7:I:4:PHE:CZ	7:I:13:MET:HE2	2.22	0.72
2:B:25:ILE:CG2	2:B:25:ILE:CG1	2.67	0.72
2:B:227:LYS:CE	2:B:227:LYS:CG	2.68	0.72
6:H:59:ILE:HG22	6:H:60:ALA:H	1.54	0.72
1:A:571:LEU:CD2	1:A:571:LEU:HG	2.16	0.72
1:A:1148:ILE:CD1	1:A:1148:ILE:CB	2.67	0.72
1:A:423:ASP:CG	1:A:423:ASP:O	2.33	0.72
2:B:368:GLU:CB	2:B:368:GLU:C	2.63	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
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
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.26	0.71
1:A:351:THR:HG23	2:B:1103:ILE:HG12	1.70	0.71
1:A:711:ARG:HE	7:I:95:THR:CG2	2.02	0.71
2:B:424:LEU:HD23	2:B:424:LEU:C	2.15	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
5:F:77:ASP:O	5:F:78:GLN:HB2	1.89	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:30:ARG:CG	7:I:30:ARG:NE	2.54	0.71
7:I:71:SER:O	7:I:83:ASN:ND2	2.24	0.71
9:K:56:VAL:CA	9:K:56:VAL:CG1	2.67	0.71
1:A:120:GLU:HG2	1:A:123:ARG:HH22	1.56	0.71
1:A:35:ILE:H	1:A:35:ILE:HD12	1.54	0.71
1:A:11:LEU:HD11	2:B:1195:HIS:CD2	2.26	0.71
3:C:196:ASP:CB	3:C:199:LYS:HG3	2.21	0.71
2:B:1128:LEU:HG	2:B:1128:LEU:O	1.89	0.71
3:C:50:GLU:HB3	10:L:64:LEU:CD1	2.20	0.71
2:B:169:ARG:O	2:B:457:LEU:HD12	1.89	0.70
2:B:1150:ARG:NH1	2:B:1150:ARG:CD	2.54	0.70
2:B:846:ILE:CA	2:B:846:ILE:HB	2.11	0.70
2:B:436:VAL:CA	2:B:436:VAL:HB	2.15	0.70
2:B:914:LYS:H	2:B:938:SER:HB2	1.56	0.70
1:A:101:LYS:NZ	1:A:101:LYS:CD	2.53	0.70
1:A:903:ASN:HD22	1:A:905:ASP:H	1.40	0.70
1:A:1162:VAL:O	1:A:1162:VAL:HG12	1.92	0.70
2:B:768:THR:C	2:B:768:THR:HG22	2.16	0.70
2:B:1182:CYS:O	2:B:1183:LYS:C	2.34	0.70
3:C:86:CYS:HG	12:C:3002:ZN:ZN	1.06	0.70
1:A:212:LYS:CD	1:A:212:LYS:CB	2.70	0.70
1:A:1081:LEU:CD2	1:A:1081:LEU:CD1	2.69	0.70
2:B:129:PHE:CE2	2:B:166:PHE:HB2	2.25	0.70
2:B:498:THR:HG21	2:B:537:LYS:HB2	1.73	0.70
2:B:542:MET:HG3	2:B:747:MET:HE3	1.73	0.70
2:B:1222:ARG:HH11	2:B:1222:ARG:CB	2.03	0.70
6:H:32:THR:CG2	6:H:33:GLN:OE1	2.40	0.70
1:A:99:ILE:HG13	1:A:234:MET:HE3	1.72	0.70
2:B:662:MET:CE	2:B:662:MET:CG	2.70	0.70
2:B:1195:HIS:C	2:B:1196:ILE:HG23	2.16	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
4:E:28:TYR:CE1	4:E:75:MET:CE	2.75	0.70
10:L:40:LEU:CD2	10:L:40:LEU:CD1	2.69	0.70
1:A:243:PRO:O	1:A:243:PRO:HG2	1.91	0.70
1:A:1364:ASN:ND2	1:A:1366:ARG:CD	2.54	0.70
3:C:252:GLN:HE22	9:K:99:GLY:HA2	1.56	0.70
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.21	0.70
2:B:446:LEU:CD2	2:B:446:LEU:CD1	2.70	0.70
2:B:999:MET:CG	2:B:999:MET:HE2	2.12	0.70
1:A:187:LYS:CB	1:A:194:ALA:HB3	2.22	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:GLU:O	1:A:210:ILE:HD13	1.92	0.69
1:A:535:THR:HG23	1:A:616:VAL:HA	1.72	0.69
2:B:515:HIS:H	2:B:518:HIS:CD2	2.03	0.69
2:B:723:VAL:CG2	2:B:723:VAL:HB	2.16	0.69
2:B:724:ASP:O	2:B:725:PRO:C	2.31	0.69
8:J:1:MET:HE3	8:J:1:MET:HB2	1.74	0.69
9:K:111:LEU:N	9:K:111:LEU:HD23	2.07	0.69
6:H:103:LYS:HZ2	6:H:105:GLU:CD	2.00	0.69
1:A:353:ILE:HD13	1:A:487:MET:SD	2.31	0.69
1:A:636:GLU:OE2	1:A:962:ARG:HD2	1.92	0.69
2:B:323:VAL:O	2:B:323:VAL:HG12	1.92	0.69
6:H:130:ARG:C	6:H:130:ARG:CD	2.59	0.69
1:A:741:ASN:HD22	1:A:741:ASN:C	2.00	0.69
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.27	0.69
1:A:838:GLN:CB	1:A:838:GLN:CD	2.65	0.69
6:H:59:ILE:H	6:H:59:ILE:HD12	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
1:A:1004:ASN:CG	4:E:167:ARG:HG3	2.17	0.69
1:A:1385:THR:C	1:A:1385:THR:HG22	2.18	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: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
7:I:65:ASP:C	7:I:65:ASP:OD1	2.32	0.69
1:A:1213:GLY:HA3	1:A:1228:TRP:CZ3	2.28	0.69
2:B:736:THR:CG2	2:B:736:THR:CA	2.67	0.69
6:H:26:ILE:HD12	6:H:42:ILE:HD12	1.75	0.69
6:H:131:ASN:CB	6:H:131:ASN:HA	2.11	0.69
1:A:42:ASP:OD2	1:A:47:ARG:CA	2.41	0.69
1:A:1064:VAL:C	1:A:1066:VAL:H	1.96	0.69
2:B:324:ILE:HD12	2:B:324:ILE:N	2.08	0.69
6:H:18:GLY:O	6:H:19:ARG:HB2	1.93	0.69
1:A:31:SER:HB3	1:A:83:HIS:HD2	1.58	0.68
2:B:94:LYS:CG	2:B:94:LYS:CA	2.69	0.68
2:B:1166:CYS:SG	2:B:1182:CYS:SG	2.91	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
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.28	0.68
5:F:80:ALA:CB	5:F:80:ALA:N	2.51	0.68
6:H:113:ALA:HA	6:H:125:LEU:O	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:1:MET:C	8:J:2:ILE:HD12	2.19	0.68
1:A:46:THR:CB	1:A:46:THR:C	2.63	0.68
2:B:217:ARG:HD3	2:B:407:ASP:OD2	1.93	0.68
2:B:345:LYS:CE	2:B:345:LYS:CG	2.72	0.68
2:B:578:THR:OG1	2:B:593:PRO:HG3	1.93	0.68
1:A:1146:VAL:O	1:A:1146:VAL:CG1	2.38	0.68
2:B:542:MET:HG3	2:B:747:MET:CE	2.23	0.68
4:E:7:ARG:O	4:E:8:ASN:C	2.36	0.68
7:I:35:VAL:HG23	7:I:35:VAL:O	1.81	0.68
1:A:827:THR:CG2	1:A:827:THR:CA	2.69	0.68
2:B:227:LYS:CD	2:B:227:LYS:CB	2.68	0.68
2:B:431:TYR:HD2	2:B:431:TYR:O	1.76	0.68
2:B:916:THR:HB	2:B:935:ARG:HB2	1.76	0.68
1:A:751:SER:OG	2:B:1015:HIS:HE1	1.76	0.68
1:A:931:GLU:CD	1:A:931:GLU:CB	2.67	0.68
2:B:381:MET:CE	2:B:381:MET:HG3	2.22	0.68
5:F:73:ALA:HB2	5:F:143:PHE:CZ	2.28	0.68
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.09	0.67
2:B:282:ILE:HD13	2:B:282:ILE:H	1.59	0.67
2:B:1163:CYS:HB3	2:B:1166:CYS:SG	2.35	0.67
2:B:172:ILE:CD1	2:B:172:ILE:CB	2.71	0.67
1:A:55:ASP:H	1:A:56:PRO:HD3	1.59	0.67
1:A:1146:VAL:O	1:A:1146:VAL:HG13	1.93	0.67
2:B:417:PHE:CD2	2:B:417:PHE:C	2.71	0.67
2:B:772:ALA:O	2:B:775:LYS:HB2	1.94	0.67
4:E:156:LEU:HB3	4:E:160:GLU:HB3	1.75	0.67
5:F:105:ALA:HB1	5:F:106:PRO:HD2	1.76	0.67
10:L:65:VAL:CG2	10:L:65:VAL:HB	2.15	0.67
1:A:32:VAL:CG2	1:A:33:ALA:H	2.02	0.67
3:C:167:HIS:HE1	10:L:70:ARG:O	1.77	0.67
10:L:38:LEU:O	10:L:39:SER:CB	2.42	0.67
1:A:132:LYS:CG	1:A:132:LYS:CE	2.70	0.67
1:A:658:LEU:HD12	1:A:658:LEU:O	1.95	0.67
2:B:98:THR:OG1	2:B:127:GLY:O	2.12	0.67
2:B:1189:ILE:CG2	2:B:1189:ILE:CA	2.72	0.67
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
1:A:912:LEU:HD23	1:A:912:LEU:N	2.10	0.67
2:B:680:THR:HG22	2:B:682:SER:N	2.08	0.67
2:B:789:MET:HE3	2:B:965:LYS:CB	2.22	0.67
2:B:424:LEU:O	2:B:424:LEU:CG	2.43	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:864:LYS:HB3	2:B:872:GLU:H	1.60	0.67
3:C:86:CYS:HG	3:C:95:CYS:HG	0.68	0.67
5:F:76:LYS:CD	5:F:76:LYS:CB	2.72	0.67
1:A:199:LEU:CD1	1:A:199:LEU:CD2	2.72	0.67
1:A:840:ARG:CG	1:A:840:ARG:NE	2.57	0.67
1:A:150:THR:HA	1:A:166:GLY:HA2	1.75	0.67
1:A:566:ILE:CG2	1:A:566:ILE:CA	2.71	0.67
1:A:1109:LYS:CG	1:A:1109:LYS:CA	2.71	0.67
2:B:884:ARG:CG	2:B:884:ARG:NE	2.57	0.67
3:C:19:ASP:C	3:C:19:ASP:OD1	2.33	0.67
6:H:83:GLN:C	6:H:85:GLY:N	2.48	0.67
10:L:25:ALA:CB	10:L:25:ALA:C	2.65	0.67
1:A:199:LEU:CD1	1:A:199:LEU:HG	2.15	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
2:B:736:THR:CG2	2:B:736:THR:OG1	2.42	0.66
4:E:116:ILE:HG22	4:E:120:ALA:CB	2.25	0.66
1:A:55:ASP:O	1:A:55:ASP:OD1	2.12	0.66
1:A:216:VAL:HG22	1:A:219:PHE:CZ	2.30	0.66
2:B:431:TYR:O	2:B:431:TYR:CD2	2.48	0.66
3:C:18:VAL:HG23	3:C:240:VAL:HG11	1.77	0.66
9:K:101:LEU:C	9:K:101:LEU:CD1	2.68	0.66
1:A:858:ASN:C	1:A:858:ASN:ND2	2.53	0.66
1:A:1350:LYS:CD	1:A:1350:LYS:CB	2.72	0.66
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.31	0.66
3:C:86:CYS:SG	3:C:92:CYS:SG	2.94	0.66
4:E:66:GLU:O	4:E:67:GLU:C	2.35	0.66
4:E:127:ILE:N	4:E:128:PRO:HD3	2.10	0.66
8:J:1:MET:HG3	8:J:1:MET:HE2	1.77	0.66
2:B:90:ILE:N	2:B:90:ILE:CD1	2.59	0.66
2:B:393:LYS:CD	2:B:393:LYS:CB	2.72	0.66
6:H:6:PHE:CG	6:H:7:ASP:N	2.60	0.66
6:H:89:LEU:O	6:H:91:ASP:N	2.28	0.66
1:A:55:ASP:N	1:A:56:PRO:HD2	2.10	0.66
1:A:966:ASN:O	1:A:967:ALA:C	2.39	0.66
2:B:1189:ILE:CG2	2:B:1189:ILE:C	2.67	0.66
3:C:88:CYS:HG	3:C:95:CYS:HG	1.36	0.66
7:I:45:ARG:HG2	7:I:45:ARG:NH1	2.08	0.66
1:A:72:GLU:OE2	2:B:1175:LEU:HD11	1.96	0.66
2:B:106:ASP:CB	2:B:106:ASP:OD1	2.41	0.66
2:B:228:LYS:O	2:B:261:ARG:NH2	2.21	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:GLU:HB2	1:A:156:ASP:OD2	1.96	0.66
2:B:705:MET:CG	2:B:705:MET:HE3	2.25	0.66
3:C:133:ILE:C	3:C:134:ILE:HG12	2.19	0.66
3:C:181:ASP:N	3:C:182:PRO:CD	2.58	0.66
6:H:63:LEU:HB2	6:H:90:ALA:HB2	1.76	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
1:A:601:LYS:CD	1:A:601:LYS:NZ	2.59	0.66
2:B:137:TYR:CG	2:B:137:TYR:HB2	2.21	0.66
2:B:360:PHE:O	2:B:361:LEU:C	2.33	0.66
2:B:1012:ILE:C	2:B:1012:ILE:HD12	2.21	0.66
4:E:191:LYS:O	4:E:192:ARG:C	2.36	0.66
2:B:305:VAL:CG1	2:B:305:VAL:CA	2.71	0.66
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.03	0.65
2:B:129:PHE:HD2	2:B:165:VAL:C	2.04	0.65
2:B:890:TYR:OH	2:B:936:ASP:OD1	2.11	0.65
4:E:71:LYS:NZ	4:E:160:GLU:OE2	2.24	0.65
1:A:64:ASN:O	1:A:66:LYS:N	2.29	0.65
1:A:531:ILE:O	1:A:535:THR:HB	1.95	0.65
1:A:1166:ASP:O	1:A:1170:ILE:HD13	1.96	0.65
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.77	0.65
3:C:239:PRO:O	3:C:242:GLN:HB2	1.97	0.65
7:I:45:ARG:CD	7:I:45:ARG:CB	2.71	0.65
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.78	0.65
1:A:903:ASN:HD22	1:A:905:ASP:N	1.94	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
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.77	0.65
6:H:105:GLU:CD	6:H:105:GLU:H	2.05	0.65
6:H:123:MET:HE1	6:H:142:LEU:HD13	1.77	0.65
1:A:53:LEU:CD1	1:A:53:LEU:HG	2.15	0.65
1:A:555:ASP:OD1	9:K:26:LYS:NZ	2.30	0.65
4:E:94:LYS:CG	4:E:94:LYS:CE	2.75	0.65
4:E:117:THR:OG1	4:E:120:ALA:CB	2.45	0.65
1:A:551:TYR:CD2	9:K:62:LYS:HD3	2.32	0.65
1:A:1236:LEU:C	1:A:1237:ILE:HD12	2.20	0.65
4:E:76:GLY:HA3	4:E:106:GLN:HB3	1.77	0.65
4:E:213:ILE:CD1	4:E:213:ILE:CB	2.71	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:89:PRO:HB2	1:A:204:THR:CG2	2.26	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:CG	6:H:95:TYR:HA	2.25	0.65
1:A:751:SER:CB	1:A:751:SER:HG	2.07	0.65
2:B:213:ILE:HD12	2:B:213:ILE:N	2.10	0.65
1:A:208:LEU:HB2	1:A:235:ILE:HG21	1.79	0.65
2:B:294:ASP:N	7:I:12:ASN:HD22	1.92	0.65
2:B:916:THR:HB	2:B:935:ARG:CB	2.25	0.65
2:B:1097:HIS:CB	2:B:1097:HIS:N	2.57	0.65
1:A:894:GLU:HB2	1:A:933:TYR:OH	1.96	0.65
1:A:903:ASN:HD22	1:A:903:ASN:C	2.05	0.65
1:A:1293:SER:HB2	1:A:1294:PRO:HD2	1.78	0.65
2:B:431:TYR:O	2:B:432:MET:HG3	1.97	0.65
2:B:995:ARG:HD2	2:B:997:GLU:OE2	1.97	0.65
2:B:1022:THR:HG23	2:B:1022:THR:O	1.97	0.65
4:E:71:LYS:CG	4:E:71:LYS:CA	2.72	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
1:A:752:LYS:CE	1:A:752:LYS:CG	2.74	0.64
2:B:789:MET:CE	2:B:789:MET:CG	2.75	0.64
6:H:89:LEU:C	6:H:91:ASP:N	2.54	0.64
10:L:65:VAL:CG2	10:L:65:VAL:N	2.61	0.64
1:A:46:THR:HB	1:A:46:THR:O	1.96	0.64
1:A:1064:VAL:O	1:A:1065:GLY:CA	2.44	0.64
2:B:906:SER:O	2:B:907:GLY:C	2.40	0.64
4:E:52:ARG:CG	4:E:53:PRO:HD3	2.27	0.64
6:H:51:ALA:CB	6:H:51:ALA:HA	2.16	0.64
4:E:28:TYR:CE1	4:E:75:MET:HE2	2.33	0.64
1:A:23:SER:O	1:A:27:VAL:HG23	1.96	0.64
1:A:1194:ARG:CB	1:A:1194:ARG:CD	2.74	0.64
2:B:328:GLU:CG	2:B:328:GLU:CA	2.73	0.64
2:B:516:ASN:H	2:B:516:ASN:ND2	1.85	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:O	2:B:323:VAL:CG1	2.46	0.64
1:A:551:TYR:CE2	9:K:62:LYS:HD3	2.33	0.64
1:A:66:LYS:CB	1:A:66:LYS:CD	2.74	0.64
1:A:1208:THR:O	1:A:1209:MET:C	2.36	0.64
2:B:645:SER:OG	2:B:646:LEU:N	2.27	0.64
2:B:864:LYS:HG3	2:B:865:LYS:N	2.12	0.64
2:B:1148:LYS:CD	2:B:1148:LYS:NZ	2.60	0.64
10:L:32:ALA:HB2	10:L:55:ILE:HG22	1.79	0.64
2:B:110:HIS:C	2:B:110:HIS:HA	2.11	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1058:LEU:CD1	2:B:1058:LEU:CB	2.72	0.64
1:A:356:ASP:OD2	1:A:469:ARG:HD3	1.98	0.64
1:A:703:THR:CG2	1:A:703:THR:CA	2.77	0.64
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.61	0.64
4:E:157:SER:O	4:E:160:GLU:HB2	1.97	0.64
10:L:38:LEU:HD23	10:L:39:SER:H	1.62	0.64
2:B:167:ILE:HG22	2:B:167:ILE:O	1.98	0.63
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
9:K:46:ILE:O	9:K:47:ARG:C	2.32	0.63
1:A:107:CYS:HB2	1:A:148:CYS:HB2	1.79	0.63
1:A:1290:LYS:HA	1:A:1299:VAL:O	1.98	0.63
1:A:26:GLU:HA	1:A:29:ALA:HB3	1.79	0.63
1:A:909:ASP:CG	1:A:910:PRO:HD2	2.22	0.63
1:A:1176:LEU:CD2	1:A:1176:LEU:HG	2.14	0.63
2:B:999:MET:CG	2:B:999:MET:HE3	2.12	0.63
3:C:40:GLU:OE1	3:C:254:LYS:NZ	2.31	0.63
9:K:56:VAL:CA	9:K:56:VAL:HB	2.13	0.63
3:C:100:THR:HG22	3:C:101:LEU:N	2.14	0.63
3:C:253:LYS:CE	3:C:253:LYS:CG	2.71	0.63
2:B:653:VAL:O	2:B:654:ARG:HD3	1.98	0.63
1:A:601:LYS:CD	1:A:601:LYS:CB	2.69	0.63
1:A:720:ARG:O	1:A:724:GLU:HB3	1.98	0.63
2:B:1097:HIS:ND1	2:B:1097:HIS:C	2.57	0.63
3:C:240:VAL:C	3:C:242:GLN:N	2.46	0.63
1:A:1151:GLU:HG3	7:I:45:ARG:HD2	1.80	0.63
2:B:775:LYS:CG	2:B:775:LYS:CA	2.74	0.63
3:C:167:HIS:CD2	3:C:169:LYS:H	2.10	0.63
4:E:44:ALA:CB	4:E:44:ALA:C	2.68	0.63
4:E:156:LEU:N	4:E:156:LEU:HD23	2.13	0.63
6:H:142:LEU:HG	6:H:143:LEU:N	2.12	0.63
8:J:7:CYS:HA	8:J:49:MET:HE3	1.79	0.63
1:A:599:SER:O	1:A:600:PRO:C	2.37	0.63
6:H:63:LEU:C	6:H:63:LEU:HA	2.09	0.63
2:B:97:VAL:HG12	2:B:178:ASN:HD21	1.62	0.63
2:B:104:GLU:HB2	2:B:108:VAL:HA	1.80	0.63
2:B:381:MET:HE3	2:B:381:MET:CG	2.21	0.63
2:B:531:GLN:CD	2:B:531:GLN:H	2.07	0.63
2:B:595:ARG:CD	2:B:595:ARG:CB	2.77	0.63
2:B:915:THR:CB	2:B:915:THR:C	2.67	0.63
2:B:1172:ILE:CG2	2:B:1172:ILE:HG12	2.29	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:25:ALA:CB	10:L:25:ALA:HA	2.14	0.63
10:L:26:THR:CG2	10:L:27:LEU:H	2.12	0.63
1:A:860:LEU:CD2	1:A:860:LEU:CB	2.76	0.62
4:E:117:THR:C	4:E:119:SER:N	2.54	0.62
7:I:10:CYS:SG	7:I:29:CYS:SG	2.97	0.62
10:L:38:LEU:HD21	10:L:40:LEU:HB2	1.80	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
2:B:863:GLU:OE1	2:B:962:LYS:HD3	1.99	0.62
9:K:103:THR:C	9:K:105:PHE:N	2.52	0.62
1:A:274:ILE:CA	1:A:274:ILE:HB	2.16	0.62
2:B:435:THR:C	2:B:435:THR:HA	2.11	0.62
2:B:987:LYS:NZ	2:B:987:LYS:CD	2.62	0.62
1:A:203:SER:OG	1:A:206:GLU:CG	2.46	0.62
1:A:1039:LYS:HG3	1:A:1039:LYS:O	1.99	0.62
1:A:1080:THR:CB	1:A:1080:THR:N	2.61	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
2:B:662:MET:CE	2:B:662:MET:HG3	2.30	0.62
2:B:768:THR:C	2:B:768:THR:CG2	2.72	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
1:A:571:LEU:CD2	1:A:571:LEU:CD1	2.72	0.62
1:A:982:THR:HB	1:A:985:ASP:CG	2.24	0.62
1:A:1004:ASN:OD1	4:E:167:ARG:HG3	1.98	0.62
1:A:1366:ARG:HB3	1:A:1366:ARG:HH11	1.63	0.62
2:B:552:MET:O	2:B:553:PRO:C	2.34	0.62
2:B:775:LYS:CB	2:B:775:LYS:CD	2.75	0.62
2:B:958:GLN:HG2	2:B:958:GLN:H	1.65	0.62
1:A:446:ARG:HB2	1:A:487:MET:HE3	1.82	0.62
1:A:1242:VAL:C	1:A:1243:VAL:HG12	2.20	0.62
6:H:27:GLU:CA	6:H:28:ALA:N	2.55	0.62
1:A:1165:GLU:C	1:A:1167:GLU:H	2.05	0.62
7:I:64:SER:O	7:I:66:PRO:HD3	1.99	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
4:E:58:MET:O	4:E:59:SER:C	2.43	0.62
6:H:32:THR:HG22	6:H:33:GLN:CD	2.24	0.62
1:A:133:LYS:O	1:A:136:ALA:HB3	1.99	0.62
1:A:1222:ASN:CB	1:A:1222:ASN:HA	2.13	0.62
1:A:719:VAL:O	1:A:719:VAL:HG12	1.95	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:SER:HG	1:A:206:GLU:HG2	1.65	0.61
1:A:1055:ARG:CD	1:A:1055:ARG:CB	2.76	0.61
2:B:341:LEU:HD12	2:B:342:GLY:H	1.65	0.61
2:B:381:MET:CG	2:B:381:MET:HE2	2.21	0.61
1:A:752:LYS:NZ	2:B:1019:SER:N	2.47	0.61
2:B:25:ILE:HD11	2:B:651:LEU:HD12	1.80	0.61
4:E:44:ALA:CB	4:E:45:LYS:N	2.63	0.61
6:H:6:PHE:CD2	6:H:6:PHE:C	2.73	0.61
1:A:1348:LEU:HG	1:A:1372:VAL:CG2	2.30	0.61
2:B:1166:CYS:CB	2:B:1185:CYS:SG	2.87	0.61
6:H:138:GLU:C	6:H:140:ALA:N	2.51	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: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
2:B:1128:LEU:C	2:B:1128:LEU:CD1	2.53	0.61
4:E:91:LYS:CB	4:E:91:LYS:CD	2.74	0.61
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:1077:THR:HG22	1:A:1078:GLN:NE2	2.16	0.61
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	2.00	0.61
1:A:1259:MET:SD	1:A:1259:MET:CB	2.89	0.61
2:B:127:GLY:HA2	2:B:168:GLY:O	2.00	0.61
3:C:120:ILE:CD1	3:C:120:ILE:HB	2.30	0.61
1:A:567:LYS:CD	1:A:567:LYS:HE3	2.18	0.61
1:A:1100:ARG:O	1:A:1103:GLU:HB3	2.01	0.61
1:A:1445:ILE:CD1	1:A:1445:ILE:CB	2.77	0.61
7:I:1:MET:CB	7:I:1:MET:HA	2.18	0.61
1:A:120:GLU:HG2	1:A:123:ARG:NH2	2.15	0.61
1:A:587:HIS:CE1	1:A:609:ASP:H	2.19	0.61
2:B:129:PHE:CE2	2:B:166:PHE:CB	2.83	0.61
2:B:846:ILE:CB	2:B:846:ILE:C	2.71	0.61
6:H:84:ALA:O	6:H:88:SER:OG	2.09	0.61
1:A:217:LYS:CD	1:A:217:LYS:NZ	2.63	0.61
2:B:266:ALA:CB	2:B:266:ALA:C	2.73	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
1:A:545:GLN:O	1:A:546:VAL:C	2.36	0.61
1:A:901:LEU:HD22	1:A:919:ILE:HD13	1.83	0.61
1:A:914:GLU:C	1:A:916:GLY:H	2.08	0.61
2:B:307:ASP:O	2:B:308:TRP:C	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1002:THR:CG2	2:B:1006:ILE:HB	2.31	0.61
2:B:1221:SER:OG	5:F:72:LYS:HD2	2.00	0.61
6:H:7:ASP:OD1	6:H:8:ASP:N	2.34	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
1:A:1208:THR:OG1	1:A:1211:GLN:CD	2.44	0.60
1:A:1383:SER:OG	1:A:1384:VAL:N	2.32	0.60
2:B:282:ILE:H	2:B:282:ILE:CD1	2.14	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
6:H:32:THR:CA	6:H:32:THR:CG2	2.72	0.60
8:J:1:MET:HE3	8:J:1:MET:CA	2.30	0.60
1:A:595:THR:CG2	1:A:596:THR:N	2.64	0.60
1:A:1098:VAL:N	1:A:1099:PRO:CD	2.64	0.60
2:B:39:ARG:CB	2:B:39:ARG:CD	2.75	0.60
2:B:428:ILE:HG12	2:B:448:ILE:CD1	2.30	0.60
2:B:705:MET:CG	2:B:705:MET:HE2	2.25	0.60
4:E:153:HIS:CE1	4:E:184:VAL:HG11	2.36	0.60
1:A:1450:LEU:CD2	1:A:1450:LEU:HG	2.22	0.60
2:B:120:ARG:NH2	2:B:956:THR:O	2.29	0.60
2:B:193:LYS:CE	2:B:193:LYS:CG	2.77	0.60
2:B:624:LEU:HD12	2:B:625:LYS:N	2.16	0.60
6:H:111:LEU:CD1	6:H:111:LEU:HG	2.17	0.60
4:E:6:GLU:OE2	4:E:43:LYS:NZ	2.34	0.60
4:E:127:ILE:H	4:E:128:PRO:HD3	1.65	0.60
10:L:43:THR:CB	10:L:43:THR:C	2.72	0.60
1:A:567:LYS:HD3	6:H:95:TYR:CD2	2.34	0.60
1:A:1226:VAL:HG12	1:A:1227:ILE:N	2.01	0.60
1:A:1265:ASN:O	1:A:1266:THR:C	2.44	0.60
1:A:1283:VAL:HG12	1:A:1284:MET:O	2.01	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
9:K:110:ASN:CB	9:K:110:ASN:ND2	2.60	0.60
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.00	0.60
6:H:56:THR:HG21	6:H:145:ARG:NE	2.16	0.60
9:K:110:ASN:CG	9:K:110:ASN:CA	2.71	0.60
1:A:1166:ASP:OD2	1:A:1239:ARG:NH2	2.31	0.60
2:B:961:LEU:CD1	2:B:961:LEU:CD2	2.76	0.60
2:B:1177:HIS:HB2	2:B:1179:GLN:NE2	2.17	0.60
6:H:103:LYS:HG2	6:H:105:GLU:CD	2.26	0.60
1:A:605:MET:CE	1:A:607:ILE:HG13	2.32	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:GLY:N	1:A:674:PRO:HD2	2.17	0.60
1:A:1239:ARG:CG	1:A:1239:ARG:NE	2.64	0.60
1:A:1272:THR:CG2	1:A:1272:THR:CA	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:215:SER:OG	1:A:218:ASP:HB2	2.02	0.60
7:I:98:VAL:HG22	7:I:99:LEU:N	2.15	0.60
2:B:55:VAL:HG12	2:B:56:ASP:N	2.17	0.59
3:C:11:ARG:NE	3:C:209:TYR:CE2	2.70	0.59
6:H:17:PRO:HB3	6:H:24:CYS:SG	2.42	0.59
6:H:93:TYR:CD1	6:H:93:TYR:N	2.70	0.59
1:A:1366:ARG:HB3	1:A:1366:ARG:CZ	2.30	0.59
2:B:846:ILE:CB	2:B:846:ILE:N	2.58	0.59
6:H:107:VAL:CG1	6:H:107:VAL:CG2	2.76	0.59
10:L:58:LYS:O	10:L:59:ALA:CB	2.33	0.59
1:A:31:SER:HB2	1:A:83:HIS:HD2	1.63	0.59
1:A:947:PHE:CE2	1:A:954:TRP:CE2	2.90	0.59
1:A:1293:SER:CB	1:A:1294:PRO:HD2	2.33	0.59
2:B:28:GLU:CD	2:B:807:ARG:HH22	2.10	0.59
2:B:100:PRO:O	2:B:111:ALA:HA	2.02	0.59
2:B:986:GLN:NE2	2:B:987:LYS:O	2.31	0.59
1:A:567:LYS:CB	6:H:96:VAL:N	2.46	0.59
1:A:588:LEU:C	1:A:588:LEU:CD2	2.70	0.59
2:B:807:ARG:CB	2:B:807:ARG:CD	2.74	0.59
2:B:900:ALA:O	2:B:901:PRO:C	2.40	0.59
2:B:1189:ILE:HG22	2:B:1190:ASP:H	1.66	0.59
3:C:15:LYS:NZ	3:C:15:LYS:CD	2.64	0.59
4:E:123:LEU:O	4:E:126:SER:HB2	2.02	0.59
5:F:109:VAL:HG22	5:F:127:GLU:OE1	2.02	0.59
6:H:7:ASP:OD1	6:H:7:ASP:C	2.45	0.59
10:L:26:THR:CA	10:L:26:THR:HB	2.20	0.59
1:A:567:LYS:HG2	6:H:96:VAL:H	1.66	0.59
6:H:77:ARG:C	6:H:78:SER:O	2.38	0.59
7:I:49:ILE:HG22	7:I:49:ILE:O	2.01	0.59
1:A:325:ILE:C	1:A:327:ALA:H	2.11	0.59
1:A:533:LYS:NZ	1:A:745:GLN:HE22	2.00	0.59
1:A:804:TYR:O	2:B:761:HIS:ND1	2.33	0.59
2:B:768:THR:C	2:B:768:THR:N	2.57	0.59
2:B:1189:ILE:CG2	2:B:1190:ASP:N	2.64	0.59
1:A:274:ILE:CG1	1:A:274:ILE:CG2	2.76	0.59
1:A:1151:GLU:OE2	7:I:45:ARG:HD3	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1359:ASP:CG	1:A:1359:ASP:CA	2.72	0.59
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.85	0.59
2:B:39:ARG:CG	2:B:39:ARG:CA	2.78	0.59
2:B:871:THR:CA	2:B:871:THR:HB	2.16	0.59
3:C:10:ILE:H	3:C:10:ILE:HD13	1.68	0.59
6:H:103:LYS:O	6:H:115:TYR:CD1	2.50	0.59
9:K:78:THR:HG22	9:K:79:GLU:H	1.66	0.59
9:K:111:LEU:CD1	9:K:111:LEU:CB	2.77	0.59
10:L:68:GLU:O	10:L:69:ALA:HB3	2.03	0.59
1:A:751:SER:OG	2:B:1015:HIS:CE1	2.55	0.59
3:C:197:SER:CB	3:C:197:SER:HG	2.08	0.59
3:C:218:PRO:O	3:C:218:PRO:HG2	2.02	0.59
9:K:65:HIS:CD2	9:K:67:PHE:H	2.13	0.59
1:A:50:ILE:HG22	1:A:52:GLY:H	1.65	0.59
1:A:1349:TYR:C	1:A:1349:TYR:CD2	2.80	0.59
2:B:100:PRO:CD	2:B:180:TYR:CE1	2.69	0.59
2:B:999:MET:HE3	2:B:999:MET:HG2	1.83	0.59
2:B:1152:MET:HE3	2:B:1152:MET:CA	2.33	0.59
3:C:92:CYS:SG	3:C:95:CYS:SG	3.00	0.59
1:A:676:MET:SD	1:A:676:MET:CB	2.90	0.59
2:B:428:ILE:CG1	2:B:448:ILE:HD11	2.33	0.59
4:E:41:ASP:O	4:E:42:PHE:C	2.45	0.59
1:A:369:SER:CB	9:K:2:ASN:ND2	2.66	0.58
1:A:446:ARG:CG	1:A:446:ARG:HH11	2.14	0.58
1:A:852:TYR:CE2	5:F:136:ARG:HD3	2.37	0.58
1:A:1134:ILE:HG22	1:A:1306:LEU:HD11	1.84	0.58
1:A:1155:ASP:O	1:A:1241:ARG:NH2	2.33	0.58
1:A:1267:MET:O	1:A:1268:LEU:C	2.41	0.58
2:B:68:THR:HG23	2:B:91:SER:HB3	1.84	0.58
2:B:744:HIS:CD2	2:B:746:SER:H	2.17	0.58
2:B:754:SER:O	2:B:806:THR:HG21	2.03	0.58
4:E:7:ARG:O	4:E:9:ILE:N	2.36	0.58
8:J:1:MET:CE	8:J:1:MET:HB2	2.30	0.58
9:K:65:HIS:HD2	9:K:67:PHE:N	1.97	0.58
1:A:325:ILE:O	1:A:325:ILE:HG22	2.03	0.58
1:A:1027:ALA:O	1:A:1030:ARG:HB2	2.03	0.58
2:B:787:VAL:O	2:B:787:VAL:HG12	2.02	0.58
4:E:43:LYS:CB	4:E:43:LYS:CD	2.78	0.58
6:H:48:PRO:C	6:H:49:VAL:HG23	2.28	0.58
1:A:188:ASP:C	1:A:188:ASP:HA	2.15	0.58
1:A:200:ARG:NH2	1:A:206:GLU:OE2	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1148:ILE:HG21	1:A:1148:ILE:HD13	1.85	0.58
2:B:121:ASN:N	2:B:121:ASN:HD22	2.01	0.58
2:B:357:GLN:NE2	2:B:368:GLU:HG2	2.18	0.58
3:C:97:VAL:HG12	3:C:98:VAL:N	2.14	0.58
1:A:378:GLU:OE1	1:A:434:ARG:HD3	2.03	0.58
1:A:596:THR:HG22	1:A:597:LEU:HD12	1.86	0.58
1:A:938:LYS:CE	1:A:938:LYS:CG	2.81	0.58
2:B:353:LYS:CD	2:B:353:LYS:CB	2.78	0.58
3:C:234:SER:OG	3:C:235:VAL:N	2.35	0.58
6:H:47:PHE:CD2	6:H:47:PHE:O	2.56	0.58
1:A:243:PRO:CB	1:A:245:PRO:HD2	2.33	0.58
2:B:70:ILE:CD1	2:B:70:ILE:CB	2.80	0.58
2:B:110:HIS:C	2:B:110:HIS:CB	2.73	0.58
2:B:549:THR:HG22	2:B:628:THR:HB	1.85	0.58
2:B:870:ILE:CB	2:B:870:ILE:HA	2.20	0.58
2:B:879:ARG:NH2	2:B:885:MET:HE1	2.18	0.58
5:F:77:ASP:O	5:F:78:GLN:CB	2.48	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
4:E:44:ALA:CB	4:E:44:ALA:N	2.64	0.58
9:K:103:THR:C	9:K:105:PHE:H	2.11	0.58
2:B:294:ASP:N	7:I:12:ASN:ND2	2.39	0.58
2:B:886:LYS:C	2:B:888:GLY:H	2.11	0.58
3:C:73:GLN:HE21	3:C:75:MET:N	2.00	0.58
2:B:1098:MET:O	2:B:1099:VAL:C	2.40	0.58
2:B:1098:MET:O	2:B:1100:ASP:N	2.36	0.58
3:C:66:ARG:O	3:C:67:LEU:C	2.45	0.58
3:C:102:GLN:CG	3:C:102:GLN:CA	2.75	0.58
1:A:45:GLN:C	1:A:45:GLN:HA	2.13	0.58
2:B:1162:ILE:HD11	2:B:1169:MET:HG2	1.85	0.58
3:C:95:CYS:HG	12:C:3002:ZN:ZN	1.13	0.58
6:H:7:ASP:HB2	6:H:58:THR:OG1	2.04	0.58
1:A:61:ILE:CA	1:A:61:ILE:CG1	2.78	0.58
1:A:243:PRO:CG	1:A:245:PRO:HD2	2.34	0.58
1:A:741:ASN:C	1:A:741:ASN:ND2	2.60	0.58
1:A:1162:VAL:CG1	1:A:1162:VAL:O	2.51	0.58
2:B:859:TYR:N	2:B:859:TYR:CD1	2.71	0.58
2:B:879:ARG:NH2	2:B:885:MET:CE	2.67	0.58
3:C:148:ARG:HH12	8:J:64:ASN:CG	2.12	0.58
3:C:196:ASP:CG	3:C:199:LYS:HG3	2.29	0.58
9:K:26:LYS:CD	9:K:26:LYS:CB	2.81	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:82:ASP:OD1	9:K:83:PRO:HG2	2.04	0.58
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.38	0.57
1:A:541:ILE:HD12	1:A:541:ILE:N	2.19	0.57
2:B:733:HIS:CA	2:B:734:HIS:N	2.59	0.57
6:H:103:LYS:HG2	6:H:105:GLU:OE2	2.03	0.57
7:I:45:ARG:CG	7:I:45:ARG:NH1	2.67	0.57
1:A:1425:SER:CB	1:A:1425:SER:HG	2.08	0.57
2:B:542:MET:HE2	2:B:747:MET:HG3	1.85	0.57
3:C:214:ASN:O	3:C:216:GLY:N	2.37	0.57
9:K:110:ASN:C	9:K:112:GLN:H	2.00	0.57
10:L:47:ARG:HG2	10:L:48:CYS:N	2.16	0.57
1:A:1282:VAL:HG12	1:A:1283:VAL:N	2.14	0.57
6:H:32:THR:CA	6:H:32:THR:HB	2.17	0.57
1:A:565:ILE:HD12	6:H:97:MET:HG2	1.87	0.57
4:E:112:TYR:CE2	4:E:116:ILE:HD11	2.39	0.57
9:K:40:HIS:O	9:K:41:THR:C	2.43	0.57
1:A:53:LEU:HD23	1:A:54:ASN:N	2.20	0.57
1:A:347:PHE:H	2:B:1107:ALA:HA	1.69	0.57
1:A:633:VAL:O	1:A:634:THR:C	2.41	0.57
1:A:834:THR:HG21	1:A:1077:THR:HA	1.86	0.57
1:A:1127:ASP:HB3	1:A:1130:GLN:H	1.70	0.57
2:B:324:ILE:N	2:B:324:ILE:CD1	2.67	0.57
2:B:446:LEU:CD2	2:B:446:LEU:CB	2.78	0.57
7:I:32:CYS:HB2	7:I:34:TYR:H	1.69	0.57
1:A:98:LYS:C	1:A:100:LYS:N	2.54	0.57
1:A:895:LYS:CD	1:A:895:LYS:NZ	2.68	0.57
2:B:113:TYR:CD2	2:B:192:LEU:CD2	2.87	0.57
2:B:249:ARG:CZ	2:B:415:GLN:HG3	2.34	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:724:ASP:HB3	2:B:727:LYS:HG3	1.86	0.57
2:B:1182:CYS:O	2:B:1184:GLY:N	2.37	0.57
1:A:567:LYS:HB2	6:H:95:TYR:HA	1.86	0.57
2:B:418:LYS:CD	2:B:418:LYS:CB	2.79	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
1:A:1176:LEU:CD2	1:A:1176:LEU:CD1	2.81	0.57
2:B:414:ALA:O	2:B:415:GLN:C	2.47	0.57
5:F:76:LYS:CG	5:F:76:LYS:CE	2.79	0.57
5:F:76:LYS:O	5:F:79:ARG:HD2	2.04	0.57
6:H:102:TYR:O	6:H:104:PHE:N	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:61:THR:CG2	10:L:61:THR:OG1	2.46	0.57
1:A:571:LEU:HD22	6:H:46:LEU:HD11	1.87	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:243:PRO:HB2	1:A:245:PRO:CD	2.34	0.57
1:A:920:LEU:CD2	1:A:921:GLY:N	2.67	0.57
2:B:367:LEU:CD1	2:B:367:LEU:CD2	2.79	0.57
1:A:869:GLY:O	4:E:204:THR:HG21	2.05	0.56
2:B:121:ASN:HD22	2:B:121:ASN:H	1.53	0.56
3:C:56:THR:HG22	3:C:58:LEU:H	1.70	0.56
3:C:156:THR:HG22	3:C:157:CYS:N	2.20	0.56
1:A:567:LYS:CE	6:H:95:TYR:CE2	2.85	0.56
1:A:830:LYS:NZ	1:A:830:LYS:CD	2.66	0.56
1:A:1146:VAL:HG12	1:A:1197:LEU:HD22	1.87	0.56
2:B:134:LYS:HB2	2:B:134:LYS:CE	2.34	0.56
2:B:192:LEU:CD2	2:B:192:LEU:HG	2.19	0.56
2:B:369:GLY:N	2:B:370:PHE:CD1	2.73	0.56
2:B:914:LYS:CD	2:B:937:ALA:HB3	2.36	0.56
3:C:66:ARG:CG	3:C:66:ARG:NH1	2.58	0.56
4:E:83:CYS:O	4:E:113:GLN:NE2	2.37	0.56
7:I:55:THR:CG2	7:I:55:THR:HB	2.24	0.56
1:A:244:PRO:HA	1:A:247:ARG:HG3	1.86	0.56
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.41	0.56
1:A:1203:ASN:C	1:A:1205:LYS:N	2.62	0.56
1:A:1238:ILE:CG2	1:A:1238:ILE:CG1	2.81	0.56
1:A:1449:SER:HB2	5:F:149:GLU:OE2	2.05	0.56
2:B:114:PRO:HD3	2:B:124:TYR:HE1	1.60	0.56
2:B:663:ALA:O	2:B:667:GLN:HG3	2.05	0.56
3:C:11:ARG:NH2	3:C:206:ASN:OD1	2.30	0.56
3:C:40:GLU:O	3:C:163:ILE:HD11	2.06	0.56
5:F:80:ALA:CB	5:F:80:ALA:C	2.71	0.56
8:J:53:HIS:ND1	8:J:53:HIS:C	2.63	0.56
10:L:47:ARG:CG	10:L:48:CYS:H	2.17	0.56
1:A:507:VAL:HB	1:A:508:PRO:HD3	1.88	0.56
1:A:689:LYS:O	1:A:693:VAL:HG23	2.05	0.56
2:B:431:TYR:CE1	2:B:447:ALA:HB1	2.40	0.56
2:B:467:GLY:H	2:B:477:ALA:CB	2.18	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
10:L:61:THR:HB	10:L:63:ARG:H	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.41	0.56
2:B:830:TYR:O	2:B:831:SER:OG	2.21	0.56
3:C:25:VAL:CG1	3:C:29:MET:HG2	2.34	0.56
4:E:28:TYR:CZ	4:E:75:MET:CE	2.88	0.56
8:J:14:VAL:HG13	8:J:50:ILE:HD11	1.88	0.56
1:A:1127:ASP:O	1:A:1128:GLN:C	2.49	0.56
2:B:90:ILE:HA	2:B:133:LYS:O	2.05	0.56
2:B:544:CYS:HB2	2:B:634:TYR:CE1	2.40	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:11:ARG:O	3:C:12:GLU:CB	2.45	0.56
3:C:242:GLN:O	3:C:246:ARG:HB2	2.06	0.56
1:A:557:ASP:O	1:A:559:VAL:N	2.39	0.56
2:B:227:LYS:HG3	2:B:395:GLN:NE2	2.20	0.56
2:B:733:HIS:C	2:B:733:HIS:CB	2.76	0.56
3:C:26:ASP:O	3:C:27:LEU:C	2.47	0.56
3:C:116:LYS:CD	3:C:116:LYS:NZ	2.67	0.56
6:H:10:PHE:HD1	6:H:57:VAL:HG23	1.71	0.56
6:H:76:THR:O	6:H:76:THR:HG22	2.06	0.56
10:L:38:LEU:CG	10:L:39:SER:H	2.19	0.56
1:A:351:THR:CG2	2:B:1103:ILE:HG13	2.36	0.56
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.35	0.56
1:A:606:LEU:HD23	1:A:613:ILE:HG21	1.87	0.56
2:B:453:ILE:HG22	2:B:454:THR:N	2.20	0.56
2:B:594:ALA:HB2	2:B:617:ARG:HH12	1.71	0.56
2:B:1128:LEU:O	2:B:1128:LEU:CG	2.54	0.56
2:B:1163:CYS:HB2	2:B:1182:CYS:SG	2.46	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
2:B:870:ILE:CG2	2:B:870:ILE:HB	2.17	0.56
1:A:189:ARG:HG2	1:A:189:ARG:O	2.06	0.56
1:A:216:VAL:HA	1:A:219:PHE:CZ	2.40	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
2:B:347:LYS:CD	2:B:347:LYS:CB	2.83	0.56
2:B:458:LYS:O	2:B:459:TYR:C	2.49	0.56
3:C:80:LEU:HD12	3:C:94:LYS:O	2.06	0.56
4:E:117:THR:C	4:E:119:SER:H	2.12	0.56
10:L:38:LEU:CD2	10:L:39:SER:H	2.18	0.56
1:A:154:SER:C	1:A:155:GLU:O	2.49	0.55
1:A:324:SER:O	1:A:327:ALA:HB2	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:ALA:CB	2:B:122:LEU:HB2	2.37	0.55
2:B:296:GLU:O	2:B:300:HIS:CD2	2.59	0.55
2:B:755:ILE:O	2:B:755:ILE:HG22	2.05	0.55
4:E:61:GLN:HB2	4:E:79:TRP:HE3	1.70	0.55
4:E:161:LYS:NZ	4:E:193:GLY:O	2.39	0.55
9:K:83:PRO:C	9:K:85:ASP:N	2.62	0.55
10:L:31:CYS:SG	10:L:34:CYS:SG	3.04	0.55
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.41	0.55
1:A:903:ASN:HD21	1:A:905:ASP:HB2	1.69	0.55
2:B:296:GLU:O	2:B:300:HIS:HD2	1.89	0.55
3:C:120:ILE:C	3:C:121:VAL:HG23	2.31	0.55
3:C:260:LEU:HD12	3:C:260:LEU:O	2.06	0.55
6:H:81:PRO:HB2	6:H:82:PRO:HD3	1.87	0.55
8:J:53:HIS:HD1	8:J:54:VAL:N	2.04	0.55
1:A:555:ASP:OD1	9:K:26:LYS:HE3	2.05	0.55
1:A:1232:ASN:CB	1:A:1232:ASN:ND2	2.65	0.55
1:A:1419:ASP:CG	1:A:1419:ASP:CA	2.76	0.55
2:B:89:GLU:C	2:B:90:ILE:HD12	2.31	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
1:A:4:GLN:CG	1:A:4:GLN:N	2.68	0.55
1:A:1341:ILE:HD13	1:A:1379:GLY:O	2.06	0.55
2:B:658:ILE:O	2:B:658:ILE:HG22	2.04	0.55
3:C:267:GLN:CA	3:C:268:ASP:N	2.63	0.55
4:E:65:THR:OG1	4:E:68:SER:OG	2.23	0.55
4:E:116:ILE:CD1	4:E:116:ILE:N	2.68	0.55
6:H:83:GLN:O	6:H:84:ALA:C	2.49	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
10:L:60:ARG:O	10:L:61:THR:C	2.42	0.55
1:A:286:HIS:O	1:A:287:HIS:C	2.46	0.55
1:A:1150:SER:OG	7:I:46:HIS:HB3	2.07	0.55
1:A:1264:GLU:OE1	7:I:44:TYR:HE2	1.89	0.55
2:B:424:LEU:O	2:B:424:LEU:HD23	2.06	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
1:A:446:ARG:HH11	1:A:446:ARG:HG2	1.72	0.55
2:B:424:LEU:O	2:B:424:LEU:CD2	2.54	0.55
2:B:643:ASP:CG	2:B:644:GLU:O	2.50	0.55
2:B:904:ARG:C	2:B:905:VAL:HG13	2.32	0.55
6:H:27:GLU:HA	6:H:28:ALA:N	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:195:GLN:CD	3:C:195:GLN:CB	2.77	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
1:A:274:ILE:CG1	1:A:274:ILE:CA	2.81	0.55
2:B:423:LYS:CD	2:B:423:LYS:CB	2.80	0.55
2:B:451:LYS:HA	2:B:454:THR:HB	1.88	0.55
2:B:592:ASN:O	2:B:593:PRO:C	2.47	0.55
3:C:127:ARG:N	3:C:127:ARG:C	2.57	0.55
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.88	0.55
5:F:129:LYS:CD	5:F:129:LYS:CB	2.78	0.55
7:I:120:GLN:O	7:I:121:PHE:CD1	2.60	0.55
9:K:83:PRO:O	9:K:84:LYS:C	2.46	0.55
1:A:274:ILE:CB	1:A:274:ILE:C	2.74	0.55
1:A:1165:GLU:C	1:A:1167:GLU:N	2.62	0.55
2:B:458:LYS:CE	2:B:458:LYS:CG	2.83	0.55
4:E:177:ARG:HD3	4:E:215:MET:HE2	1.87	0.55
6:H:10:PHE:CD1	6:H:57:VAL:HG23	2.41	0.55
6:H:118:PHE:C	6:H:120:GLY:N	2.63	0.55
1:A:34:LYS:HG2	1:A:83:HIS:HE1	1.72	0.55
1:A:203:SER:H	1:A:206:GLU:HG3	1.72	0.55
1:A:1172:LEU:O	1:A:1173:HIS:CD2	2.60	0.55
1:A:1203:ASN:C	1:A:1205:LYS:H	2.14	0.55
2:B:269:ILE:HB	2:B:282:ILE:HD12	1.88	0.55
2:B:561:TRP:O	2:B:590:HIS:CE1	2.55	0.55
2:B:830:TYR:O	2:B:831:SER:CB	2.52	0.55
3:C:102:GLN:CG	3:C:102:GLN:N	2.70	0.55
4:E:14:ARG:O	4:E:15:ALA:C	2.43	0.55
9:K:55:LYS:HB3	9:K:81:TYR:HD1	1.72	0.55
2:B:120:ARG:CG	2:B:120:ARG:CA	2.79	0.54
2:B:657:HIS:O	2:B:658:ILE:C	2.45	0.54
2:B:1159:ARG:HG2	2:B:1160:VAL:H	1.72	0.54
4:E:65:THR:O	4:E:66:GLU:C	2.48	0.54
7:I:4:PHE:CZ	7:I:13:MET:CE	2.88	0.54
1:A:562:THR:HG22	6:H:98:TYR:CD2	2.42	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
4:E:213:ILE:CD1	4:E:213:ILE:HG21	2.37	0.54
1:A:976:THR:O	1:A:977:LYS:HG3	2.06	0.54
1:A:1132:LYS:O	1:A:1133:LEU:C	2.46	0.54
2:B:531:GLN:CG	2:B:531:GLN:CA	2.78	0.54
10:L:50:ASP:CA	10:L:51:CYS:N	2.62	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:THR:HG21	2:B:1149:GLU:OE1	2.08	0.54
1:A:752:LYS:HE2	2:B:1019:SER:HG	1.67	0.54
2:B:100:PRO:HD2	2:B:180:TYR:HE1	1.61	0.54
3:C:55:THR:O	3:C:55:THR:HG22	2.07	0.54
6:H:131:ASN:CA	6:H:132:LEU:N	2.64	0.54
8:J:53:HIS:CE1	8:J:54:VAL:C	2.85	0.54
1:A:464:PRO:O	1:A:465:TYR:O	2.24	0.54
2:B:169:ARG:HG3	2:B:454:THR:OG1	2.07	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
3:C:11:ARG:HE	3:C:209:TYR:HE2	1.48	0.54
6:H:138:GLU:HG2	6:H:139:ASN:N	2.22	0.54
8:J:2:ILE:O	8:J:3:VAL:C	2.50	0.54
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.89	0.54
1:A:1259:MET:O	1:A:1260:LEU:C	2.47	0.54
1:A:1313:LEU:O	1:A:1314:SER:C	2.43	0.54
2:B:417:PHE:C	2:B:417:PHE:HD2	2.15	0.54
2:B:705:MET:CE	2:B:705:MET:HG3	2.33	0.54
2:B:820:GLY:HA3	2:B:1091:TYR:CZ	2.43	0.54
3:C:47:ASP:CG	3:C:47:ASP:O	2.51	0.54
6:H:59:ILE:H	6:H:59:ILE:CD1	2.20	0.54
6:H:130:ARG:HB2	6:H:133:ASN:HB3	1.89	0.54
1:A:274:ILE:CD1	1:A:274:ILE:HA	2.37	0.54
1:A:913:LEU:C	1:A:913:LEU:HD12	2.31	0.54
1:A:1411:GLU:O	1:A:1412:ALA:C	2.48	0.54
2:B:26:THR:O	2:B:27:ALA:C	2.49	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
10:L:48:CYS:CA	10:L:49:LYS:N	2.64	0.54
1:A:278:THR:O	1:A:278:THR:HG22	2.07	0.54
1:A:849:MET:HE2	1:A:1061:GLY:HA2	1.89	0.54
2:B:25:ILE:CG2	2:B:25:ILE:HD12	2.38	0.54
2:B:345:LYS:O	2:B:346:GLU:C	2.46	0.54
2:B:414:ALA:O	2:B:418:LYS:N	2.41	0.54
2:B:520:GLY:O	2:B:521:LEU:HD23	2.07	0.54
2:B:903:VAL:HG12	2:B:904:ARG:N	2.16	0.54
2:B:914:LYS:HD3	2:B:937:ALA:HB3	1.89	0.54
6:H:2:SER:CA	6:H:3:ASN:N	2.65	0.54
9:K:49:GLU:CG	9:K:94:ILE:HD11	2.38	0.54
1:A:120:GLU:CG	1:A:123:ARG:HH22	2.19	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ARG:HG2	1:A:430:TRP:CZ3	2.43	0.54
2:B:369:GLY:CA	2:B:370:PHE:CD1	2.91	0.54
2:B:960:GLY:O	2:B:961:LEU:C	2.47	0.54
2:B:991:GLY:O	2:B:992:ILE:HB	2.08	0.54
9:K:26:LYS:CG	9:K:26:LYS:CA	2.80	0.54
1:A:182:VAL:HG22	1:A:201:VAL:HG22	1.90	0.54
1:A:274:ILE:CD1	1:A:274:ILE:CB	2.80	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:605:MET:HE3	1:A:607:ILE:HG13	1.89	0.54
1:A:1258:HIS:O	1:A:1259:MET:C	2.51	0.54
2:B:129:PHE:CD2	2:B:166:PHE:N	2.75	0.54
2:B:172:ILE:HD13	2:B:172:ILE:HG21	1.90	0.54
2:B:705:MET:HE3	2:B:745:PRO:HG3	1.90	0.54
6:H:81:PRO:C	6:H:82:PRO:O	2.44	0.54
1:A:216:VAL:HA	1:A:219:PHE:CE2	2.43	0.53
1:A:325:ILE:C	1:A:327:ALA:N	2.67	0.53
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.72	0.53
1:A:884:ASP:O	1:A:886:ILE:N	2.41	0.53
1:A:1172:LEU:O	1:A:1173:HIS:CG	2.60	0.53
3:C:63:ILE:O	3:C:66:ARG:HB2	2.08	0.53
1:A:191:THR:HB	1:A:192:GLY:N	2.22	0.53
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.90	0.53
1:A:534:LEU:O	1:A:574:GLY:HA3	2.08	0.53
4:E:47:CYS:HA	4:E:48:ASP:N	2.23	0.53
4:E:213:ILE:CD1	4:E:213:ILE:CG2	2.86	0.53
1:A:420:ARG:O	1:A:421:ALA:C	2.37	0.53
1:A:537:ARG:NH2	1:A:600:PRO:O	2.41	0.53
2:B:103:ASN:HB2	2:B:169:ARG:HH22	1.73	0.53
3:C:40:GLU:HA	3:C:163:ILE:HG12	1.91	0.53
4:E:47:CYS:CA	4:E:48:ASP:N	2.61	0.53
6:H:136:LYS:CA	6:H:137:GLN:N	2.61	0.53
8:J:53:HIS:HE1	8:J:55:ASP:CA	2.21	0.53
1:A:92:HIS:HD2	1:A:94:GLY:H	1.56	0.53
1:A:387:ARG:O	1:A:388:LEU:C	2.52	0.53
1:A:418:SER:C	1:A:420:ARG:N	2.60	0.53
1:A:1203:ASN:O	1:A:1205:LYS:N	2.41	0.53
2:B:958:GLN:CG	2:B:958:GLN:CA	2.83	0.53
3:C:56:THR:CG2	3:C:57:VAL:N	2.67	0.53
3:C:99:LEU:N	3:C:99:LEU:CD1	2.68	0.53
3:C:233:GLU:OE1	8:J:12:LYS:HE2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.44	0.53
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.90	0.53
2:B:864:LYS:N	2:B:872:GLU:HB2	2.24	0.53
2:B:879:ARG:HH21	2:B:885:MET:HE1	1.73	0.53
3:C:10:ILE:HD13	3:C:10:ILE:N	2.20	0.53
4:E:65:THR:O	4:E:69:ILE:HG13	2.07	0.53
7:I:20:LYS:CD	7:I:20:LYS:CB	2.80	0.53
1:A:119:ASN:O	1:A:120:GLU:HB2	2.07	0.53
1:A:274:ILE:CB	1:A:274:ILE:HA	2.20	0.53
1:A:1287:TYR:O	1:A:1302:PRO:HA	2.08	0.53
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.89	0.53
2:B:282:ILE:HD11	2:B:317:CYS:SG	2.48	0.53
2:B:910:VAL:C	2:B:911:ILE:HD12	2.33	0.53
3:C:252:GLN:HE22	9:K:99:GLY:CA	2.22	0.53
6:H:93:TYR:N	6:H:93:TYR:HD1	2.07	0.53
1:A:1039:LYS:HE3	1:A:1043:ASP:OD2	2.08	0.53
2:B:807:ARG:CG	2:B:807:ARG:CA	2.80	0.53
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.74	0.53
4:E:80:VAL:HG22	4:E:109:ILE:HD12	1.91	0.53
8:J:42:LYS:HG3	8:J:43:ARG:N	2.23	0.53
1:A:295:LEU:CD2	1:A:295:LEU:CB	2.82	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
2:B:60:GLN:O	2:B:60:GLN:HG3	1.98	0.53
1:A:28:ARG:CG	1:A:28:ARG:NE	2.67	0.53
1:A:476:SER:N	1:A:477:PRO:HD2	2.24	0.53
1:A:1450:LEU:CD1	1:A:1450:LEU:CB	2.83	0.53
2:B:137:TYR:CG	2:B:137:TYR:HB3	2.21	0.53
2:B:307:ASP:C	2:B:309:GLN:N	2.64	0.53
2:B:806:THR:HG23	2:B:808:ALA:H	1.73	0.53
8:J:43:ARG:O	8:J:47:ARG:HG3	2.09	0.53
10:L:65:VAL:CG2	10:L:65:VAL:CG1	2.78	0.53
1:A:7:SER:O	1:A:8:SER:C	2.48	0.53
1:A:567:LYS:CE	1:A:567:LYS:CG	2.82	0.53
1:A:596:THR:CG2	1:A:597:LEU:N	2.72	0.53
2:B:705:MET:CE	2:B:745:PRO:HG3	2.39	0.53
3:C:126:GLY:C	3:C:127:ARG:CA	2.70	0.53
5:F:111:LEU:C	5:F:113:GLY:N	2.67	0.53
6:H:4:THR:C	6:H:5:LEU:CD2	2.70	0.53
6:H:10:PHE:O	6:H:55:LEU:N	2.39	0.53
6:H:105:GLU:CD	6:H:105:GLU:N	2.66	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLN:CG	1:A:4:GLN:H	2.22	0.52
1:A:98:LYS:O	1:A:99:ILE:C	2.52	0.52
1:A:271:LYS:CD	1:A:271:LYS:CB	2.80	0.52
1:A:353:ILE:HG21	1:A:487:MET:SD	2.49	0.52
1:A:518:LYS:CE	1:A:518:LYS:CG	2.83	0.52
1:A:547:LEU:HB3	9:K:58:PHE:HE1	1.71	0.52
1:A:915:SER:O	1:A:916:GLY:C	2.50	0.52
2:B:600:LEU:O	2:B:601:ARG:C	2.50	0.52
2:B:864:LYS:CB	2:B:872:GLU:H	2.22	0.52
3:C:56:THR:HG23	3:C:57:VAL:N	2.22	0.52
3:C:253:LYS:CD	3:C:253:LYS:NZ	2.67	0.52
8:J:2:ILE:HD11	8:J:57:ILE:HD12	1.91	0.52
2:B:127:GLY:C	2:B:128:LEU:HD13	2.34	0.52
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.91	0.52
2:B:999:MET:HE2	2:B:999:MET:CB	2.37	0.52
2:B:1182:CYS:HB3	2:B:1185:CYS:HB2	1.91	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: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
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:778:MET:HE2	2:B:794:ASN:OD1	2.09	0.52
3:C:35:ARG:HH11	9:K:41:THR:H	1.58	0.52
3:C:66:ARG:CG	3:C:66:ARG:HH11	2.00	0.52
8:J:53:HIS:C	8:J:53:HIS:HD1	2.16	0.52
1:A:567:LYS:HB3	6:H:96:VAL:HG23	1.92	0.52
1:A:1408:ILE:O	1:A:1408:ILE:HG22	2.09	0.52
2:B:502:ILE:HA	2:B:502:ILE:CD1	2.37	0.52
2:B:625:LYS:NZ	2:B:625:LYS:HD2	2.22	0.52
2:B:845:SER:O	2:B:846:ILE:C	2.49	0.52
2:B:914:LYS:N	2:B:938:SER:HB2	2.22	0.52
2:B:962:LYS:CD	2:B:962:LYS:CB	2.80	0.52
4:E:85:GLU:OE2	4:E:92:THR:OG1	2.22	0.52
6:H:32:THR:CG2	6:H:33:GLN:CD	2.83	0.52
9:K:49:GLU:C	9:K:51:LEU:N	2.67	0.52
1:A:7:SER:O	1:A:9:ALA:N	2.42	0.52
1:A:11:LEU:CD1	2:B:1195:HIS:CD2	2.92	0.52
10:L:51:CYS:SG	10:L:51:CYS:O	2.68	0.52
1:A:7:SER:C	1:A:9:ALA:H	2.18	0.52
1:A:103:CYS:SG	1:A:207:ILE:HD12	2.50	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:205:LYS:O	3:C:207:CYS:N	2.42	0.52
8:J:7:CYS:SG	8:J:46:CYS:N	2.82	0.52
9:K:111:LEU:CD1	9:K:111:LEU:HG	2.25	0.52
1:A:555:ASP:OD1	9:K:26:LYS:CE	2.58	0.52
1:A:744:LYS:HD3	1:A:748:MET:SD	2.49	0.52
1:A:768:GLN:NE2	1:A:816:HIS:HA	2.25	0.52
2:B:117:ALA:O	2:B:207:GLY:HA2	2.10	0.52
2:B:205:ILE:O	2:B:205:ILE:HG22	2.06	0.52
2:B:1152:MET:HA	2:B:1152:MET:HE2	1.92	0.52
2:B:1172:ILE:CG2	2:B:1172:ILE:CA	2.75	0.52
4:E:140:LEU:O	4:E:141:VAL:C	2.49	0.52
8:J:42:LYS:CD	8:J:42:LYS:CB	2.80	0.52
1:A:384:ASN:OD1	1:A:384:ASN:C	2.53	0.52
1:A:606:LEU:HD23	1:A:613:ILE:CG2	2.40	0.52
1:A:1122:PRO:O	1:A:1123:GLY:C	2.49	0.52
2:B:875:GLU:O	2:B:876:LYS:C	2.52	0.52
2:B:958:GLN:CG	2:B:958:GLN:H	2.23	0.52
2:B:1008:PRO:HG2	2:B:1011:ILE:HD11	1.91	0.52
2:B:1172:ILE:O	2:B:1180:PHE:HA	2.08	0.52
2:B:1222:ARG:HD3	2:B:1222:ARG:N	2.25	0.52
4:E:90:VAL:CG1	4:E:90:VAL:CA	2.80	0.52
1:A:4:GLN:N	1:A:4:GLN:HG2	2.24	0.52
1:A:180:LYS:CG	1:A:180:LYS:CA	2.80	0.52
1:A:786:HIS:H	1:A:786:HIS:CD2	2.25	0.52
1:A:1264:GLU:OE2	7:I:46:HIS:HD2	1.92	0.52
2:B:965:LYS:CD	2:B:965:LYS:NZ	2.72	0.52
2:B:1006:ILE:HD12	2:B:1006:ILE:N	2.25	0.52
1:A:934:LYS:CD	1:A:934:LYS:NZ	2.73	0.52
3:C:112:ASN:HB2	3:C:114:TYR:CE1	2.45	0.52
1:A:1146:VAL:CG1	1:A:1197:LEU:HD22	2.40	0.51
2:B:563:MET:SD	2:B:563:MET:CB	2.91	0.51
1:A:39:GLU:HB3	1:A:50:ILE:CD1	2.40	0.51
1:A:134:ARG:HD2	1:A:221:SER:O	2.10	0.51
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.45	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
1:A:894:GLU:HB2	1:A:933:TYR:HH	1.75	0.51
1:A:1315:GLU:O	1:A:1318:THR:HG22	2.09	0.51
2:B:25:ILE:HD12	2:B:25:ILE:HG23	1.92	0.51
2:B:89:GLU:C	2:B:90:ILE:CD1	2.83	0.51
2:B:249:ARG:CD	2:B:249:ARG:CB	2.86	0.51

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:NH1	2.25	0.51
6:H:95:TYR:HB3	6:H:144:ILE:HB	1.92	0.51
9:K:77:THR:OG1	9:K:83:PRO:HD3	2.10	0.51
1:A:93:VAL:HG22	1:A:304:MET:HE3	1.92	0.51
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:809:THR:OG1	1:A:812:GLU:HG3	2.11	0.51
1:A:901:LEU:N	1:A:926:GLN:NE2	2.50	0.51
1:A:976:THR:O	1:A:977:LYS:CG	2.58	0.51
2:B:130:VAL:CG2	2:B:167:ILE:HD11	2.41	0.51
2:B:372:SER:O	2:B:373:ARG:C	2.53	0.51
2:B:884:ARG:O	2:B:936:ASP:HB3	2.09	0.51
3:C:56:THR:CG2	3:C:58:LEU:H	2.23	0.51
4:E:7:ARG:CG	4:E:7:ARG:CA	2.82	0.51
4:E:156:LEU:HB3	4:E:160:GLU:CB	2.40	0.51
1:A:143:LYS:CG	1:A:143:LYS:CE	2.81	0.51
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.74	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
1:A:844:ALA:HB2	1:A:1384:VAL:HG12	1.92	0.51
2:B:25:ILE:HD13	2:B:25:ILE:H	1.75	0.51
2:B:893:LEU:HD13	2:B:897:GLY:C	2.34	0.51
3:C:69:LEU:HB2	8:J:5:VAL:HG11	1.93	0.51
3:C:166:GLU:O	3:C:167:HIS:HB2	2.10	0.51
5:F:147:SER:O	5:F:148:VAL:C	2.50	0.51
7:I:30:ARG:CD	7:I:30:ARG:CB	2.80	0.51
9:K:103:THR:O	9:K:105:PHE:N	2.42	0.51
10:L:38:LEU:HG	10:L:39:SER:N	2.25	0.51
1:A:1172:LEU:C	1:A:1173:HIS:CD2	2.88	0.51
1:A:1364:ASN:HD22	1:A:1365:TYR:N	2.08	0.51
2:B:1163:CYS:CB	2:B:1166:CYS:SG	2.98	0.51
3:C:43:THR:CG2	3:C:44:LEU:N	2.74	0.51
1:A:53:LEU:O	1:A:56:PRO:HD3	2.11	0.51
2:B:35:SER:HA	2:B:811:TYR:CE2	2.46	0.51
2:B:165:VAL:HG12	2:B:165:VAL:O	2.11	0.51
2:B:692:TYR:O	2:B:693:ILE:HD13	2.10	0.51
7:I:40:SER:HB2	7:I:41:PRO:CD	2.41	0.51
9:K:28:PRO:O	9:K:29:ASN:HB2	2.09	0.51
1:A:351:THR:HG21	2:B:1103:ILE:CG1	2.36	0.51
1:A:902:LEU:HD23	1:A:902:LEU:N	2.25	0.51
2:B:609:ILE:HG22	2:B:610:ASN:N	2.20	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:863:GLU:C	2:B:864:LYS:O	2.54	0.51
2:B:1002:THR:HG22	2:B:1006:ILE:N	2.25	0.51
2:B:1065:GLN:NE2	2:B:1067:ARG:N	2.58	0.51
3:C:131:HIS:O	3:C:132:PRO:C	2.47	0.51
4:E:154:ILE:N	4:E:154:ILE:HD12	2.26	0.51
1:A:706:HIS:O	1:A:707:GLY:C	2.53	0.51
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
6:H:32:THR:HG22	6:H:33:GLN:OE1	2.10	0.51
7:I:120:GLN:O	7:I:121:PHE:CG	2.63	0.51
1:A:46:THR:C	1:A:46:THR:HB	2.35	0.51
1:A:176:LYS:CG	1:A:176:LYS:CE	2.82	0.51
1:A:557:ASP:OD1	1:A:557:ASP:C	2.51	0.51
1:A:834:THR:HG21	1:A:1077:THR:CA	2.41	0.51
1:A:1205:LYS:O	1:A:1206:ASP:C	2.50	0.51
2:B:206:ASN:OD1	2:B:458:LYS:HE3	2.10	0.51
3:C:167:HIS:CE1	10:L:70:ARG:O	2.62	0.51
3:C:230:MET:SD	3:C:230:MET:CB	2.98	0.51
6:H:40:LEU:HD12	6:H:41:ASP:H	1.76	0.51
6:H:98:TYR:C	6:H:118:PHE:HD2	2.19	0.51
7:I:1:MET:CB	7:I:1:MET:C	2.77	0.51
1:A:187:LYS:O	1:A:188:ASP:CG	2.54	0.50
1:A:1204:ASP:CG	1:A:1204:ASP:O	2.54	0.50
1:A:1256:GLU:HG2	1:A:1259:MET:HE1	1.94	0.50
2:B:129:PHE:CE2	2:B:166:PHE:N	2.79	0.50
2:B:419:THR:O	2:B:419:THR:HG22	2.09	0.50
2:B:654:ARG:H	2:B:657:HIS:CD2	2.22	0.50
2:B:1020:ARG:O	2:B:1021:MET:HB2	2.10	0.50
3:C:124:LEU:O	3:C:127:ARG:HG3	2.11	0.50
8:J:24:LEU:HD22	8:J:30:LEU:HD12	1.93	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
1:A:941:LYS:CD	1:A:941:LYS:CB	2.78	0.50
2:B:121:ASN:HD21	2:B:965:LYS:NZ	2.09	0.50
2:B:599:THR:O	2:B:600:LEU:C	2.51	0.50
2:B:1081:LEU:O	2:B:1082:MET:C	2.50	0.50
3:C:33:LEU:HD13	3:C:248:ILE:HD13	1.93	0.50
4:E:57:MET:SD	4:E:57:MET:CE	2.99	0.50
4:E:93:MET:CG	4:E:93:MET:CE	2.89	0.50
6:H:11:GLN:HB3	6:H:29:ALA:HB3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:48:ARG:C	8:J:48:ARG:CD	2.83	0.50
9:K:82:ASP:OD1	9:K:83:PRO:N	2.43	0.50
9:K:88:LYS:O	9:K:89:ASN:C	2.51	0.50
1:A:950:GLY:CA	1:A:1298:TYR:CZ	2.95	0.50
1:A:1259:MET:SD	1:A:1259:MET:HB2	2.51	0.50
2:B:235:SER:C	2:B:236:HIS:CD2	2.89	0.50
2:B:341:LEU:HD12	2:B:342:GLY:N	2.27	0.50
4:E:97:VAL:HG13	4:E:127:ILE:HD13	1.93	0.50
6:H:10:PHE:HB3	6:H:29:ALA:O	2.12	0.50
7:I:41:PRO:HD2	7:I:42:LEU:H	1.76	0.50
1:A:35:ILE:HD12	1:A:35:ILE:N	2.25	0.50
1:A:50:ILE:HG22	1:A:51:GLY:N	2.21	0.50
1:A:365:GLY:HA2	1:A:461:LYS:O	2.11	0.50
1:A:722:LEU:HD22	1:A:799:PHE:CD1	2.47	0.50
3:C:181:ASP:N	3:C:182:PRO:HD2	2.26	0.50
3:C:209:TYR:N	3:C:209:TYR:CD1	2.80	0.50
3:C:218:PRO:O	3:C:218:PRO:CG	2.59	0.50
6:H:103:LYS:HG2	6:H:105:GLU:OE1	2.08	0.50
9:K:88:LYS:CD	9:K:88:LYS:CB	2.85	0.50
9:K:110:ASN:C	9:K:112:GLN:N	2.60	0.50
1:A:191:THR:CA	1:A:191:THR:HB	2.20	0.50
1:A:844:ALA:CB	1:A:1384:VAL:HG12	2.40	0.50
2:B:373:ARG:HD2	2:B:567:GLU:OE1	2.12	0.50
4:E:39:LEU:O	4:E:43:LYS:N	2.45	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:213:ILE:HG21	4:E:213:ILE:HD13	1.92	0.50
8:J:1:MET:HG3	8:J:60:PHE:HE2	1.77	0.50
2:B:235:SER:OG	2:B:236:HIS:HD2	1.94	0.50
4:E:63:ASN:C	4:E:64:PRO:O	2.54	0.50
6:H:63:LEU:H	6:H:63:LEU:HD12	1.77	0.50
1:A:1135:ARG:CG	1:A:1135:ARG:NE	2.70	0.50
2:B:520:GLY:C	2:B:521:LEU:HD23	2.37	0.50
2:B:609:ILE:O	2:B:610:ASN:C	2.52	0.50
2:B:643:ASP:HB3	2:B:644:GLU:C	2.36	0.50
3:C:180:TYR:CD1	3:C:180:TYR:C	2.89	0.50
3:C:241:ASP:CG	3:C:242:GLN:N	2.69	0.50
6:H:48:PRO:O	6:H:49:VAL:CG2	2.59	0.50
1:A:853:ASP:OD2	1:A:857:ARG:NH2	2.42	0.50
1:A:982:THR:O	1:A:985:ASP:HB2	2.12	0.50
1:A:1271:ILE:HG22	1:A:1272:THR:N	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1184:GLY:H	2:B:1186:ASP:H	1.58	0.50
3:C:121:VAL:O	3:C:121:VAL:HG12	2.11	0.50
3:C:181:ASP:CG	3:C:181:ASP:O	2.49	0.50
3:C:181:ASP:OD2	3:C:186:LEU:HB2	2.11	0.50
7:I:7:CYS:SG	7:I:29:CYS:SG	3.10	0.50
2:B:68:THR:CG2	2:B:91:SER:HB3	2.41	0.50
2:B:130:VAL:HG23	2:B:167:ILE:HD11	1.94	0.50
3:C:29:MET:CE	3:C:29:MET:HB2	2.42	0.50
4:E:1:MET:CG	4:E:1:MET:CA	2.82	0.50
1:A:265:LYS:HZ3	1:A:302:THR:CG2	2.24	0.49
1:A:265:LYS:HZ3	1:A:302:THR:HG21	1.77	0.49
1:A:295:LEU:CD2	1:A:295:LEU:CD1	2.88	0.49
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.94	0.49
2:B:99:LYS:CB	2:B:100:PRO:CD	2.85	0.49
2:B:502:ILE:CA	2:B:502:ILE:CG1	2.85	0.49
2:B:1101:ASP:CA	2:B:1102:LYS:N	2.62	0.49
3:C:180:TYR:OH	3:C:188:HIS:ND1	2.30	0.49
4:E:44:ALA:HB3	4:E:45:LYS:H	1.77	0.49
7:I:40:SER:HB2	7:I:41:PRO:HD3	1.94	0.49
9:K:105:PHE:C	9:K:107:THR:N	2.67	0.49
1:A:50:ILE:CG2	1:A:51:GLY:N	2.71	0.49
1:A:920:LEU:HD22	1:A:921:GLY:H	1.74	0.49
1:A:950:GLY:HA2	1:A:1298:TYR:CZ	2.46	0.49
1:A:1318:THR:CG2	1:A:1318:THR:HB	2.20	0.49
3:C:100:THR:CG2	3:C:101:LEU:N	2.71	0.49
3:C:102:GLN:N	3:C:102:GLN:HG2	2.27	0.49
6:H:97:MET:HE3	6:H:118:PHE:CG	2.47	0.49
1:A:418:SER:C	1:A:420:ARG:H	2.19	0.49
1:A:982:THR:HG22	1:A:984:LYS:N	2.27	0.49
1:A:1012:ARG:CD	1:A:1012:ARG:CB	2.85	0.49
1:A:1194:ARG:CG	1:A:1194:ARG:C	2.85	0.49
1:A:1198:ASP:OD1	1:A:1200:ALA:HB3	2.13	0.49
3:C:44:LEU:HG	3:C:45:ALA:N	2.26	0.49
9:K:23:PRO:HD2	9:K:23:PRO:O	2.12	0.49
1:A:219:PHE:CD1	1:A:219:PHE:C	2.88	0.49
1:A:535:THR:CG2	1:A:617:VAL:N	2.55	0.49
1:A:1142:THR:C	1:A:1144:LYS:N	2.68	0.49
2:B:225:VAL:CG1	2:B:226:PHE:N	2.74	0.49
2:B:516:ASN:ND2	2:B:516:ASN:N	2.59	0.49
2:B:711:GLU:CD	2:B:711:GLU:CB	2.76	0.49
3:C:19:ASP:OD1	3:C:20:PHE:N	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:260:LEU:CD2	3:C:260:LEU:CD1	2.87	0.49
4:E:37:LEU:C	4:E:38:PRO:O	2.54	0.49
4:E:118:PRO:CG	4:E:118:PRO:CA	2.88	0.49
1:A:125:ALA:O	1:A:126:LEU:C	2.47	0.49
1:A:516:SER:O	1:A:517:ASN:C	2.51	0.49
1:A:1217:LYS:NZ	1:A:1217:LYS:CD	2.67	0.49
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.12	0.49
2:B:118:ARG:HH22	2:B:194:GLU:CG	2.24	0.49
6:H:17:PRO:O	6:H:18:GLY:C	2.50	0.49
7:I:83:ASN:HA	7:I:102:VAL:O	2.13	0.49
9:K:49:GLU:HG3	9:K:94:ILE:CD1	2.42	0.49
1:A:67:CYS:SG	1:A:77:CYS:SG	3.08	0.49
4:E:58:MET:O	4:E:59:SER:O	2.31	0.49
4:E:118:PRO:O	4:E:121:MET:SD	2.70	0.49
5:F:123:LYS:NZ	5:F:123:LYS:HD2	2.27	0.49
7:I:109:ILE:HD12	7:I:109:ILE:N	2.28	0.49
8:J:57:ILE:O	8:J:60:PHE:N	2.46	0.49
1:A:132:LYS:CD	1:A:132:LYS:CB	2.83	0.49
1:A:1151:GLU:HG2	7:I:45:ARG:CD	2.43	0.49
1:A:1405:THR:CB	1:A:1405:THR:C	2.82	0.49
2:B:365:THR:HG22	2:B:366:GLN:N	2.27	0.49
2:B:578:THR:HG23	2:B:622:LYS:C	2.37	0.49
2:B:739:THR:O	2:B:740:HIS:CG	2.66	0.49
2:B:1006:ILE:CD1	8:J:43:ARG:HD2	2.42	0.49
6:H:33:GLN:O	6:H:34:ASP:C	2.54	0.49
6:H:118:PHE:O	6:H:119:GLY:C	2.52	0.49
1:A:672:ASP:HB2	1:A:736:ASN:ND2	2.28	0.49
3:C:77:ILE:O	3:C:77:ILE:HG13	2.11	0.49
10:L:30:ILE:CD1	10:L:30:ILE:CB	2.78	0.49
1:A:636:GLU:OE2	1:A:962:ARG:CD	2.60	0.49
3:C:208:GLU:O	3:C:210:GLU:N	2.45	0.49
4:E:97:VAL:O	4:E:97:VAL:HG12	2.13	0.49
4:E:112:TYR:CZ	4:E:116:ILE:HD11	2.47	0.49
1:A:35:ILE:HG23	1:A:53:LEU:HB2	1.95	0.48
1:A:116:ASP:OD2	1:A:116:ASP:C	2.55	0.48
1:A:265:LYS:HE2	1:A:299:HIS:O	2.13	0.48
1:A:325:ILE:O	1:A:325:ILE:CG2	2.61	0.48
1:A:1264:GLU:OE1	7:I:44:TYR:CE2	2.66	0.48
2:B:64:CYS:C	2:B:65:GLU:O	2.49	0.48
2:B:421:PHE:O	2:B:425:THR:HB	2.13	0.48
2:B:724:ASP:C	2:B:726:ALA:H	2.19	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:769:TYR:O	2:B:770:GLN:C	2.55	0.48
4:E:137:GLU:O	4:E:138:ALA:C	2.53	0.48
8:J:2:ILE:HD12	8:J:2:ILE:N	2.25	0.48
1:A:373:THR:O	1:A:373:THR:HG22	2.10	0.48
1:A:567:LYS:HD3	6:H:95:TYR:C	2.36	0.48
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.78	0.48
1:A:971:PHE:O	1:A:972:HIS:C	2.49	0.48
1:A:1148:ILE:CD1	1:A:1148:ILE:HG21	2.43	0.48
1:A:1262:LYS:C	1:A:1264:GLU:N	2.70	0.48
2:B:134:LYS:CB	2:B:134:LYS:HE3	2.39	0.48
2:B:276:ILE:HD11	2:B:355:ILE:HG13	1.94	0.48
2:B:515:HIS:N	2:B:518:HIS:HD2	1.98	0.48
2:B:705:MET:SD	2:B:705:MET:HB2	2.50	0.48
1:A:125:ALA:HA	1:A:128:ILE:HG12	1.95	0.48
1:A:156:ASP:O	1:A:158:PRO:CD	2.57	0.48
1:A:567:LYS:CE	6:H:95:TYR:CG	2.89	0.48
2:B:864:LYS:HD2	2:B:871:THR:OG1	2.13	0.48
2:B:1162:ILE:HA	2:B:1162:ILE:HD13	1.54	0.48
3:C:180:TYR:HH	3:C:188:HIS:HD1	1.55	0.48
7:I:3:THR:CG2	7:I:3:THR:C	2.86	0.48
1:A:44:THR:CG2	1:A:44:THR:OG1	2.57	0.48
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.95	0.48
2:B:206:ASN:OD1	2:B:458:LYS:HE2	2.12	0.48
2:B:408:LEU:O	2:B:409:ALA:C	2.52	0.48
4:E:61:GLN:HB2	4:E:79:TRP:CE3	2.47	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
2:B:890:TYR:C	2:B:892:LYS:H	2.22	0.48
3:C:266:ASP:OD1	3:C:266:ASP:N	2.45	0.48
4:E:98:ILE:CG1	4:E:98:ILE:HA	2.42	0.48
7:I:50:THR:O	7:I:50:THR:HG23	2.12	0.48
1:A:1106:ASN:O	1:A:1107:VAL:C	2.49	0.48
2:B:25:ILE:CG2	2:B:25:ILE:CD1	2.91	0.48
2:B:710:LEU:N	2:B:710:LEU:HD23	2.29	0.48
2:B:816:GLU:C	2:B:818:PRO:HD3	2.38	0.48
2:B:1176:ASN:CB	2:B:1176:ASN:ND2	2.69	0.48
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.49	0.48
5:F:138:LEU:HB3	5:F:139:PRO:CD	2.44	0.48
9:K:47:ARG:O	9:K:48:ALA:C	2.50	0.48
1:A:533:LYS:HZ3	1:A:745:GLN:HE22	1.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:THR:HG22	1:A:984:LYS:H	1.78	0.48
7:I:50:THR:O	7:I:50:THR:CG2	2.61	0.48
1:A:560:ILE:O	1:A:561:PRO:C	2.49	0.48
1:A:870:GLU:HG2	4:E:208:TYR:CD1	2.48	0.48
1:A:896:ARG:CD	1:A:897:TYR:CE1	2.97	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:51:ALA:CB	6:H:51:ALA:C	2.77	0.48
1:A:445:ASN:HA	1:A:454:SER:O	2.13	0.48
1:A:567:LYS:HB3	6:H:95:TYR:C	2.32	0.48
1:A:650:GLN:O	1:A:654:ASN:HB2	2.14	0.48
1:A:826:ASP:O	1:A:827:THR:C	2.44	0.48
1:A:1052:GLN:O	1:A:1053:PHE:C	2.52	0.48
2:B:737:THR:O	2:B:738:PHE:C	2.55	0.48
2:B:755:ILE:N	2:B:755:ILE:HD13	2.26	0.48
2:B:933:SER:CA	2:B:934:LYS:N	2.67	0.48
6:H:123:MET:HG2	6:H:124:ARG:N	2.28	0.48
7:I:98:VAL:O	7:I:98:VAL:CG1	2.61	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
1:A:852:TYR:CD2	5:F:136:ARG:HD3	2.49	0.48
1:A:926:GLN:HG3	1:A:926:GLN:O	2.13	0.48
1:A:1112:LYS:CG	1:A:1112:LYS:CA	2.78	0.48
1:A:1239:ARG:O	1:A:1239:ARG:HG3	2.13	0.48
1:A:1272:THR:CG2	1:A:1272:THR:OG1	2.55	0.48
1:A:1287:TYR:O	1:A:1303:GLU:N	2.37	0.48
2:B:357:GLN:HE21	2:B:368:GLU:HG2	1.77	0.48
2:B:515:HIS:CD2	2:B:517:THR:H	2.32	0.48
2:B:794:ASN:O	2:B:795:ILE:HD13	2.13	0.48
4:E:43:LYS:CG	4:E:43:LYS:CA	2.83	0.48
5:F:135:ARG:CD	5:F:135:ARG:CB	2.82	0.48
6:H:81:PRO:HB2	6:H:82:PRO:HD2	1.93	0.48
6:H:101:ALA:HB2	6:H:116:TYR:CD2	2.49	0.48
8:J:26:GLN:CG	8:J:26:GLN:CA	2.84	0.48
1:A:296:LEU:HA	1:A:296:LEU:HD12	1.42	0.47
1:A:566:ILE:CG2	1:A:566:ILE:HD12	2.43	0.47
1:A:861:GLY:O	1:A:862:ASN:C	2.50	0.47
2:B:311:LEU:O	2:B:312:GLU:C	2.53	0.47
3:C:209:TYR:N	3:C:209:TYR:HD1	2.10	0.47
6:H:32:THR:CB	6:H:33:GLN:OE1	2.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:39:ASP:HB2	9:K:40:HIS:H	1.36	0.47
1:A:44:THR:CA	1:A:44:THR:HB	2.30	0.47
1:A:187:LYS:CA	1:A:188:ASP:N	2.68	0.47
1:A:705:LYS:CB	1:A:705:LYS:C	2.79	0.47
1:A:1066:VAL:O	1:A:1067:LEU:C	2.51	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
2:B:287:ARG:O	2:B:327:ARG:HG3	2.13	0.47
7:I:59:VAL:O	7:I:60:GLN:C	2.55	0.47
1:A:217:LYS:O	1:A:221:SER:HB2	2.14	0.47
1:A:503:GLN:HE21	5:F:90:ARG:NH2	2.07	0.47
1:A:827:THR:CG2	1:A:827:THR:C	2.87	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
2:B:984:HIS:CD2	2:B:1025:HIS:CA	2.96	0.47
4:E:160:GLU:O	4:E:161:LYS:C	2.57	0.47
6:H:130:ARG:HB2	6:H:133:ASN:CB	2.44	0.47
9:K:11:LEU:CD1	9:K:11:LEU:CB	2.81	0.47
1:A:857:ARG:NH2	5:F:139:PRO:HG2	2.29	0.47
1:A:858:ASN:ND2	1:A:862:ASN:H	2.13	0.47
1:A:970:THR:O	1:A:970:THR:HG22	2.14	0.47
1:A:1153:TYR:CZ	7:I:42:LEU:HD13	2.50	0.47
2:B:34:ILE:O	2:B:35:SER:C	2.56	0.47
2:B:642:ASP:HA	2:B:643:ASP:HA	1.28	0.47
2:B:668:ASP:CG	2:B:668:ASP:CA	2.77	0.47
4:E:57:MET:CG	4:E:57:MET:CA	2.84	0.47
6:H:8:ASP:OD2	6:H:9:ILE:N	2.37	0.47
6:H:10:PHE:CD1	6:H:57:VAL:CG2	2.97	0.47
6:H:15:VAL:HG12	6:H:15:VAL:O	2.14	0.47
6:H:138:GLU:O	6:H:139:ASN:O	2.27	0.47
10:L:26:THR:CG2	10:L:26:THR:OG1	2.58	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
2:B:224:GLN:HB3	2:B:226:PHE:CZ	2.49	0.47
2:B:1058:LEU:O	2:B:1062:HIS:HD2	1.96	0.47
2:B:1205:GLN:O	2:B:1206:GLU:C	2.55	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
1:A:1004:ASN:ND2	4:E:167:ARG:HG3	2.30	0.47
2:B:487:THR:HG23	2:B:488:TYR:N	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:827:ILE:HG21	2:B:827:ILE:HD13	1.23	0.47
2:B:1003:ALA:C	2:B:1005:GLY:H	2.22	0.47
3:C:148:ARG:O	3:C:149:LYS:C	2.57	0.47
4:E:161:LYS:O	4:E:162:ARG:C	2.55	0.47
6:H:123:MET:CE	6:H:142:LEU:HD22	2.45	0.47
1:A:78:PRO:HB2	1:A:79:GLY:O	2.14	0.47
1:A:187:LYS:CG	1:A:194:ALA:CB	2.91	0.47
1:A:470:LEU:HD11	1:A:487:MET:SD	2.54	0.47
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.94	0.47
1:A:1217:LYS:O	1:A:1221:LYS:N	2.47	0.47
1:A:1220:PHE:CE2	1:A:1263:ILE:HD12	2.50	0.47
2:B:65:GLU:HG2	2:B:66:ASP:H	1.80	0.47
2:B:172:ILE:CD1	2:B:172:ILE:HG21	2.44	0.47
2:B:801:LYS:CG	2:B:801:LYS:CE	2.83	0.47
2:B:1079:LYS:HE3	3:C:188:HIS:CE1	2.50	0.47
2:B:1082:MET:HA	3:C:189:THR:HA	1.95	0.47
2:B:1173:ALA:HA	2:B:1180:PHE:HD2	1.80	0.47
3:C:11:ARG:O	3:C:12:GLU:HB2	2.13	0.47
6:H:4:THR:O	6:H:5:LEU:CB	2.60	0.47
6:H:47:PHE:CD2	6:H:47:PHE:C	2.91	0.47
8:J:53:HIS:C	8:J:54:VAL:HG23	2.37	0.47
1:A:71:GLN:CG	1:A:71:GLN:NE2	2.69	0.47
1:A:216:VAL:HG22	1:A:219:PHE:HZ	1.80	0.47
1:A:571:LEU:HA	1:A:571:LEU:HD12	1.68	0.47
1:A:843:LYS:CD	1:A:843:LYS:NZ	2.69	0.47
1:A:1109:LYS:CG	1:A:1109:LYS:HA	2.43	0.47
1:A:1148:ILE:CD1	1:A:1148:ILE:CG2	2.92	0.47
2:B:199:MET:HE2	2:B:492:LEU:CD2	2.44	0.47
2:B:502:ILE:CA	2:B:502:ILE:CD1	2.93	0.47
2:B:661:LEU:HD23	2:B:679:TYR:CD2	2.50	0.47
7:I:16:PRO:O	7:I:17:ARG:CD	2.57	0.47
1:A:620:LYS:CG	1:A:620:LYS:CE	2.91	0.47
1:A:829:VAL:CG2	1:A:829:VAL:HB	2.20	0.47
2:B:240:ILE:HG13	2:B:241:ARG:N	2.30	0.47
2:B:772:ALA:O	2:B:773:MET:C	2.57	0.47
2:B:789:MET:CE	2:B:965:LYS:CB	2.88	0.47
2:B:882:THR:HG1	2:B:933:SER:N	2.13	0.47
7:I:118:ARG:CD	7:I:118:ARG:CB	2.85	0.47
1:A:31:SER:HB2	1:A:83:HIS:CD2	2.46	0.47
1:A:92:HIS:HD2	1:A:94:GLY:N	2.12	0.47
1:A:418:SER:O	1:A:419:LYS:C	2.56	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:CD	1:A:568:PRO:CD	2.88	0.47
2:B:307:ASP:C	2:B:307:ASP:OD1	2.57	0.47
2:B:916:THR:HB	2:B:935:ARG:HB3	1.96	0.47
3:C:9:LYS:CD	3:C:9:LYS:CB	2.77	0.47
6:H:48:PRO:O	6:H:49:VAL:HG23	2.14	0.47
1:A:58:LEU:HB3	1:A:80:HIS:O	2.14	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
1:A:868:TYR:HE1	1:A:1064:VAL:HG13	1.81	0.46
2:B:189:LEU:HD23	2:B:189:LEU:HA	1.46	0.46
2:B:225:VAL:O	2:B:226:PHE:CD2	2.68	0.46
2:B:1182:CYS:HB3	2:B:1185:CYS:CB	2.43	0.46
3:C:207:CYS:O	3:C:208:GLU:C	2.59	0.46
4:E:48:ASP:HB3	4:E:54:GLN:HG2	1.97	0.46
4:E:74:ASP:N	4:E:74:ASP:OD1	2.48	0.46
6:H:100:THR:HG22	6:H:101:ALA:N	2.29	0.46
6:H:131:ASN:H	6:H:131:ASN:HD22	1.63	0.46
1:A:984:LYS:HG2	1:A:988:LEU:HD11	1.97	0.46
2:B:281:PRO:HB2	2:B:284:ILE:HD13	1.97	0.46
2:B:355:ILE:HG23	2:B:355:ILE:HD12	1.45	0.46
2:B:582:VAL:O	2:B:583:ASN:C	2.55	0.46
2:B:1176:ASN:CG	2:B:1176:ASN:CA	2.78	0.46
3:C:120:ILE:H	3:C:120:ILE:HD12	1.80	0.46
3:C:199:LYS:CG	3:C:199:LYS:N	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
4:E:96:PHE:O	4:E:97:VAL:C	2.52	0.46
1:A:523:ILE:CB	1:A:622:VAL:HG13	2.43	0.46
1:A:567:LYS:CB	6:H:95:TYR:CA	2.90	0.46
1:A:596:THR:CG2	1:A:596:THR:C	2.88	0.46
1:A:1143:LEU:O	1:A:1144:LYS:C	2.57	0.46
2:B:286:PHE:HB3	2:B:297:ILE:HD12	1.96	0.46
2:B:409:ALA:O	2:B:410:GLY:C	2.54	0.46
2:B:773:MET:C	2:B:775:LYS:N	2.69	0.46
4:E:13:TRP:CE3	4:E:39:LEU:HD13	2.50	0.46
5:F:140:ASP:C	5:F:140:ASP:OD1	2.56	0.46
6:H:105:GLU:C	6:H:107:VAL:N	2.70	0.46
7:I:51:ASN:HB2	7:I:118:ARG:CZ	2.46	0.46
8:J:62:ARG:HE	8:J:62:ARG:HB3	1.24	0.46
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.96	0.46
1:A:31:SER:HB3	1:A:83:HIS:CD2	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:LYS:HD3	1:A:748:MET:HE2	1.97	0.46
1:A:1358:SER:C	1:A:1360:GLY:H	2.23	0.46
2:B:416:LEU:HB3	2:B:420:LEU:HD12	1.97	0.46
2:B:880:THR:CG2	2:B:880:THR:CA	2.82	0.46
2:B:1045:SER:HB3	2:B:1046:PRO:HD2	1.98	0.46
3:C:239:PRO:O	3:C:240:VAL:C	2.51	0.46
6:H:48:PRO:C	6:H:49:VAL:CG2	2.88	0.46
1:A:243:PRO:C	1:A:245:PRO:HD2	2.40	0.46
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.97	0.46
1:A:599:SER:HA	1:A:600:PRO:HD2	1.58	0.46
1:A:860:LEU:CD1	1:A:860:LEU:CB	2.86	0.46
1:A:890:ASP:O	1:A:891:ALA:C	2.56	0.46
1:A:1023:ARG:HH21	1:A:1023:ARG:HD3	1.60	0.46
1:A:1132:LYS:C	1:A:1134:ILE:N	2.68	0.46
1:A:1364:ASN:HB3	1:A:1366:ARG:HG2	1.97	0.46
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.15	0.46
6:H:32:THR:HB	6:H:33:GLN:OE1	2.16	0.46
6:H:62:SER:O	6:H:63:LEU:C	2.58	0.46
1:A:567:LYS:CB	1:A:568:PRO:CD	2.90	0.46
1:A:920:LEU:CD2	1:A:921:GLY:H	2.28	0.46
2:B:393:LYS:HZ1	2:B:621:GLU:CD	2.15	0.46
6:H:56:THR:HG21	6:H:145:ARG:HE	1.79	0.46
6:H:101:ALA:HA	6:H:116:TYR:HA	1.97	0.46
9:K:103:THR:O	9:K:104:ASN:C	2.58	0.46
1:A:34:LYS:HG2	1:A:83:HIS:CE1	2.50	0.46
1:A:54:ASN:C	1:A:56:PRO:HD2	2.40	0.46
1:A:144:THR:O	1:A:146:MET:HG2	2.16	0.46
1:A:191:THR:CB	1:A:191:THR:C	2.84	0.46
1:A:1112:LYS:CD	1:A:1112:LYS:CB	2.90	0.46
2:B:400:HIS:CE1	2:B:517:THR:HG21	2.51	0.46
2:B:547:VAL:O	2:B:547:VAL:HG13	2.16	0.46
3:C:252:GLN:HB2	9:K:98:LEU:HD12	1.98	0.46
4:E:78:LEU:HD21	4:E:80:VAL:CG2	2.45	0.46
9:K:105:PHE:C	9:K:107:THR:H	2.23	0.46
1:A:46:THR:O	1:A:48:ALA:N	2.49	0.46
1:A:566:ILE:CG2	1:A:566:ILE:CD1	2.94	0.46
1:A:635:ARG:HH11	1:A:635:ARG:HD3	1.59	0.46
1:A:767:GLN:HA	1:A:799:PHE:HA	1.98	0.46
1:A:922:ASP:OD1	1:A:922:ASP:C	2.58	0.46
2:B:393:LYS:NZ	2:B:621:GLU:CD	2.72	0.46
2:B:736:THR:CG2	2:B:736:THR:HA	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:864:LYS:NZ	2:B:865:LYS:H	2.13	0.46
5:F:109:VAL:CG1	5:F:110:ASP:N	2.76	0.46
8:J:56:LEU:O	8:J:57:ILE:C	2.56	0.46
1:A:42:ASP:OD2	1:A:47:ARG:HA	2.16	0.46
1:A:135:PHE:CD1	1:A:222:LEU:HD22	2.51	0.46
1:A:356:ASP:OD2	1:A:469:ARG:CD	2.62	0.46
1:A:567:LYS:CE	6:H:95:TYR:CD2	2.99	0.46
1:A:999:VAL:HG12	1:A:1000:LEU:HG	1.98	0.46
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.80	0.46
1:A:1225:PHE:CG	1:A:1225:PHE:CA	2.90	0.46
2:B:773:MET:O	2:B:774:GLY:C	2.51	0.46
2:B:1006:ILE:HG22	2:B:1007:VAL:N	2.29	0.46
3:C:145:CYS:SG	3:C:146:LYS:N	2.89	0.46
5:F:125:LEU:HA	5:F:130:ILE:HD12	1.97	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:418:LYS:CG	2:B:418:LYS:CE	2.92	0.46
2:B:758:PHE:N	2:B:759:PRO:CD	2.79	0.46
2:B:1182:CYS:CB	2:B:1185:CYS:HB2	2.39	0.46
2:B:1195:HIS:C	2:B:1196:ILE:CG2	2.87	0.46
1:A:860:LEU:CD1	1:A:860:LEU:HG	2.21	0.45
1:A:1063:MET:C	1:A:1064:VAL:C	2.84	0.45
2:B:130:VAL:O	2:B:164:LYS:O	2.33	0.45
2:B:242:SER:OG	2:B:363:HIS:ND1	2.49	0.45
2:B:404:LYS:C	2:B:405:ARG:HG2	2.41	0.45
4:E:98:ILE:CG2	4:E:98:ILE:HG12	2.39	0.45
1:A:466:SER:HB3	2:B:1103:ILE:HD11	1.98	0.45
1:A:489:LEU:HD23	1:A:489:LEU:C	2.40	0.45
1:A:553:VAL:O	1:A:554:PRO:C	2.56	0.45
1:A:588:LEU:HD23	1:A:589:GLN:N	2.29	0.45
1:A:1120:LEU:HD21	1:A:1131:ALA:HB2	1.99	0.45
2:B:245:GLU:CA	2:B:246:LYS:N	2.67	0.45
2:B:521:LEU:CD2	2:B:635:ARG:HD3	2.45	0.45
3:C:195:GLN:CG	3:C:195:GLN:NE2	2.73	0.45
4:E:44:ALA:HB3	4:E:45:LYS:N	2.31	0.45
4:E:161:LYS:CE	4:E:161:LYS:CG	2.77	0.45
1:A:300:VAL:O	1:A:304:MET:HE2	2.16	0.45
1:A:974:ASP:OD1	1:A:974:ASP:N	2.49	0.45
1:A:1003:LYS:CG	1:A:1003:LYS:CE	2.91	0.45
2:B:344:LYS:O	2:B:345:LYS:C	2.59	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:LEU:HD12	3:C:80:LEU:HA	1.55	0.45
9:K:83:PRO:C	9:K:85:ASP:H	2.25	0.45
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.52	0.45
1:A:878:ILE:HG23	1:A:878:ILE:HD12	1.60	0.45
1:A:1225:PHE:C	1:A:1226:VAL:HG23	2.41	0.45
2:B:259:TYR:HB2	2:B:268:THR:HG22	1.98	0.45
2:B:900:ALA:O	2:B:903:VAL:HG23	2.17	0.45
5:F:89:GLU:O	5:F:90:ARG:C	2.56	0.45
6:H:22:LYS:C	6:H:23:VAL:HG23	2.38	0.45
1:A:108:MET:HE3	1:A:108:MET:HB3	1.50	0.45
1:A:589:GLN:HB2	1:A:961:ARG:HH22	1.80	0.45
1:A:1134:ILE:HG22	1:A:1306:LEU:CD1	2.46	0.45
2:B:118:ARG:NH2	2:B:194:GLU:CD	2.73	0.45
2:B:232:SER:OG	2:B:233:PRO:HD2	2.16	0.45
2:B:552:MET:N	2:B:553:PRO:HD2	2.31	0.45
2:B:999:MET:HB3	2:B:1000:PRO:CD	2.40	0.45
3:C:179:GLU:CG	3:C:180:TYR:N	2.79	0.45
3:C:230:MET:CG	3:C:230:MET:CE	2.82	0.45
4:E:2:ASP:HB3	4:E:6:GLU:HB2	1.98	0.45
8:J:14:VAL:HG13	8:J:14:VAL:O	2.13	0.45
2:B:69:LEU:O	2:B:70:ILE:HD13	2.17	0.45
2:B:423:LYS:CD	2:B:423:LYS:NZ	2.69	0.45
2:B:768:THR:O	2:B:769:TYR:C	2.50	0.45
3:C:169:LYS:NZ	10:L:69:ALA:O	2.44	0.45
3:C:205:LYS:H	3:C:205:LYS:HG3	1.64	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
1:A:1166:ASP:O	1:A:1167:GLU:C	2.58	0.45
1:A:1348:LEU:CG	1:A:1372:VAL:HG22	2.40	0.45
1:A:1364:ASN:ND2	1:A:1365:TYR:N	2.65	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:1131:GLY:C	2:B:1133:MET:N	2.74	0.45
4:E:37:LEU:HA	4:E:38:PRO:HD2	1.61	0.45
6:H:138:GLU:CG	6:H:139:ASN:N	2.80	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:903:ASN:HD21	1:A:905:ASP:H	1.57	0.45
2:B:343:ILE:CD1	2:B:343:ILE:CB	2.83	0.45
2:B:827:ILE:HG12	2:B:1012:ILE:HD11	1.99	0.45
2:B:1144:ALA:O	2:B:1145:SER:C	2.56	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1162:ILE:HD12	2:B:1162:ILE:HG23	1.54	0.45
6:H:47:PHE:O	6:H:47:PHE:HD2	2.00	0.45
6:H:105:GLU:HG2	6:H:136:LYS:HZ2	1.82	0.45
9:K:7:PHE:CD1	9:K:7:PHE:C	2.93	0.45
9:K:35:PHE:CD1	9:K:71:PHE:CE1	3.04	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
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.46	0.45
1:A:899:VAL:CG1	1:A:929:LEU:HD13	2.47	0.45
1:A:1162:VAL:CG1	1:A:1162:VAL:C	2.90	0.45
1:A:1322:ILE:O	1:A:1324:PRO:HD3	2.16	0.45
1:A:1405:THR:CA	1:A:1405:THR:HB	2.23	0.45
2:B:25:ILE:CG2	2:B:25:ILE:CA	2.86	0.45
2:B:134:LYS:CB	2:B:134:LYS:CE	2.94	0.45
2:B:416:LEU:HD11	2:B:466:TRP:CZ2	2.52	0.45
2:B:498:THR:HG22	2:B:537:LYS:H	1.81	0.45
2:B:958:GLN:HG2	2:B:958:GLN:N	2.30	0.45
3:C:116:LYS:C	3:C:118:LEU:H	2.25	0.45
3:C:262:LEU:HA	3:C:262:LEU:HD23	1.62	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
6:H:10:PHE:O	6:H:54:SER:HB2	2.16	0.45
1:A:848:ILE:HA	1:A:857:ARG:O	2.17	0.45
1:A:909:ASP:CG	1:A:910:PRO:CD	2.90	0.45
1:A:913:LEU:HD12	1:A:914:GLU:N	2.32	0.45
3:C:127:ARG:N	3:C:127:ARG:CG	2.80	0.45
6:H:114:VAL:HG11	6:H:134:ASN:ND2	2.32	0.45
1:A:70:CYS:O	1:A:72:GLU:OE1	2.34	0.44
1:A:80:HIS:O	1:A:243:PRO:HB3	2.17	0.44
1:A:524:VAL:O	1:A:525:GLN:C	2.58	0.44
1:A:878:ILE:HA	1:A:878:ILE:HD13	1.35	0.44
1:A:880:LYS:CD	1:A:880:LYS:CB	2.88	0.44
1:A:920:LEU:HA	1:A:920:LEU:HD23	1.45	0.44
2:B:92:PHE:CD1	2:B:92:PHE:N	2.85	0.44
2:B:531:GLN:CG	2:B:531:GLN:H	2.30	0.44
2:B:644:GLU:HA	2:B:645:SER:HB3	1.99	0.44
4:E:115:ASN:CB	4:E:115:ASN:ND2	2.67	0.44
4:E:123:LEU:O	4:E:126:SER:CB	2.64	0.44
4:E:171:LYS:O	4:E:172:GLU:C	2.60	0.44
9:K:88:LYS:C	9:K:90:ALA:N	2.70	0.44
1:A:138:ILE:HD12	1:A:142:CYS:SG	2.57	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ILE:HG22	1:A:542:GLU:N	2.32	0.44
1:A:548:ASN:O	1:A:549:MET:C	2.56	0.44
1:A:557:ASP:O	1:A:558:GLY:C	2.41	0.44
1:A:964:ILE:HA	1:A:964:ILE:HD13	1.70	0.44
1:A:1112:LYS:CG	1:A:1112:LYS:CE	2.92	0.44
2:B:68:THR:C	2:B:69:LEU:HG	2.41	0.44
2:B:249:ARG:HB2	2:B:418:LYS:NZ	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
4:E:47:CYS:SG	4:E:52:ARG:C	3.01	0.44
9:K:98:LEU:C	9:K:100:ALA:N	2.73	0.44
1:A:184:SER:HB2	1:A:199:LEU:HD23	2.00	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
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	1.99	0.44
1:A:1425:SER:O	1:A:1428:VAL:HB	2.17	0.44
2:B:129:PHE:HE2	2:B:166:PHE:CB	2.18	0.44
2:B:361:LEU:N	2:B:362:PRO:CD	2.79	0.44
2:B:916:THR:CG2	2:B:916:THR:CA	2.86	0.44
5:F:148:VAL:O	5:F:149:GLU:C	2.61	0.44
6:H:11:GLN:CB	6:H:11:GLN:CD	2.78	0.44
10:L:30:ILE:CD1	10:L:30:ILE:HG21	2.47	0.44
1:A:138:ILE:HG12	1:A:222:LEU:HD23	1.99	0.44
1:A:268:ASP:HA	1:A:271:LYS:HB2	1.99	0.44
1:A:1266:THR:O	1:A:1267:MET:C	2.61	0.44
1:A:1415:SER:O	1:A:1416:ALA:HB3	2.17	0.44
2:B:384:ARG:O	2:B:385:LEU:C	2.60	0.44
2:B:864:LYS:HZ2	2:B:865:LYS:C	2.25	0.44
2:B:893:LEU:N	2:B:893:LEU:HD23	2.33	0.44
2:B:958:GLN:CG	2:B:958:GLN:N	2.80	0.44
2:B:1050:ILE:H	2:B:1050:ILE:HD12	1.82	0.44
2:B:1163:CYS:SG	2:B:1165:ILE:HG12	2.58	0.44
6:H:123:MET:HG2	6:H:124:ARG:H	1.83	0.44
7:I:69:PRO:C	7:I:70:ARG:HG2	2.40	0.44
1:A:203:SER:O	1:A:204:THR:C	2.58	0.44
1:A:633:VAL:HG21	1:A:645:LEU:HD22	1.98	0.44
1:A:1208:THR:OG1	1:A:1211:GLN:NE2	2.50	0.44
1:A:1310:GLY:C	1:A:1311:VAL:HG23	2.42	0.44
2:B:529:GLU:O	2:B:531:GLN:NE2	2.50	0.44
2:B:904:ARG:C	2:B:905:VAL:CG1	2.90	0.44
2:B:1002:THR:O	2:B:1003:ALA:C	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1206:GLU:O	2:B:1209:ALA:HB3	2.17	0.44
3:C:94:LYS:CG	3:C:94:LYS:HB2	2.20	0.44
3:C:147:LEU:HD13	3:C:151:GLN:O	2.17	0.44
4:E:65:THR:O	4:E:69:ILE:CG1	2.66	0.44
4:E:132:ILE:HA	4:E:132:ILE:HD13	1.75	0.44
5:F:94:LEU:HD23	5:F:94:LEU:HA	1.66	0.44
6:H:16:ASP:O	6:H:24:CYS:HB3	2.17	0.44
6:H:33:GLN:C	6:H:35:GLN:N	2.75	0.44
2:B:137:TYR:CB	2:B:137:TYR:CD2	2.83	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:1131:GLY:O	2:B:1132:GLU:C	2.60	0.44
3:C:73:GLN:NE2	3:C:74:SER:H	2.16	0.44
4:E:2:ASP:O	4:E:3:GLN:C	2.61	0.44
4:E:37:LEU:CD1	4:E:37:LEU:CB	2.85	0.44
6:H:76:THR:CG2	6:H:76:THR:O	2.66	0.44
9:K:65:HIS:CD2	9:K:67:PHE:HB2	2.53	0.44
1:A:108:MET:N	1:A:171:GLN:HE22	2.09	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
2:B:269:ILE:HG13	2:B:317:CYS:SG	2.57	0.44
2:B:1172:ILE:HD12	2:B:1181:GLU:O	2.18	0.44
2:B:1188:LYS:CD	2:B:1188:LYS:CB	2.87	0.44
3:C:144:ILE:HG21	3:C:144:ILE:HD12	1.68	0.44
4:E:32:GLN:O	4:E:35:VAL:HB	2.18	0.44
9:K:65:HIS:CD2	9:K:66:PRO:HD2	2.53	0.44
1:A:463:ILE:HG21	1:A:463:ILE:HD13	1.64	0.44
1:A:606:LEU:HD11	1:A:608:ILE:HD11	1.99	0.44
1:A:1079:MET:HG2	1:A:1359:ASP:CG	2.43	0.44
1:A:1260:LEU:HD12	1:A:1260:LEU:HA	1.69	0.44
1:A:1298:TYR:O	1:A:1299:VAL:HG23	2.18	0.44
2:B:423:LYS:O	2:B:425:THR:N	2.51	0.44
2:B:772:ALA:O	2:B:775:LYS:N	2.40	0.44
3:C:250:THR:O	3:C:251:LEU:C	2.57	0.44
10:L:47:ARG:CG	10:L:48:CYS:N	2.78	0.44
1:A:39:GLU:HB3	1:A:50:ILE:HD12	2.00	0.44
1:A:92:HIS:O	1:A:93:VAL:C	2.58	0.44
1:A:509:LEU:H	1:A:509:LEU:HG	1.54	0.44
1:A:607:ILE:HG21	1:A:607:ILE:HD13	1.65	0.44
1:A:1164:PRO:O	1:A:1165:GLU:C	2.60	0.44
1:A:1172:LEU:C	1:A:1173:HIS:CG	2.96	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:319:GLU:H	2:B:319:GLU:HG3	1.66	0.44
2:B:609:ILE:CG2	2:B:610:ASN:N	2.77	0.44
2:B:1051:THR:HG22	2:B:1054:GLY:H	1.82	0.44
3:C:211:ASP:O	3:C:212:PRO:C	2.57	0.44
4:E:39:LEU:O	4:E:40:GLU:C	2.59	0.44
4:E:64:PRO:C	4:E:65:THR:HG23	2.43	0.44
8:J:4:PRO:HD3	8:J:53:HIS:HD2	1.83	0.44
1:A:187:LYS:C	1:A:187:LYS:CB	2.83	0.43
1:A:207:ILE:C	1:A:209:ASN:H	2.25	0.43
1:A:263:THR:O	1:A:264:PHE:C	2.61	0.43
1:A:407:ARG:O	1:A:408:ASP:C	2.61	0.43
1:A:672:ASP:HB2	1:A:675:THR:OG1	2.18	0.43
2:B:739:THR:C	2:B:740:HIS:CG	2.95	0.43
2:B:755:ILE:O	2:B:755:ILE:CG2	2.66	0.43
3:C:73:GLN:HB3	3:C:131:HIS:H	1.82	0.43
3:C:98:VAL:C	3:C:99:LEU:HD12	2.43	0.43
3:C:178:PHE:C	3:C:178:PHE:CD2	2.95	0.43
3:C:235:VAL:HG13	3:C:236:GLY:N	2.32	0.43
4:E:82:PHE:CD1	4:E:82:PHE:N	2.86	0.43
9:K:98:LEU:O	9:K:99:GLY:C	2.60	0.43
1:A:688:LYS:O	1:A:689:LYS:C	2.59	0.43
1:A:1164:PRO:O	1:A:1167:GLU:N	2.51	0.43
2:B:119:LEU:HD23	2:B:119:LEU:HA	1.63	0.43
2:B:958:GLN:CG	2:B:958:GLN:NE2	2.69	0.43
2:B:1010:LEU:HD12	2:B:1010:LEU:HA	1.34	0.43
3:C:251:LEU:HA	3:C:251:LEU:HD12	1.72	0.43
4:E:124:VAL:HB	4:E:125:PRO:HD3	2.01	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
1:A:247:ARG:HH11	1:A:247:ARG:HD2	1.61	0.43
1:A:264:PHE:O	1:A:267:ALA:HB3	2.18	0.43
1:A:587:HIS:NE2	1:A:969:GLN:HG2	2.33	0.43
1:A:613:ILE:HD12	1:A:613:ILE:HG23	1.75	0.43
1:A:911:SER:O	1:A:978:PRO:HB3	2.19	0.43
2:B:566:LEU:HD12	2:B:566:LEU:HA	1.71	0.43
2:B:582:VAL:C	2:B:584:GLY:N	2.75	0.43
2:B:1084:GLN:C	2:B:1085:ILE:HD12	2.44	0.43
4:E:11:ARG:HH11	4:E:11:ARG:HD2	1.32	0.43
4:E:43:LYS:CB	4:E:43:LYS:CE	2.96	0.43
6:H:100:THR:OG1	6:H:138:GLU:HG3	2.18	0.43
8:J:53:HIS:HE1	8:J:55:ASP:HA	1.82	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
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.17	0.43
1:A:587:HIS:CD2	1:A:966:ASN:OD1	2.68	0.43
1:A:1364:ASN:CG	1:A:1366:ARG:HD3	2.43	0.43
2:B:913:GLY:HA2	2:B:938:SER:HB2	1.99	0.43
3:C:255:VAL:O	3:C:255:VAL:HG12	2.18	0.43
4:E:40:GLU:O	4:E:41:ASP:C	2.61	0.43
5:F:117:PRO:O	5:F:118:LEU:C	2.57	0.43
6:H:137:GLN:CD	6:H:137:GLN:CB	2.82	0.43
10:L:32:ALA:CB	10:L:55:ILE:CG2	2.96	0.43
1:A:101:LYS:HD3	1:A:139:TRP:CE2	2.53	0.43
1:A:809:THR:HB	1:A:810:PRO:CD	2.48	0.43
2:B:59:LEU:HD12	2:B:59:LEU:HA	1.73	0.43
2:B:172:ILE:CD1	2:B:172:ILE:CG2	2.96	0.43
2:B:451:LYS:O	2:B:452:THR:C	2.60	0.43
2:B:878:GLN:H	2:B:934:LYS:HD2	1.83	0.43
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.78	0.43
3:C:66:ARG:NH2	8:J:3:VAL:O	2.51	0.43
6:H:23:VAL:HG12	6:H:24:CYS:N	2.32	0.43
1:A:31:SER:OG	1:A:83:HIS:CD2	2.72	0.43
1:A:269:ILE:HD13	1:A:269:ILE:HG21	1.82	0.43
1:A:518:LYS:HE3	1:A:624:SER:O	2.18	0.43
1:A:550:LEU:HD13	1:A:556:TRP:CZ2	2.53	0.43
2:B:129:PHE:HD2	2:B:166:PHE:N	2.15	0.43
2:B:817:LEU:N	2:B:818:PRO:HD3	2.33	0.43
2:B:1161:HIS:HA	2:B:1192:TYR:O	2.19	0.43
3:C:19:ASP:HA	3:C:231:ASN:HA	2.00	0.43
3:C:34:ARG:O	3:C:35:ARG:C	2.57	0.43
3:C:204:SER:O	3:C:205:LYS:C	2.60	0.43
4:E:37:LEU:HD23	4:E:42:PHE:HB2	1.99	0.43
4:E:45:LYS:C	4:E:46:TYR:CG	2.96	0.43
4:E:100:ILE:CG2	4:E:101:GLN:N	2.39	0.43
6:H:99:GLY:HA3	6:H:118:PHE:CD2	2.53	0.43
9:K:49:GLU:CG	9:K:94:ILE:CD1	2.96	0.43
1:A:11:LEU:O	1:A:12:ARG:HG2	2.18	0.43
1:A:289:ILE:HD13	1:A:289:ILE:HA	1.80	0.43
1:A:535:THR:CG2	1:A:616:VAL:CA	2.92	0.43
1:A:567:LYS:O	1:A:568:PRO:C	2.57	0.43
1:A:1059:HIS:CD2	1:A:1059:HIS:N	2.85	0.43
1:A:1111:MET:HE1	1:A:1331:SER:CB	2.48	0.43
1:A:1328:TYR:CG	1:A:1329:THR:N	2.87	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:1204:PHE:O	2:B:1205:GLN:C	2.58	0.43
3:C:73:GLN:HA	3:C:133:ILE:HD11	1.99	0.43
1:A:64:ASN:O	1:A:64:ASN:CG	2.60	0.43
1:A:177:ASP:CG	1:A:177:ASP:CA	2.80	0.43
1:A:827:THR:O	1:A:828:ALA:C	2.56	0.43
1:A:977:LYS:HA	1:A:978:PRO:HD2	1.79	0.43
1:A:1213:GLY:HA3	1:A:1228:TRP:CE3	2.53	0.43
2:B:122:LEU:HD23	2:B:122:LEU:HA	1.56	0.43
2:B:228:LYS:CG	2:B:228:LYS:HA	2.47	0.43
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.72	0.43
2:B:987:LYS:NZ	2:B:987:LYS:HD2	2.34	0.43
3:C:9:LYS:O	3:C:10:ILE:C	2.60	0.43
7:I:41:PRO:CD	7:I:42:LEU:H	2.31	0.43
1:A:64:ASN:C	1:A:66:LYS:N	2.76	0.43
1:A:83:HIS:ND1	1:A:83:HIS:C	2.77	0.43
1:A:203:SER:N	1:A:206:GLU:HG3	2.33	0.43
1:A:243:PRO:O	1:A:243:PRO:CG	2.61	0.43
1:A:423:ASP:CG	1:A:423:ASP:CA	2.76	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
2:B:106:ASP:O	10:L:47:ARG:NH2	2.52	0.43
2:B:179:CYS:O	2:B:180:TYR:C	2.55	0.43
2:B:187:SER:O	2:B:188:ASP:C	2.57	0.43
2:B:353:LYS:CG	2:B:353:LYS:CE	2.88	0.43
4:E:78:LEU:HD21	4:E:80:VAL:HG23	2.01	0.43
5:F:97:ARG:NH2	5:F:124:GLU:OE2	2.46	0.43
6:H:142:LEU:HD12	6:H:142:LEU:HA	1.74	0.43
9:K:65:HIS:CD2	9:K:66:PRO:N	2.86	0.43
1:A:247:ARG:HA	1:A:248:PRO:HD3	1.70	0.43
1:A:263:THR:C	1:A:265:LYS:N	2.77	0.43
1:A:993:LEU:O	1:A:994:GLN:C	2.56	0.43
1:A:1053:PHE:O	1:A:1054:LEU:C	2.58	0.43
2:B:120:ARG:HB2	2:B:122:LEU:HG	2.01	0.43
2:B:373:ARG:H	2:B:373:ARG:HG3	1.66	0.43
2:B:557:PHE:CZ	2:B:561:TRP:CD1	3.06	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
2:B:770:GLN:OE1	2:B:770:GLN:HA	2.18	0.43
3:C:55:THR:O	3:C:151:GLN:HG2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:84:ARG:CG	3:C:84:ARG:CA	2.82	0.43
3:C:156:THR:CG2	3:C:156:THR:C	2.90	0.43
4:E:63:ASN:OD1	4:E:77:SER:HB3	2.19	0.43
5:F:120:ILE:HD12	5:F:120:ILE:HG23	1.66	0.43
6:H:108:SER:O	6:H:109:LYS:C	2.61	0.43
10:L:58:LYS:O	10:L:59:ALA:O	2.36	0.43
1:A:274:ILE:CD1	1:A:274:ILE:CA	2.97	0.42
1:A:423:ASP:CG	1:A:423:ASP:C	2.87	0.42
1:A:670:ILE:HG21	1:A:670:ILE:HD12	1.77	0.42
1:A:1166:ASP:O	1:A:1170:ILE:CD1	2.64	0.42
1:A:1446:ASP:OD1	1:A:1448:GLU:HG3	2.19	0.42
2:B:98:THR:HB	2:B:99:LYS:O	2.19	0.42
2:B:121:ASN:HA	2:B:207:GLY:HA3	2.01	0.42
2:B:190:TYR:O	2:B:191:LYS:C	2.61	0.42
2:B:279:ASP:CG	2:B:279:ASP:CA	2.82	0.42
2:B:557:PHE:O	2:B:558:LEU:C	2.61	0.42
2:B:975:GLN:O	2:B:976:ILE:C	2.62	0.42
3:C:185:LYS:HB2	3:C:185:LYS:HE2	1.90	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
1:A:973:ILE:HD11	1:A:1038:THR:HG23	2.01	0.42
2:B:186:GLU:O	2:B:187:SER:C	2.61	0.42
2:B:202:TYR:CD2	2:B:202:TYR:N	2.84	0.42
2:B:648:HIS:ND1	2:B:648:HIS:N	2.67	0.42
2:B:764:SER:HB3	2:B:765:PRO:HD3	2.01	0.42
2:B:1031:LEU:O	2:B:1031:LEU:HG	2.17	0.42
2:B:1191:ILE:HG21	2:B:1191:ILE:HD13	1.74	0.42
3:C:241:ASP:OD1	3:C:241:ASP:N	2.51	0.42
4:E:43:LYS:O	4:E:47:CYS:HB3	2.19	0.42
4:E:103:LYS:CE	4:E:103:LYS:CG	2.83	0.42
4:E:176:PRO:O	4:E:212:ARG:HA	2.19	0.42
9:K:58:PHE:HB3	9:K:76:GLN:CB	2.50	0.42
10:L:55:ILE:HG21	10:L:55:ILE:HD12	1.82	0.42
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.55	0.42
1:A:842:VAL:O	1:A:846:GLU:HB2	2.20	0.42
1:A:882:SER:CB	1:A:953:ASN:OD1	2.68	0.42
2:B:37:PHE:CD2	2:B:37:PHE:C	2.97	0.42
2:B:215:GLN:HE21	2:B:215:GLN:HB3	1.62	0.42
2:B:1008:PRO:CG	2:B:1011:ILE:HD11	2.49	0.42
4:E:23:VAL:HG11	4:E:30:ILE:HD11	2.01	0.42
5:F:128:LYS:HD3	5:F:128:LYS:HA	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:44:VAL:O	6:H:44:VAL:HG13	2.18	0.42
1:A:366:VAL:O	1:A:367:PRO:C	2.60	0.42
1:A:816:HIS:HE2	2:B:763:GLN:HA	1.84	0.42
1:A:885:THR:O	1:A:940:ARG:HG3	2.20	0.42
1:A:1157:ASP:O	1:A:1159:ARG:N	2.52	0.42
1:A:1161:THR:CG2	1:A:1162:VAL:N	2.77	0.42
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.29	0.42
1:A:1364:ASN:O	1:A:1365:TYR:C	2.62	0.42
2:B:92:PHE:HZ	2:B:428:ILE:HD12	1.84	0.42
2:B:130:VAL:HB	2:B:131:ASP:H	1.80	0.42
2:B:197:PHE:O	2:B:198:ASP:C	2.59	0.42
2:B:705:MET:CE	2:B:745:PRO:CG	2.97	0.42
2:B:789:MET:CE	2:B:789:MET:HG3	2.50	0.42
2:B:864:LYS:O	2:B:961:LEU:CD2	2.67	0.42
3:C:33:LEU:O	3:C:34:ARG:C	2.59	0.42
6:H:33:GLN:C	6:H:35:GLN:H	2.28	0.42
9:K:18:LYS:HE3	9:K:38:GLU:HG2	2.00	0.42
1:A:53:LEU:HD23	1:A:54:ASN:H	1.84	0.42
1:A:829:VAL:CG2	1:A:829:VAL:CA	2.80	0.42
1:A:884:ASP:O	1:A:885:THR:C	2.62	0.42
3:C:181:ASP:OD2	3:C:185:LYS:N	2.49	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
9:K:94:ILE:HD12	9:K:94:ILE:HG23	1.88	0.42
10:L:29:TYR:O	10:L:30:ILE:HG13	2.19	0.42
10:L:61:THR:HG21	10:L:63:ARG:HD3	2.02	0.42
1:A:636:GLU:OE1	1:A:966:ASN:ND2	2.52	0.42
1:A:853:ASP:O	1:A:854:ASN:HB2	2.20	0.42
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.20	0.42
2:B:978:ASP:O	2:B:989:THR:HA	2.20	0.42
3:C:31:ASN:O	3:C:32:SER:C	2.59	0.42
3:C:43:THR:HG23	3:C:44:LEU:N	2.33	0.42
3:C:186:LEU:HA	3:C:186:LEU:HD12	1.57	0.42
4:E:44:ALA:C	4:E:46:TYR:N	2.77	0.42
1:A:870:GLU:HG2	4:E:208:TYR:CG	2.54	0.42
1:A:920:LEU:HD22	1:A:920:LEU:C	2.36	0.42
1:A:1150:SER:C	1:A:1151:GLU:HG3	2.45	0.42
1:A:1209:MET:O	1:A:1210:GLY:C	2.59	0.42
1:A:1430:LEU:O	1:A:1432:GLN:HG3	2.19	0.42
2:B:521:LEU:HD21	2:B:635:ARG:HD3	2.01	0.42
2:B:646:LEU:HG	2:B:646:LEU:CA	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:949:VAL:HG12	2:B:950:ASP:N	2.31	0.42
4:E:73:PRO:HD2	4:E:74:ASP:H	1.84	0.42
6:H:31:THR:O	6:H:32:THR:OG1	2.27	0.42
6:H:41:ASP:CG	6:H:41:ASP:CA	2.83	0.42
9:K:21:ILE:HD13	9:K:21:ILE:HG21	1.78	0.42
9:K:55:LYS:HB2	9:K:81:TYR:CE1	2.54	0.42
1:A:388:LEU:O	1:A:392:VAL:HG23	2.20	0.42
1:A:562:THR:CG2	6:H:98:TYR:CD2	3.02	0.42
2:B:27:ALA:O	2:B:28:GLU:C	2.59	0.42
2:B:791:THR:O	2:B:857:ARG:HA	2.20	0.42
2:B:846:ILE:CD1	2:B:974:PRO:CB	2.94	0.42
3:C:63:ILE:HD12	3:C:63:ILE:HG23	1.43	0.42
4:E:69:ILE:O	4:E:70:SER:C	2.56	0.42
4:E:72:PHE:HA	4:E:73:PRO:HD3	1.74	0.42
9:K:29:ASN:HB3	9:K:77:THR:O	2.20	0.42
1:A:613:ILE:HD13	1:A:613:ILE:HA	1.81	0.42
1:A:913:LEU:O	1:A:914:GLU:C	2.62	0.42
1:A:926:GLN:HE21	1:A:926:GLN:HB2	1.38	0.42
1:A:1305:VAL:HG12	1:A:1306:LEU:N	2.34	0.42
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.54	0.42
2:B:639:ILE:CG2	2:B:640:VAL:N	2.81	0.42
2:B:784:ASN:OD1	2:B:784:ASN:C	2.61	0.42
2:B:984:HIS:HD2	2:B:1025:HIS:HA	1.81	0.42
2:B:1051:THR:O	2:B:1055:ILE:HG12	2.20	0.42
2:B:1191:ILE:HG22	2:B:1192:TYR:N	2.34	0.42
3:C:88:CYS:SG	3:C:92:CYS:SG	3.17	0.42
4:E:153:HIS:C	4:E:154:ILE:HD12	2.44	0.42
1:A:241:VAL:HA	1:A:242:PRO:HD2	1.96	0.42
1:A:705:LYS:CG	1:A:705:LYS:CE	2.87	0.42
1:A:820:GLY:O	1:A:821:ARG:C	2.54	0.42
1:A:867:ILE:HG21	1:A:867:ILE:HD13	1.73	0.42
1:A:1116:LEU:HD12	1:A:1116:LEU:HA	1.71	0.42
2:B:416:LEU:C	2:B:418:LYS:N	2.74	0.42
2:B:492:LEU:HD23	2:B:492:LEU:HA	1.81	0.42
2:B:846:ILE:CA	2:B:846:ILE:CG1	2.81	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:119:ASN:O	1:A:120:GLU:CB	2.68	0.41
1:A:644:LYS:HE3	1:A:644:LYS:HB3	1.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:884:ASP:C	1:A:886:ILE:N	2.78	0.41
1:A:924:LYS:HE2	1:A:924:LYS:HB2	1.60	0.41
1:A:1044:TRP:CZ2	1:A:1048:ASN:ND2	2.88	0.41
1:A:1258:HIS:C	1:A:1260:LEU:N	2.73	0.41
1:A:1316:VAL:O	1:A:1317:MET:C	2.61	0.41
2:B:98:THR:OG1	2:B:127:GLY:N	2.52	0.41
2:B:571:PRO:O	2:B:573:GLN:N	2.53	0.41
2:B:620:ARG:CG	2:B:620:ARG:N	2.83	0.41
2:B:661:LEU:HD23	2:B:679:TYR:HD2	1.85	0.41
2:B:956:THR:CG2	2:B:961:LEU:O	2.68	0.41
3:C:15:LYS:CG	3:C:15:LYS:CA	2.89	0.41
3:C:72:LEU:O	3:C:73:GLN:C	2.60	0.41
3:C:220:ASP:CG	3:C:220:ASP:CA	2.80	0.41
4:E:78:LEU:HG	4:E:79:TRP:N	2.32	0.41
1:A:40:THR:CB	1:A:40:THR:C	2.83	0.41
1:A:158:PRO:HA	1:A:160:GLN:H	1.85	0.41
1:A:270:LEU:HD13	1:A:270:LEU:HA	1.86	0.41
1:A:399:HIS:HE1	1:A:436:ILE:O	2.04	0.41
1:A:752:LYS:CE	1:A:752:LYS:HG2	2.48	0.41
1:A:793:SER:O	1:A:794:PRO:C	2.56	0.41
1:A:1217:LYS:O	1:A:1221:LYS:HA	2.20	0.41
1:A:1362:TYR:CD2	1:A:1362:TYR:C	2.95	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
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
4:E:43:LYS:CB	4:E:43:LYS:HE2	2.50	0.41
5:F:147:SER:OG	5:F:150:GLU:HB2	2.19	0.41
6:H:9:ILE:HA	6:H:55:LEU:O	2.19	0.41
6:H:18:GLY:O	6:H:19:ARG:CB	2.54	0.41
9:K:23:PRO:O	9:K:23:PRO:CD	2.68	0.41
1:A:353:ILE:HD13	1:A:353:ILE:HG21	1.12	0.41
1:A:393:ARG:CG	1:A:393:ARG:NE	2.75	0.41
2:B:1035:ALA:HB1	2:B:1040:ASN:O	2.21	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
3:C:114:TYR:HB3	3:C:140:ASN:O	2.20	0.41
6:H:47:PHE:CB	6:H:95:TYR:HD1	2.32	0.41
1:A:709:THR:CG2	1:A:712:GLU:HG3	2.50	0.41
1:A:910:PRO:HA	1:A:916:GLY:HA3	2.03	0.41
1:A:1154:TYR:CZ	1:A:1156:PRO:HB3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1424:VAL:O	1:A:1428:VAL:HG23	2.20	0.41
1:A:1433:MET:HB3	1:A:1433:MET:HE3	1.71	0.41
2:B:123:THR:O	2:B:123:THR:HG22	2.09	0.41
2:B:134:LYS:CB	2:B:134:LYS:CD	2.86	0.41
2:B:170:LEU:HA	2:B:171:PRO:HD3	1.76	0.41
2:B:179:CYS:C	2:B:181:LEU:H	2.28	0.41
2:B:424:LEU:CD2	2:B:428:ILE:HD11	2.41	0.41
4:E:7:ARG:C	4:E:9:ILE:N	2.77	0.41
10:L:48:CYS:HB3	10:L:51:CYS:O	2.21	0.41
1:A:150:THR:HG22	1:A:151:ASP:OD2	2.21	0.41
1:A:275:SER:O	1:A:279:LEU:HG	2.21	0.41
1:A:516:SER:O	1:A:517:ASN:CG	2.64	0.41
1:A:962:ARG:O	1:A:963:ILE:C	2.59	0.41
1:A:1354:ASN:O	1:A:1355:VAL:C	2.62	0.41
2:B:387:LEU:HD12	2:B:387:LEU:HA	1.73	0.41
2:B:416:LEU:HD23	2:B:416:LEU:HA	1.51	0.41
2:B:515:HIS:HD2	2:B:517:THR:H	1.67	0.41
2:B:646:LEU:CD2	2:B:646:LEU:HG	2.32	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
3:C:26:ASP:OD1	3:C:26:ASP:N	2.50	0.41
4:E:182:ASP:O	4:E:183:PRO:C	2.61	0.41
6:H:47:PHE:CZ	6:H:146:ARG:HD2	2.55	0.41
6:H:95:TYR:CD2	6:H:95:TYR:C	2.99	0.41
1:A:542:GLU:O	1:A:546:VAL:HG23	2.20	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
2:B:28:GLU:OE1	2:B:807:ARG:NH2	2.54	0.41
2:B:292:ILE:N	2:B:293:PRO:CD	2.83	0.41
2:B:571:PRO:C	2:B:573:GLN:N	2.76	0.41
2:B:694:ASP:O	2:B:695:ALA:C	2.58	0.41
2:B:705:MET:HB3	2:B:706:GLN:HE21	1.85	0.41
2:B:820:GLY:HA3	2:B:1091:TYR:CE2	2.56	0.41
2:B:879:ARG:NH2	2:B:885:MET:HE2	2.35	0.41
2:B:1007:VAL:HA	2:B:1008:PRO:HD3	1.97	0.41
3:C:15:LYS:NZ	3:C:15:LYS:HD2	2.36	0.41
4:E:36:GLU:O	4:E:38:PRO:N	2.53	0.41
8:J:5:VAL:HG12	8:J:6:ARG:HG2	2.03	0.41
8:J:38:ARG:C	8:J:40:GLY:H	2.27	0.41
9:K:33:ILE:CD1	9:K:87:LEU:HD22	2.51	0.41
1:A:186:LYS:CG	1:A:186:LYS:CA	2.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ILE:C	1:A:209:ASN:N	2.75	0.41
1:A:414:ASP:OD1	1:A:414:ASP:C	2.63	0.41
1:A:1111:MET:CE	1:A:1111:MET:CB	2.99	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
2:B:940:PRO:O	2:B:941:LEU:C	2.60	0.41
3:C:53:THR:HB	3:C:154:LYS:HG3	2.02	0.41
7:I:14:LEU:HB3	7:I:27:PHE:HB3	2.03	0.41
10:L:30:ILE:HG21	10:L:30:ILE:HD13	2.02	0.41
10:L:30:ILE:CG2	10:L:31:CYS:N	2.83	0.41
1:A:1107:VAL:O	1:A:1107:VAL:HG12	2.20	0.41
2:B:170:LEU:HA	2:B:170:LEU:HD12	1.83	0.41
2:B:877:PRO:O	2:B:878:GLN:HG2	2.21	0.41
2:B:1013:ASN:OD1	2:B:1013:ASN:C	2.63	0.41
2:B:1163:CYS:CB	2:B:1163:CYS:C	2.77	0.41
3:C:22:LEU:HD23	3:C:22:LEU:HA	1.82	0.41
3:C:124:LEU:N	3:C:124:LEU:HD23	2.36	0.41
4:E:88:VAL:HG12	4:E:116:ILE:HG23	2.02	0.41
4:E:167:ARG:HD3	4:E:167:ARG:HA	1.92	0.41
5:F:74:ILE:HG23	5:F:74:ILE:HD12	1.80	0.41
1:A:40:THR:CB	1:A:40:THR:HA	2.21	0.41
1:A:456:MET:HB2	1:A:478:TYR:OH	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
2:B:999:MET:HE2	2:B:999:MET:HA	2.03	0.41
2:B:1006:ILE:CG2	2:B:1007:VAL:N	2.83	0.41
2:B:1096:ARG:C	2:B:1097:HIS:CB	2.93	0.41
3:C:116:LYS:C	3:C:118:LEU:N	2.79	0.41
3:C:211:ASP:C	3:C:212:PRO:O	2.58	0.41
3:C:240:VAL:C	3:C:242:GLN:H	2.20	0.41
4:E:79:TRP:HE1	4:E:81:GLU:HB2	1.86	0.41
6:H:51:ALA:CB	6:H:51:ALA:N	2.67	0.41
6:H:118:PHE:O	6:H:120:GLY:N	2.54	0.41
6:H:138:GLU:CG	6:H:139:ASN:H	2.33	0.41
7:I:111:THR:HB	7:I:113:ASP:H	1.86	0.41
7:I:111:THR:HG21	7:I:113:ASP:HB2	2.02	0.41
10:L:38:LEU:HD13	10:L:48:CYS:HA	2.02	0.41
1:A:7:SER:C	1:A:9:ALA:N	2.76	0.41
1:A:11:LEU:HD11	2:B:1195:HIS:HD2	1.82	0.41
1:A:34:LYS:O	1:A:35:ILE:C	2.63	0.41
1:A:84:ILE:HD13	1:A:270:LEU:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:GLN:O	1:A:526:ASP:C	2.62	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
2:B:237:VAL:CG1	2:B:238:ALA:N	2.71	0.41
2:B:539:LEU:H	2:B:539:LEU:HG	1.69	0.41
2:B:1196:ILE:O	2:B:1197:PRO:C	2.60	0.41
4:E:78:LEU:CD2	4:E:80:VAL:HG23	2.51	0.41
5:F:79:ARG:HH22	5:F:150:GLU:CD	2.29	0.41
6:H:11:GLN:NE2	6:H:52:GLN:HG2	2.35	0.41
6:H:103:LYS:CG	6:H:105:GLU:CD	2.90	0.41
8:J:36:LEU:HD13	8:J:47:ARG:HB3	2.03	0.41
9:K:21:ILE:HG12	9:K:33:ILE:HG12	2.03	0.41
9:K:56:VAL:CB	9:K:56:VAL:C	2.80	0.41
9:K:58:PHE:HB3	9:K:76:GLN:HB3	2.03	0.41
1:A:370:ILE:HD11	2:B:1103:ILE:HG23	2.02	0.40
1:A:577:ILE:HD12	1:A:577:ILE:HG23	1.83	0.40
1:A:606:LEU:HB3	1:A:614:PHE:CD2	2.56	0.40
1:A:1111:MET:HE1	1:A:1331:SER:HB2	2.03	0.40
1:A:1130:GLN:NE2	1:A:1134:ILE:CD1	2.84	0.40
1:A:1207:LEU:HD23	1:A:1207:LEU:HA	2.00	0.40
1:A:1318:THR:CG2	4:E:11:ARG:HH12	2.27	0.40
2:B:310:MET:O	2:B:311:LEU:C	2.61	0.40
2:B:423:LYS:O	2:B:426:LYS:N	2.47	0.40
2:B:764:SER:HB3	2:B:765:PRO:CD	2.51	0.40
2:B:787:VAL:O	2:B:787:VAL:HG13	2.20	0.40
3:C:15:LYS:O	3:C:240:VAL:CG2	2.70	0.40
3:C:216:GLY:O	3:C:217:ASP:C	2.64	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:903:ASN:ND2	1:A:903:ASN:C	2.75	0.40
1:A:970:THR:O	1:A:970:THR:CG2	2.68	0.40
1:A:1267:MET:HB3	1:A:1267:MET:HE3	1.47	0.40
1:A:1327:ILE:HD13	1:A:1327:ILE:HG21	1.90	0.40
2:B:56:ASP:N	2:B:56:ASP:OD1	2.53	0.40
2:B:117:ALA:HB1	2:B:122:LEU:HB2	2.03	0.40
2:B:119:LEU:O	2:B:965:LYS:NZ	2.49	0.40
2:B:121:ASN:ND2	2:B:965:LYS:NZ	2.69	0.40
2:B:423:LYS:O	2:B:424:LEU:C	2.63	0.40
2:B:435:THR:CA	2:B:436:VAL:N	2.69	0.40
2:B:723:VAL:CG1	2:B:723:VAL:CA	2.92	0.40
3:C:73:GLN:HG3	3:C:74:SER:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:143:PHE:CD1	5:F:143:PHE:C	2.99	0.40
6:H:95:TYR:HB3	6:H:144:ILE:CG2	2.52	0.40
7:I:45:ARG:HG3	7:I:46:HIS:N	2.35	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
1:A:1293:SER:OG	1:A:1294:PRO:N	2.45	0.40
2:B:199:MET:HE2	2:B:492:LEU:HD23	2.03	0.40
2:B:328:GLU:CG	2:B:328:GLU:HA	2.50	0.40
2:B:405:ARG:HA	2:B:631:GLY:O	2.20	0.40
2:B:565:PRO:O	2:B:566:LEU:C	2.58	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
6:H:43:ASN:OD1	6:H:43:ASN:C	2.65	0.40
7:I:104:LEU:HA	7:I:104:LEU:HD23	1.90	0.40
9:K:74:ARG:HH11	9:K:74:ARG:HD2	1.50	0.40
1:A:300:VAL:O	1:A:303:TYR:HB3	2.20	0.40
1:A:446:ARG:HB2	1:A:487:MET:CE	2.48	0.40
2:B:422:LYS:HD3	2:B:422:LYS:HA	1.95	0.40
2:B:1151:LEU:O	2:B:1152:MET:C	2.63	0.40
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.86	0.40
3:C:167:HIS:CD2	3:C:169:LYS:HG2	2.56	0.40
6:H:2:SER:HA	6:H:3:ASN:N	2.32	0.40
7:I:15:TYR:CD1	7:I:30:ARG:HG3	2.57	0.40
1:A:64:ASN:OD1	1:A:64:ASN:C	2.61	0.40
1:A:187:LYS:CG	1:A:194:ALA:HB3	2.51	0.40
1:A:215:SER:HG	1:A:218:ASP:HB2	1.86	0.40
1:A:282:ASN:CG	1:A:282:ASN:CA	2.84	0.40
1:A:567:LYS:HB2	1:A:568:PRO:HD3	2.03	0.40
1:A:605:MET:HE1	1:A:612:ILE:HG23	2.04	0.40
1:A:616:VAL:HG12	1:A:617:VAL:N	2.35	0.40
2:B:101:MET:O	2:B:101:MET:CG	2.69	0.40
2:B:191:LYS:CG	2:B:191:LYS:CE	2.94	0.40
2:B:245:GLU:C	2:B:245:GLU:CB	2.81	0.40
2:B:973:ILE:HD13	2:B:973:ILE:HG21	1.91	0.40
8:J:16:ASP:OD1	8:J:17:LYS:HE2	2.22	0.40
9:K:110:ASN:O	9:K:111:LEU:C	2.53	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%)	1 10
2	B	1071/1224 (88%)	914 (85%)	110 (10%)	47 (4%)	2 13
3	C	264/318 (83%)	230 (87%)	22 (8%)	12 (4%)	2 12
4	E	213/215 (99%)	182 (85%)	20 (9%)	11 (5%)	1 10
5	F	81/155 (52%)	72 (89%)	7 (9%)	2 (2%)	4 21
6	H	129/146 (88%)	82 (64%)	21 (16%)	26 (20%)	0 0
7	I	119/122 (98%)	107 (90%)	11 (9%)	1 (1%)	16 44
8	J	62/70 (89%)	58 (94%)	3 (5%)	1 (2%)	7 29
9	K	112/120 (93%)	99 (88%)	9 (8%)	4 (4%)	2 16
10	L	44/70 (63%)	24 (54%)	9 (20%)	11 (25%)	0 0
All	All	3427/4173 (82%)	2941 (86%)	305 (9%)	181 (5%)	1 10

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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 (i)

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%)	936 (79%)	245 (21%)	1	4
2	B	947/1061 (89%)	756 (80%)	191 (20%)	1	4
3	C	234/274 (85%)	186 (80%)	48 (20%)	1	4
4	E	197/197 (100%)	138 (70%)	59 (30%)	0	1
5	F	73/137 (53%)	61 (84%)	12 (16%)	2	10
6	H	117/128 (91%)	65 (56%)	52 (44%)	0	0
7	I	115/116 (99%)	85 (74%)	30 (26%)	0	1
8	J	59/65 (91%)	43 (73%)	16 (27%)	0	1
9	K	99/102 (97%)	76 (77%)	23 (23%)	1	2
10	L	40/57 (70%)	21 (52%)	19 (48%)	0	0
All	All	3062/3657 (84%)	2367 (77%)	695 (23%)	1	3

All (695) 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	21	LEU
1	A	22	PHE
1	A	28	ARG
1	A	34	LYS
1	A	36	ARG
1	A	39	GLU
1	A	41	MET
1	A	46	THR
1	A	49	LYS
1	A	54	ASN
1	A	57	ARG
1	A	58	LEU
1	A	60	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	65	LEU
1	A	66	LYS
1	A	68	GLN
1	A	70	CYS
1	A	72	GLU
1	A	84	ILE
1	A	85	ASP
1	A	90	VAL
1	A	93	VAL
1	A	98	LYS
1	A	99	ILE
1	A	106	VAL
1	A	107	CYS
1	A	110	CYS
1	A	112	LYS
1	A	114	LEU
1	A	120	GLU
1	A	123	ARG
1	A	129	LYS
1	A	132	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
1	A	176	LYS
1	A	181	LEU
1	A	184	SER
1	A	186	LYS
1	A	191	THR
1	A	198	GLU
1	A	201	VAL
1	A	205	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	206	GLU
1	A	210	ILE
1	A	225	ASN
1	A	226	GLU
1	A	236	LEU
1	A	237	THR
1	A	239	LEU
1	A	246	VAL
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	286	HIS
1	A	289	ILE
1	A	294	SER
1	A	299	HIS
1	A	302	THR
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	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
1	A	475	THR
1	A	493	GLN
1	A	495	GLU
1	A	497	THR
1	A	498	ARG
1	A	504	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	508	PRO
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	590	ARG
1	A	597	LEU
1	A	599	SER
1	A	613	ILE
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	682	THR
1	A	688	LYS
1	A	695	LYS
1	A	702	LEU
1	A	703	THR
1	A	708	MET
1	A	709	THR
1	A	710	LEU
1	A	720	ARG
1	A	724	GLU
1	A	728	LYS
1	A	737	LEU
1	A	741	ASN
1	A	744	LYS
1	A	752	LYS
1	A	794	PRO
1	A	810	PRO
1	A	827	THR
1	A	830	LYS
1	A	834	THR
1	A	840	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	913	LEU
1	A	918	GLU
1	A	919	ILE
1	A	920	LEU
1	A	924	LYS
1	A	960	ILE
1	A	969	GLN
1	A	973	ILE
1	A	974	ASP
1	A	978	PRO
1	A	979	SER
1	A	982	THR
1	A	983	ILE
1	A	1001	ARG
1	A	1006	ILE
1	A	1015	VAL
1	A	1030	ARG
1	A	1039	LYS
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	1116	LEU
1	A	1118	VAL
1	A	1120	LEU
1	A	1127	ASP
1	A	1129	GLU
1	A	1133	LEU
1	A	1134	ILE
1	A	1135	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1138	ILE
1	A	1141	THR
1	A	1146	VAL
1	A	1161	THR
1	A	1165	GLU
1	A	1168	GLU
1	A	1170	ILE
1	A	1171	GLN
1	A	1176	LEU
1	A	1187	GLN
1	A	1208	THR
1	A	1217	LYS
1	A	1221	LYS
1	A	1222	ASN
1	A	1225	PHE
1	A	1230	GLU
1	A	1235	LYS
1	A	1236	LEU
1	A	1237	ILE
1	A	1239	ARG
1	A	1243	VAL
1	A	1255	GLU
1	A	1258	HIS
1	A	1259	MET
1	A	1260	LEU
1	A	1263	ILE
1	A	1269	GLU
1	A	1271	ILE
1	A	1277	GLU
1	A	1279	ILE
1	A	1280	GLU
1	A	1281	ARG
1	A	1290	LYS
1	A	1291	VAL
1	A	1293	SER
1	A	1299	VAL
1	A	1309	ASP
1	A	1314	SER
1	A	1318	THR
1	A	1322	ILE
1	A	1325	THR
1	A	1336	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1350	LYS
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	1382	THR
1	A	1384	VAL
1	A	1405	THR
1	A	1424	VAL
1	A	1426	GLU
1	A	1433	MET
1	A	1436	ILE
1	A	1438	THR
1	A	1444	MET
1	A	1445	ILE
1	A	1448	GLU
1	A	1449	SER
2	B	18	PHE
2	B	20	ASP
2	B	25	ILE
2	B	46	GLN
2	B	63	ILE
2	B	65	GLU
2	B	68	THR
2	B	69	LEU
2	B	89	GLU
2	B	90	ILE
2	B	92	PHE
2	B	95	ILE
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	169	ARG
2	B	172	ILE
2	B	178	ASN
2	B	179	CYS
2	B	183	GLU
2	B	199	MET
2	B	204	ILE
2	B	205	ILE
2	B	228	LYS
2	B	239	GLU
2	B	240	ILE
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	272	THR
2	B	276	ILE
2	B	277	LYS
2	B	282	ILE
2	B	283	VAL
2	B	284	ILE
2	B	305	VAL
2	B	306	ASN
2	B	315	LYS
2	B	347	LYS
2	B	357	GLN
2	B	367	LEU
2	B	371	GLU
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	422	LYS
2	B	423	LYS
2	B	425	THR
2	B	426	LYS
2	B	434	ARG
2	B	435	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	502	ILE
2	B	513	GLN
2	B	516	ASN
2	B	522	VAL
2	B	524	PRO
2	B	531	GLN
2	B	541	LEU
2	B	547	VAL
2	B	549	THR
2	B	552	MET
2	B	566	LEU
2	B	567	GLU
2	B	574	SER
2	B	589	VAL
2	B	591	ARG
2	B	595	ARG
2	B	598	GLU
2	B	604	ARG
2	B	606	LYS
2	B	612	GLU
2	B	614	SER
2	B	615	MET
2	B	619	ILE
2	B	624	LEU
2	B	640	VAL
2	B	641	GLU
2	B	648	HIS
2	B	653	VAL
2	B	662	MET
2	B	680	THR
2	B	690	VAL
2	B	691	GLU
2	B	693	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	706	GLN
2	B	710	LEU
2	B	723	VAL
2	B	733	HIS
2	B	736	THR
2	B	768	THR
2	B	775	LYS
2	B	780	VAL
2	B	787	VAL
2	B	806	THR
2	B	838	SER
2	B	839	MET
2	B	860	MET
2	B	863	GLU
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	885	MET
2	B	889	THR
2	B	893	LEU
2	B	895	ASP
2	B	896	ASP
2	B	901	PRO
2	B	908	GLU
2	B	911	ILE
2	B	933	SER
2	B	938	SER
2	B	944	THR
2	B	948	ILE
2	B	955	THR
2	B	956	THR
2	B	958	GLN
2	B	964	VAL
2	B	971	THR
2	B	973	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	974	PRO
2	B	975	GLN
2	B	983	ARG
2	B	987	LYS
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1034	VAL
2	B	1045	SER
2	B	1051	THR
2	B	1056	SER
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	1103	ILE
2	B	1106	ARG
2	B	1147	LEU
2	B	1150	ARG
2	B	1152	MET
2	B	1155	SER
2	B	1156	ASP
2	B	1159	ARG
2	B	1162	ILE
2	B	1165	ILE
2	B	1174	LYS
2	B	1175	LEU
2	B	1177	HIS
2	B	1178	ASN
2	B	1179	GLN
2	B	1183	LYS
2	B	1185	CYS
2	B	1187	ASN
2	B	1189	ILE
2	B	1190	ASP
2	B	1211	ASN
2	B	1218	THR
2	B	1222	ARG
2	B	1224	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	3	GLU
3	C	4	GLU
3	C	11	ARG
3	C	14	SER
3	C	23	SER
3	C	25	VAL
3	C	26	ASP
3	C	29	MET
3	C	33	LEU
3	C	38	ILE
3	C	43	THR
3	C	56	THR
3	C	57	VAL
3	C	62	PHE
3	C	83	SER
3	C	86	CYS
3	C	93	ASP
3	C	102	GLN
3	C	110	THR
3	C	119	VAL
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	137	LYS
3	C	154	LYS
3	C	156	THR
3	C	163	ILE
3	C	184	ASN
3	C	185	LYS
3	C	186	LEU
3	C	197	SER
3	C	199	LYS
3	C	205	LYS
3	C	209	TYR
3	C	214	ASN
3	C	218	PRO
3	C	235	VAL
3	C	238	ILE
3	C	240	VAL
3	C	241	ASP
3	C	242	GLN
3	C	245	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	246	ARG
3	C	252	GLN
3	C	258	ILE
3	C	260	LEU
3	C	265	MET
3	C	266	ASP
4	E	3	GLN
4	E	4	GLU
4	E	6	GLU
4	E	8	ASN
4	E	10	SER
4	E	14	ARG
4	E	30	ILE
4	E	33	GLU
4	E	34	GLU
4	E	36	GLU
4	E	37	LEU
4	E	39	LEU
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	66	GLU
4	E	69	ILE
4	E	70	SER
4	E	74	ASP
4	E	78	LEU
4	E	81	GLU
4	E	82	PHE
4	E	84	ASP
4	E	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	E	117	THR
4	E	118	PRO
4	E	121	MET
4	E	123	LEU
4	E	127	ILE
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	162	ARG
4	E	167	ARG
4	E	169	ARG
4	E	179	GLN
4	E	183	PRO
4	E	192	ARG
4	E	198	ILE
4	E	200	ARG
4	E	201	LYS
4	E	204	THR
4	E	212	ARG
5	F	72	LYS
5	F	74	ILE
5	F	77	ASP
5	F	81	THR
5	F	82	THR
5	F	97	ARG
5	F	109	VAL
5	F	110	ASP
5	F	111	LEU
5	F	117	PRO
5	F	119	ARG
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	15	VAL
6	H	17	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	H	19	ARG
6	H	22	LYS
6	H	34	ASP
6	H	35	GLN
6	H	36	CYS
6	H	37	LYS
6	H	40	LEU
6	H	42	ILE
6	H	44	VAL
6	H	45	GLU
6	H	52	GLN
6	H	53	ASP
6	H	54	SER
6	H	56	THR
6	H	57	VAL
6	H	59	ILE
6	H	63	LEU
6	H	77	ARG
6	H	78	SER
6	H	80	ARG
6	H	83	GLN
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
6	H	131	ASN
6	H	135	LEU
6	H	136	LYS
6	H	137	GLN
6	H	138	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	H	143	LEU
6	H	144	ILE
6	H	145	ARG
7	I	1	MET
7	I	2	THR
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	55	THR
7	I	58	VAL
7	I	59	VAL
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	82	GLU
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	119	THR
7	I	120	GLN
8	J	1	MET
8	J	2	ILE
8	J	3	VAL
8	J	7	CYS
8	J	9	SER
8	J	13	VAL
8	J	14	VAL
8	J	20	SER
8	J	25	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	6	ARG
9	K	11	LEU
9	K	12	LEU
9	K	14	GLU
9	K	20	LYS
9	K	31	VAL
9	K	42	LEU
9	K	47	ARG
9	K	51	LEU
9	K	54	ARG
9	K	55	LYS
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	106	GLU
9	K	107	THR
9	K	112	GLN
9	K	113	THR
9	K	114	LEU
10	L	27	LEU
10	L	28	LYS
10	L	33	GLU
10	L	36	SER
10	L	42	ARG
10	L	43	THR
10	L	46	VAL
10	L	47	ARG
10	L	49	LYS
10	L	51	CYS
10	L	53	HIS
10	L	54	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	64	ASN
1	A	83	HIS
1	A	92	HIS
1	A	171	GLN
1	A	209	ASN
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	517	ASN
1	A	587	HIS
1	A	589	GLN
1	A	660	ASN
1	A	736	ASN
1	A	741	ASN
1	A	742	ASN
1	A	745	GLN
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	994	GLN
1	A	1078	GLN
1	A	1128	GLN
1	A	1130	GLN
1	A	1140	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1173	HIS
1	A	1203	ASN
1	A	1364	ASN
1	A	1378	GLN
1	A	1432	GLN
2	B	60	GLN
2	B	121	ASN
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS
2	B	300	HIS
2	B	325	GLN
2	B	357	GLN
2	B	366	GLN
2	B	383	ASN
2	B	395	GLN
2	B	499	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	531	GLN
2	B	538	ASN
2	B	573	GLN
2	B	590	HIS
2	B	657	HIS
2	B	667	GLN
2	B	706	GLN
2	B	744	HIS
2	B	763	GLN
2	B	951	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	1176	ASN
2	B	1177	HIS
2	B	1178	ASN
2	B	1179	GLN
2	B	1193	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	73	GLN
3	C	112	ASN
3	C	128	ASN
3	C	131	HIS
3	C	167	HIS
3	C	184	ASN
3	C	242	GLN
3	C	252	GLN
4	E	3	GLN
4	E	5	ASN
4	E	101	GLN
4	E	104	ASN
4	E	113	GLN
4	E	146	HIS
4	E	147	HIS
6	H	11	GLN
6	H	131	ASN
6	H	134	ASN
6	H	137	GLN
6	H	139	ASN
7	I	12	ASN
7	I	46	HIS
7	I	83	ASN
7	I	89	GLN
7	I	108	HIS
7	I	116	ASN
8	J	26	GLN
9	K	2	ASN
9	K	65	HIS
9	K	76	GLN
9	K	110	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	ATP	A	3011	11	31,32,33	1.08	2 (6%)	46,50,52	1.92	6 (13%)

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	5/22/34/38	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	C4-N3	3.32	1.40	1.34
13	A	3011	ATP	PA-O3A	2.03	1.61	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	3011	ATP	O4'-C1'-N9	9.59	125.18	107.96
13	A	3011	ATP	C1'-N9-C8	-4.72	110.45	126.95
13	A	3011	ATP	O4'-C1'-C2'	3.66	113.08	106.25
13	A	3011	ATP	C4-N9-C1'	2.89	138.10	126.50
13	A	3011	ATP	C2'-C1'-N9	2.47	120.42	114.63
13	A	3011	ATP	C2'-C3'-C4'	2.21	107.29	102.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	3011	ATP	C1'

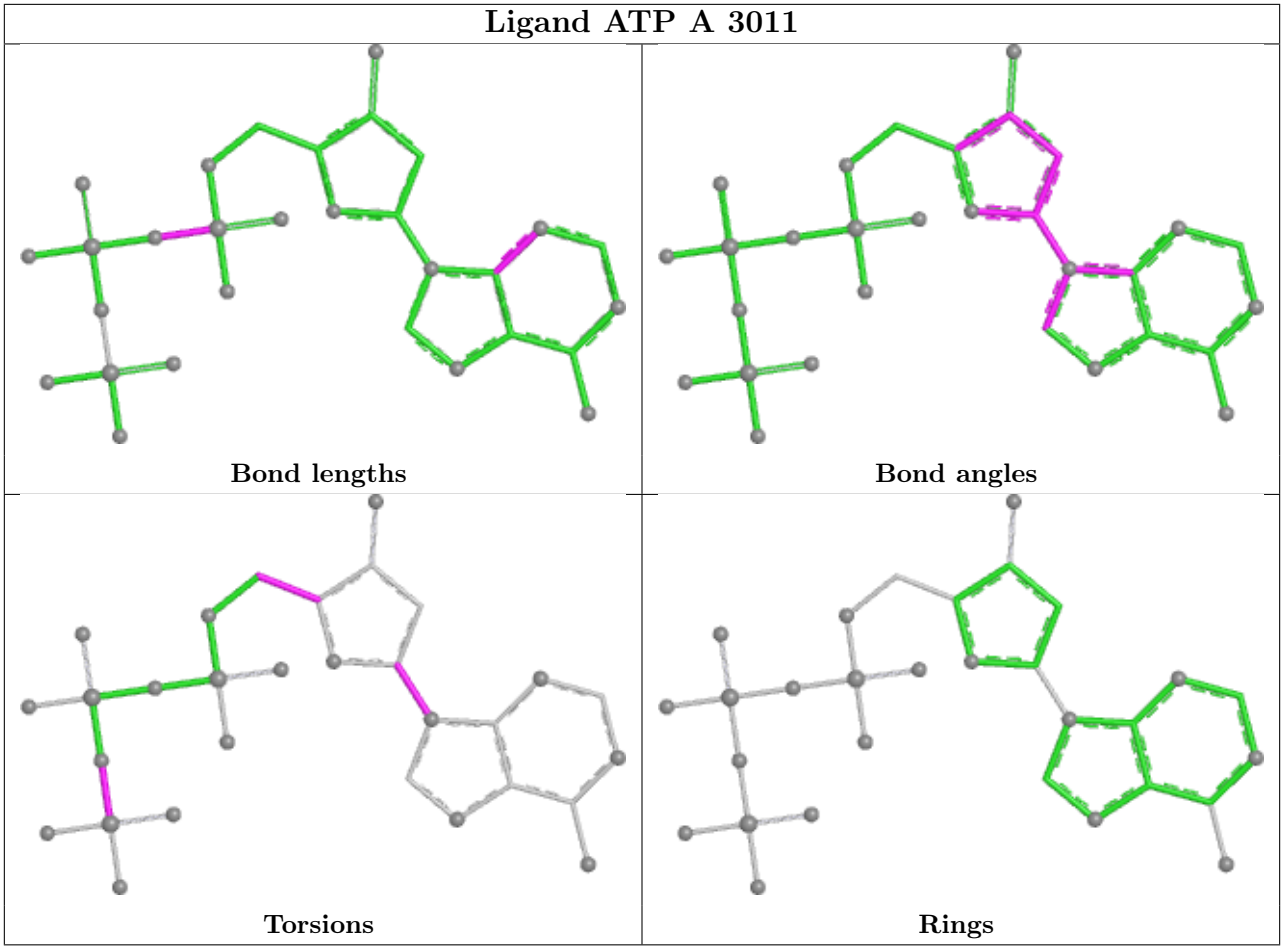
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	3011	ATP	O4'-C4'-C5'-O5'
13	A	3011	ATP	C3'-C4'-C5'-O5'
13	A	3011	ATP	C2'-C1'-N9-C4
13	A	3011	ATP	PB-O3B-PG-O2G
13	A	3011	ATP	PB-O3B-PG-O3G

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	12
1	A	8
3	C	2
7	I	2
5	F	1
9	K	1
8	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1014:ALA	C	1015:VAL	N	1.20
1	A	1378:GLN	C	1379:GLY	N	1.20
1	B	49:ASP	C	50:SER	N	1.20
1	B	586:TRP	C	587:HIS	N	1.20
1	B	724:ASP	C	725:PRO	N	1.20
1	B	763:GLN	C	764:SER	N	1.20
1	B	976:ILE	C	977:GLY	N	1.20
1	B	1203:LEU	C	1204:PHE	N	1.20
1	C	70:ILE	C	71:PRO	N	1.20
1	C	123:ASN	C	124:LEU	N	1.20
1	F	121:ALA	C	122:MET	N	1.20
1	I	41:PRO	C	42:LEU	N	1.20
1	I	62:ILE	C	63:GLY	N	1.20
1	A	748:MET	C	749:ALA	N	1.19
1	B	639:ILE	C	640:VAL	N	1.19
1	B	810:GLU	C	811:TYR	N	1.19
1	B	845:SER	C	846:ILE	N	1.19
1	A	529:CYS	C	530:GLY	N	1.18
1	A	912:LEU	C	913:LEU	N	1.18
1	B	813:LYS	C	814:PHE	N	1.18
1	K	34:THR	C	35:PHE	N	1.18
1	A	482:PHE	C	483:ASP	N	1.17
1	B	1150:ARG	C	1151:LEU	N	1.17
1	B	1193:GLN	C	1194:ILE	N	1.17
1	A	942:PHE	C	943:LEU	N	1.16
1	J	24:LEU	C	25:LEU	N	1.15
1	A	464:PRO	C	465:TYR	N	1.14

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, 95^{th} 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%)	-0.25	21 (1%) 70 56	1, 22, 99, 165	0
2	B	1091/1224 (89%)	-0.20	22 (2%) 65 49	1, 22, 107, 155	0
3	C	266/318 (83%)	-0.20	0 100 100	1, 22, 72, 145	0
4	E	215/215 (100%)	-0.14	1 (0%) 87 78	1, 40, 102, 138	0
5	F	83/155 (53%)	-0.38	0 100 100	1, 21, 63, 88	0
6	H	133/146 (91%)	0.62	12 (9%) 15 14	14, 65, 120, 167	0
7	I	121/122 (99%)	-0.13	1 (0%) 82 71	1, 30, 79, 120	0
8	J	64/70 (91%)	-0.29	0 100 100	3, 18, 64, 91	0
9	K	114/120 (95%)	-0.17	1 (0%) 81 68	1, 32, 72, 103	0
10	L	46/70 (65%)	0.56	1 (2%) 62 47	16, 72, 123, 140	0
All	All	3482/4173 (83%)	-0.18	59 (1%) 69 54	1, 25, 103, 167	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	PRO	4.8
6	H	104	PHE	4.3
2	B	882	THR	4.1
6	H	85	GLY	3.9
1	A	33	ALA	3.8
1	A	1176	LEU	3.8
9	K	114	LEU	3.7
2	B	869	SER	3.4
2	B	866	TYR	3.2
4	E	102	GLU	3.1
2	B	1110	PRO	3.0
2	B	883	LEU	3.0
10	L	27	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1366	ARG	3.0
6	H	136	LYS	3.0
1	A	1080	THR	2.9
1	A	707	GLY	2.9
6	H	107	VAL	2.8
2	B	451	LYS	2.8
2	B	432	MET	2.8
1	A	975	HIS	2.8
2	B	250	PHE	2.7
1	A	194	ALA	2.7
2	B	646	LEU	2.7
1	A	487	MET	2.6
6	H	63	LEU	2.6
2	B	986	GLN	2.6
2	B	106	ASP	2.6
1	A	56	PRO	2.5
1	A	37	PHE	2.4
1	A	49	LYS	2.4
7	I	118	ARG	2.4
1	A	35	ILE	2.4
2	B	509	ALA	2.4
1	A	48	ALA	2.3
2	B	733	HIS	2.3
1	A	1450	LEU	2.3
1	A	1254	ALA	2.3
2	B	105	SER	2.3
6	H	135	LEU	2.3
2	B	433	GLN	2.3
1	A	1256	GLU	2.2
2	B	870	ILE	2.2
2	B	735	ALA	2.2
6	H	106	GLU	2.2
6	H	146	ARG	2.2
2	B	732	SER	2.2
6	H	139	ASN	2.2
1	A	1129	GLU	2.2
2	B	369	GLY	2.1
6	H	131	ASN	2.1
1	A	196	GLU	2.1
1	A	1232	ASN	2.1
2	B	370	PHE	2.1
6	H	82	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	69	THR	2.1
6	H	129	TYR	2.1
2	B	1224	PHE	2.0
2	B	868	MET	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

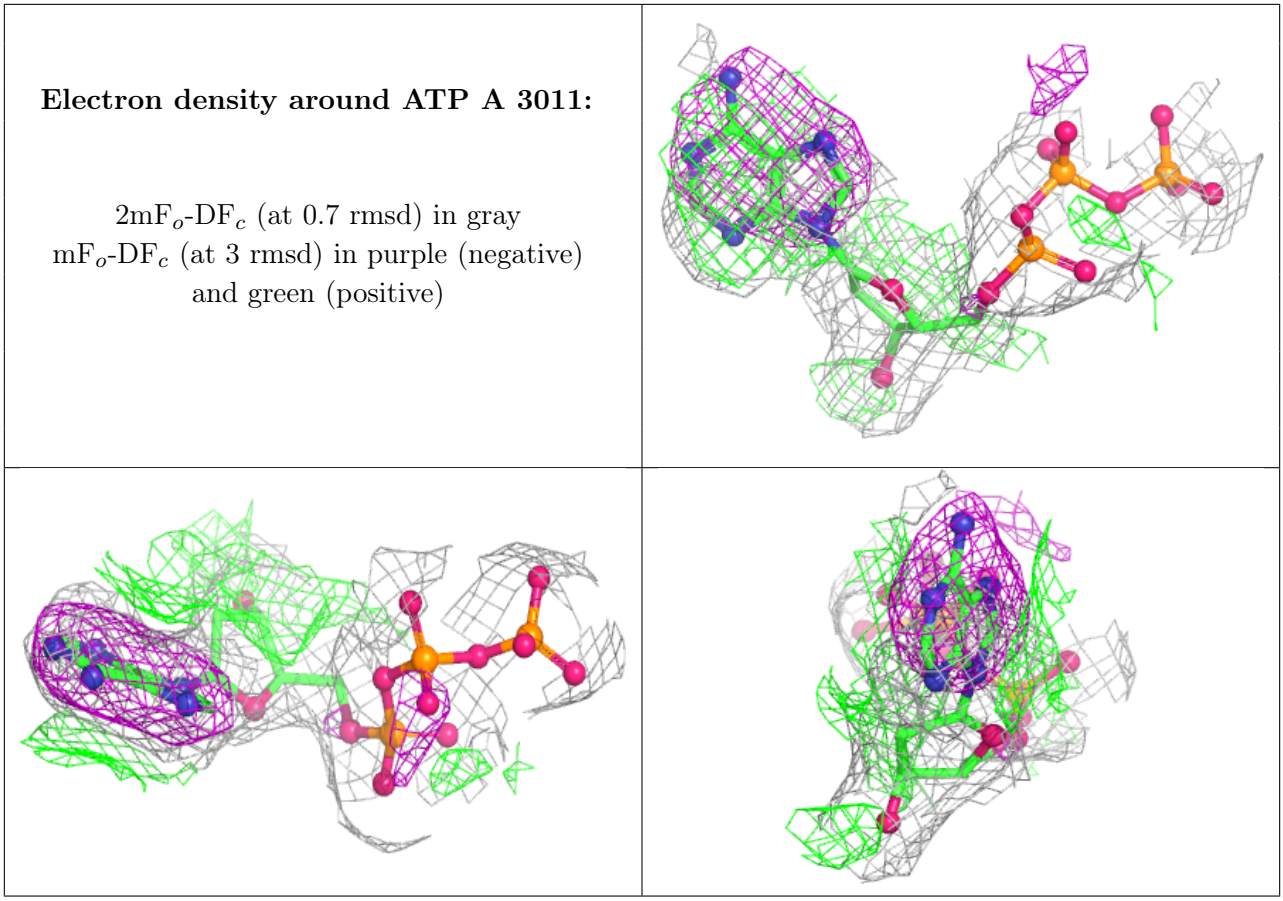
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	ATP	A	3011	30/31	0.80	0.16	5,46,82,85	0
12	ZN	I	3004	1/1	0.95	0.09	66,66,66,66	0
12	ZN	J	3001	1/1	0.97	0.13	34,34,34,34	0
12	ZN	A	3008	1/1	0.97	0.05	91,91,91,91	0
12	ZN	I	3003	1/1	0.98	0.07	46,46,46,46	0
12	ZN	A	3006	1/1	0.98	0.10	47,47,47,47	0
12	ZN	B	3007	1/1	0.99	0.08	57,57,57,57	0
12	ZN	C	3002	1/1	0.99	0.12	42,42,42,42	0
12	ZN	L	3005	1/1	0.99	0.12	90,90,90,90	0
11	MN	A	3010	1/1	0.99	0.05	12,12,12,12	0
11	MN	A	3009	1/1	1.00	0.02	4,4,4,4	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP A 3011:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.