



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:01 PM GMT

PDB ID : 1DLP  
Title : STRUCTURAL CHARACTERIZATION OF THE NATIVE FETUIN-BINDING PROTEIN SCILLA CAMPANULATA AGGLUTININ (SCAFET): A NOVEL TWO-DOMAIN LECTIN  
Authors : Wright, L.M.; Reynolds, C.D.; Rizkallah, P.J.; Allen, A.K.; VanDamme, E.J.M.; Donovan, M.J.; Peumans, W.J.  
Deposited on : 1999-12-11  
Resolution : 3.30 Å(reported)

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

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

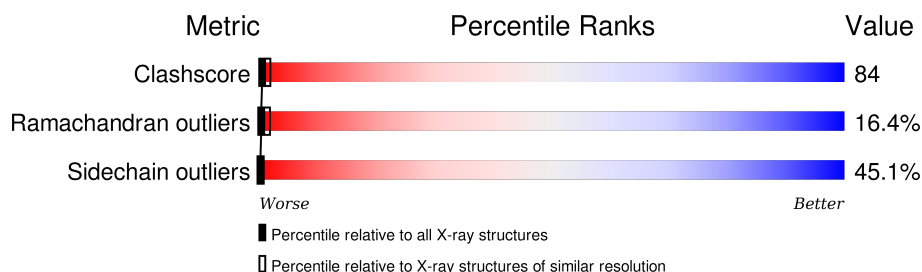
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	236	
1	B	236	
1	C	236	
1	D	236	
1	E	236	
1	F	236	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10431 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 LECTIN SCAFET PRECURSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	18	0	0
			1778	1102	322	347	7			
1	B	221	Total	C	N	O	S	21	0	0
			1694	1053	305	329	7			
1	C	234	Total	C	N	O	S	25	0	0
			1772	1097	323	345	7			
1	D	223	Total	C	N	O	S	28	0	0
			1702	1057	307	331	7			
1	E	231	Total	C	N	O	S	17	0	0
			1759	1093	318	341	7			
1	F	216	Total	C	N	O	S	40	0	0
			1659	1034	298	320	7			

- Molecule 2 is water.

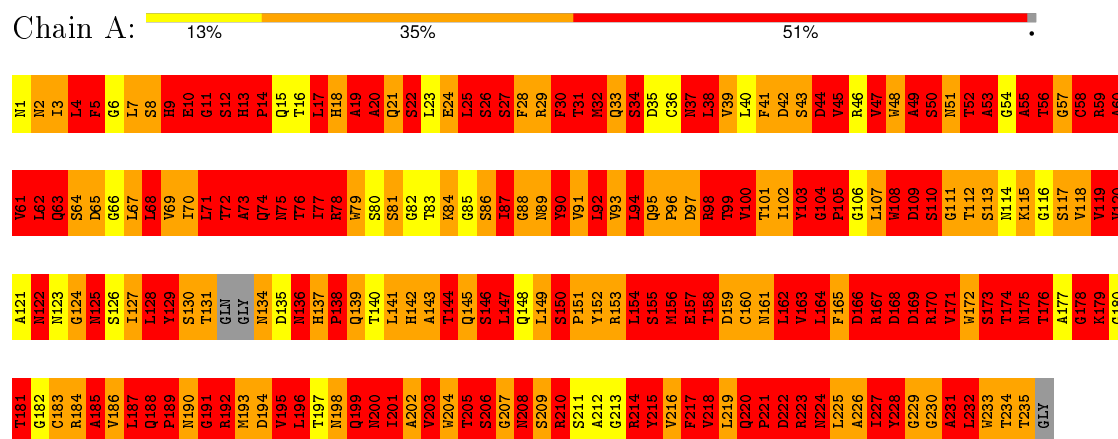
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	O	0	0
			19	19		
2	B	15	Total	O	0	0
			15	15		
2	C	6	Total	O	0	0
			6	6		
2	D	8	Total	O	0	0
			8	8		
2	E	8	Total	O	0	0
			8	8		
2	F	11	Total	O	0	0
			11	11		

### 3 Residue-property plots

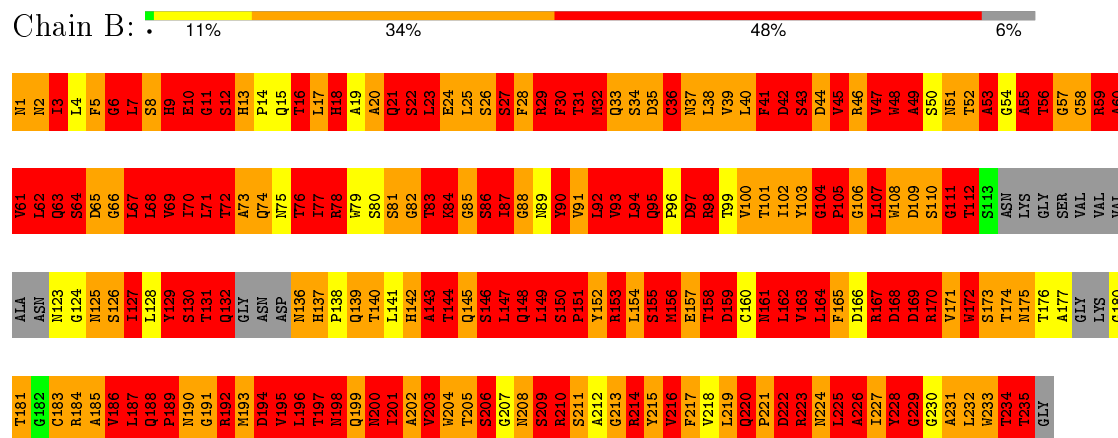
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

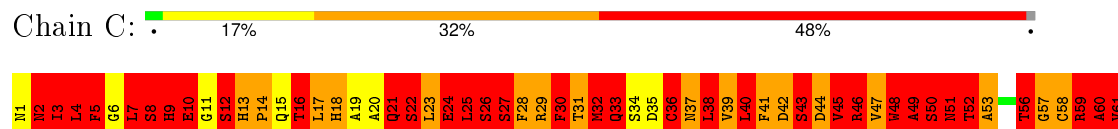
#### • Molecule 1: LECTIN SCAFET PRECURSOR

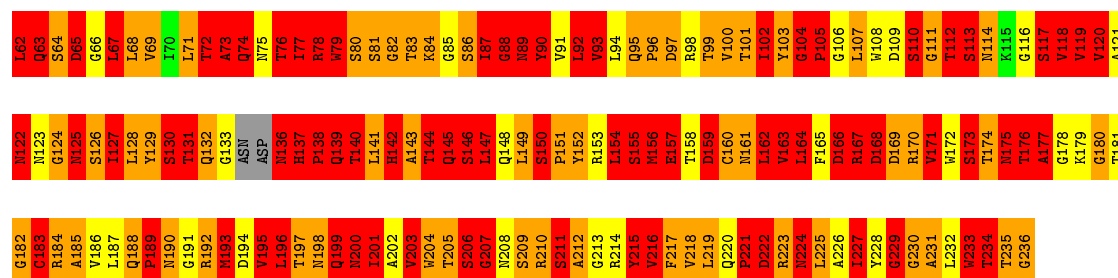


#### • Molecule 1: LECTIN SCAFET PRECURSOR



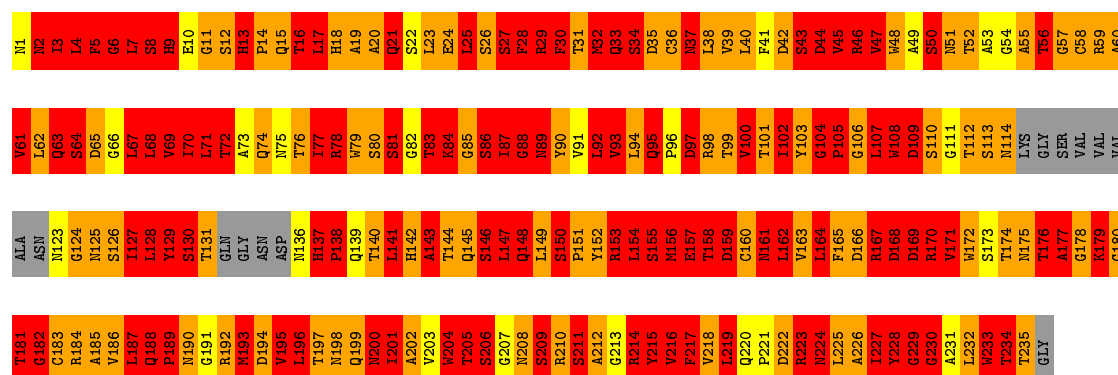
#### • Molecule 1: LECTIN SCAFET PRECURSOR





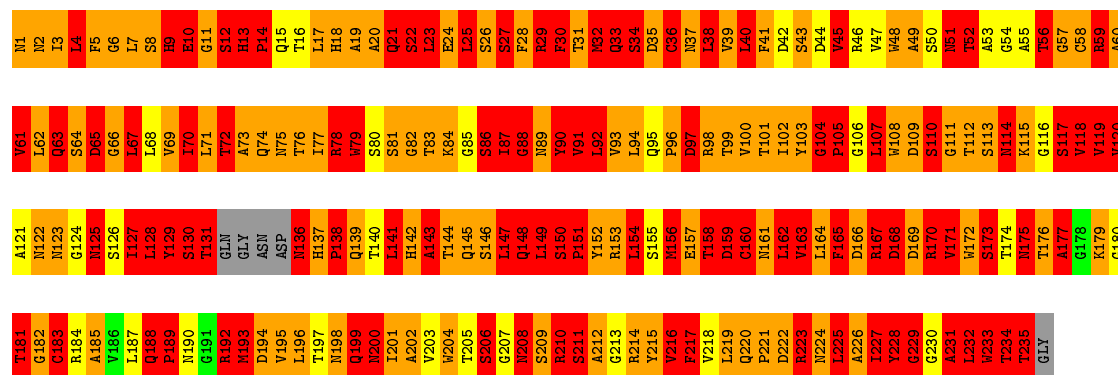
### • Molecule 1: LECTIN SCAFET PRECURSOR

Chain D: 11% 35% 49% 6%



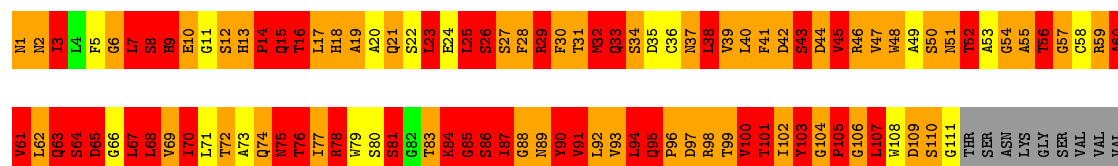
### • Molecule 1: LECTIN SCAFET PRECURSOR

Chain E: 14% 39% 43%



### • Molecule 1: LECTIN SCAFET PRECURSOR

Chain F: 14% 37% 40% 8%



ALA	T181	G182	T182	ASN	G124	N125	S126	L127	L128	Y129	S130	T131	GLN	GLY	ASN	ASP	N136	H137	P138	Q139	T140	L141	H142	A143	T144	T205	S146	L147	Q148	L149	S150	P151	Y152	R153	L154	S155	M156	E157	F158	D159	C160	N161	L162	V163	L164	F165	D166	R167	D168	D169	R170	V171	W172	S173	T174	N175	T176	ALA	GLY	LYS	G180
G182	R183	R184	A185	V186	L187	Q188	P189	N190	G191	R192	M193	D194	V195	L196	T197	N198	Q199	N200	L201	A202	V203	W204	T205	S206	G207	N208	S209	R210	S211	A212	G213	R214	Y215	V216	F217	V218	L219	Q220	P221	D222	R223	W224	L225	A226	I227	Y228	G229	G230	A231	L232	W233	T234	T235	GLY							

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	277.94Å 164.10Å 53.60Å 90.00° 95.38° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30	Depositor
% Data completeness (in resolution range)	95.3 (20.00-3.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.189 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10431	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	2.62	91/1812 (5.0%)	6.89	912/2470 (36.9%)
1	B	2.44	80/1726 (4.6%)	6.84	897/2351 (38.2%)
1	C	2.34	58/1805 (3.2%)	6.48	838/2459 (34.1%)
1	D	3.14	88/1735 (5.1%)	7.13	928/2365 (39.2%)
1	E	2.06	35/1793 (2.0%)	5.99	765/2444 (31.3%)
1	F	2.14	38/1691 (2.2%)	6.60	810/2303 (35.2%)
All	All	2.48	390/10562 (3.7%)	6.66	5150/14392 (35.8%)

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	2	60
1	B	2	73
1	C	0	66
1	D	0	51
1	E	0	39
1	F	2	53
All	All	6	342

All (390) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1	ASN	CG-ND2	50.13	2.58	1.32
1	D	78	ARG	CG-CD	46.82	2.69	1.51
1	A	44	ASP	CB-CG	-34.10	0.80	1.51
1	C	168	ASP	CG-OD1	30.06	1.94	1.25
1	D	167	ARG	CD-NE	-29.28	0.96	1.46
1	A	136	ASN	CB-CG	-23.90	0.96	1.51
1	C	9	HIS	CB-CG	-20.03	1.14	1.50
1	F	224	ASN	CA-CB	-19.84	1.01	1.53

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	12	SER	CB-OG	-19.60	1.16	1.42
1	D	64	SER	CB-OG	19.02	1.67	1.42
1	D	230	GLY	N-CA	-18.84	1.17	1.46
1	F	59	ARG	CD-NE	-18.77	1.14	1.46
1	E	168	ASP	CA-CB	-17.48	1.15	1.53
1	D	210	ARG	CB-CG	-17.09	1.06	1.52
1	D	84	LYS	CG-CD	-16.43	0.96	1.52
1	A	59	ARG	CZ-NH1	16.11	1.53	1.33
1	C	44	ASP	CA-CB	16.02	1.89	1.53
1	D	233	TRP	CG-CD1	-14.94	1.15	1.36
1	E	136	ASN	CA-CB	13.41	1.88	1.53
1	C	130	SER	CB-OG	-13.16	1.25	1.42
1	D	233	TRP	CB-CG	-12.90	1.27	1.50
1	D	8	SER	C-O	12.59	1.47	1.23
1	E	46	ARG	CA-CB	-12.06	1.27	1.53
1	D	12	SER	C-O	-12.00	1.00	1.23
1	D	105	PRO	N-CD	11.92	1.64	1.47
1	E	131	THR	C-O	11.90	1.46	1.23
1	B	57	GLY	N-CA	-11.78	1.28	1.46
1	F	81	SER	CB-OG	-11.73	1.27	1.42
1	F	170	ARG	CB-CG	-11.38	1.21	1.52
1	A	207	GLY	N-CA	-11.34	1.29	1.46
1	D	229	GLY	N-CA	-11.24	1.29	1.46
1	B	90	TYR	CG-CD1	-10.88	1.25	1.39
1	A	126	SER	CB-OG	-10.88	1.28	1.42
1	B	138	PRO	N-CD	-10.86	1.32	1.47
1	D	12	SER	CB-OG	-10.82	1.28	1.42
1	E	130	SER	CB-OG	10.78	1.56	1.42
1	A	180	GLY	N-CA	-10.74	1.29	1.46
1	A	131	THR	CB-OG1	10.45	1.64	1.43
1	C	215	TYR	CG-CD2	-10.27	1.25	1.39
1	F	105	PRO	N-CA	-10.23	1.29	1.47
1	C	59	ARG	CZ-NH1	10.08	1.46	1.33
1	C	167	ARG	CA-CB	-10.02	1.31	1.53
1	C	46	ARG	CA-CB	-9.97	1.32	1.53
1	A	215	TYR	CG-CD2	-9.87	1.26	1.39
1	E	231	ALA	CA-CB	-9.85	1.31	1.52
1	C	136	ASN	N-CA	9.79	1.66	1.46
1	B	150	SER	CA-CB	-9.62	1.38	1.52
1	A	187	LEU	N-CA	-9.58	1.27	1.46
1	C	168	ASP	CG-OD2	9.42	1.47	1.25
1	A	157	GLU	CD-OE1	9.41	1.36	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	126	SER	CB-OG	-9.37	1.30	1.42
1	B	235	THR	C-O	9.31	1.41	1.23
1	B	61	VAL	N-CA	9.20	1.64	1.46
1	D	105	PRO	N-CA	-9.17	1.31	1.47
1	E	160	CYS	CB-SG	-9.14	1.66	1.82
1	B	66	GLY	C-O	9.10	1.38	1.23
1	A	59	ARG	CZ-NH2	9.08	1.44	1.33
1	B	60	ALA	C-O	9.00	1.40	1.23
1	B	54	GLY	C-O	8.96	1.38	1.23
1	E	110	SER	CB-OG	-8.88	1.30	1.42
1	D	98	ARG	CZ-NH1	8.84	1.44	1.33
1	E	131	THR	CA-C	8.82	1.75	1.52
1	A	206	SER	CB-OG	8.79	1.53	1.42
1	B	61	VAL	C-N	8.79	1.54	1.34
1	F	34	SER	CA-CB	8.78	1.66	1.52
1	A	48	TRP	CG-CD1	-8.73	1.24	1.36
1	D	89	ASN	CG-ND2	8.64	1.54	1.32
1	A	194	ASP	CA-CB	-8.62	1.34	1.53
1	B	22	SER	CA-CB	8.61	1.65	1.52
1	B	61	VAL	C-O	-8.60	1.07	1.23
1	A	215	TYR	N-CA	-8.59	1.29	1.46
1	D	126	SER	CA-CB	-8.52	1.40	1.52
1	E	232	LEU	CA-C	-8.43	1.31	1.52
1	B	34	SER	CB-OG	-8.43	1.31	1.42
1	D	217	PHE	C-O	-8.40	1.07	1.23
1	A	101	THR	CB-OG1	-8.39	1.26	1.43
1	A	235	THR	C-O	8.39	1.39	1.23
1	A	26	SER	CB-OG	-8.30	1.31	1.42
1	B	225	LEU	C-N	-8.28	1.15	1.34
1	F	8	SER	C-O	8.28	1.39	1.23
1	B	64	SER	N-CA	8.27	1.62	1.46
1	F	131	THR	C-O	8.26	1.39	1.23
1	D	136	ASN	N-CA	8.24	1.62	1.46
1	E	167	ARG	CB-CG	-8.19	1.30	1.52
1	D	106	GLY	C-O	8.17	1.36	1.23
1	B	98	ARG	CZ-NH2	8.15	1.43	1.33
1	C	28	PHE	CG-CD2	-8.14	1.26	1.38
1	A	131	THR	C-O	8.09	1.38	1.23
1	D	130	SER	CB-OG	8.02	1.52	1.42
1	F	78	ARG	CG-CD	-8.01	1.31	1.51
1	C	150	SER	CB-OG	7.99	1.52	1.42
1	D	221	PRO	CA-CB	-7.99	1.37	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	61	VAL	N-CA	7.98	1.62	1.46
1	F	210	ARG	CB-CG	7.81	1.73	1.52
1	A	139	GLN	C-N	7.81	1.52	1.34
1	B	18	HIS	N-CA	-7.79	1.30	1.46
1	B	191	GLY	CA-C	-7.67	1.39	1.51
1	F	14	PRO	N-CA	-7.65	1.34	1.47
1	C	215	TYR	CE1-CZ	-7.61	1.28	1.38
1	D	157	GLU	CD-OE1	7.61	1.34	1.25
1	C	88	GLY	N-CA	7.60	1.57	1.46
1	A	217	PHE	CE1-CZ	-7.58	1.23	1.37
1	A	59	ARG	NE-CZ	7.57	1.42	1.33
1	D	209	SER	CA-CB	7.56	1.64	1.52
1	B	30	PHE	C-N	-7.52	1.16	1.34
1	C	229	GLY	C-N	-7.43	1.19	1.33
1	C	165	PHE	CB-CG	-7.42	1.38	1.51
1	F	129	TYR	CD2-CE2	-7.41	1.28	1.39
1	D	168	ASP	CA-CB	7.40	1.70	1.53
1	F	98	ARG	CZ-NH1	7.37	1.42	1.33
1	A	12	SER	CA-CB	-7.35	1.42	1.52
1	A	6	GLY	N-CA	7.29	1.56	1.46
1	A	138	PRO	N-CD	7.28	1.58	1.47
1	E	15	GLN	C-O	7.26	1.37	1.23
1	D	217	PHE	CD2-CE2	-7.25	1.24	1.39
1	A	209	SER	CB-OG	7.23	1.51	1.42
1	D	21	GLN	CA-CB	-7.21	1.38	1.53
1	A	86	SER	CB-OG	-7.18	1.32	1.42
1	F	66	GLY	C-O	7.18	1.35	1.23
1	B	184	ARG	CD-NE	-7.14	1.34	1.46
1	B	192	ARG	CD-NE	-7.13	1.34	1.46
1	B	129	TYR	N-CA	-7.12	1.32	1.46
1	A	30	PHE	CG-CD1	-7.11	1.28	1.38
1	C	5	PHE	CB-CG	-7.07	1.39	1.51
1	F	129	TYR	CZ-OH	7.07	1.49	1.37
1	B	5	PHE	C-O	7.06	1.36	1.23
1	D	14	PRO	N-CA	-7.04	1.35	1.47
1	B	152	TYR	CE2-CZ	-7.04	1.29	1.38
1	D	198	ASN	CA-CB	-6.95	1.35	1.53
1	D	230	GLY	C-O	6.89	1.34	1.23
1	A	92	LEU	C-O	-6.88	1.10	1.23
1	C	59	ARG	NE-CZ	6.87	1.42	1.33
1	C	104	GLY	N-CA	-6.86	1.35	1.46
1	B	105	PRO	N-CA	-6.85	1.35	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	11	GLY	CA-C	-6.84	1.41	1.51
1	E	104	GLY	N-CA	-6.81	1.35	1.46
1	D	108	TRP	CB-CG	-6.79	1.38	1.50
1	A	100	VAL	CA-CB	6.78	1.69	1.54
1	B	110	SER	N-CA	-6.78	1.32	1.46
1	D	216	VAL	CB-CG2	-6.76	1.38	1.52
1	A	182	GLY	CA-C	-6.75	1.41	1.51
1	D	233	TRP	CA-CB	-6.73	1.39	1.53
1	B	60	ALA	CA-C	-6.73	1.35	1.52
1	D	194	ASP	N-CA	-6.72	1.32	1.46
1	A	229	GLY	N-CA	-6.70	1.36	1.46
1	D	217	PHE	CA-CB	-6.67	1.39	1.53
1	A	233	TRP	CZ2-CH2	-6.65	1.24	1.37
1	C	231	ALA	N-CA	-6.65	1.33	1.46
1	A	124	GLY	N-CA	-6.64	1.36	1.46
1	D	64	SER	CA-CB	-6.64	1.43	1.52
1	B	29	ARG	CZ-NH1	6.63	1.41	1.33
1	B	98	ARG	CZ-NH1	6.63	1.41	1.33
1	E	6	GLY	N-CA	6.56	1.55	1.46
1	C	90	TYR	CE1-CZ	-6.54	1.30	1.38
1	C	28	PHE	CE1-CZ	6.54	1.49	1.37
1	B	194	ASP	N-CA	-6.53	1.33	1.46
1	A	155	SER	CA-CB	-6.53	1.43	1.52
1	A	189	PRO	CA-CB	-6.48	1.40	1.53
1	D	229	GLY	CA-C	-6.47	1.41	1.51
1	B	87	ILE	N-CA	-6.46	1.33	1.46
1	E	66	GLY	N-CA	-6.45	1.36	1.46
1	B	84	LYS	C-N	-6.44	1.21	1.33
1	B	55	ALA	C-O	6.42	1.35	1.23
1	A	48	TRP	CB-CG	-6.41	1.38	1.50
1	A	146	SER	CB-OG	6.39	1.50	1.42
1	D	131	THR	C-O	6.37	1.35	1.23
1	E	136	ASN	N-CA	6.37	1.59	1.46
1	B	54	GLY	C-N	6.36	1.48	1.34
1	C	180	GLY	N-CA	-6.33	1.36	1.46
1	C	110	SER	CB-OG	-6.33	1.34	1.42
1	B	214	ARG	NE-CZ	6.33	1.41	1.33
1	E	215	TYR	CG-CD2	-6.32	1.30	1.39
1	A	204	TRP	CD2-CE2	-6.31	1.33	1.41
1	C	48	TRP	CG-CD1	-6.31	1.27	1.36
1	E	233	TRP	N-CA	6.31	1.58	1.46
1	D	146	SER	C-O	6.30	1.35	1.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	150	SER	N-CA	6.27	1.58	1.46
1	F	98	ARG	NE-CZ	6.26	1.41	1.33
1	B	223	ARG	N-CA	-6.26	1.33	1.46
1	B	8	SER	C-N	-6.24	1.19	1.34
1	C	126	SER	CA-CB	6.21	1.62	1.52
1	F	136	ASN	N-CA	6.21	1.58	1.46
1	D	191	GLY	N-CA	-6.20	1.36	1.46
1	A	25	LEU	C-N	-6.20	1.19	1.34
1	D	174	THR	N-CA	-6.19	1.33	1.46
1	E	85	GLY	C-N	-6.19	1.19	1.34
1	D	20	ALA	N-CA	6.18	1.58	1.46
1	A	48	TRP	CA-CB	-6.18	1.40	1.53
1	B	231	ALA	N-CA	-6.18	1.33	1.46
1	B	228	TYR	C-N	-6.18	1.22	1.33
1	A	232	LEU	N-CA	-6.17	1.34	1.46
1	D	105	PRO	CA-CB	6.16	1.65	1.53
1	A	233	TRP	NE1-CE2	-6.13	1.29	1.37
1	A	229	GLY	C-N	-6.09	1.22	1.33
1	B	59	ARG	CA-CB	-6.09	1.40	1.53
1	B	29	ARG	CZ-NH2	6.09	1.41	1.33
1	D	142	HIS	N-CA	-6.08	1.34	1.46
1	B	147	LEU	CB-CG	-6.08	1.34	1.52
1	A	170	ARG	CZ-NH2	6.08	1.41	1.33
1	A	214	ARG	CB-CG	-6.07	1.36	1.52
1	A	12	SER	C-O	-6.05	1.11	1.23
1	F	6	GLY	CA-C	6.04	1.61	1.51
1	F	194	ASP	N-CA	-6.04	1.34	1.46
1	C	58	CYS	CA-CB	-6.03	1.40	1.53
1	A	14	PRO	N-CD	-6.03	1.39	1.47
1	F	105	PRO	N-CD	6.03	1.56	1.47
1	C	217	PHE	CG-CD1	-6.02	1.29	1.38
1	A	138	PRO	N-CA	-6.00	1.37	1.47
1	B	191	GLY	C-O	6.00	1.33	1.23
1	A	48	TRP	CE3-CZ3	-5.98	1.28	1.38
1	F	34	SER	CB-OG	5.98	1.50	1.42
1	E	48	TRP	CG-CD1	-5.98	1.28	1.36
1	B	78	ARG	NE-CZ	5.96	1.40	1.33
1	A	188	GLN	CB-CG	5.93	1.68	1.52
1	A	9	HIS	N-CA	-5.91	1.34	1.46
1	A	231	ALA	N-CA	-5.91	1.34	1.46
1	D	66	GLY	C-O	5.90	1.33	1.23
1	F	129	TYR	CD1-CE1	-5.89	1.30	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	GLN	N-CA	-5.89	1.34	1.46
1	F	184	ARG	N-CA	-5.87	1.34	1.46
1	D	9	HIS	N-CA	-5.87	1.34	1.46
1	B	146	SER	CB-OG	-5.86	1.34	1.42
1	F	6	GLY	C-O	5.86	1.33	1.23
1	C	145	GLN	CA-CB	-5.86	1.41	1.53
1	E	183	CYS	N-CA	-5.85	1.34	1.46
1	D	235	THR	C-O	5.85	1.34	1.23
1	D	59	ARG	CA-CB	-5.85	1.41	1.53
1	C	36	CYS	CB-SG	-5.85	1.72	1.81
1	C	203	VAL	CB-CG2	-5.83	1.40	1.52
1	C	138	PRO	C-N	5.83	1.47	1.34
1	F	12	SER	CB-OG	5.83	1.49	1.42
1	A	129	TYR	CZ-OH	-5.82	1.27	1.37
1	D	27	SER	CA-CB	5.82	1.61	1.52
1	A	90	TYR	C-N	-5.81	1.20	1.34
1	E	66	GLY	C-O	5.79	1.32	1.23
1	D	203	VAL	CB-CG2	5.79	1.65	1.52
1	A	57	GLY	N-CA	-5.78	1.37	1.46
1	C	57	GLY	N-CA	-5.78	1.37	1.46
1	B	184	ARG	CZ-NH1	5.78	1.40	1.33
1	E	20	ALA	CA-CB	-5.77	1.40	1.52
1	B	129	TYR	CE2-CZ	-5.76	1.31	1.38
1	B	72	THR	N-CA	-5.76	1.34	1.46
1	D	160	CYS	CB-SG	-5.76	1.72	1.81
1	D	11	GLY	N-CA	5.75	1.54	1.46
1	A	85	GLY	C-O	5.73	1.32	1.23
1	B	138	PRO	CA-CB	-5.72	1.42	1.53
1	D	13	HIS	C-N	-5.72	1.23	1.34
1	D	148	GLN	CA-CB	-5.72	1.41	1.53
1	B	1	ASN	CG-OD1	5.71	1.36	1.24
1	B	14	PRO	N-CA	-5.70	1.37	1.47
1	E	10	GLU	N-CA	-5.70	1.34	1.46
1	C	141	LEU	CA-CB	-5.70	1.40	1.53
1	D	183	CYS	CB-SG	-5.69	1.72	1.81
1	F	7	LEU	C-O	5.68	1.34	1.23
1	B	222	ASP	C-N	-5.68	1.21	1.34
1	B	10	GLU	CD-OE1	5.67	1.31	1.25
1	D	187	LEU	C-O	-5.67	1.12	1.23
1	A	61	VAL	CB-CG1	-5.67	1.41	1.52
1	B	225	LEU	CA-CB	-5.65	1.40	1.53
1	A	80	SER	CB-OG	-5.65	1.34	1.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	34	SER	CA-C	-5.65	1.38	1.52
1	A	83	THR	C-N	-5.64	1.21	1.34
1	D	88	GLY	N-CA	5.64	1.54	1.46
1	C	83	THR	C-N	-5.63	1.21	1.34
1	B	230	GLY	N-CA	-5.63	1.37	1.46
1	C	124	GLY	N-CA	-5.63	1.37	1.46
1	A	192	ARG	CZ-NH2	-5.63	1.25	1.33
1	C	196	LEU	CB-CG	-5.63	1.36	1.52
1	F	98	ARG	CZ-NH2	5.63	1.40	1.33
1	F	67	LEU	CG-CD2	5.63	1.72	1.51
1	A	68	LEU	C-O	-5.61	1.12	1.23
1	D	146	SER	CA-CB	5.61	1.61	1.52
1	B	74	GLN	N-CA	-5.61	1.35	1.46
1	A	217	PHE	CD1-CE1	5.57	1.50	1.39
1	C	192	ARG	CA-CB	-5.57	1.41	1.53
1	F	130	SER	C-N	5.56	1.46	1.34
1	A	170	ARG	CZ-NH1	5.54	1.40	1.33
1	A	221	PRO	N-CA	5.53	1.56	1.47
1	E	5	PHE	C-O	5.53	1.33	1.23
1	B	193	MET	CA-CB	-5.52	1.41	1.53
1	A	218	VAL	CB-CG2	5.52	1.64	1.52
1	A	114	ASN	N-CA	-5.51	1.35	1.46
1	A	214	ARG	CZ-NH2	5.51	1.40	1.33
1	C	27	SER	CA-CB	-5.51	1.44	1.52
1	C	183	CYS	CB-SG	-5.51	1.72	1.81
1	A	156	MET	CG-SD	-5.50	1.66	1.81
1	D	15	GLN	CA-CB	-5.50	1.41	1.53
1	D	196	LEU	CA-CB	-5.49	1.41	1.53
1	A	60	ALA	C-O	5.49	1.33	1.23
1	D	52	THR	N-CA	-5.47	1.35	1.46
1	D	183	CYS	C-N	-5.46	1.21	1.34
1	D	48	TRP	CA-CB	-5.45	1.42	1.53
1	A	186	VAL	C-N	5.44	1.46	1.34
1	C	139	GLN	CA-CB	-5.44	1.42	1.53
1	D	61	VAL	C-N	-5.44	1.21	1.34
1	A	104	GLY	N-CA	-5.44	1.37	1.46
1	B	160	CYS	N-CA	-5.43	1.35	1.46
1	F	139	GLN	CB-CG	-5.42	1.38	1.52
1	E	129	TYR	CE1-CZ	-5.41	1.31	1.38
1	C	207	GLY	CA-C	-5.41	1.43	1.51
1	F	128	LEU	C-N	-5.41	1.21	1.34
1	B	109	ASP	N-CA	-5.40	1.35	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	8	SER	CB-OG	5.39	1.49	1.42
1	F	129	TYR	CB-CG	5.39	1.59	1.51
1	B	98	ARG	NE-CZ	5.39	1.40	1.33
1	D	227	ILE	C-N	-5.38	1.21	1.34
1	A	125	ASN	N-CA	-5.38	1.35	1.46
1	D	44	ASP	C-N	-5.38	1.21	1.34
1	E	138	PRO	N-CA	-5.37	1.38	1.47
1	D	139	GLN	CB-CG	-5.36	1.38	1.52
1	B	89	ASN	CG-ND2	5.35	1.46	1.32
1	A	230	GLY	C-N	-5.34	1.21	1.34
1	E	11	GLY	CA-C	-5.34	1.43	1.51
1	C	88	GLY	C-O	-5.34	1.15	1.23
1	A	105	PRO	N-CA	-5.34	1.38	1.47
1	B	60	ALA	C-N	-5.33	1.21	1.34
1	E	146	SER	CA-CB	5.32	1.60	1.52
1	B	78	ARG	CZ-NH2	5.31	1.40	1.33
1	C	205	THR	C-O	5.29	1.33	1.23
1	A	30	PHE	CA-CB	-5.29	1.42	1.53
1	D	221	PRO	N-CD	-5.29	1.40	1.47
1	D	28	PHE	N-CA	-5.28	1.35	1.46
1	D	139	GLN	CA-CB	-5.28	1.42	1.53
1	C	133	GLY	CA-C	5.26	1.60	1.51
1	B	149	LEU	N-CA	-5.26	1.35	1.46
1	B	183	CYS	CB-SG	-5.26	1.73	1.81
1	A	25	LEU	CA-CB	-5.25	1.41	1.53
1	B	28	PHE	CB-CG	-5.25	1.42	1.51
1	D	147	LEU	N-CA	5.25	1.56	1.46
1	C	172	TRP	CD2-CE2	-5.24	1.35	1.41
1	C	138	PRO	C-O	5.24	1.33	1.23
1	B	1	ASN	N-CA	5.23	1.56	1.46
1	C	143	ALA	CA-CB	-5.22	1.41	1.52
1	D	69	VAL	C-N	-5.22	1.22	1.34
1	B	190	ASN	N-CA	-5.22	1.35	1.46
1	A	137	HIS	ND1-CE1	-5.22	1.21	1.34
1	A	125	ASN	CG-OD1	5.21	1.35	1.24
1	E	13	HIS	C-N	-5.21	1.24	1.34
1	A	50	SER	CB-OG	5.21	1.49	1.42
1	A	96	PRO	N-CD	-5.20	1.40	1.47
1	C	199	GLN	N-CA	-5.20	1.35	1.46
1	A	29	ARG	CA-CB	-5.19	1.42	1.53
1	A	186	VAL	CB-CG1	-5.19	1.42	1.52
1	D	92	LEU	C-O	5.19	1.33	1.23

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	167	ARG	CA-CB	5.19	1.65	1.53
1	B	28	PHE	CG-CD1	-5.18	1.30	1.38
1	F	61	VAL	N-CA	5.18	1.56	1.46
1	D	21	GLN	CB-CG	-5.17	1.38	1.52
1	B	211	SER	CB-OG	5.17	1.49	1.42
1	D	184	ARG	NE-CZ	5.16	1.39	1.33
1	C	130	SER	C-O	-5.16	1.13	1.23
1	A	103	TYR	C-O	-5.15	1.13	1.23
1	D	84	LYS	C-N	-5.15	1.23	1.33
1	D	152	TYR	CE1-CZ	-5.15	1.31	1.38
1	C	65	ASP	CA-CB	-5.15	1.42	1.53
1	D	57	GLY	N-CA	-5.14	1.38	1.46
1	E	86	SER	N-CA	-5.14	1.36	1.46
1	D	107	LEU	C-O	-5.13	1.13	1.23
1	F	89	ASN	CG-ND2	5.12	1.45	1.32
1	A	14	PRO	CG-CD	-5.12	1.33	1.50
1	A	140	THR	C-O	-5.12	1.13	1.23
1	A	17	LEU	CA-CB	-5.12	1.42	1.53
1	C	165	PHE	CA-CB	-5.11	1.42	1.53
1	D	66	GLY	N-CA	-5.11	1.38	1.46
1	B	184	ARG	CZ-NH2	5.11	1.39	1.33
1	D	172	TRP	CB-CG	-5.10	1.41	1.50
1	B	216	VAL	CA-C	-5.10	1.39	1.52
1	B	95	GLN	C-N	-5.09	1.24	1.34
1	A	128	LEU	N-CA	-5.09	1.36	1.46
1	E	24	GLU	CD-OE1	5.08	1.31	1.25
1	F	86	SER	CB-OG	5.08	1.48	1.42
1	B	59	ARG	NE-CZ	5.08	1.39	1.33
1	D	224	ASN	CA-CB	5.08	1.66	1.53
1	C	197	THR	CB-OG1	5.07	1.53	1.43
1	F	110	SER	CB-OG	-5.07	1.35	1.42
1	A	146	SER	CA-CB	5.07	1.60	1.52
1	C	224	ASN	CB-CG	5.07	1.62	1.51
1	C	59	ARG	CZ-NH2	5.06	1.39	1.33
1	E	129	TYR	CE2-CZ	5.05	1.45	1.38
1	A	23	LEU	CB-CG	-5.04	1.38	1.52
1	C	188	GLN	CD-NE2	5.03	1.45	1.32
1	D	85	GLY	N-CA	5.03	1.53	1.46
1	B	107	LEU	N-CA	5.03	1.56	1.46
1	D	5	PHE	CD1-CE1	5.02	1.49	1.39
1	B	63	GLN	C-O	-5.02	1.13	1.23
1	B	97	ASP	CA-CB	-5.02	1.43	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	125	ASN	C-O	-5.01	1.13	1.23
1	E	157	GLU	CB-CG	5.01	1.61	1.52
1	B	191	GLY	N-CA	-5.00	1.38	1.46
1	F	126	SER	CB-OG	-5.00	1.35	1.42

All (5150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	214	ARG	NE-CZ-NH2	59.84	150.22	120.30
1	E	59	ARG	NE-CZ-NH2	-55.14	92.73	120.30
1	B	184	ARG	NE-CZ-NH2	-53.22	93.69	120.30
1	F	223	ARG	NE-CZ-NH2	-49.78	95.41	120.30
1	A	184	ARG	NE-CZ-NH1	48.82	144.71	120.30
1	A	59	ARG	NE-CZ-NH2	-48.03	96.28	120.30
1	C	223	ARG	NE-CZ-NH1	-47.86	96.37	120.30
1	F	184	ARG	NE-CZ-NH2	-47.40	96.60	120.30
1	F	46	ARG	NE-CZ-NH1	47.06	143.83	120.30
1	A	184	ARG	NE-CZ-NH2	-46.93	96.84	120.30
1	A	59	ARG	NE-CZ-NH1	45.23	142.91	120.30
1	E	59	ARG	NE-CZ-NH1	43.99	142.30	120.30
1	A	78	ARG	NE-CZ-NH2	42.42	141.51	120.30
1	F	129	TYR	CB-CG-CD2	41.91	146.15	121.00
1	D	59	ARG	NE-CZ-NH1	-41.20	99.70	120.30
1	F	129	TYR	CB-CG-CD1	-40.14	96.91	121.00
1	D	184	ARG	NE-CZ-NH2	-39.63	100.48	120.30
1	E	170	ARG	NE-CZ-NH2	39.53	140.06	120.30
1	A	44	ASP	CB-CG-OD1	-37.95	84.14	118.30
1	D	214	ARG	NE-CZ-NH2	37.90	139.25	120.30
1	C	159	ASP	CB-CG-OD2	37.73	152.26	118.30
1	A	65	ASP	CB-CG-OD2	37.37	151.93	118.30
1	C	59	ARG	NE-CZ-NH2	-36.93	101.84	120.30
1	C	168	ASP	CB-CG-OD1	-36.83	85.15	118.30
1	E	29	ARG	CD-NE-CZ	36.56	174.78	123.60
1	D	214	ARG	CD-NE-CZ	35.79	173.70	123.60
1	F	192	ARG	CD-NE-CZ	35.76	173.66	123.60
1	D	170	ARG	NE-CZ-NH2	34.66	137.63	120.30
1	C	214	ARG	NE-CZ-NH1	-34.65	102.97	120.30
1	D	97	ASP	CB-CG-OD2	34.19	149.07	118.30
1	D	97	ASP	CB-CG-OD1	-34.15	87.56	118.30
1	B	214	ARG	CD-NE-CZ	33.20	170.07	123.60
1	A	222	ASP	CB-CG-OD2	33.16	148.15	118.30
1	A	170	ARG	NE-CZ-NH2	33.01	136.81	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	153	ARG	NE-CZ-NH2	-32.57	104.01	120.30
1	C	167	ARG	CD-NE-CZ	32.51	169.12	123.60
1	A	153	ARG	NE-CZ-NH2	31.88	136.24	120.30
1	A	170	ARG	CD-NE-CZ	31.85	168.19	123.60
1	C	170	ARG	CD-NE-CZ	31.51	167.72	123.60
1	D	167	ARG	NE-CZ-NH1	-31.49	104.55	120.30
1	B	193	MET	CG-SD-CE	31.36	150.38	100.20
1	C	97	ASP	CB-CG-OD2	30.72	145.95	118.30
1	A	222	ASP	CB-CG-OD1	-30.63	90.74	118.30
1	D	174	THR	CA-CB-CG2	-30.62	69.54	112.40
1	E	157	GLU	OE1-CD-OE2	30.46	159.85	123.30
1	B	192	ARG	CD-NE-CZ	30.33	166.06	123.60
1	A	214	ARG	CD-NE-CZ	30.23	165.93	123.60
1	B	128	LEU	CB-CG-CD1	29.63	161.38	111.00
1	A	138	PRO	CA-N-CD	-29.61	70.05	111.50
1	A	215	TYR	CB-CG-CD2	29.11	138.47	121.00
1	D	212	ALA	CB-CA-C	29.06	153.69	110.10
1	E	167	ARG	NE-CZ-NH1	28.99	134.79	120.30
1	A	98	ARG	NE-CZ-NH2	-28.48	106.06	120.30
1	F	109	ASP	CA-CB-CG	28.11	175.25	113.40
1	D	167	ARG	NE-CZ-NH2	27.31	133.95	120.30
1	D	152	TYR	CB-CG-CD1	27.28	137.37	121.00
1	E	98	ARG	NE-CZ-NH1	-27.24	106.68	120.30
1	B	59	ARG	CA-CB-CG	27.03	172.87	113.40
1	B	28	PHE	CB-CG-CD1	26.99	139.69	120.80
1	C	60	ALA	CA-C-N	26.98	176.57	117.20
1	D	1	ASN	OD1-CG-ND2	-26.79	60.28	121.90
1	E	146	SER	CA-C-N	26.73	176.01	117.20
1	B	184	ARG	NH1-CZ-NH2	26.52	148.57	119.40
1	D	46	ARG	CD-NE-CZ	26.43	160.61	123.60
1	E	228	TYR	C-N-CA	26.23	177.39	122.30
1	B	152	TYR	CB-CG-CD2	26.06	136.63	121.00
1	A	78	ARG	CA-CB-CG	26.05	170.71	113.40
1	C	152	TYR	CB-CG-CD2	26.00	136.60	121.00
1	D	128	LEU	CA-C-N	25.90	174.18	117.20
1	C	223	ARG	NH1-CZ-NH2	25.88	147.87	119.40
1	B	214	ARG	NE-CZ-NH2	25.85	133.23	120.30
1	C	168	ASP	CB-CG-OD2	-25.82	95.06	118.30
1	C	8	SER	O-C-N	-25.72	81.54	122.70
1	B	167	ARG	CA-CB-CG	25.65	169.83	113.40
1	A	90	TYR	CB-CG-CD1	25.65	136.39	121.00
1	C	215	TYR	CB-CG-CD1	-25.63	105.62	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	214	ARG	CD-NE-CZ	25.59	159.43	123.60
1	E	29	ARG	NE-CZ-NH1	25.44	133.02	120.30
1	F	210	ARG	CD-NE-CZ	25.44	159.21	123.60
1	B	170	ARG	CD-NE-CZ	25.36	159.10	123.60
1	F	46	ARG	NE-CZ-NH2	-25.26	107.67	120.30
1	B	98	ARG	NE-CZ-NH2	25.26	132.93	120.30
1	D	198	ASN	N-CA-CB	-25.08	65.46	110.60
1	D	31	THR	CA-CB-CG2	25.04	147.46	112.40
1	A	194	ASP	CB-CG-OD2	24.88	140.69	118.30
1	D	1	ASN	CB-CG-OD1	24.77	171.15	121.60
1	E	1	ASN	CA-CB-CG	24.77	167.89	113.40
1	C	210	ARG	NE-CZ-NH1	24.73	132.67	120.30
1	D	128	LEU	CA-C-O	-24.73	68.17	120.10
1	A	44	ASP	CB-CG-OD2	24.72	140.55	118.30
1	D	152	TYR	CB-CG-CD2	-24.58	106.25	121.00
1	B	153	ARG	NE-CZ-NH1	-24.54	108.03	120.30
1	D	16	THR	CA-CB-CG2	-24.16	78.57	112.40
1	F	60	ALA	CA-C-N	24.16	170.35	117.20
1	E	129	TYR	CG-CD1-CE1	24.06	140.54	121.30
1	B	230	GLY	O-C-N	23.98	161.07	122.70
1	F	9	HIS	CA-CB-CG	23.95	154.31	113.60
1	D	154	LEU	CB-CG-CD1	23.91	151.65	111.00
1	C	132	GLN	C-N-CA	23.81	172.30	122.30
1	F	98	ARG	NE-CZ-NH2	-23.80	108.40	120.30
1	F	100	VAL	CA-CB-CG2	23.76	146.54	110.90
1	A	157	GLU	CG-CD-OE1	23.74	165.78	118.30
1	B	98	ARG	CG-CD-NE	23.67	161.51	111.80
1	B	28	PHE	CB-CG-CD2	-23.60	104.28	120.80
1	B	72	THR	CA-CB-CG2	23.58	145.41	112.40
1	E	217	PHE	CB-CG-CD1	-23.46	104.38	120.80
1	A	19	ALA	CB-CA-C	23.45	145.27	110.10
1	E	138	PRO	N-CA-CB	23.43	131.42	103.30
1	C	159	ASP	CB-CG-OD1	-23.43	97.21	118.30
1	C	168	ASP	OD1-CG-OD2	-23.42	78.81	123.30
1	D	146	SER	CA-C-N	23.39	168.66	117.20
1	D	107	LEU	CB-CG-CD1	23.30	150.61	111.00
1	C	170	ARG	NE-CZ-NH1	-23.26	108.67	120.30
1	F	166	ASP	CB-CG-OD1	23.25	139.22	118.30
1	B	65	ASP	CB-CG-OD2	23.24	139.22	118.30
1	C	138	PRO	CA-N-CD	-23.21	79.01	111.50
1	C	117	SER	C-N-CA	23.17	179.63	121.70
1	C	153	ARG	NH1-CZ-NH2	23.14	144.85	119.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	ASP	CB-CG-OD2	-23.07	97.54	118.30
1	B	55	ALA	O-C-N	-23.02	85.86	122.70
1	A	129	TYR	C-N-CA	23.02	179.24	121.70
1	F	153	ARG	NE-CZ-NH1	-23.00	108.80	120.30
1	B	162	LEU	CB-CG-CD1	22.92	149.97	111.00
1	B	64	SER	N-CA-CB	-22.90	76.15	110.50
1	F	184	ARG	NH1-CZ-NH2	22.87	144.55	119.40
1	F	90	TYR	CB-CG-CD1	22.82	134.69	121.00
1	C	130	SER	N-CA-CB	22.80	144.70	110.50
1	F	92	LEU	CB-CG-CD1	22.77	149.71	111.00
1	C	230	GLY	CA-C-O	-22.76	79.63	120.60
1	D	20	ALA	CB-CA-C	22.76	144.25	110.10
1	D	99	THR	CA-CB-CG2	22.69	144.16	112.40
1	D	72	THR	CA-CB-CG2	22.65	144.11	112.40
1	C	59	ARG	NE-CZ-NH1	22.64	131.62	120.30
1	B	59	ARG	NE-CZ-NH2	-22.57	109.01	120.30
1	B	228	TYR	CB-CG-CD1	22.53	134.52	121.00
1	B	60	ALA	CA-C-O	-22.49	72.87	120.10
1	A	210	ARG	NE-CZ-NH1	-22.45	109.07	120.30
1	A	228	TYR	CB-CG-CD2	22.37	134.42	121.00
1	D	67	LEU	CA-CB-CG	22.31	166.62	115.30
1	B	67	LEU	CB-CG-CD1	-22.23	73.22	111.00
1	E	130	SER	C-N-CA	22.22	177.26	121.70
1	D	214	ARG	CA-CB-CG	22.20	162.23	113.40
1	D	185	ALA	N-CA-CB	-22.14	79.10	110.10
1	C	215	TYR	CB-CG-CD2	22.13	134.28	121.00
1	B	148	GLN	CA-CB-CG	22.12	162.07	113.40
1	A	167	ARG	NE-CZ-NH1	22.09	131.35	120.30
1	B	126	SER	N-CA-CB	-22.03	77.45	110.50
1	D	83	THR	CA-C-N	22.03	165.68	117.20
1	C	60	ALA	O-C-N	-22.03	87.45	122.70
1	E	223	ARG	NE-CZ-NH2	22.01	131.31	120.30
1	E	33	GLN	C-N-CA	21.96	176.60	121.70
1	F	1	ASN	C-N-CA	21.95	176.56	121.70
1	A	9	HIS	N-CA-C	21.88	170.07	111.00
1	B	87	ILE	CA-CB-CG1	21.86	152.54	111.00
1	F	124	GLY	C-N-CA	21.79	176.16	121.70
1	D	109	ASP	CB-CG-OD1	-21.76	98.71	118.30
1	F	173	SER	CA-CB-OG	21.76	169.94	111.20
1	F	152	TYR	CB-CG-CD1	-21.75	107.95	121.00
1	E	217	PHE	CB-CG-CD2	21.72	136.00	120.80
1	B	123	ASN	C-N-CA	21.67	167.80	122.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	170	ARG	CA-CB-CG	21.58	160.88	113.40
1	A	152	TYR	CB-CG-CD2	21.57	133.94	121.00
1	F	128	LEU	C-N-CA	21.55	175.56	121.70
1	A	129	TYR	CB-CG-CD2	21.43	133.85	121.00
1	C	145	GLN	C-N-CA	21.33	175.02	121.70
1	D	141	LEU	C-N-CA	21.32	175.00	121.70
1	E	113	SER	CA-CB-OG	21.32	168.76	111.20
1	D	193	MET	C-N-CA	21.31	174.98	121.70
1	D	209	SER	N-CA-CB	-21.27	78.60	110.50
1	E	231	ALA	N-CA-CB	21.26	139.87	110.10
1	F	214	ARG	CG-CD-NE	21.24	156.41	111.80
1	B	60	ALA	CA-C-N	21.16	163.75	117.20
1	B	60	ALA	N-CA-CB	21.16	139.72	110.10
1	B	152	TYR	CB-CG-CD1	-21.14	108.32	121.00
1	B	109	ASP	CB-CG-OD1	-21.12	99.29	118.30
1	B	215	TYR	CB-CG-CD1	20.99	133.59	121.00
1	F	210	ARG	NE-CZ-NH1	-20.88	109.86	120.30
1	B	47	VAL	CA-CB-CG1	-20.86	79.61	110.90
1	B	223	ARG	NE-CZ-NH1	-20.85	109.88	120.30
1	D	65	ASP	CB-CG-OD2	-20.84	99.54	118.30
1	D	202	ALA	CB-CA-C	20.79	141.28	110.10
1	B	109	ASP	OD1-CG-OD2	20.76	162.74	123.30
1	A	153	ARG	CD-NE-CZ	20.68	152.55	123.60
1	D	29	ARG	NE-CZ-NH1	-20.68	109.96	120.30
1	B	5	PHE	CE1-CZ-CE2	-20.67	82.79	120.00
1	F	73	ALA	C-N-CA	20.67	173.38	121.70
1	C	184	ARG	NE-CZ-NH1	-20.66	109.97	120.30
1	D	76	THR	C-N-CA	20.51	172.99	121.70
1	B	56	THR	C-N-CA	20.41	165.16	122.30
1	C	128	LEU	O-C-N	-20.31	90.20	122.70
1	F	193	MET	C-N-CA	20.24	172.29	121.70
1	D	60	ALA	CA-C-O	-20.23	77.61	120.10
1	D	219	LEU	CB-CG-CD2	20.21	145.37	111.00
1	C	190	ASN	N-CA-CB	-20.15	74.32	110.60
1	F	154	LEU	CA-CB-CG	20.14	161.63	115.30
1	C	44	ASP	N-CA-CB	-20.12	74.38	110.60
1	A	215	TYR	CB-CG-CD1	-20.10	108.94	121.00
1	A	131	THR	CA-CB-OG1	20.08	151.17	109.00
1	B	193	MET	C-N-CA	20.08	171.89	121.70
1	C	230	GLY	O-C-N	-20.06	90.61	122.70
1	E	33	GLN	CG-CD-OE1	20.04	161.67	121.60
1	D	56	THR	N-CA-CB	20.00	148.31	110.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	203	VAL	CG1-CB-CG2	-19.97	78.95	110.90
1	B	137	HIS	CA-C-O	-19.86	78.40	120.10
1	F	59	ARG	NE-CZ-NH1	19.84	130.22	120.30
1	F	202	ALA	CB-CA-C	19.77	139.76	110.10
1	C	128	LEU	CB-CG-CD2	19.74	144.56	111.00
1	F	128	LEU	CB-CA-C	19.67	147.57	110.20
1	C	123	ASN	CA-CB-CG	19.65	156.64	113.40
1	F	70	ILE	CA-CB-CG1	-19.59	73.78	111.00
1	B	30	PHE	CB-CG-CD2	-19.46	107.18	120.80
1	E	158	THR	OG1-CB-CG2	19.45	154.73	110.00
1	B	22	SER	N-CA-CB	-19.45	81.33	110.50
1	B	123	ASN	CA-CB-CG	19.40	156.07	113.40
1	E	35	ASP	CB-CG-OD2	19.32	135.69	118.30
1	B	46	ARG	NE-CZ-NH2	-19.24	110.68	120.30
1	A	92	LEU	N-CA-CB	19.07	148.54	110.40
1	B	187	LEU	O-C-N	19.04	153.17	122.70
1	C	89	ASN	CB-CG-OD1	-19.02	83.56	121.60
1	F	223	ARG	NH1-CZ-NH2	18.99	140.29	119.40
1	F	7	LEU	CA-C-O	18.99	159.98	120.10
1	A	221	PRO	O-C-N	-18.97	92.34	122.70
1	E	138	PRO	CA-N-CD	-18.95	84.96	111.50
1	B	228	TYR	CG-CD2-CE2	18.95	136.46	121.30
1	B	154	LEU	CA-CB-CG	18.94	158.87	115.30
1	F	67	LEU	CB-CG-CD1	-18.94	78.80	111.00
1	A	100	VAL	CG1-CB-CG2	-18.93	80.61	110.90
1	D	174	THR	CA-CB-OG1	18.91	148.71	109.00
1	B	64	SER	O-C-N	-18.84	92.56	122.70
1	B	166	ASP	CB-CG-OD1	18.82	135.24	118.30
1	A	170	ARG	NH1-CZ-NH2	-18.80	98.72	119.40
1	C	58	CYS	CA-CB-SG	18.79	147.81	114.00
1	D	144	THR	N-CA-CB	18.78	145.97	110.30
1	A	223	ARG	CG-CD-NE	18.77	151.21	111.80
1	A	40	LEU	CB-CG-CD1	18.74	142.86	111.00
1	D	203	VAL	CA-CB-CG1	18.73	138.99	110.90
1	E	76	THR	CA-CB-OG1	-18.71	69.72	109.00
1	F	97	ASP	CB-CG-OD1	-18.66	101.50	118.30
1	B	5	PHE	CZ-CE2-CD2	18.66	142.49	120.10
1	A	157	GLU	CG-CD-OE2	-18.65	81.00	118.30
1	E	33	GLN	O-C-N	-18.65	92.86	122.70
1	F	102	ILE	CB-CG1-CD1	18.59	165.97	113.90
1	C	46	ARG	CD-NE-CZ	18.52	149.53	123.60
1	A	231	ALA	C-N-CA	18.52	168.00	121.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	222	ASP	CB-CG-OD2	18.51	134.96	118.30
1	B	202	ALA	CB-CA-C	18.51	137.86	110.10
1	C	192	ARG	CD-NE-CZ	18.46	149.44	123.60
1	F	103	TYR	O-C-N	-18.45	91.83	123.20
1	A	128	LEU	CA-C-N	18.44	157.77	117.20
1	E	98	ARG	NH1-CZ-NH2	18.40	139.64	119.40
1	B	100	VAL	O-C-N	-18.34	93.35	122.70
1	C	153	ARG	NE-CZ-NH1	-18.34	111.13	120.30
1	A	84	LYS	CD-CE-NZ	18.27	153.72	111.70
1	B	147	LEU	CB-CG-CD1	18.26	142.04	111.00
1	A	169	ASP	CA-CB-CG	18.18	153.41	113.40
1	A	60	ALA	CA-C-N	18.18	157.19	117.20
1	D	6	GLY	C-N-CA	18.15	167.07	121.70
1	F	214	ARG	O-C-N	-18.15	93.66	122.70
1	F	129	TYR	N-CA-CB	-18.14	77.94	110.60
1	B	222	ASP	C-N-CA	18.11	166.99	121.70
1	B	137	HIS	CA-C-N	18.11	167.81	117.10
1	A	94	LEU	CB-CG-CD2	18.06	141.70	111.00
1	C	132	GLN	O-C-N	-18.00	92.60	123.20
1	A	159	ASP	CB-CG-OD2	17.98	134.48	118.30
1	E	223	ARG	CG-CD-NE	17.96	149.51	111.80
1	E	223	ARG	NE-CZ-NH1	-17.89	111.36	120.30
1	D	167	ARG	CG-CD-NE	17.88	149.35	111.80
1	D	91	VAL	CA-CB-CG1	17.83	137.65	110.90
1	F	202	ALA	N-CA-CB	-17.80	85.18	110.10
1	D	8	SER	N-CA-CB	-17.77	83.84	110.50
1	C	210	ARG	CD-NE-CZ	-17.75	98.74	123.60
1	F	129	TYR	CE1-CZ-OH	-17.72	72.27	120.10
1	D	126	SER	CA-CB-OG	17.70	159.00	111.20
1	E	109	ASP	CB-CG-OD1	17.70	134.23	118.30
1	A	88	GLY	CA-C-O	17.67	152.40	120.60
1	D	105	PRO	CA-N-CD	-17.65	86.79	111.50
1	A	123	ASN	C-N-CA	17.64	159.34	122.30
1	A	44	ASP	CA-CB-CG	17.59	152.10	113.40
1	F	72	THR	CA-CB-CG2	17.59	137.03	112.40
1	E	125	ASN	CA-CB-CG	17.57	152.05	113.40
1	A	97	ASP	CB-CG-OD2	-17.56	102.49	118.30
1	C	210	ARG	NE-CZ-NH2	-17.56	111.52	120.30
1	F	196	LEU	C-N-CA	17.53	165.53	121.70
1	D	139	GLN	CB-CG-CD	17.52	157.16	111.60
1	D	153	ARG	NE-CZ-NH2	-17.50	111.55	120.30
1	C	175	ASN	N-CA-CB	17.47	142.04	110.60

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	5	PHE	CB-CG-CD1	17.47	133.03	120.80
1	D	89	ASN	O-C-N	-17.43	94.80	122.70
1	A	29	ARG	CA-CB-CG	17.43	151.75	113.40
1	E	20	ALA	CB-CA-C	17.41	136.22	110.10
1	F	8	SER	C-N-CA	17.41	165.22	121.70
1	C	163	VAL	CG1-CB-CG2	17.40	138.74	110.90
1	C	124	GLY	C-N-CA	17.38	165.14	121.70
1	D	229	GLY	CA-C-O	-17.37	89.34	120.60
1	F	203	VAL	CA-CB-CG2	17.37	136.95	110.90
1	F	55	ALA	CB-CA-C	17.36	136.14	110.10
1	C	36	CYS	CA-CB-SG	-17.35	82.78	114.00
1	E	175	ASN	CA-CB-CG	17.35	151.57	113.40
1	B	5	PHE	CD1-CG-CD2	-17.31	95.79	118.30
1	B	192	ARG	NE-CZ-NH2	17.31	128.96	120.30
1	D	12	SER	CB-CA-C	17.29	142.95	110.10
1	A	208	ASN	O-C-N	17.29	150.36	122.70
1	A	14	PRO	CA-N-CD	-17.28	87.31	111.50
1	A	18	HIS	CA-C-O	17.27	156.38	120.10
1	D	65	ASP	CB-CG-OD1	17.25	133.83	118.30
1	E	60	ALA	CA-C-N	17.24	155.13	117.20
1	A	230	GLY	C-N-CA	17.23	164.78	121.70
1	A	124	GLY	C-N-CA	17.15	164.58	121.70
1	B	87	ILE	CB-CG1-CD1	17.14	161.88	113.90
1	A	229	GLY	C-N-CA	17.11	158.24	122.30
1	C	214	ARG	O-C-N	-17.10	95.34	122.70
1	F	104	GLY	C-N-CD	-17.09	82.99	120.60
1	D	189	PRO	N-CA-CB	17.09	123.81	103.30
1	A	194	ASP	OD1-CG-OD2	-17.08	90.85	123.30
1	D	7	LEU	CA-C-O	17.05	155.91	120.10
1	F	104	GLY	O-C-N	17.04	153.48	121.10
1	D	107	LEU	CB-CG-CD2	-17.04	82.03	111.00
1	E	192	ARG	NE-CZ-NH2	-17.04	111.78	120.30
1	D	65	ASP	N-CA-CB	-17.03	79.94	110.60
1	D	12	SER	N-CA-CB	-17.03	84.96	110.50
1	D	171	VAL	CA-CB-CG2	16.97	136.35	110.90
1	D	103	TYR	CB-CG-CD1	16.95	131.17	121.00
1	D	166	ASP	CB-CG-OD1	16.94	133.55	118.30
1	D	47	VAL	CA-CB-CG1	-16.93	85.50	110.90
1	B	210	ARG	CA-C-O	-16.93	84.56	120.10
1	F	90	TYR	CG-CD2-CE2	16.93	134.84	121.30
1	E	145	GLN	CB-CG-CD	16.92	155.59	111.60
1	B	124	GLY	C-N-CA	16.90	163.95	121.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	136	ASN	CA-CB-CG	16.89	150.56	113.40
1	F	7	LEU	O-C-N	-16.88	95.70	122.70
1	B	167	ARG	N-CA-CB	16.87	140.97	110.60
1	D	51	ASN	C-N-CA	16.87	163.87	121.70
1	D	158	THR	CA-C-N	16.87	154.31	117.20
1	E	99	THR	CA-CB-CG2	16.83	135.96	112.40
1	D	196	LEU	CA-CB-CG	16.83	154.00	115.30
1	F	154	LEU	CB-CG-CD1	16.82	139.60	111.00
1	D	188	GLN	O-C-N	-16.82	89.15	121.10
1	B	1	ASN	CA-CB-CG	16.81	150.39	113.40
1	D	169	ASP	CB-CG-OD1	-16.80	103.18	118.30
1	F	67	LEU	CB-CG-CD2	16.78	139.53	111.00
1	D	106	GLY	CA-C-N	16.78	154.12	117.20
1	E	146	SER	O-C-N	-16.75	95.90	122.70
1	B	105	PRO	CA-N-CD	-16.74	88.06	111.50
1	B	143	ALA	CA-C-N	16.73	154.01	117.20
1	C	197	THR	CA-CB-CG2	16.73	135.82	112.40
1	B	229	GLY	CA-C-N	-16.73	82.75	116.20
1	B	124	GLY	N-CA-C	16.71	154.87	113.10
1	C	38	LEU	O-C-N	-16.70	95.99	122.70
1	C	78	ARG	NE-CZ-NH2	16.70	128.65	120.30
1	E	182	GLY	C-N-CA	16.69	163.42	121.70
1	C	132	GLN	CA-CB-CG	16.68	150.10	113.40
1	A	98	ARG	NH1-CZ-NH2	16.68	137.74	119.40
1	A	182	GLY	CA-C-O	-16.68	90.58	120.60
1	B	108	TRP	O-C-N	-16.67	96.03	122.70
1	D	169	ASP	CB-CG-OD2	16.67	133.30	118.30
1	D	56	THR	C-N-CA	16.67	157.30	122.30
1	F	189	PRO	C-N-CA	16.65	163.33	121.70
1	F	65	ASP	N-CA-CB	-16.65	80.63	110.60
1	C	130	SER	CA-C-O	16.64	155.05	120.10
1	E	33	GLN	CA-CB-CG	16.63	149.98	113.40
1	B	201	ILE	O-C-N	-16.63	96.10	122.70
1	D	129	TYR	CZ-CE2-CD2	-16.62	104.84	119.80
1	A	105	PRO	CA-N-CD	-16.58	88.28	111.50
1	E	1	ASN	OD1-CG-ND2	-16.58	83.76	121.90
1	B	184	ARG	CD-NE-CZ	16.57	146.80	123.60
1	E	9	HIS	C-N-CA	16.56	163.09	121.70
1	B	107	LEU	CA-C-N	16.53	153.57	117.20
1	B	147	LEU	CB-CG-CD2	-16.53	82.90	111.00
1	A	128	LEU	CA-C-O	-16.52	85.40	120.10
1	B	194	ASP	CB-CG-OD2	-16.50	103.45	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	128	LEU	CB-CA-C	16.50	141.54	110.20
1	C	78	ARG	NE-CZ-NH1	-16.49	112.06	120.30
1	E	167	ARG	CD-NE-CZ	16.47	146.66	123.60
1	D	64	SER	CB-CA-C	16.45	141.35	110.10
1	E	131	THR	CA-C-O	16.45	154.64	120.10
1	D	146	SER	CA-C-O	-16.43	85.60	120.10
1	D	168	ASP	CA-CB-CG	16.43	149.53	113.40
1	B	89	ASN	CB-CG-OD1	-16.42	88.75	121.60
1	D	21	GLN	CA-CB-CG	16.42	149.52	113.40
1	D	89	ASN	CB-CG-OD1	-16.41	88.78	121.60
1	F	86	SER	CA-C-O	-16.41	85.64	120.10
1	D	233	TRP	CA-CB-CG	16.41	144.87	113.70
1	B	21	GLN	C-N-CA	16.40	162.70	121.70
1	E	59	ARG	CD-NE-CZ	16.39	146.55	123.60
1	E	89	ASN	CB-CG-OD1	-16.36	88.89	121.60
1	B	54	GLY	CA-C-O	-16.34	91.18	120.60
1	A	124	GLY	N-CA-C	16.29	153.83	113.10
1	C	150	SER	N-CA-CB	16.28	134.92	110.50
1	C	214	ARG	CA-CB-CG	16.25	149.16	113.40
1	D	124	GLY	C-N-CA	16.25	162.31	121.70
1	E	225	LEU	N-CA-CB	-16.25	77.91	110.40
1	B	22	SER	O-C-N	-16.24	96.72	122.70
1	E	128	LEU	CB-CG-CD1	16.23	138.59	111.00
1	A	206	SER	O-C-N	-16.21	95.64	123.20
1	D	210	ARG	CA-CB-CG	16.21	149.07	113.40
1	B	209	SER	O-C-N	16.15	148.54	122.70
1	E	128	LEU	O-C-N	-16.14	96.88	122.70
1	A	143	ALA	CB-CA-C	16.14	134.30	110.10
1	B	142	HIS	CA-CB-CG	16.09	140.95	113.60
1	A	198	ASN	C-N-CA	16.09	161.91	121.70
1	E	59	ARG	CA-CB-CG	16.07	148.75	113.40
1	F	109	ASP	CB-CG-OD1	16.05	132.75	118.30
1	C	174	THR	O-C-N	-16.05	97.02	122.70
1	F	85	GLY	O-C-N	-16.03	97.05	122.70
1	D	154	LEU	CA-CB-CG	16.02	152.15	115.30
1	A	180	GLY	CA-C-O	-16.02	91.77	120.60
1	F	78	ARG	CG-CD-NE	16.02	145.44	111.80
1	F	111	GLY	CA-C-O	16.01	149.41	120.60
1	B	82	GLY	CA-C-O	15.98	149.37	120.60
1	C	152	TYR	CG-CD2-CE2	15.97	134.08	121.30
1	C	206	SER	O-C-N	-15.94	96.09	123.20
1	C	103	TYR	CD1-CE1-CZ	-15.94	105.46	119.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	224	ASN	C-N-CA	15.92	161.50	121.70
1	B	5	PHE	CB-CG-CD1	15.89	131.93	120.80
1	D	39	VAL	CA-CB-CG2	15.89	134.74	110.90
1	B	230	GLY	CA-C-N	-15.89	82.25	117.20
1	A	113	SER	CA-C-O	15.87	153.43	120.10
1	B	104	GLY	C-N-CD	-15.87	85.70	120.60
1	F	194	ASP	CB-CG-OD2	15.86	132.57	118.30
1	D	210	ARG	CD-NE-CZ	15.82	145.74	123.60
1	E	214	ARG	O-C-N	-15.79	97.43	122.70
1	C	128	LEU	C-N-CA	15.79	161.18	121.70
1	B	91	VAL	CA-CB-CG1	15.78	134.56	110.90
1	A	203	VAL	CA-CB-CG1	15.76	134.54	110.90
1	E	158	THR	CA-CB-CG2	-15.74	90.36	112.40
1	A	129	TYR	CD1-CE1-CZ	15.74	133.97	119.80
1	F	8	SER	CB-CA-C	15.74	140.00	110.10
1	D	159	ASP	CB-CG-OD1	-15.72	104.15	118.30
1	F	24	GLU	CA-CB-CG	15.69	147.93	113.40
1	F	54	GLY	O-C-N	-15.68	97.61	122.70
1	A	142	HIS	O-C-N	-15.68	97.62	122.70
1	C	124	GLY	N-CA-C	15.67	152.28	113.10
1	D	214	ARG	NH1-CZ-NH2	-15.67	102.16	119.40
1	B	209	SER	CA-C-O	-15.65	87.23	120.10
1	A	47	VAL	CA-CB-CG1	-15.65	87.43	110.90
1	C	40	LEU	O-C-N	-15.65	97.66	122.70
1	C	212	ALA	CB-CA-C	-15.65	86.63	110.10
1	F	32	MET	CG-SD-CE	15.64	125.22	100.20
1	B	222	ASP	CA-C-N	15.63	151.59	117.20
1	B	64	SER	CB-CA-C	15.63	139.79	110.10
1	C	28	PHE	CD1-CE1-CZ	-15.62	101.36	120.10
1	D	217	PHE	CB-CA-C	15.60	141.60	110.40
1	B	5	PHE	CD1-CE1-CZ	15.58	138.80	120.10
1	E	35	ASP	O-C-N	-15.57	97.79	122.70
1	C	228	TYR	CB-CG-CD1	15.55	130.33	121.00
1	F	190	ASN	OD1-CG-ND2	-15.55	86.14	121.90
1	D	148	GLN	O-C-N	-15.53	97.85	122.70
1	A	81	SER	CA-C-N	15.53	147.26	116.20
1	E	124	GLY	C-N-CA	15.53	160.52	121.70
1	F	128	LEU	O-C-N	-15.53	97.86	122.70
1	D	35	ASP	O-C-N	-15.52	97.87	122.70
1	F	109	ASP	CB-CG-OD2	-15.52	104.33	118.30
1	D	221	PRO	O-C-N	-15.51	97.88	122.70
1	F	141	LEU	N-CA-CB	-15.50	79.39	110.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	ARG	CG-CD-NE	15.49	144.33	111.80
1	B	71	LEU	CB-CG-CD1	-15.48	84.68	111.00
1	A	169	ASP	CB-CG-OD2	15.48	132.23	118.30
1	A	145	GLN	CA-CB-CG	15.45	147.40	113.40
1	C	123	ASN	C-N-CA	15.43	154.71	122.30
1	A	170	ARG	CB-CG-CD	15.41	151.67	111.60
1	A	99	THR	CA-CB-OG1	-15.40	76.65	109.00
1	C	2	ASN	CB-CG-ND2	15.40	153.67	116.70
1	B	5	PHE	CB-CG-CD2	15.40	131.58	120.80
1	F	55	ALA	O-C-N	-15.39	98.08	122.70
1	B	55	ALA	CA-C-O	15.38	152.41	120.10
1	C	61	VAL	CB-CA-C	-15.38	82.17	111.40
1	A	55	ALA	CB-CA-C	15.36	133.13	110.10
1	A	214	ARG	O-C-N	-15.35	98.14	122.70
1	C	13	HIS	CA-C-O	-15.34	87.89	120.10
1	C	128	LEU	CB-CA-C	15.33	139.34	110.20
1	C	230	GLY	CA-C-N	15.32	150.91	117.20
1	B	107	LEU	O-C-N	-15.32	98.19	122.70
1	F	210	ARG	CA-C-N	15.30	150.85	117.20
1	E	90	TYR	CB-CG-CD2	15.28	130.17	121.00
1	E	146	SER	CA-C-O	-15.28	88.02	120.10
1	B	192	ARG	CG-CD-NE	15.27	143.87	111.80
1	B	100	VAL	CA-CB-CG2	15.26	133.78	110.90
1	D	213	GLY	CA-C-O	-15.24	93.18	120.60
1	B	217	PHE	O-C-N	15.22	147.05	122.70
1	F	225	LEU	N-CA-CB	15.22	140.84	110.40
1	A	170	ARG	O-C-N	-15.21	98.37	122.70
1	D	198	ASN	CA-CB-CG	-15.21	79.94	113.40
1	C	189	PRO	C-N-CA	15.20	159.69	121.70
1	B	202	ALA	O-C-N	-15.19	98.39	122.70
1	E	5	PHE	CA-C-N	-15.18	85.84	116.20
1	A	174	THR	CA-CB-CG2	-15.17	91.17	112.40
1	D	130	SER	C-N-CA	15.16	159.59	121.70
1	C	210	ARG	O-C-N	-15.15	98.45	122.70
1	F	131	THR	N-CA-C	15.15	151.90	111.00
1	D	224	ASN	N-CA-CB	-15.14	83.35	110.60
1	A	33	GLN	C-N-CA	15.14	159.55	121.70
1	F	129	TYR	OH-CZ-CE2	15.14	160.97	120.10
1	F	54	GLY	C-N-CA	15.13	159.53	121.70
1	D	106	GLY	O-C-N	-15.10	98.54	122.70
1	D	1	ASN	C-N-CA	15.10	159.45	121.70
1	F	190	ASN	O-C-N	-15.08	97.56	123.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	130	SER	C-N-CA	15.06	159.34	121.70
1	A	99	THR	CA-CB-CG2	15.02	133.43	112.40
1	F	195	VAL	CA-CB-CG1	15.01	133.41	110.90
1	A	166	ASP	N-CA-CB	14.99	137.59	110.60
1	D	83	THR	CA-CB-CG2	-14.99	91.41	112.40
1	A	61	VAL	CA-CB-CG2	-14.99	88.42	110.90
1	D	59	ARG	NH1-CZ-NH2	14.99	135.88	119.40
1	A	113	SER	O-C-N	-14.98	98.73	122.70
1	A	110	SER	CA-C-O	14.97	151.54	120.10
1	E	170	ARG	NH1-CZ-NH2	-14.96	102.94	119.40
1	F	101	THR	N-CA-C	14.93	151.31	111.00
1	F	153	ARG	CG-CD-NE	14.91	143.11	111.80
1	E	170	ARG	CB-CG-CD	14.90	150.35	111.60
1	F	26	SER	C-N-CA	14.87	158.88	121.70
1	F	152	TYR	CB-CG-CD2	14.85	129.91	121.00
1	F	137	HIS	CA-C-O	-14.84	88.93	120.10
1	C	41	PHE	CB-CG-CD2	-14.83	110.42	120.80
1	A	127	ILE	CA-CB-CG1	14.83	139.17	111.00
1	B	19	ALA	CB-CA-C	14.78	132.26	110.10
1	B	22	SER	CB-CA-C	-14.78	82.03	110.10
1	D	196	LEU	C-N-CA	14.77	158.62	121.70
1	A	7	LEU	CA-C-N	14.76	149.66	117.20
1	A	88	GLY	N-CA-C	14.76	149.99	113.10
1	D	62	LEU	CA-C-O	14.75	151.07	120.10
1	C	118	VAL	C-N-CA	14.74	158.56	121.70
1	D	34	SER	N-CA-CB	14.74	132.61	110.50
1	F	60	ALA	CA-C-O	-14.73	89.17	120.10
1	D	223	ARG	O-C-N	-14.72	99.14	122.70
1	A	92	LEU	CA-CB-CG	14.72	149.15	115.30
1	A	5	PHE	CA-C-N	14.71	145.62	116.20
1	A	164	LEU	CB-CG-CD1	14.71	136.01	111.00
1	F	210	ARG	NH1-CZ-NH2	14.71	135.58	119.40
1	C	206	SER	C-N-CA	14.70	153.18	122.30
1	D	75	ASN	OD1-CG-ND2	14.71	155.72	121.90
1	F	60	ALA	O-C-N	-14.70	99.18	122.70
1	D	193	MET	CA-C-N	14.70	149.53	117.20
1	A	193	MET	CA-CB-CG	14.69	138.28	113.30
1	C	217	PHE	CB-CG-CD1	14.69	131.08	120.80
1	D	216	VAL	CB-CA-C	14.67	139.27	111.40
1	A	19	ALA	CA-C-N	14.65	149.44	117.20
1	E	102	ILE	O-C-N	14.65	146.15	122.70
1	B	59	ARG	CB-CA-C	-14.64	81.12	110.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	86	SER	N-CA-CB	-14.64	88.54	110.50
1	C	73	ALA	CB-CA-C	14.61	132.01	110.10
1	D	15	GLN	CG-CD-OE1	-14.60	92.40	121.60
1	A	68	LEU	C-N-CA	14.55	158.08	121.70
1	E	152	TYR	CG-CD2-CE2	14.54	132.93	121.30
1	C	192	ARG	NE-CZ-NH2	-14.53	113.03	120.30
1	A	58	CYS	N-CA-CB	-14.53	84.45	110.60
1	A	78	ARG	NH1-CZ-NH2	-14.53	103.42	119.40
1	F	136	ASN	O-C-N	-14.52	99.47	122.70
1	A	20	ALA	N-CA-CB	14.51	130.42	110.10
1	B	7	LEU	O-C-N	-14.49	99.52	122.70
1	A	135	ASP	CB-CG-OD1	-14.49	105.26	118.30
1	D	35	ASP	CB-CG-OD2	-14.49	105.26	118.30
1	A	94	LEU	C-N-CA	14.48	157.90	121.70
1	D	83	THR	CA-C-O	-14.48	89.69	120.10
1	C	218	VAL	CG1-CB-CG2	-14.47	87.74	110.90
1	F	87	ILE	CA-C-N	14.47	145.15	116.20
1	A	146	SER	N-CA-C	14.47	150.07	111.00
1	D	104	GLY	O-C-N	14.45	148.55	121.10
1	A	167	ARG	CD-NE-CZ	14.44	143.81	123.60
1	C	105	PRO	CA-N-CD	-14.44	91.29	111.50
1	F	26	SER	CA-CB-OG	14.43	150.16	111.20
1	D	91	VAL	O-C-N	-14.42	99.63	122.70
1	B	205	THR	CA-CB-CG2	14.41	132.58	112.40
1	D	46	ARG	CB-CG-CD	14.40	149.04	111.60
1	C	125	ASN	CA-CB-CG	14.40	145.08	113.40
1	C	37	ASN	CB-CG-OD1	-14.39	92.82	121.60
1	C	74	GLN	OE1-CD-NE2	14.38	154.98	121.90
1	D	21	GLN	CB-CG-CD	14.38	148.99	111.60
1	A	210	ARG	NH1-CZ-NH2	14.37	135.21	119.40
1	C	46	ARG	NE-CZ-NH2	14.37	127.49	120.30
1	D	29	ARG	NE-CZ-NH2	14.37	127.48	120.30
1	D	129	TYR	CB-CG-CD1	-14.37	112.38	121.00
1	A	200	ASN	O-C-N	-14.37	99.72	122.70
1	E	193	MET	CG-SD-CE	14.37	123.18	100.20
1	F	83	THR	O-C-N	-14.32	99.78	122.70
1	D	35	ASP	CA-C-N	14.32	148.71	117.20
1	F	78	ARG	CB-CG-CD	14.32	148.82	111.60
1	C	201	ILE	O-C-N	-14.31	99.80	122.70
1	E	46	ARG	CB-CA-C	14.31	139.03	110.40
1	D	25	LEU	CB-CG-CD2	14.31	135.32	111.00
1	F	164	LEU	CA-C-O	-14.30	90.07	120.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	65	ASP	CB-CG-OD2	14.29	131.17	118.30
1	D	213	GLY	O-C-N	14.24	145.49	122.70
1	B	100	VAL	CA-C-O	14.24	150.01	120.10
1	F	149	LEU	N-CA-CB	14.24	138.88	110.40
1	B	222	ASP	CB-CG-OD2	-14.24	105.49	118.30
1	B	129	TYR	CB-CG-CD2	-14.22	112.47	121.00
1	B	196	LEU	CA-C-O	14.22	149.97	120.10
1	F	195	VAL	CB-CA-C	14.22	138.42	111.40
1	B	73	ALA	C-N-CA	14.20	157.21	121.70
1	D	130	SER	O-C-N	-14.20	99.98	122.70
1	B	183	CYS	CA-CB-SG	14.19	139.54	114.00
1	D	13	HIS	CA-C-O	-14.19	90.31	120.10
1	B	105	PRO	CA-C-O	-14.18	86.16	120.20
1	A	4	LEU	CB-CA-C	14.17	137.12	110.20
1	E	153	ARG	CD-NE-CZ	14.15	143.41	123.60
1	D	100	VAL	CG1-CB-CG2	-14.13	88.29	110.90
1	E	34	SER	CB-CA-C	14.12	136.93	110.10
1	D	76	THR	O-C-N	-14.11	100.12	122.70
1	A	32	MET	CG-SD-CE	-14.10	77.65	100.20
1	D	234	THR	CA-CB-CG2	14.07	132.09	112.40
1	B	140	THR	CA-CB-CG2	14.06	132.09	112.40
1	B	17	LEU	CB-CG-CD1	-14.04	87.12	111.00
1	B	203	VAL	CA-CB-CG2	14.04	131.96	110.90
1	E	42	ASP	CB-CG-OD2	-14.03	105.68	118.30
1	F	166	ASP	CB-CG-OD2	-14.02	105.68	118.30
1	F	61	VAL	CB-CA-C	-14.02	84.76	111.40
1	D	129	TYR	CG-CD1-CE1	-14.00	110.10	121.30
1	C	184	ARG	NH1-CZ-NH2	13.99	134.79	119.40
1	A	94	LEU	CA-CB-CG	13.98	147.47	115.30
1	D	8	SER	CB-CA-C	13.98	136.67	110.10
1	A	48	TRP	CG-CD1-NE1	13.98	124.08	110.10
1	F	129	TYR	C-N-CA	13.98	156.65	121.70
1	A	60	ALA	O-C-N	-13.97	100.34	122.70
1	D	177	ALA	N-CA-CB	13.97	129.66	110.10
1	D	74	GLN	CA-CB-CG	-13.97	82.67	113.40
1	A	187	LEU	CA-CB-CG	13.96	147.40	115.30
1	B	220	GLN	CG-CD-NE2	13.96	150.20	116.70
1	B	64	SER	CA-C-N	13.95	147.90	117.20
1	E	129	TYR	CB-CG-CD2	13.95	129.37	121.00
1	E	1	ASN	O-C-N	-13.95	100.39	122.70
1	D	166	ASP	CB-CG-OD2	-13.94	105.75	118.30
1	B	9	HIS	CB-CA-C	-13.91	82.58	110.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	184	ARG	CD-NE-CZ	13.90	143.06	123.60
1	A	95	GLN	CB-CG-CD	13.88	147.70	111.60
1	B	77	ILE	CB-CA-C	-13.88	83.83	111.60
1	C	131	THR	CA-CB-OG1	13.88	138.14	109.00
1	D	192	ARG	CD-NE-CZ	13.87	143.02	123.60
1	D	76	THR	CA-CB-CG2	13.87	131.82	112.40
1	D	34	SER	O-C-N	-13.87	100.52	122.70
1	D	15	GLN	CG-CD-NE2	13.86	149.96	116.70
1	E	10	GLU	CB-CA-C	13.85	138.09	110.40
1	F	220	GLN	CA-CB-CG	-13.84	82.95	113.40
1	F	8	SER	N-CA-CB	-13.81	89.78	110.50
1	D	107	LEU	CA-C-O	-13.80	91.13	120.10
1	D	226	ALA	CB-CA-C	13.79	130.79	110.10
1	C	28	PHE	CG-CD1-CE1	13.79	135.97	120.80
1	B	215	TYR	CB-CG-CD2	-13.79	112.73	121.00
1	A	109	ASP	N-CA-CB	13.76	135.37	110.60
1	A	5	PHE	CB-CG-CD2	13.75	130.43	120.80
1	D	224	ASN	N-CA-C	13.75	148.13	111.00
1	A	129	TYR	CA-C-O	-13.74	91.25	120.10
1	D	223	ARG	CG-CD-NE	13.74	140.65	111.80
1	E	136	ASN	N-CA-CB	13.73	135.31	110.60
1	F	194	ASP	CA-CB-CG	-13.72	83.21	113.40
1	E	128	LEU	CD1-CG-CD2	-13.71	69.35	110.50
1	E	64	SER	O-C-N	-13.71	100.76	122.70
1	E	214	ARG	CD-NE-CZ	13.70	142.78	123.60
1	F	187	LEU	CA-CB-CG	13.70	146.81	115.30
1	B	109	ASP	CB-CA-C	-13.69	83.02	110.40
1	A	19	ALA	N-CA-CB	-13.68	90.95	110.10
1	A	62	LEU	CA-CB-CG	13.68	146.76	115.30
1	A	65	ASP	OD1-CG-OD2	-13.68	97.32	123.30
1	F	104	GLY	C-N-CA	13.65	179.33	122.00
1	C	62	LEU	CB-CG-CD2	13.65	134.20	111.00
1	A	173	SER	CA-C-N	13.64	147.22	117.20
1	D	187	LEU	N-CA-CB	13.64	137.69	110.40
1	D	176	THR	N-CA-CB	-13.64	84.38	110.30
1	A	7	LEU	CB-CA-C	13.63	136.10	110.20
1	E	188	GLN	CA-CB-CG	-13.63	83.41	113.40
1	A	188	GLN	CG-CD-NE2	13.62	149.39	116.70
1	F	210	ARG	CA-C-O	-13.62	91.50	120.10
1	B	143	ALA	CA-C-O	-13.62	91.50	120.10
1	C	71	LEU	CB-CG-CD2	-13.62	87.85	111.00
1	F	138	PRO	N-CA-CB	13.62	119.64	103.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	TRP	CB-CG-CD2	13.60	144.28	126.60
1	F	192	ARG	CA-CB-CG	13.60	143.32	113.40
1	D	105	PRO	CA-C-O	-13.60	87.56	120.20
1	A	131	THR	N-CA-CB	13.59	136.12	110.30
1	D	27	SER	C-N-CA	13.59	155.67	121.70
1	D	104	GLY	C-N-CA	13.57	178.98	122.00
1	F	59	ARG	CD-NE-CZ	-13.56	104.62	123.60
1	D	3	ILE	CA-CB-CG2	-13.55	83.80	110.90
1	D	170	ARG	NH1-CZ-NH2	-13.55	104.50	119.40
1	E	159	ASP	O-C-N	-13.54	101.03	122.70
1	D	130	SER	CA-C-O	13.54	148.54	120.10
1	C	234	THR	O-C-N	-13.54	101.04	122.70
1	D	53	ALA	N-CA-CB	13.54	129.05	110.10
1	B	92	LEU	N-CA-CB	13.52	137.44	110.40
1	E	163	VAL	O-C-N	13.51	144.32	122.70
1	B	48	TRP	N-CA-CB	-13.50	86.31	110.60
1	B	101	THR	CA-CB-OG1	-13.49	80.68	109.00
1	A	134	ASN	CA-CB-CG	13.48	143.06	113.40
1	A	212	ALA	CB-CA-C	-13.48	89.88	110.10
1	D	42	ASP	CB-CG-OD2	-13.48	106.17	118.30
1	F	125	ASN	CA-CB-CG	13.47	143.04	113.40
1	A	110	SER	C-N-CA	13.46	150.58	122.30
1	D	217	PHE	CB-CG-CD2	13.46	130.22	120.80
1	D	34	SER	CA-CB-OG	-13.46	74.86	111.20
1	C	107	LEU	CA-C-O	-13.46	91.84	120.10
1	C	127	ILE	CA-CB-CG1	13.44	136.54	111.00
1	E	152	TYR	CB-CG-CD1	13.44	129.06	121.00
1	C	188	GLN	CA-CB-CG	-13.44	83.84	113.40
1	E	129	TYR	CD1-CE1-CZ	-13.43	107.71	119.80
1	A	220	GLN	CA-CB-CG	-13.43	83.85	113.40
1	B	78	ARG	NE-CZ-NH2	13.43	127.01	120.30
1	B	146	SER	CA-C-N	13.40	146.69	117.20
1	A	8	SER	C-N-CA	13.39	155.18	121.70
1	A	29	ARG	NE-CZ-NH1	-13.37	113.61	120.30
1	C	58	CYS	CB-CA-C	13.35	137.11	110.40
1	F	224	ASN	CA-C-N	13.35	146.58	117.20
1	C	138	PRO	C-N-CA	-13.34	88.35	121.70
1	C	20	ALA	CB-CA-C	13.34	130.11	110.10
1	A	1	ASN	N-CA-CB	13.32	134.59	110.60
1	D	196	LEU	CB-CG-CD2	13.32	133.65	111.00
1	F	190	ASN	CB-CG-ND2	13.32	148.66	116.70
1	E	62	LEU	CB-CG-CD2	13.31	133.63	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	98	ARG	NE-CZ-NH2	-13.31	113.64	120.30
1	B	142	HIS	CG-ND1-CE1	13.30	126.82	108.20
1	E	184	ARG	NE-CZ-NH2	-13.29	113.65	120.30
1	A	92	LEU	O-C-N	-13.29	101.44	122.70
1	C	90	TYR	CA-C-O	-13.28	92.22	120.10
1	B	15	GLN	CA-CB-CG	13.27	142.60	113.40
1	B	226	ALA	N-CA-CB	13.27	128.68	110.10
1	B	170	ARG	NE-CZ-NH1	13.27	126.94	120.30
1	B	59	ARG	NH1-CZ-NH2	13.27	133.99	119.40
1	C	197	THR	CA-CB-OG1	-13.25	81.18	109.00
1	E	222	ASP	CB-CG-OD2	13.25	130.22	118.30
1	B	84	LYS	CB-CG-CD	13.24	146.02	111.60
1	D	19	ALA	N-CA-CB	13.23	128.63	110.10
1	A	128	LEU	CB-CG-CD1	13.23	133.48	111.00
1	A	206	SER	C-N-CA	13.22	150.06	122.30
1	A	15	GLN	CB-CA-C	13.21	136.82	110.40
1	E	149	LEU	C-N-CA	-13.21	88.67	121.70
1	D	212	ALA	N-CA-CB	-13.21	91.61	110.10
1	B	194	ASP	OD1-CG-OD2	13.20	148.38	123.30
1	E	128	LEU	CB-CG-CD2	13.20	133.44	111.00
1	A	214	ARG	CA-CB-CG	13.20	142.43	113.40
1	D	96	PRO	CA-C-N	13.20	146.23	117.20
1	D	197	THR	CA-CB-OG1	-13.19	81.31	109.00
1	E	110	SER	N-CA-CB	13.18	130.27	110.50
1	D	196	LEU	O-C-N	-13.17	101.63	122.70
1	F	234	THR	OG1-CB-CG2	-13.17	79.72	110.00
1	C	8	SER	CA-C-O	13.16	147.74	120.10
1	D	152	TYR	OH-CZ-CE2	-13.15	84.59	120.10
1	B	71	LEU	C-N-CA	13.14	154.55	121.70
1	D	138	PRO	CA-N-CD	-13.14	93.11	111.50
1	E	215	TYR	CB-CG-CD1	-13.12	113.13	121.00
1	A	229	GLY	CA-C-O	13.11	144.20	120.60
1	C	167	ARG	N-CA-C	-13.09	75.66	111.00
1	B	6	GLY	O-C-N	-13.07	101.78	122.70
1	D	95	GLN	CG-CD-OE1	13.07	147.74	121.60
1	A	14	PRO	N-CD-CG	13.06	122.80	103.20
1	C	45	VAL	CA-CB-CG2	13.06	130.50	110.90
1	F	89	ASN	CB-CG-OD1	-13.06	95.48	121.60
1	B	21	GLN	CG-CD-NE2	13.04	147.99	116.70
1	B	50	SER	CB-CA-C	13.03	134.85	110.10
1	B	62	LEU	CB-CG-CD1	13.03	133.14	111.00
1	B	31	THR	CA-CB-CG2	13.02	130.62	112.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	15	GLN	CB-CA-C	13.01	136.43	110.40
1	B	210	ARG	O-C-N	13.01	143.51	122.70
1	E	144	THR	CA-CB-CG2	-13.01	94.19	112.40
1	C	142	HIS	O-C-N	-12.99	101.92	122.70
1	D	131	THR	N-CA-C	12.97	146.03	111.00
1	A	168	ASP	CB-CG-OD1	-12.97	106.63	118.30
1	C	112	THR	CA-CB-CG2	12.97	130.56	112.40
1	B	220	GLN	CG-CD-OE1	-12.97	95.66	121.60
1	A	46	ARG	NE-CZ-NH1	12.96	126.78	120.30
1	B	132	GLN	CA-C-O	12.96	147.32	120.10
1	A	88	GLY	CA-C-N	-12.95	88.71	117.20
1	A	221	PRO	N-CA-CB	-12.94	87.77	103.30
1	C	122	ASN	CA-CB-CG	12.94	141.86	113.40
1	A	221	PRO	CB-CA-C	12.93	144.32	112.00
1	D	194	ASP	CB-CG-OD2	12.92	129.93	118.30
1	C	29	ARG	NE-CZ-NH2	12.92	126.76	120.30
1	D	193	MET	CA-CB-CG	12.91	135.25	113.30
1	A	56	THR	CA-C-O	12.91	147.21	120.10
1	A	181	THR	C-N-CA	-12.91	95.20	122.30
1	D	202	ALA	CA-C-N	12.90	145.59	117.20
1	A	92	LEU	CB-CG-CD1	-12.90	89.07	111.00
1	B	170	ARG	NE-CZ-NH2	-12.90	113.85	120.30
1	C	193	MET	CG-SD-CE	-12.89	79.57	100.20
1	E	111	GLY	O-C-N	12.89	143.32	122.70
1	E	26	SER	CA-C-N	12.89	145.55	117.20
1	B	87	ILE	CA-CB-CG2	-12.88	85.14	110.90
1	F	101	THR	CA-CB-OG1	-12.88	81.96	109.00
1	B	89	ASN	CB-CG-ND2	12.86	147.56	116.70
1	D	224	ASN	CA-CB-CG	-12.86	85.11	113.40
1	B	73	ALA	N-CA-CB	12.85	128.09	110.10
1	D	107	LEU	CB-CA-C	-12.84	85.80	110.20
1	E	166	ASP	CB-CG-OD1	-12.84	106.74	118.30
1	B	11	GLY	C-N-CA	12.83	153.78	121.70
1	D	13	HIS	CA-CB-CG	-12.83	91.78	113.60
1	B	137	HIS	N-CA-C	12.83	145.63	111.00
1	E	210	ARG	NE-CZ-NH1	-12.82	113.89	120.30
1	B	139	GLN	CG-CD-OE1	12.82	147.24	121.60
1	B	108	TRP	CA-C-N	12.82	145.40	117.20
1	B	217	PHE	CA-C-O	-12.82	93.18	120.10
1	B	44	ASP	CB-CG-OD1	-12.81	106.77	118.30
1	E	87	ILE	CG1-CB-CG2	12.80	139.56	111.40
1	D	101	THR	CA-CB-OG1	-12.79	82.13	109.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	GLY	O-C-N	-12.79	102.23	122.70
1	D	189	PRO	CA-N-CD	-12.79	93.59	111.50
1	E	160	CYS	CA-CB-SG	12.78	137.00	114.00
1	D	108	TRP	CZ3-CH2-CZ2	-12.77	106.27	121.60
1	F	125	ASN	CA-C-N	12.76	145.27	117.20
1	A	15	GLN	CG-CD-NE2	12.75	147.30	116.70
1	E	105	PRO	CA-N-CD	-12.75	93.66	111.50
1	E	7	LEU	CA-C-N	12.74	145.23	117.20
1	B	75	ASN	O-C-N	12.74	143.08	122.70
1	C	57	GLY	O-C-N	12.73	143.06	122.70
1	A	25	LEU	CB-CG-CD2	-12.72	89.38	111.00
1	A	190	ASN	O-C-N	-12.71	101.59	123.20
1	C	44	ASP	CB-CG-OD2	-12.71	106.87	118.30
1	F	94	LEU	CB-CG-CD2	12.71	132.60	111.00
1	C	166	ASP	CB-CG-OD1	-12.70	106.87	118.30
1	F	184	ARG	N-CA-CB	12.69	133.45	110.60
1	B	169	ASP	CB-CG-OD1	-12.69	106.88	118.30
1	B	194	ASP	CB-CG-OD1	-12.69	106.88	118.30
1	F	140	THR	CA-CB-CG2	12.69	130.16	112.40
1	B	190	ASN	CB-CG-ND2	12.68	147.12	116.70
1	C	103	TYR	CG-CD1-CE1	12.67	131.44	121.30
1	C	107	LEU	CB-CG-CD2	-12.67	89.46	111.00
1	D	184	ARG	NH1-CZ-NH2	12.66	133.33	119.40
1	E	5	PHE	CA-C-O	12.66	146.69	120.10
1	F	157	GLU	OE1-CD-OE2	-12.66	108.11	123.30
1	A	189	PRO	N-CA-CB	12.65	118.48	103.30
1	D	70	ILE	CA-CB-CG1	-12.64	86.97	111.00
1	F	230	GLY	O-C-N	-12.63	102.49	122.70
1	D	88	GLY	C-N-CA	12.63	153.27	121.70
1	A	138	PRO	N-CA-CB	12.63	118.45	103.30
1	D	172	TRP	CD1-CG-CD2	-12.61	96.21	106.30
1	A	182	GLY	O-C-N	12.57	142.82	122.70
1	B	211	SER	CA-C-O	-12.57	93.70	120.10
1	B	202	ALA	CA-C-N	12.56	144.84	117.20
1	E	33	GLN	OE1-CD-NE2	-12.56	93.02	121.90
1	F	100	VAL	CG1-CB-CG2	-12.56	90.81	110.90
1	C	232	LEU	CA-C-N	12.55	144.81	117.20
1	D	26	SER	C-N-CA	12.55	153.07	121.70
1	D	69	VAL	CA-CB-CG1	12.54	129.71	110.90
1	A	129	TYR	CA-C-N	12.54	144.78	117.20
1	A	171	VAL	CA-CB-CG2	12.53	129.69	110.90
1	F	214	ARG	CB-CA-C	12.53	135.45	110.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	48	TRP	O-C-N	12.52	142.73	122.70
1	D	232	LEU	O-C-N	12.51	142.72	122.70
1	B	214	ARG	NH1-CZ-NH2	-12.51	105.64	119.40
1	C	156	MET	O-C-N	12.51	142.71	122.70
1	C	25	LEU	CB-CA-C	-12.51	86.44	110.20
1	A	15	GLN	CA-CB-CG	12.50	140.90	113.40
1	B	93	VAL	O-C-N	12.50	142.70	122.70
1	E	167	ARG	NH1-CZ-NH2	-12.49	105.66	119.40
1	F	106	GLY	O-C-N	-12.48	102.73	122.70
1	E	103	TYR	N-CA-CB	-12.48	88.13	110.60
1	E	156	MET	CG-SD-CE	12.48	120.16	100.20
1	A	15	GLN	CG-CD-OE1	-12.47	96.66	121.60
1	A	146	SER	CA-CB-OG	-12.47	77.53	111.20
1	A	233	TRP	CZ3-CH2-CZ2	-12.47	106.64	121.60
1	D	60	ALA	CA-C-N	12.46	144.61	117.20
1	C	219	LEU	O-C-N	-12.45	102.78	122.70
1	D	188	GLN	OE1-CD-NE2	-12.45	93.26	121.90
1	A	206	SER	CA-C-N	12.43	141.07	116.20
1	B	31	THR	CA-CB-OG1	-12.43	82.89	109.00
1	A	233	TRP	CH2-CZ2-CE2	12.43	129.83	117.40
1	F	131	THR	CA-C-O	12.42	146.19	120.10
1	F	232	LEU	CA-C-O	-12.42	94.02	120.10
1	D	192	ARG	C-N-CA	12.42	152.74	121.70
1	B	70	ILE	CB-CA-C	-12.41	86.77	111.60
1	D	90	TYR	CB-CG-CD1	12.41	128.45	121.00
1	F	125	ASN	C-N-CA	12.41	152.72	121.70
1	A	44	ASP	CA-C-N	12.40	144.47	117.20
1	A	20	ALA	O-C-N	12.39	142.52	122.70
1	C	130	SER	O-C-N	-12.39	102.88	122.70
1	D	62	LEU	CA-C-N	-12.39	89.95	117.20
1	B	81	SER	N-CA-CB	-12.39	91.92	110.50
1	D	80	SER	O-C-N	-12.38	102.89	122.70
1	C	38	LEU	C-N-CA	12.38	152.64	121.70
1	B	33	GLN	CG-CD-NE2	12.37	146.39	116.70
1	C	32	MET	CG-SD-CE	-12.37	80.41	100.20
1	D	223	ARG	C-N-CA	12.37	152.62	121.70
1	E	19	ALA	CB-CA-C	12.36	128.64	110.10
1	F	30	PHE	C-N-CA	12.36	152.61	121.70
1	C	170	ARG	NE-CZ-NH2	12.35	126.47	120.30
1	F	90	TYR	CD1-CG-CD2	-12.34	104.33	117.90
1	F	143	ALA	N-CA-CB	12.34	127.37	110.10
1	B	71	LEU	N-CA-CB	-12.33	85.73	110.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42	ASP	CB-CG-OD2	12.33	129.40	118.30
1	E	157	GLU	CG-CD-OE2	-12.33	93.64	118.30
1	F	176	THR	CA-CB-CG2	-12.33	95.14	112.40
1	C	106	GLY	CA-C-O	12.32	142.78	120.60
1	E	61	VAL	CA-CB-CG2	-12.32	92.42	110.90
1	F	192	ARG	CB-CA-C	12.31	135.02	110.40
1	B	224	ASN	N-CA-CB	-12.31	88.44	110.60
1	C	158	THR	CA-CB-CG2	-12.30	95.18	112.40
1	A	42	ASP	O-C-N	-12.30	103.02	122.70
1	A	145	GLN	C-N-CA	12.30	152.45	121.70
1	B	65	ASP	OD1-CG-OD2	-12.30	99.93	123.30
1	C	143	ALA	CB-CA-C	12.29	128.54	110.10
1	D	125	ASN	O-C-N	-12.29	103.04	122.70
1	F	224	ASN	O-C-N	-12.29	103.04	122.70
1	A	40	LEU	CA-CB-CG	12.27	143.52	115.30
1	B	234	THR	C-N-CA	12.27	152.37	121.70
1	E	129	TYR	CZ-CE2-CD2	12.26	130.84	119.80
1	F	125	ASN	O-C-N	-12.26	103.08	122.70
1	D	176	THR	CA-C-N	12.25	144.16	117.20
1	B	214	ARG	N-CA-CB	-12.25	88.55	110.60
1	E	13	HIS	CA-C-O	-12.25	94.37	120.10
1	B	139	GLN	CB-CA-C	12.24	134.87	110.40
1	A	72	THR	CA-CB-CG2	12.23	129.52	112.40
1	D	136	ASN	CA-C-N	12.23	144.11	117.20
1	A	114	ASN	CB-CG-OD1	-12.23	97.14	121.60
1	D	46	ARG	NE-CZ-NH1	12.23	126.41	120.30
1	A	129	TYR	CD1-CG-CD2	-12.23	104.45	117.90
1	A	181	THR	N-CA-CB	12.23	133.53	110.30
1	D	104	GLY	C-N-CD	-12.21	93.74	120.60
1	D	129	TYR	CA-C-N	12.20	144.04	117.20
1	B	216	VAL	CA-CB-CG2	-12.19	92.62	110.90
1	C	137	HIS	CB-CA-C	-12.18	86.03	110.40
1	B	105	PRO	N-CD-CG	12.18	121.47	103.20
1	F	193	MET	CA-CB-CG	12.18	134.00	113.30
1	B	56	THR	CA-CB-OG1	12.18	134.57	109.00
1	D	131	THR	CA-C-O	12.17	145.66	120.10
1	B	194	ASP	CA-CB-CG	-12.17	86.63	113.40
1	D	71	LEU	O-C-N	12.16	142.16	122.70
1	A	2	ASN	CB-CG-OD1	12.16	145.92	121.60
1	B	125	ASN	CA-C-N	12.16	143.95	117.20
1	E	60	ALA	CA-C-O	-12.16	94.57	120.10
1	E	185	ALA	N-CA-CB	-12.15	93.08	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	223	ARG	CA-C-N	12.15	143.92	117.20
1	D	224	ASN	OD1-CG-ND2	12.14	149.82	121.90
1	F	125	ASN	CB-CG-OD1	-12.13	97.33	121.60
1	E	18	HIS	N-CA-CB	12.13	132.43	110.60
1	B	126	SER	O-C-N	-12.12	103.31	122.70
1	A	59	ARG	N-CA-CB	12.12	132.41	110.60
1	D	163	VAL	CA-CB-CG1	-12.11	92.73	110.90
1	D	60	ALA	N-CA-CB	12.10	127.04	110.10
1	D	72	THR	CA-CB-OG1	-12.10	83.59	109.00
1	B	27	SER	CA-CB-OG	-12.09	78.56	111.20
1	C	128	LEU	CD1-CG-CD2	-12.09	74.23	110.50
1	A	125	ASN	CB-CA-C	-12.08	86.25	110.40
1	C	232	LEU	CA-C-O	-12.07	94.76	120.10
1	C	100	VAL	CA-CB-CG1	12.06	128.99	110.90
1	D	32	MET	N-CA-CB	12.06	132.31	110.60
1	E	122	ASN	CA-CB-CG	12.06	139.93	113.40
1	A	2	ASN	OD1-CG-ND2	-12.05	94.19	121.90
1	E	40	LEU	CA-CB-CG	12.05	143.01	115.30
1	C	103	TYR	C-N-CA	12.04	147.59	122.30
1	D	146	SER	N-CA-C	12.03	143.48	111.00
1	F	29	ARG	NE-CZ-NH1	-12.03	114.28	120.30
1	F	192	ARG	N-CA-CB	-12.03	88.95	110.60
1	A	180	GLY	O-C-N	12.03	141.94	122.70
1	E	137	HIS	CB-CA-C	-12.02	86.36	110.40
1	F	138	PRO	CA-CB-CG	-12.01	81.17	104.00
1	E	183	CYS	CA-CB-SG	-12.01	92.38	114.00
1	E	168	ASP	CB-CG-OD2	12.01	129.10	118.30
1	D	225	LEU	CA-C-O	-12.00	94.90	120.10
1	A	128	LEU	CB-CA-C	11.99	132.98	110.20
1	B	45	VAL	CB-CA-C	11.99	134.18	111.40
1	E	138	PRO	N-CD-CG	11.98	121.17	103.20
1	A	169	ASP	CB-CG-OD1	-11.97	107.53	118.30
1	B	100	VAL	CB-CA-C	11.97	134.15	111.40
1	D	15	GLN	CA-CB-CG	11.97	139.74	113.40
1	B	29	ARG	CD-NE-CZ	11.96	140.35	123.60
1	D	61	VAL	CB-CA-C	-11.96	88.69	111.40
1	F	73	ALA	O-C-N	-11.95	103.58	122.70
1	F	219	LEU	CB-CG-CD1	11.95	131.31	111.00
1	A	190	ASN	C-N-CA	11.95	147.39	122.30
1	B	112	THR	C-N-CA	11.94	151.54	121.70
1	D	34	SER	CA-C-N	11.93	143.44	117.20
1	B	86	SER	O-C-N	-11.93	103.62	122.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	147	LEU	CB-CG-CD2	-11.93	90.72	111.00
1	F	183	CYS	C-N-CA	11.93	151.52	121.70
1	D	184	ARG	O-C-N	-11.92	103.62	122.70
1	D	57	GLY	CA-C-O	11.91	142.04	120.60
1	D	123	ASN	CA-CB-CG	11.90	139.59	113.40
1	D	210	ARG	CA-C-O	-11.90	95.11	120.10
1	E	129	TYR	CA-C-N	11.90	143.38	117.20
1	A	98	ARG	CG-CD-NE	11.89	136.77	111.80
1	F	83	THR	CB-CA-C	11.89	143.70	111.60
1	D	5	PHE	CZ-CE2-CD2	11.88	134.36	120.10
1	A	108	TRP	CA-C-O	-11.88	95.15	120.10
1	E	130	SER	CA-C-O	-11.88	95.16	120.10
1	E	230	GLY	CA-C-O	-11.88	99.22	120.60
1	F	16	THR	CA-CB-CG2	-11.88	95.78	112.40
1	D	156	MET	CA-CB-CG	11.87	133.48	113.30
1	A	137	HIS	C-N-CA	11.87	171.84	122.00
1	F	187	LEU	CA-C-N	-11.87	91.10	117.20
1	C	218	VAL	CA-CB-CG2	11.86	128.69	110.90
1	B	159	ASP	CB-CG-OD2	-11.86	107.63	118.30
1	B	222	ASP	CA-C-O	-11.86	95.20	120.10
1	C	165	PHE	CG-CD1-CE1	11.84	133.83	120.80
1	D	18	HIS	CA-C-O	-11.84	95.24	120.10
1	D	194	ASP	O-C-N	11.83	141.63	122.70
1	D	139	GLN	O-C-N	11.83	141.63	122.70
1	C	97	ASP	CB-CG-OD1	-11.83	107.66	118.30
1	A	181	THR	CA-CB-OG1	-11.83	84.17	109.00
1	F	217	PHE	N-CA-CB	-11.82	89.32	110.60
1	F	139	GLN	CB-CA-C	11.82	134.04	110.40
1	E	222	ASP	CB-CG-OD1	-11.81	107.67	118.30
1	F	84	LYS	CB-CG-CD	11.81	142.32	111.60
1	B	235	THR	CA-C-O	11.81	144.90	120.10
1	D	69	VAL	CG1-CB-CG2	-11.81	92.01	110.90
1	C	176	THR	O-C-N	-11.80	103.82	122.70
1	B	138	PRO	N-CA-CB	11.80	117.45	103.30
1	A	90	TYR	CA-CB-CG	-11.79	90.99	113.40
1	A	223	ARG	NE-CZ-NH1	-11.79	114.41	120.30
1	B	81	SER	CA-C-N	11.79	139.77	116.20
1	F	60	ALA	N-CA-CB	11.78	126.59	110.10
1	F	216	VAL	O-C-N	-11.78	103.86	122.70
1	A	9	HIS	CB-CA-C	-11.77	86.85	110.40
1	F	2	ASN	CB-CA-C	-11.77	86.86	110.40
1	A	190	ASN	N-CA-CB	-11.75	89.45	110.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	98	ARG	CD-NE-CZ	-11.75	107.16	123.60
1	A	228	TYR	CG-CD1-CE1	11.74	130.69	121.30
1	B	146	SER	N-CA-CB	-11.74	92.88	110.50
1	C	19	ALA	CA-C-N	11.74	143.04	117.20
1	B	106	GLY	CA-C-O	-11.74	99.47	120.60
1	A	171	VAL	N-CA-CB	11.74	137.32	111.50
1	B	109	ASP	N-CA-CB	11.74	131.73	110.60
1	D	169	ASP	CA-C-N	-11.73	91.39	117.20
1	B	223	ARG	NH1-CZ-NH2	11.73	132.30	119.40
1	D	229	GLY	O-C-N	-11.73	103.26	123.20
1	C	138	PRO	N-CA-CB	11.73	117.37	103.30
1	C	174	THR	C-N-CA	11.71	150.99	121.70
1	B	125	ASN	O-C-N	-11.71	103.96	122.70
1	F	29	ARG	NE-CZ-NH2	11.71	126.15	120.30
1	B	137	HIS	O-C-N	-11.70	98.87	121.10
1	C	162	LEU	CB-CG-CD2	11.70	130.89	111.00
1	D	158	THR	CA-C-O	-11.70	95.53	120.10
1	A	65	ASP	CB-CA-C	11.70	133.79	110.40
1	D	190	ASN	CA-C-N	11.69	139.58	116.20
1	B	195	VAL	CA-C-O	-11.69	95.56	120.10
1	E	193	MET	CA-CB-CG	11.69	133.17	113.30
1	A	129	TYR	CG-CD2-CE2	11.69	130.65	121.30
1	B	12	SER	CA-CB-OG	11.69	142.75	111.20
1	D	67	LEU	CB-CG-CD1	11.68	130.86	111.00
1	C	139	GLN	CB-CA-C	11.68	133.76	110.40
1	D	16	THR	C-N-CA	-11.67	92.53	121.70
1	D	7	LEU	N-CA-CB	11.66	133.72	110.40
1	D	7	LEU	CA-C-N	-11.65	91.57	117.20
1	C	198	ASN	CB-CG-OD1	-11.65	98.31	121.60
1	E	20	ALA	CA-C-O	11.64	144.54	120.10
1	E	125	ASN	CB-CA-C	-11.64	87.12	110.40
1	D	41	PHE	CB-CG-CD1	11.63	128.94	120.80
1	B	190	ASN	CA-C-N	11.62	139.45	116.20
1	D	73	ALA	N-CA-CB	11.62	126.38	110.10
1	A	202	ALA	N-CA-CB	-11.62	93.83	110.10
1	B	153	ARG	NE-CZ-NH2	11.62	126.11	120.30
1	F	9	HIS	CB-CA-C	-11.61	87.17	110.40
1	D	126	SER	O-C-N	11.61	141.27	122.70
1	B	23	LEU	N-CA-CB	11.61	133.61	110.40
1	B	101	THR	CA-CB-CG2	11.59	128.63	112.40
1	C	222	ASP	CA-C-N	11.59	142.69	117.20
1	C	5	PHE	CB-CG-CD2	-11.58	112.69	120.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	47	VAL	CA-CB-CG2	11.57	128.25	110.90
1	E	56	THR	CA-CB-CG2	-11.57	96.20	112.40
1	D	148	GLN	CB-CG-CD	11.57	141.68	111.60
1	E	154	LEU	N-CA-CB	11.56	133.52	110.40
1	D	141	LEU	CB-CG-CD2	-11.56	91.35	111.00
1	E	141	LEU	CB-CG-CD2	11.55	130.63	111.00
1	A	90	TYR	CG-CD1-CE1	11.55	130.54	121.30
1	F	50	SER	O-C-N	-11.53	104.25	122.70
1	F	209	SER	N-CA-CB	-11.53	93.21	110.50
1	C	60	ALA	CA-C-O	-11.52	95.90	120.10
1	E	85	GLY	C-N-CA	11.52	150.50	121.70
1	F	37	ASN	CB-CA-C	-11.52	87.36	110.40
1	A	26	SER	CA-C-N	11.52	142.54	117.20
1	D	151	PRO	O-C-N	-11.51	104.28	122.70
1	B	231	ALA	CB-CA-C	11.51	127.36	110.10
1	F	210	ARG	NE-CZ-NH2	-11.50	114.55	120.30
1	D	26	SER	CA-C-O	11.49	144.24	120.10
1	D	27	SER	O-C-N	-11.49	104.31	122.70
1	A	46	ARG	NE-CZ-NH2	-11.48	114.56	120.30
1	E	137	HIS	N-CA-C	11.48	142.01	111.00
1	B	45	VAL	CA-CB-CG1	11.47	128.10	110.90
1	B	187	LEU	CA-C-O	-11.46	96.02	120.10
1	C	172	TRP	CH2-CZ2-CE2	11.47	128.87	117.40
1	D	78	ARG	O-C-N	-11.46	104.36	122.70
1	D	144	THR	CA-CB-OG1	11.46	133.07	109.00
1	D	184	ARG	NE-CZ-NH1	11.46	126.03	120.30
1	A	75	ASN	CB-CG-OD1	-11.45	98.70	121.60
1	C	214	ARG	NH1-CZ-NH2	-11.45	106.80	119.40
1	E	131	THR	OG1-CB-CG2	11.45	136.34	110.00
1	D	149	LEU	C-N-CA	-11.45	93.08	121.70
1	E	167	ARG	CG-CD-NE	11.45	135.84	111.80
1	E	201	ILE	CB-CG1-CD1	11.45	145.96	113.90
1	C	2	ASN	CB-CG-OD1	-11.44	98.71	121.60
1	F	149	LEU	CA-C-O	-11.45	96.07	120.10
1	C	210	ARG	CA-C-O	11.44	144.12	120.10
1	A	120	VAL	CA-CB-CG1	11.44	128.05	110.90
1	B	125	ASN	CB-CG-ND2	11.43	144.14	116.70
1	F	31	THR	CA-CB-OG1	11.43	133.00	109.00
1	B	98	ARG	CA-CB-CG	11.42	138.52	113.40
1	E	144	THR	CA-CB-OG1	11.42	132.98	109.00
1	F	15	GLN	CA-CB-CG	11.42	138.52	113.40
1	E	157	GLU	CA-C-N	11.42	142.32	117.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	TYR	O-C-N	-11.41	103.80	123.20
1	F	152	TYR	CZ-CE2-CD2	-11.41	109.53	119.80
1	B	192	ARG	O-C-N	11.40	140.93	122.70
1	B	223	ARG	CD-NE-CZ	-11.40	107.64	123.60
1	E	103	TYR	CB-CG-CD1	11.40	127.84	121.00
1	D	43	SER	CB-CA-C	-11.39	88.45	110.10
1	B	149	LEU	CB-CG-CD2	11.39	130.37	111.00
1	B	228	TYR	CZ-CE2-CD2	-11.39	109.55	119.80
1	B	85	GLY	C-N-CA	11.39	150.17	121.70
1	B	165	PHE	N-CA-CB	-11.39	90.11	110.60
1	D	229	GLY	N-CA-C	11.38	141.56	113.10
1	B	216	VAL	O-C-N	-11.38	104.49	122.70
1	D	58	CYS	N-CA-CB	-11.38	90.11	110.60
1	F	67	LEU	CA-CB-CG	11.38	141.46	115.30
1	B	235	THR	CA-CB-OG1	11.37	132.88	109.00
1	A	87	ILE	O-C-N	-11.37	103.88	123.20
1	C	216	VAL	CA-CB-CG2	-11.36	93.86	110.90
1	D	83	THR	O-C-N	-11.36	104.53	122.70
1	F	83	THR	C-N-CA	11.36	150.09	121.70
1	A	61	VAL	CA-CB-CG1	11.35	127.92	110.90
1	B	223	ARG	CA-CB-CG	11.35	138.36	113.40
1	D	81	SER	O-C-N	-11.35	103.91	123.20
1	C	152	TYR	CD1-CG-CD2	-11.34	105.43	117.90
1	D	142	HIS	CA-C-N	11.33	142.13	117.20
1	B	15	GLN	CG-CD-OE1	-11.33	98.94	121.60
1	B	104	GLY	C-N-CA	11.33	169.57	122.00
1	A	44	ASP	N-CA-CB	11.32	130.98	110.60
1	C	148	GLN	CA-CB-CG	11.32	138.31	113.40
1	D	184	ARG	CD-NE-CZ	-11.32	107.75	123.60
1	C	136	ASN	CB-CA-C	-11.32	87.77	110.40
1	C	46	ARG	CA-C-N	11.31	142.08	117.20
1	D	217	PHE	CA-C-O	-11.31	96.35	120.10
1	E	60	ALA	CB-CA-C	11.31	127.06	110.10
1	E	58	CYS	N-CA-CB	-11.30	90.25	110.60
1	B	198	ASN	CA-CB-CG	-11.30	88.53	113.40
1	D	131	THR	CA-CB-CG2	-11.29	96.59	112.40
1	F	147	LEU	CB-CG-CD1	11.29	130.19	111.00
1	D	163	VAL	CG1-CB-CG2	11.29	128.96	110.90
1	C	89	ASN	OD1-CG-ND2	11.28	147.85	121.90
1	C	219	LEU	CA-CB-CG	11.28	141.25	115.30
1	D	55	ALA	N-CA-CB	11.28	125.89	110.10
1	D	64	SER	O-C-N	-11.28	104.65	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	TRP	CB-CG-CD1	-11.28	112.34	127.00
1	C	105	PRO	N-CA-CB	11.27	116.82	103.30
1	A	154	LEU	CB-CG-CD2	11.27	130.16	111.00
1	A	90	TYR	CB-CG-CD2	-11.27	114.24	121.00
1	E	99	THR	CA-CB-OG1	-11.27	85.34	109.00
1	A	191	GLY	C-N-CA	11.26	149.85	121.70
1	A	196	LEU	CB-CG-CD2	-11.26	91.85	111.00
1	A	159	ASP	O-C-N	-11.26	104.69	122.70
1	D	183	CYS	C-N-CA	11.25	149.82	121.70
1	E	62	LEU	O-C-N	11.24	140.69	122.70
1	E	232	LEU	N-CA-CB	-11.24	87.91	110.40
1	D	100	VAL	O-C-N	-11.24	104.71	122.70
1	E	169	ASP	N-CA-CB	11.24	130.83	110.60
1	E	225	LEU	CB-CA-C	11.24	131.56	110.20
1	A	193	MET	CG-SD-CE	-11.24	82.22	100.20
1	A	95	GLN	CG-CD-OE1	11.23	144.06	121.60
1	F	131	THR	CB-CA-C	-11.23	81.29	111.60
1	E	100	VAL	CA-CB-CG2	11.22	127.73	110.90
1	A	64	SER	CA-CB-OG	-11.22	80.91	111.20
1	A	30	PHE	C-N-CA	11.22	149.75	121.70
1	D	234	THR	C-N-CA	11.22	149.74	121.70
1	E	137	HIS	CA-C-O	-11.21	96.56	120.10
1	F	27	SER	CA-CB-OG	-11.21	80.93	111.20
1	B	44	ASP	CB-CG-OD2	11.21	128.39	118.30
1	E	123	ASN	N-CA-C	11.21	141.25	111.00
1	B	125	ASN	CB-CG-OD1	-11.20	99.20	121.60
1	B	224	ASN	O-C-N	-11.20	104.78	122.70
1	C	99	THR	O-C-N	-11.20	104.78	122.70
1	A	151	PRO	N-CD-CG	-11.20	86.41	103.20
1	E	1	ASN	CA-C-O	11.19	143.60	120.10
1	F	5	PHE	CB-CG-CD1	11.19	128.63	120.80
1	A	94	LEU	CB-CG-CD1	-11.19	91.98	111.00
1	E	103	TYR	CA-CB-CG	11.19	134.66	113.40
1	D	202	ALA	O-C-N	-11.19	104.80	122.70
1	B	232	LEU	O-C-N	-11.18	104.81	122.70
1	C	117	SER	O-C-N	-11.18	104.81	122.70
1	F	5	PHE	CD1-CG-CD2	-11.18	103.77	118.30
1	D	216	VAL	CA-CB-CG1	-11.17	94.14	110.90
1	F	187	LEU	O-C-N	11.17	140.58	122.70
1	B	168	ASP	CB-CA-C	11.17	132.74	110.40
1	B	109	ASP	O-C-N	11.17	140.57	122.70
1	D	59	ARG	CA-C-O	11.17	143.55	120.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	188	GLN	CG-CD-NE2	11.16	143.50	116.70
1	A	194	ASP	CA-CB-CG	11.15	137.93	113.40
1	A	214	ARG	N-CA-CB	-11.14	90.54	110.60
1	E	159	ASP	CB-CG-OD2	11.14	128.33	118.30
1	A	128	LEU	CD1-CG-CD2	-11.14	77.09	110.50
1	F	69	VAL	CG1-CB-CG2	-11.13	93.08	110.90
1	B	29	ARG	N-CA-CB	11.13	130.64	110.60
1	B	164	LEU	CB-CA-C	-11.13	89.05	110.20
1	C	108	TRP	CA-CB-CG	11.13	134.85	113.70
1	B	138	PRO	CA-N-CD	-11.12	95.93	111.50
1	F	214	ARG	CA-C-N	11.12	141.66	117.20
1	F	41	PHE	CB-CG-CD1	11.11	128.58	120.80
1	B	181	THR	CA-CB-CG2	11.11	127.95	112.40
1	D	158	THR	O-C-N	-11.10	104.93	122.70
1	F	199	GLN	O-C-N	-11.10	104.94	122.70
1	E	125	ASN	N-CA-C	11.10	140.97	111.00
1	E	129	TYR	CG-CD2-CE2	-11.10	112.42	121.30
1	C	197	THR	OG1-CB-CG2	-11.10	84.48	110.00
1	A	94	LEU	CB-CA-C	-11.09	89.13	110.20
1	E	24	GLU	O-C-N	-11.08	104.97	122.70
1	C	137	HIS	N-CA-C	11.08	140.91	111.00
1	F	46	ARG	CG-CD-NE	11.07	135.05	111.80
1	B	53	ALA	CB-CA-C	11.07	126.70	110.10
1	C	189	PRO	O-C-N	-11.07	104.99	122.70
1	C	142	HIS	CA-C-N	11.07	141.54	117.20
1	B	124	GLY	O-C-N	-11.06	105.01	122.70
1	A	137	HIS	N-CA-CB	-11.05	90.71	110.60
1	E	46	ARG	N-CA-CB	-11.05	90.72	110.60
1	C	98	ARG	O-C-N	-11.04	105.03	122.70
1	D	217	PHE	CD1-CE1-CZ	-11.04	106.85	120.10
1	E	130	SER	CA-C-N	11.04	141.49	117.20
1	A	196	LEU	O-C-N	11.04	140.36	122.70
1	E	122	ASN	C-N-CA	11.04	149.30	121.70
1	C	46	ARG	C-N-CA	11.04	149.29	121.70
1	E	34	SER	CA-CB-OG	11.04	141.00	111.20
1	B	149	LEU	CB-CG-CD1	-11.03	92.25	111.00
1	C	147	LEU	N-CA-CB	11.03	132.45	110.40
1	F	100	VAL	CA-C-N	11.02	141.45	117.20
1	B	69	VAL	CA-CB-CG2	11.02	127.43	110.90
1	B	235	THR	CA-CB-CG2	-11.02	96.97	112.40
1	C	73	ALA	N-CA-C	-11.02	81.26	111.00
1	A	194	ASP	CB-CG-OD1	11.01	128.21	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	54	GLY	CA-C-O	11.01	140.42	120.60
1	F	209	SER	CA-CB-OG	11.01	140.93	111.20
1	C	60	ALA	CB-CA-C	11.01	126.61	110.10
1	E	62	LEU	CA-C-N	-11.00	93.00	117.20
1	F	124	GLY	O-C-N	-11.00	105.10	122.70
1	B	33	GLN	OE1-CD-NE2	-11.00	96.60	121.90
1	F	5	PHE	CG-CD2-CE2	11.00	132.90	120.80
1	D	159	ASP	CB-CG-OD2	11.00	128.20	118.30
1	C	95	GLN	CG-CD-OE1	10.99	143.59	121.60
1	F	188	GLN	CA-CB-CG	10.99	137.59	113.40
1	B	90	TYR	CE1-CZ-OH	10.99	149.77	120.10
1	B	46	ARG	NH1-CZ-NH2	10.99	131.49	119.40
1	E	105	PRO	CA-CB-CG	-10.98	83.13	104.00
1	F	20	ALA	CB-CA-C	10.98	126.58	110.10
1	F	199	GLN	CA-C-O	10.98	143.16	120.10
1	D	167	ARG	O-C-N	-10.98	105.13	122.70
1	C	46	ARG	O-C-N	-10.98	105.14	122.70
1	B	8	SER	CA-CB-OG	10.97	140.82	111.20
1	C	38	LEU	CA-C-N	10.97	141.34	117.20
1	A	33	GLN	CA-C-O	10.97	143.13	120.10
1	D	6	GLY	CA-C-O	-10.96	100.86	120.60
1	F	24	GLU	N-CA-CB	-10.96	90.87	110.60
1	A	141	LEU	CB-CG-CD1	-10.96	92.37	111.00
1	D	146	SER	O-C-N	-10.95	105.17	122.70
1	C	5	PHE	CB-CG-CD1	10.95	128.46	120.80
1	A	56	THR	CA-C-N	-10.94	94.32	116.20
1	E	155	SER	N-CA-CB	-10.94	94.09	110.50
1	A	233	TRP	CE3-CZ3-CH2	10.93	133.23	121.20
1	B	61	VAL	CA-CB-CG2	-10.93	94.51	110.90
1	F	28	PHE	N-CA-CB	-10.92	90.94	110.60
1	D	210	ARG	NE-CZ-NH1	10.92	125.76	120.30
1	D	53	ALA	CB-CA-C	-10.92	93.73	110.10
1	B	189	PRO	CB-CA-C	-10.91	84.72	112.00
1	D	125	ASN	CB-CG-OD1	-10.89	99.81	121.60
1	C	39	VAL	O-C-N	-10.88	105.29	122.70
1	E	49	ALA	N-CA-CB	10.87	125.32	110.10
1	A	18	HIS	O-C-N	-10.87	105.30	122.70
1	B	110	SER	CA-C-O	-10.87	97.27	120.10
1	F	222	ASP	CB-CA-C	-10.87	88.66	110.40
1	D	162	LEU	O-C-N	-10.87	105.31	122.70
1	E	112	THR	CA-C-N	10.87	141.11	117.20
1	F	193	MET	CA-C-N	10.87	141.11	117.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	149	LEU	CB-CA-C	-10.86	89.56	110.20
1	D	19	ALA	C-N-CA	-10.86	94.54	121.70
1	D	200	ASN	N-CA-CB	-10.86	91.05	110.60
1	A	71	LEU	CA-C-N	-10.86	93.31	117.20
1	D	35	ASP	CB-CG-OD1	10.86	128.07	118.30
1	C	221	PRO	N-CA-CB	-10.86	90.27	103.30
1	D	107	LEU	N-CA-CB	10.85	132.10	110.40
1	A	30	PHE	CB-CG-CD1	-10.85	113.20	120.80
1	A	168	ASP	CB-CG-OD2	10.85	128.06	118.30
1	D	30	PHE	CD1-CE1-CZ	-10.85	107.08	120.10
1	F	192	ARG	NE-CZ-NH1	10.85	125.72	120.30
1	C	127	ILE	C-N-CA	10.84	148.81	121.70
1	A	8	SER	O-C-N	-10.84	105.36	122.70
1	A	191	GLY	CA-C-O	10.84	140.10	120.60
1	C	13	HIS	CA-C-N	10.83	147.43	117.10
1	B	169	ASP	CA-C-O	10.83	142.84	120.10
1	D	70	ILE	N-CA-CB	-10.83	85.89	110.80
1	D	143	ALA	CA-C-O	-10.83	97.36	120.10
1	D	36	CYS	N-CA-CB	10.83	130.09	110.60
1	E	63	GLN	N-CA-C	10.82	140.23	111.00
1	C	47	VAL	CB-CA-C	-10.81	90.86	111.40
1	D	214	ARG	CB-CA-C	10.81	132.02	110.40
1	A	41	PHE	CB-CA-C	-10.80	88.79	110.40
1	B	146	SER	O-C-N	-10.80	105.42	122.70
1	D	31	THR	CA-CB-OG1	-10.79	86.33	109.00
1	D	92	LEU	N-CA-CB	10.79	131.99	110.40
1	D	30	PHE	CB-CA-C	-10.78	88.84	110.40
1	F	153	ARG	CA-CB-CG	10.78	137.11	113.40
1	A	159	ASP	OD1-CG-OD2	-10.77	102.83	123.30
1	D	13	HIS	CA-C-N	10.77	147.26	117.10
1	E	141	LEU	C-N-CA	10.77	148.62	121.70
1	B	61	VAL	CA-C-O	10.77	142.71	120.10
1	C	12	SER	CB-CA-C	10.76	130.54	110.10
1	A	169	ASP	O-C-N	10.76	139.91	122.70
1	F	143	ALA	O-C-N	10.76	139.91	122.70
1	D	15	GLN	CB-CA-C	10.75	131.90	110.40
1	E	190	ASN	O-C-N	-10.75	104.92	123.20
1	A	90	TYR	O-C-N	-10.75	105.50	122.70
1	C	173	SER	CB-CA-C	-10.75	89.67	110.10
1	C	201	ILE	CA-CB-CG2	10.75	132.40	110.90
1	E	176	THR	CA-CB-CG2	-10.75	97.35	112.40
1	F	99	THR	O-C-N	10.75	139.89	122.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	79	TRP	CB-CG-CD2	10.74	140.56	126.60
1	C	16	THR	CA-C-O	-10.73	97.58	120.10
1	B	61	VAL	CA-CB-CG1	10.72	126.98	110.90
1	C	148	GLN	N-CA-CB	-10.72	91.30	110.60
1	B	165	PHE	CB-CG-CD2	10.72	128.30	120.80
1	C	154	LEU	CA-C-O	-10.71	97.61	120.10
1	B	83	THR	CA-CB-CG2	10.71	127.39	112.40
1	B	72	THR	C-N-CA	10.69	148.44	121.70
1	D	222	ASP	CA-CB-CG	10.69	136.92	113.40
1	E	131	THR	N-CA-C	10.69	139.86	111.00
1	A	139	GLN	N-CA-CB	-10.69	91.36	110.60
1	B	163	VAL	O-C-N	-10.69	105.60	122.70
1	D	22	SER	CB-CA-C	-10.68	89.80	110.10
1	C	125	ASN	N-CA-C	10.68	139.84	111.00
1	C	136	ASN	N-CA-C	10.68	139.83	111.00
1	D	89	ASN	N-CA-CB	-10.68	91.38	110.60
1	D	72	THR	N-CA-CB	-10.67	90.02	110.30
1	A	195	VAL	CA-CB-CG1	-10.67	94.89	110.90
1	B	197	THR	CA-CB-CG2	-10.67	97.46	112.40
1	C	196	LEU	CA-CB-CG	10.66	139.83	115.30
1	D	108	TRP	CE2-CD2-CE3	-10.66	105.91	118.70
1	D	192	ARG	O-C-N	-10.65	105.65	122.70
1	A	86	SER	N-CA-CB	-10.65	94.53	110.50
1	A	146	SER	N-CA-CB	-10.63	94.56	110.50
1	B	5	PHE	CB-CA-C	10.62	131.64	110.40
1	A	86	SER	CA-C-N	10.62	140.56	117.20
1	C	186	VAL	CB-CA-C	10.61	131.56	111.40
1	F	212	ALA	CB-CA-C	10.61	126.02	110.10
1	E	194	ASP	CB-CG-OD2	10.61	127.84	118.30
1	F	87	ILE	O-C-N	-10.61	105.17	123.20
1	F	188	GLN	CG-CD-OE1	10.60	142.80	121.60
1	C	90	TYR	O-C-N	10.60	139.65	122.70
1	C	9	HIS	O-C-N	10.59	139.64	122.70
1	D	1	ASN	O-C-N	-10.59	105.76	122.70
1	A	173	SER	CA-C-O	-10.58	97.88	120.10
1	C	45	VAL	CG1-CB-CG2	-10.58	93.98	110.90
1	E	232	LEU	N-CA-C	10.58	139.56	111.00
1	A	125	ASN	N-CA-C	10.57	139.55	111.00
1	D	98	ARG	CD-NE-CZ	-10.57	108.80	123.60
1	F	64	SER	CA-CB-OG	-10.57	82.65	111.20
1	B	76	THR	CA-CB-CG2	10.57	127.20	112.40
1	B	9	HIS	N-CA-CB	-10.57	91.57	110.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	SER	N-CA-CB	-10.57	94.65	110.50
1	A	153	ARG	NE-CZ-NH1	-10.56	115.02	120.30
1	B	142	HIS	N-CA-CB	-10.56	91.59	110.60
1	A	136	ASN	N-CA-C	-10.56	82.49	111.00
1	A	137	HIS	CB-CA-C	-10.56	89.29	110.40
1	D	219	LEU	CD1-CG-CD2	-10.54	78.87	110.50
1	E	128	LEU	CA-C-N	10.54	140.38	117.20
1	D	25	LEU	N-CA-CB	10.53	131.45	110.40
1	A	105	PRO	C-N-CA	-10.52	100.21	122.30
1	C	228	TYR	CG-CD2-CE2	10.52	129.72	121.30
1	D	152	TYR	CE1-CZ-OH	10.51	148.49	120.10
1	A	95	GLN	OE1-CD-NE2	-10.51	97.73	121.90
1	A	78	ARG	NE-CZ-NH1	-10.51	115.05	120.30
1	C	48	TRP	CB-CG-CD2	10.51	140.26	126.60
1	A	93	VAL	CA-C-O	-10.50	98.05	120.10
1	A	46	ARG	CD-NE-CZ	10.50	138.29	123.60
1	D	87	ILE	CA-C-O	-10.49	98.07	120.10
1	E	1	ASN	CB-CG-ND2	10.49	141.87	116.70
1	A	18	HIS	C-N-CA	10.49	147.92	121.70
1	A	131	THR	OG1-CB-CG2	-10.48	85.89	110.00
1	E	107	LEU	CA-C-O	-10.48	98.09	120.10
1	A	7	LEU	CA-C-O	-10.47	98.11	120.10
1	B	214	ARG	CB-CA-C	10.47	131.35	110.40
1	D	80	SER	CA-C-N	10.47	140.22	117.20
1	E	147	LEU	O-C-N	-10.46	105.96	122.70
1	F	60	ALA	CB-CA-C	10.46	125.79	110.10
1	B	103	TYR	CB-CG-CD2	10.46	127.28	121.00
1	E	20	ALA	O-C-N	-10.46	105.96	122.70
1	C	1	ASN	CA-CB-CG	10.46	136.41	113.40
1	A	40	LEU	O-C-N	10.46	139.43	122.70
1	C	4	LEU	CA-C-O	-10.46	98.14	120.10
1	B	4	LEU	CA-C-N	10.45	140.20	117.20
1	E	196	LEU	CB-CG-CD2	-10.45	93.23	111.00
1	D	101	THR	N-CA-CB	-10.45	90.45	110.30
1	A	86	SER	CA-C-O	-10.43	98.19	120.10
1	E	228	TYR	CB-CG-CD2	10.43	127.26	121.00
1	D	193	MET	O-C-N	-10.43	106.02	122.70
1	E	157	GLU	CA-C-O	-10.43	98.20	120.10
1	C	105	PRO	CA-CB-CG	-10.42	84.21	104.00
1	C	24	GLU	O-C-N	-10.41	106.04	122.70
1	C	146	SER	CA-C-O	-10.41	98.23	120.10
1	A	41	PHE	CD1-CE1-CZ	-10.40	107.62	120.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	GLY	N-CA-C	-10.40	87.09	113.10
1	B	193	MET	O-C-N	-10.40	106.06	122.70
1	D	21	GLN	N-CA-CB	-10.40	91.89	110.60
1	F	189	PRO	CA-C-O	-10.40	95.25	120.20
1	B	128	LEU	O-C-N	-10.38	106.09	122.70
1	D	27	SER	CA-C-O	10.38	141.89	120.10
1	D	105	PRO	CA-C-N	10.38	136.95	116.20
1	D	223	ARG	NE-CZ-NH2	10.38	125.49	120.30
1	D	149	LEU	N-CA-CB	10.37	131.14	110.40
1	D	188	GLN	N-CA-CB	-10.36	91.95	110.60
1	E	157	GLU	CB-CG-CD	-10.36	86.23	114.20
1	F	98	ARG	NH1-CZ-NH2	10.36	130.80	119.40
1	D	25	LEU	O-C-N	10.36	139.27	122.70
1	A	8	SER	CA-C-O	10.35	141.84	120.10
1	C	69	VAL	CA-CB-CG1	-10.35	95.38	110.90
1	A	198	ASN	CA-CB-CG	-10.34	90.65	113.40
1	D	92	LEU	CA-C-O	-10.33	98.41	120.10
1	D	160	CYS	CA-CB-SG	10.33	132.59	114.00
1	F	143	ALA	CA-C-O	-10.33	98.41	120.10
1	F	61	VAL	O-C-N	10.32	139.22	122.70
1	E	58	CYS	CA-C-O	10.32	141.77	120.10
1	D	45	VAL	N-CA-C	-10.31	83.15	111.00
1	E	149	LEU	CB-CG-CD2	10.31	128.54	111.00
1	E	114	ASN	CA-CB-CG	-10.31	90.71	113.40
1	B	137	HIS	CB-CG-ND1	10.31	148.97	123.20
1	A	149	LEU	C-N-CA	-10.31	95.94	121.70
1	A	48	TRP	CE3-CZ3-CH2	-10.30	109.86	121.20
1	B	105	PRO	CB-CA-C	-10.30	86.24	112.00
1	B	71	LEU	CA-CB-CG	10.30	138.99	115.30
1	A	150	SER	N-CA-CB	10.30	125.95	110.50
1	C	9	HIS	CA-CB-CG	10.30	131.11	113.60
1	D	18	HIS	CA-C-N	10.30	139.86	117.20
1	E	2	ASN	CB-CG-ND2	10.30	141.42	116.70
1	E	189	PRO	CA-CB-CG	-10.30	84.43	104.00
1	B	31	THR	OG1-CB-CG2	10.29	133.66	110.00
1	B	30	PHE	O-C-N	-10.28	106.25	122.70
1	E	33	GLN	CA-C-O	10.28	141.69	120.10
1	C	227	ILE	CA-CB-CG2	-10.28	90.34	110.90
1	D	142	HIS	N-CA-C	10.28	138.75	111.00
1	C	48	TRP	CB-CG-CD1	-10.27	113.65	127.00
1	C	221	PRO	CA-C-N	10.27	139.79	117.20
1	D	204	TRP	CB-CG-CD2	10.27	139.95	126.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	SER	O-C-N	10.26	140.60	121.10
1	B	150	SER	CA-C-O	-10.26	98.55	120.10
1	F	30	PHE	CB-CG-CD2	-10.26	113.62	120.80
1	E	38	LEU	CA-C-N	10.25	139.74	117.20
1	D	219	LEU	CA-CB-CG	10.24	138.86	115.30
1	C	205	THR	OG1-CB-CG2	10.24	133.55	110.00
1	A	107	LEU	CA-C-O	-10.23	98.61	120.10
1	C	90	TYR	CB-CG-CD2	10.23	127.14	121.00
1	F	226	ALA	CB-CA-C	10.23	125.44	110.10
1	A	176	THR	N-CA-CB	-10.23	90.87	110.30
1	C	171	VAL	CA-C-O	-10.23	98.62	120.10
1	C	184	ARG	NE-CZ-NH2	-10.21	115.19	120.30
1	B	42	ASP	CA-C-N	10.21	139.66	117.20
1	F	20	ALA	O-C-N	-10.20	106.38	122.70
1	C	145	GLN	CB-CA-C	10.20	130.79	110.40
1	E	131	THR	CB-CA-C	-10.20	84.07	111.60
1	D	223	ARG	NE-CZ-NH1	-10.19	115.20	120.30
1	A	72	THR	CA-CB-OG1	-10.19	87.61	109.00
1	F	9	HIS	O-C-N	-10.18	106.42	122.70
1	F	63	GLN	CG-CD-NE2	10.18	141.12	116.70
1	A	90	TYR	CB-CA-C	-10.17	90.05	110.40
1	E	11	GLY	O-C-N	-10.17	106.42	122.70
1	F	17	LEU	O-C-N	10.17	138.97	122.70
1	C	169	ASP	CA-CB-CG	10.16	135.76	113.40
1	D	194	ASP	CB-CA-C	-10.16	90.08	110.40
1	E	211	SER	CA-C-N	10.16	139.56	117.20
1	A	103	TYR	CB-CG-CD2	-10.15	114.91	121.00
1	E	52	THR	CA-CB-CG2	10.15	126.61	112.40
1	F	2	ASN	N-CA-C	10.15	138.40	111.00
1	A	36	CYS	CA-CB-SG	-10.15	95.73	114.00
1	D	165	PHE	CB-CG-CD2	10.15	127.90	120.80
1	E	233	TRP	CD1-NE1-CE2	-10.15	99.87	109.00
1	D	231	ALA	CB-CA-C	-10.14	94.89	110.10
1	A	200	ASN	CB-CG-OD1	10.14	141.88	121.60
1	E	51	ASN	N-CA-CB	10.14	128.85	110.60
1	B	174	THR	CA-CB-CG2	-10.14	98.21	112.40
1	C	216	VAL	CA-CB-CG1	10.14	126.11	110.90
1	E	62	LEU	CB-CA-C	-10.14	90.94	110.20
1	B	152	TYR	CB-CA-C	-10.14	90.12	110.40
1	D	195	VAL	CG1-CB-CG2	10.13	127.11	110.90
1	E	26	SER	O-C-N	-10.13	106.49	122.70
1	B	82	GLY	O-C-N	-10.13	106.49	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	VAL	O-C-N	10.11	138.88	122.70
1	D	105	PRO	N-CD-CG	10.11	118.37	103.20
1	A	90	TYR	C-N-CA	10.11	146.96	121.70
1	D	8	SER	CA-CB-OG	10.10	138.47	111.20
1	D	224	ASN	CB-CG-OD1	-10.10	101.40	121.60
1	E	38	LEU	O-C-N	-10.09	106.55	122.70
1	C	205	THR	CA-CB-CG2	-10.09	98.28	112.40
1	F	31	THR	N-CA-CB	-10.09	91.13	110.30
1	D	233	TRP	CG-CD1-NE1	10.09	120.19	110.10
1	A	208	ASN	CA-CB-CG	10.08	135.58	113.40
1	B	13	HIS	O-C-N	-10.08	101.95	121.10
1	B	71	LEU	CA-C-N	10.07	139.36	117.20
1	C	56	THR	CA-C-N	-10.07	96.05	116.20
1	E	169	ASP	CB-CG-OD2	-10.07	109.23	118.30
1	A	110	SER	O-C-N	-10.07	106.08	123.20
1	D	9	HIS	CA-CB-CG	10.07	130.72	113.60
1	D	13	HIS	O-C-N	-10.06	101.99	121.10
1	E	61	VAL	N-CA-C	10.06	138.16	111.00
1	E	22	SER	CA-CB-OG	-10.05	84.07	111.20
1	D	99	THR	O-C-N	10.04	138.77	122.70
1	A	128	LEU	CA-CB-CG	10.04	138.40	115.30
1	B	13	HIS	N-CA-C	10.04	138.12	111.00
1	C	25	LEU	N-CA-CB	10.04	130.48	110.40
1	A	49	ALA	CB-CA-C	10.04	125.16	110.10
1	A	90	TYR	CA-C-N	10.04	139.28	117.20
1	B	159	ASP	C-N-CA	10.04	146.79	121.70
1	C	98	ARG	NE-CZ-NH2	10.04	125.32	120.30
1	A	15	GLN	N-CA-C	-10.03	83.92	111.00
1	D	148	GLN	CA-CB-CG	10.02	135.45	113.40
1	A	81	SER	O-C-N	-10.02	106.16	123.20
1	D	64	SER	CA-C-O	10.02	141.15	120.10
1	E	156	MET	C-N-CA	-10.02	96.65	121.70
1	B	101	THR	O-C-N	10.02	138.73	122.70
1	E	167	ARG	O-C-N	-10.01	106.68	122.70
1	F	14	PRO	CA-N-CD	-10.01	97.49	111.50
1	A	217	PHE	CA-C-O	-10.01	99.08	120.10
1	A	44	ASP	CA-C-O	-10.01	99.09	120.10
1	C	112	THR	O-C-N	-10.01	106.69	122.70
1	A	105	PRO	N-CD-CG	9.99	118.19	103.20
1	B	25	LEU	N-CA-CB	9.99	130.39	110.40
1	F	230	GLY	N-CA-C	-9.99	88.12	113.10
1	F	84	LYS	C-N-CA	9.99	143.28	122.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	ARG	CD-NE-CZ	9.98	137.58	123.60
1	C	145	GLN	CB-CG-CD	9.98	137.56	111.60
1	A	104	GLY	C-N-CA	9.98	163.91	122.00
1	D	153	ARG	N-CA-CB	-9.97	92.64	110.60
1	F	1	ASN	OD1-CG-ND2	9.97	144.84	121.90
1	F	86	SER	N-CA-CB	9.97	125.46	110.50
1	D	142	HIS	O-C-N	-9.97	106.75	122.70
1	B	150	SER	CA-C-N	9.96	144.99	117.10
1	A	109	ASP	CB-CG-OD1	9.96	127.26	118.30
1	A	19	ALA	O-C-N	-9.96	106.77	122.70
1	A	61	VAL	N-CA-C	9.96	137.88	111.00
1	B	214	ARG	O-C-N	-9.95	106.78	122.70
1	F	46	ARG	NH1-CZ-NH2	-9.94	108.46	119.40
1	A	146	SER	CB-CA-C	-9.94	91.21	110.10
1	A	77	ILE	O-C-N	-9.94	106.80	122.70
1	E	100	VAL	CA-CB-CG1	-9.93	96.00	110.90
1	E	72	THR	C-N-CA	9.93	146.52	121.70
1	B	24	GLU	OE1-CD-OE2	9.92	135.21	123.30
1	B	42	ASP	CA-C-O	-9.92	99.28	120.10
1	F	110	SER	CA-C-O	-9.91	99.28	120.10
1	A	198	ASN	CB-CG-ND2	9.91	140.49	116.70
1	E	93	VAL	CA-CB-CG1	9.91	125.77	110.90
1	D	109	ASP	OD1-CG-OD2	9.91	142.13	123.30
1	A	178	GLY	O-C-N	-9.91	106.85	122.70
1	E	139	GLN	O-C-N	9.91	138.55	122.70
1	A	218	VAL	O-C-N	9.90	138.54	122.70
1	D	154	LEU	N-CA-CB	9.90	130.20	110.40
1	E	158	THR	CA-C-N	9.90	138.98	117.20
1	B	5	PHE	N-CA-CB	-9.90	92.78	110.60
1	C	27	SER	O-C-N	-9.90	106.87	122.70
1	C	89	ASN	CB-CA-C	-9.89	90.61	110.40
1	D	225	LEU	CA-C-N	9.88	138.95	117.20
1	E	43	SER	C-N-CA	9.88	146.41	121.70
1	F	55	ALA	N-CA-CB	-9.88	96.26	110.10
1	D	27	SER	CA-CB-OG	-9.88	84.52	111.20
1	A	48	TRP	CZ3-CH2-CZ2	9.88	133.46	121.60
1	A	141	LEU	CA-CB-CG	9.88	138.03	115.30
1	D	94	LEU	CB-CG-CD2	9.88	127.80	111.00
1	F	105	PRO	CA-N-CD	-9.88	97.67	111.50
1	B	105	PRO	C-N-CA	9.88	143.04	122.30
1	C	143	ALA	N-CA-CB	-9.88	96.27	110.10
1	D	172	TRP	CG-CD1-NE1	9.88	119.98	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	235	THR	CA-CB-OG1	9.88	129.74	109.00
1	C	67	LEU	CA-CB-CG	9.87	138.00	115.30
1	E	123	ASN	CB-CA-C	-9.87	90.66	110.40
1	D	30	PHE	CG-CD1-CE1	9.87	131.65	120.80
1	E	139	GLN	CA-C-O	-9.86	99.39	120.10
1	E	43	SER	CB-CA-C	9.86	128.83	110.10
1	A	108	TRP	CG-CD2-CE3	-9.85	125.03	133.90
1	F	160	CYS	CB-CA-C	9.85	130.10	110.40
1	B	103	TYR	CD1-CE1-CZ	-9.85	110.94	119.80
1	E	233	TRP	CG-CD1-NE1	9.85	119.95	110.10
1	E	99	THR	N-CA-C	9.84	137.58	111.00
1	F	209	SER	CB-CA-C	9.84	128.80	110.10
1	A	94	LEU	O-C-N	-9.84	106.96	122.70
1	F	73	ALA	CA-C-O	9.84	140.75	120.10
1	A	158	THR	CA-CB-CG2	-9.83	98.63	112.40
1	A	215	TYR	O-C-N	-9.83	106.97	122.70
1	B	136	ASN	CA-C-N	9.83	138.82	117.20
1	D	8	SER	C-N-CA	9.82	146.24	121.70
1	B	148	GLN	OE1-CD-NE2	9.81	144.46	121.90
1	E	38	LEU	CB-CG-CD2	-9.81	94.33	111.00
1	A	123	ASN	CA-CB-CG	9.81	134.97	113.40
1	F	8	SER	CA-C-N	-9.81	95.62	117.20
1	A	139	GLN	CB-CA-C	9.80	130.01	110.40
1	B	149	LEU	CB-CA-C	-9.80	91.58	110.20
1	D	5	PHE	CE1-CZ-CE2	-9.80	102.36	120.00
1	E	228	TYR	O-C-N	-9.80	106.54	123.20
1	D	76	THR	CA-C-N	9.79	138.75	117.20
1	A	148	GLN	O-C-N	-9.79	107.04	122.70
1	B	5	PHE	CG-CD1-CE1	9.79	131.57	120.80
1	C	93	VAL	CA-C-O	-9.79	99.54	120.10
1	F	139	GLN	CG-CD-OE1	9.79	141.17	121.60
1	F	3	ILE	O-C-N	9.78	138.35	122.70
1	D	128	LEU	N-CA-CB	9.78	129.96	110.40
1	E	71	LEU	CB-CG-CD1	9.78	127.62	111.00
1	C	40	LEU	C-N-CA	9.78	146.14	121.70
1	B	65	ASP	N-CA-CB	-9.77	93.01	110.60
1	D	99	THR	OG1-CB-CG2	-9.77	87.52	110.00
1	B	129	TYR	CB-CA-C	-9.76	90.88	110.40
1	C	99	THR	CA-CB-OG1	-9.76	88.50	109.00
1	D	101	THR	N-CA-C	9.76	137.35	111.00
1	F	97	ASP	CB-CG-OD2	9.76	127.08	118.30
1	E	8	SER	CA-C-N	-9.75	95.75	117.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	ASP	CA-C-N	9.75	138.64	117.20
1	A	122	ASN	CA-CB-CG	9.74	134.84	113.40
1	B	222	ASP	CB-CG-OD1	9.74	127.07	118.30
1	C	228	TYR	CA-C-O	9.74	140.56	120.10
1	F	138	PRO	CA-N-CD	-9.74	97.86	111.50
1	E	102	ILE	C-N-CA	-9.74	97.35	121.70
1	A	60	ALA	CA-C-O	-9.74	99.65	120.10
1	A	92	LEU	CB-CA-C	-9.74	91.70	110.20
1	F	153	ARG	NE-CZ-NH2	9.73	125.17	120.30
1	A	223	ARG	CD-NE-CZ	-9.73	109.98	123.60
1	A	222	ASP	N-CA-C	-9.72	84.74	111.00
1	A	49	ALA	CA-C-O	-9.72	99.68	120.10
1	C	15	GLN	CG-CD-OE1	9.72	141.03	121.60
1	A	153	ARG	NH1-CZ-NH2	-9.71	108.71	119.40
1	F	52	THR	O-C-N	-9.71	107.17	122.70
1	A	48	TRP	CD1-NE1-CE2	-9.71	100.27	109.00
1	B	193	MET	N-CA-CB	9.71	128.07	110.60
1	F	129	TYR	O-C-N	-9.71	107.17	122.70
1	B	220	GLN	CA-CB-CG	9.70	134.74	113.40
1	E	151	PRO	N-CA-CB	-9.70	91.66	103.30
1	F	63	GLN	CG-CD-OE1	-9.69	102.21	121.60
1	C	221	PRO	O-C-N	-9.69	107.19	122.70
1	B	167	ARG	NE-CZ-NH2	9.69	125.14	120.30
1	B	216	VAL	CG1-CB-CG2	-9.69	95.40	110.90
1	F	137	HIS	O-C-N	9.69	139.51	121.10
1	A	100	VAL	CA-C-O	-9.68	99.76	120.10
1	F	12	SER	O-C-N	-9.68	107.21	122.70
1	B	200	ASN	C-N-CA	9.68	145.90	121.70
1	D	39	VAL	CG1-CB-CG2	-9.68	95.41	110.90
1	E	181	THR	C-N-CA	-9.68	101.97	122.30
1	D	79	TRP	CD1-NE1-CE2	9.68	117.71	109.00
1	D	158	THR	OG1-CB-CG2	9.68	132.25	110.00
1	F	124	GLY	CA-C-O	9.68	138.02	120.60
1	C	145	GLN	CA-CB-CG	9.67	134.68	113.40
1	D	130	SER	CA-CB-OG	9.67	137.31	111.20
1	A	137	HIS	CA-C-O	-9.67	99.80	120.10
1	E	34	SER	CA-C-O	-9.66	99.81	120.10
1	C	178	GLY	C-N-CA	9.66	145.85	121.70
1	D	226	ALA	N-CA-CB	9.66	123.62	110.10
1	F	43	SER	C-N-CA	9.66	145.85	121.70
1	F	164	LEU	CA-C-N	9.65	138.44	117.20
1	C	157	GLU	C-N-CA	9.65	145.83	121.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ILE	CA-CB-CG1	-9.64	92.68	111.00
1	C	124	GLY	O-C-N	-9.64	107.28	122.70
1	D	226	ALA	N-CA-C	-9.64	84.98	111.00
1	D	25	LEU	C-N-CA	-9.63	97.62	121.70
1	D	73	ALA	O-C-N	-9.63	107.28	122.70
1	F	31	THR	CA-CB-CG2	-9.63	98.91	112.40
1	D	78	ARG	CB-CG-CD	-9.63	86.57	111.60
1	D	154	LEU	CB-CG-CD2	-9.62	94.64	111.00
1	A	121	ALA	CB-CA-C	9.62	124.53	110.10
1	B	191	GLY	CA-C-O	-9.62	103.29	120.60
1	C	43	SER	CB-CA-C	9.62	128.38	110.10
1	D	164	LEU	CB-CG-CD1	9.62	127.35	111.00
1	F	167	ARG	CD-NE-CZ	9.62	137.06	123.60
1	B	10	GLU	CA-CB-CG	9.62	134.56	113.40
1	D	86	SER	CA-CB-OG	9.62	137.16	111.20
1	A	70	ILE	C-N-CA	9.61	145.73	121.70
1	F	103	TYR	CA-C-O	9.61	140.28	120.10
1	B	75	ASN	CA-CB-CG	-9.61	92.26	113.40
1	C	3	ILE	O-C-N	9.61	138.07	122.70
1	D	94	LEU	CB-CG-CD1	-9.61	94.67	111.00
1	D	130	SER	CB-CA-C	9.60	128.34	110.10
1	A	200	ASN	CB-CA-C	9.60	129.60	110.40
1	D	218	VAL	CA-CB-CG2	9.60	125.30	110.90
1	A	2	ASN	CB-CA-C	9.60	129.59	110.40
1	B	190	ASN	CA-C-O	-9.60	99.95	120.10
1	D	64	SER	CA-CB-OG	-9.60	85.29	111.20
1	E	65	ASP	CB-CG-OD1	9.59	126.93	118.30
1	F	110	SER	CA-CB-OG	-9.59	85.30	111.20
1	A	3	ILE	N-CA-CB	-9.59	88.75	110.80
1	B	169	ASP	OD1-CG-OD2	9.59	141.52	123.30
1	B	79	TRP	CD1-CG-CD2	-9.58	98.63	106.30
1	C	64	SER	N-CA-CB	-9.58	96.13	110.50
1	F	77	ILE	N-CA-CB	-9.58	88.76	110.80
1	C	146	SER	N-CA-CB	-9.58	96.13	110.50
1	D	52	THR	CA-CB-CG2	9.58	125.81	112.40
1	E	161	ASN	CB-CG-OD1	-9.58	102.45	121.60
1	E	167	ARG	CA-C-N	9.57	138.26	117.20
1	A	19	ALA	CA-C-O	-9.57	100.01	120.10
1	B	68	LEU	CB-CA-C	9.56	128.37	110.20
1	B	214	ARG	CG-CD-NE	9.55	131.86	111.80
1	B	225	LEU	N-CA-CB	9.55	129.51	110.40
1	E	137	HIS	CB-CG-ND1	9.55	147.09	123.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	44	ASP	CA-C-N	9.55	138.22	117.20
1	C	99	THR	N-CA-CB	-9.55	92.16	110.30
1	D	217	PHE	CA-C-N	9.55	138.21	117.20
1	F	180	GLY	CA-C-O	-9.54	103.43	120.60
1	A	20	ALA	CA-C-N	-9.54	96.22	117.20
1	D	230	GLY	CA-C-N	9.54	138.18	117.20
1	B	129	TYR	CB-CG-CD1	9.52	126.71	121.00
1	B	106	GLY	CA-C-N	9.52	138.14	117.20
1	C	77	ILE	CG1-CB-CG2	-9.52	90.46	111.40
1	C	118	VAL	O-C-N	-9.51	107.49	122.70
1	C	41	PHE	CB-CA-C	-9.51	91.39	110.40
1	F	72	THR	CA-CB-OG1	-9.51	89.04	109.00
1	A	188	GLN	CG-CD-OE1	-9.50	102.59	121.60
1	F	59	ARG	NH1-CZ-NH2	-9.50	108.95	119.40
1	C	165	PHE	CB-CG-CD1	9.48	127.44	120.80
1	A	158	THR	CA-C-O	-9.48	100.19	120.10
1	C	196	LEU	CB-CG-CD2	9.48	127.11	111.00
1	E	71	LEU	CA-C-O	9.48	140.00	120.10
1	A	222	ASP	N-CA-CB	9.47	127.65	110.60
1	C	195	VAL	CG1-CB-CG2	-9.47	95.75	110.90
1	E	5	PHE	C-N-CA	-9.47	102.42	122.30
1	F	53	ALA	N-CA-CB	-9.47	96.85	110.10
1	A	224	ASN	C-N-CA	-9.46	98.04	121.70
1	C	145	GLN	O-C-N	-9.46	107.56	122.70
1	A	104	GLY	C-N-CD	-9.46	99.79	120.60
1	F	105	PRO	N-CD-CG	9.46	117.39	103.20
1	A	209	SER	CA-CB-OG	-9.46	85.67	111.20
1	A	179	LYS	O-C-N	9.45	139.26	123.20
1	B	49	ALA	CB-CA-C	-9.45	95.93	110.10
1	B	152	TYR	CE1-CZ-OH	-9.45	94.59	120.10
1	B	56	THR	N-CA-C	9.45	136.50	111.00
1	B	142	HIS	CA-C-N	9.45	137.98	117.20
1	D	164	LEU	CA-C-O	-9.45	100.26	120.10
1	D	63	GLN	CA-CB-CG	-9.44	92.63	113.40
1	C	74	GLN	CG-CD-NE2	-9.44	94.05	116.70
1	A	215	TYR	CG-CD2-CE2	9.43	128.85	121.30
1	E	8	SER	N-CA-CB	9.43	124.64	110.50
1	A	136	ASN	CB-CA-C	9.42	129.25	110.40
1	E	139	GLN	OE1-CD-NE2	9.41	143.55	121.90
1	F	180	GLY	CA-C-N	9.41	137.91	117.20
1	F	12	SER	CA-C-O	9.39	139.82	120.10
1	A	139	GLN	O-C-N	9.39	137.72	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	LEU	CA-CB-CG	9.38	136.88	115.30
1	B	94	LEU	CB-CG-CD2	-9.39	95.04	111.00
1	B	108	TRP	CB-CA-C	9.39	129.17	110.40
1	B	10	GLU	C-N-CA	-9.38	102.59	122.30
1	D	156	MET	CB-CA-C	-9.38	91.63	110.40
1	D	217	PHE	CG-CD2-CE2	9.38	131.12	120.80
1	B	84	LYS	CB-CA-C	-9.37	91.66	110.40
1	D	59	ARG	O-C-N	-9.37	107.71	122.70
1	F	174	THR	CA-CB-CG2	-9.37	99.29	112.40
1	A	157	GLU	N-CA-CB	-9.37	93.74	110.60
1	A	179	LYS	CA-C-O	-9.37	100.43	120.10
1	C	228	TYR	CB-CG-CD2	-9.37	115.38	121.00
1	E	14	PRO	CA-N-CD	-9.36	98.39	111.50
1	A	204	TRP	CE2-CD2-CG	9.36	114.79	107.30
1	F	65	ASP	C-N-CA	9.36	141.95	122.30
1	A	63	GLN	CB-CA-C	-9.36	91.69	110.40
1	B	70	ILE	CA-C-O	9.35	139.74	120.10
1	F	47	VAL	CA-C-O	-9.35	100.46	120.10
1	F	55	ALA	CA-C-N	9.35	137.77	117.20
1	A	204	TRP	CB-CG-CD2	9.34	138.75	126.60
1	D	165	PHE	CB-CG-CD1	-9.34	114.26	120.80
1	D	181	THR	N-CA-C	-9.34	85.78	111.00
1	E	159	ASP	C-N-CA	9.34	145.05	121.70
1	D	190	ASN	O-C-N	-9.34	107.33	123.20
1	C	222	ASP	CA-C-O	-9.33	100.50	120.10
1	B	30	PHE	CA-CB-CG	-9.33	91.51	113.90
1	F	160	CYS	CA-C-O	9.33	139.69	120.10
1	C	125	ASN	N-CA-CB	-9.32	93.82	110.60
1	E	124	GLY	N-CA-C	9.32	136.41	113.10
1	F	138	PRO	C-N-CA	-9.32	98.39	121.70
1	F	192	ARG	O-C-N	-9.32	107.78	122.70
1	D	100	VAL	CA-CB-CG2	9.31	124.87	110.90
1	F	16	THR	OG1-CB-CG2	9.31	131.42	110.00
1	F	34	SER	CA-CB-OG	-9.31	86.05	111.20
1	A	226	ALA	O-C-N	9.31	137.59	122.70
1	A	104	GLY	O-C-N	9.30	138.77	121.10
1	D	71	LEU	N-CA-CB	-9.30	91.80	110.40
1	A	26	SER	N-CA-CB	-9.30	96.55	110.50
1	A	208	ASN	CA-C-O	-9.30	100.57	120.10
1	D	202	ALA	N-CA-CB	-9.30	97.08	110.10
1	A	41	PHE	CG-CD2-CE2	-9.29	110.58	120.80
1	F	92	LEU	CA-C-O	-9.29	100.58	120.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	102	ILE	CG1-CB-CG2	-9.29	90.96	111.40
1	F	165	PHE	CA-CB-CG	9.29	136.20	113.90
1	A	41	PHE	CB-CG-CD2	-9.29	114.30	120.80
1	A	195	VAL	CG1-CB-CG2	9.29	125.76	110.90
1	C	65	ASP	CA-C-N	9.29	134.78	116.20
1	F	84	LYS	CA-CB-CG	9.29	133.83	113.40
1	F	152	TYR	N-CA-C	9.29	136.08	111.00
1	B	24	GLU	CA-C-O	-9.29	100.60	120.10
1	F	199	GLN	C-N-CA	9.29	144.91	121.70
1	C	89	ASN	O-C-N	9.28	137.55	122.70
1	C	200	ASN	CB-CG-ND2	9.28	138.97	116.70
1	D	232	LEU	CB-CG-CD1	-9.28	95.23	111.00
1	B	68	LEU	C-N-CA	-9.27	98.52	121.70
1	A	210	ARG	NE-CZ-NH2	-9.27	115.67	120.30
1	D	35	ASP	C-N-CA	9.27	144.88	121.70
1	C	29	ARG	CB-CG-CD	9.27	135.69	111.60
1	A	184	ARG	CA-C-O	9.27	139.56	120.10
1	C	213	GLY	CA-C-O	-9.27	103.92	120.60
1	F	78	ARG	CA-C-O	9.27	139.56	120.10
1	A	184	ARG	CB-CG-CD	9.26	135.68	111.60
1	A	218	VAL	CA-CB-CG1	-9.26	97.01	110.90
1	A	196	LEU	CD1-CG-CD2	9.26	138.28	110.50
1	D	56	THR	O-C-N	-9.26	107.46	123.20
1	C	158	THR	OG1-CB-CG2	-9.26	88.71	110.00
1	D	16	THR	CA-C-O	-9.25	100.67	120.10
1	E	127	ILE	CG1-CB-CG2	9.25	131.76	111.40
1	D	37	ASN	CA-CB-CG	-9.25	93.06	113.40
1	F	146	SER	CA-C-N	9.24	137.54	117.20
1	B	33	GLN	CA-CB-CG	9.24	133.73	113.40
1	D	129	TYR	CA-CB-CG	9.24	130.96	113.40
1	C	211	SER	CA-C-N	9.24	137.53	117.20
1	D	5	PHE	N-CA-CB	-9.24	93.97	110.60
1	A	48	TRP	CB-CG-CD2	9.24	138.61	126.60
1	C	153	ARG	CA-CB-CG	-9.24	93.08	113.40
1	C	205	THR	O-C-N	-9.24	107.92	122.70
1	C	227	ILE	N-CA-CB	9.24	132.05	110.80
1	F	144	THR	CA-CB-CG2	9.24	125.33	112.40
1	A	204	TRP	CD1-CG-CD2	-9.23	98.91	106.30
1	D	158	THR	CA-CB-CG2	-9.23	99.48	112.40
1	D	129	TYR	CE1-CZ-CE2	9.23	134.57	119.80
1	A	48	TRP	CD1-CG-CD2	-9.23	98.92	106.30
1	F	143	ALA	CB-CA-C	-9.23	96.26	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	TRP	CD1-CG-CD2	-9.22	98.92	106.30
1	D	235	THR	CA-CB-OG1	9.22	128.37	109.00
1	D	47	VAL	CG1-CB-CG2	-9.22	96.15	110.90
1	A	18	HIS	CA-C-N	-9.21	96.93	117.20
1	A	118	VAL	N-CA-CB	-9.21	91.23	111.50
1	E	147	LEU	N-CA-C	9.21	135.88	111.00
1	E	99	THR	O-C-N	-9.21	107.96	122.70
1	F	152	TYR	CB-CA-C	-9.21	91.98	110.40
1	B	211	SER	O-C-N	9.21	137.43	122.70
1	C	186	VAL	CA-CB-CG2	-9.20	97.10	110.90
1	C	192	ARG	NH1-CZ-NH2	9.20	129.52	119.40
1	D	26	SER	O-C-N	-9.20	107.98	122.70
1	F	176	THR	CA-C-O	9.20	139.42	120.10
1	C	50	SER	N-CA-CB	-9.20	96.71	110.50
1	D	24	GLU	CA-C-N	9.20	137.43	117.20
1	B	30	PHE	CB-CG-CD1	9.19	127.23	120.80
1	D	129	TYR	CA-C-O	-9.19	100.81	120.10
1	E	21	GLN	N-CA-CB	-9.19	94.06	110.60
1	A	87	ILE	CB-CA-C	9.19	129.97	111.60
1	F	128	LEU	N-CA-C	-9.18	86.21	111.00
1	C	29	ARG	N-CA-CB	-9.18	94.08	110.60
1	F	5	PHE	CB-CG-CD2	9.18	127.22	120.80
1	D	38	LEU	CB-CG-CD2	-9.18	95.40	111.00
1	D	229	GLY	CA-C-N	9.17	134.54	116.20
1	E	206	SER	O-C-N	-9.17	107.61	123.20
1	C	223	ARG	NE-CZ-NH2	-9.17	115.72	120.30
1	D	86	SER	N-CA-CB	9.17	124.25	110.50
1	F	22	SER	CA-C-O	9.17	139.35	120.10
1	B	53	ALA	CA-C-N	9.16	134.53	116.20
1	D	54	GLY	C-N-CA	9.16	144.60	121.70
1	F	86	SER	CA-C-N	9.16	137.35	117.20
1	D	9	HIS	CB-CA-C	-9.16	92.08	110.40
1	C	43	SER	O-C-N	-9.15	108.05	122.70
1	C	156	MET	CG-SD-CE	9.15	114.85	100.20
1	C	87	ILE	C-N-CA	-9.15	103.08	122.30
1	C	114	ASN	N-CA-CB	-9.14	94.14	110.60
1	F	84	LYS	CB-CA-C	-9.14	92.11	110.40
1	D	5	PHE	CB-CG-CD1	9.14	127.20	120.80
1	C	41	PHE	CD1-CE1-CZ	-9.14	109.14	120.10
1	A	183	CYS	CB-CA-C	9.13	128.67	110.40
1	B	194	ASP	CB-CA-C	-9.13	92.13	110.40
1	C	65	ASP	CB-CG-OD1	-9.14	110.08	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	43	SER	CA-CB-OG	-9.14	86.53	111.20
1	F	192	ARG	C-N-CA	9.13	144.54	121.70
1	C	37	ASN	C-N-CA	9.13	144.53	121.70
1	A	118	VAL	O-C-N	-9.12	108.10	122.70
1	A	157	GLU	CA-C-O	-9.12	100.94	120.10
1	C	150	SER	CA-CB-OG	-9.12	86.56	111.20
1	B	24	GLU	CA-C-N	9.12	137.27	117.20
1	A	154	LEU	C-N-CA	-9.12	98.90	121.70
1	A	213	GLY	N-CA-C	-9.12	90.31	113.10
1	B	212	ALA	CB-CA-C	9.12	123.78	110.10
1	C	160	CYS	N-CA-CB	9.12	127.01	110.60
1	C	164	LEU	CB-CA-C	-9.11	92.89	110.20
1	F	1	ASN	O-C-N	-9.11	108.12	122.70
1	A	92	LEU	C-N-CA	9.11	144.47	121.70
1	E	69	VAL	O-C-N	9.11	137.27	122.70
1	D	136	ASN	N-CA-CB	9.10	126.98	110.60
1	B	130	SER	CB-CA-C	9.10	127.39	110.10
1	D	12	SER	CA-CB-OG	9.09	135.74	111.20
1	C	71	LEU	CB-CG-CD1	9.09	126.45	111.00
1	F	13	HIS	CA-CB-CG	-9.09	98.15	113.60
1	D	58	CYS	CA-CB-SG	-9.09	97.64	114.00
1	B	152	TYR	OH-CZ-CE2	9.08	144.62	120.10
1	C	101	THR	N-CA-CB	-9.08	93.04	110.30
1	C	128	LEU	CB-CG-CD1	9.08	126.44	111.00
1	D	217	PHE	CZ-CE2-CD2	-9.08	109.20	120.10
1	A	227	ILE	C-N-CA	9.08	144.40	121.70
1	B	14	PRO	C-N-CA	-9.08	99.00	121.70
1	D	210	ARG	NH1-CZ-NH2	-9.08	109.41	119.40
1	F	168	ASP	CB-CG-OD1	9.08	126.47	118.30
1	F	217	PHE	CA-C-N	9.08	137.17	117.20
1	A	113	SER	C-N-CA	9.07	144.38	121.70
1	E	214	ARG	NE-CZ-NH2	9.07	124.84	120.30
1	F	192	ARG	NE-CZ-NH2	9.07	124.84	120.30
1	F	61	VAL	N-CA-CB	9.07	131.45	111.50
1	A	5	PHE	CA-C-O	-9.07	101.06	120.10
1	D	125	ASN	N-CA-C	9.07	135.48	111.00
1	D	196	LEU	CA-C-O	9.07	139.14	120.10
1	E	210	ARG	CA-C-O	9.06	139.14	120.10
1	A	39	VAL	CA-CB-CG1	9.06	124.49	110.90
1	B	91	VAL	CA-CB-CG2	-9.06	97.31	110.90
1	B	104	GLY	CA-C-N	-9.06	91.73	117.10
1	F	201	ILE	CA-C-O	-9.06	101.07	120.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	17	LEU	CA-CB-CG	9.06	136.13	115.30
1	F	104	GLY	CA-C-N	-9.06	91.74	117.10
1	F	192	ARG	NH1-CZ-NH2	-9.06	109.44	119.40
1	E	235	THR	CA-CB-CG2	-9.05	99.72	112.40
1	B	217	PHE	CD1-CE1-CZ	-9.05	109.24	120.10
1	C	46	ARG	NH1-CZ-NH2	-9.05	109.44	119.40
1	C	125	ASN	CB-CA-C	-9.05	92.30	110.40
1	B	46	ARG	CD-NE-CZ	9.05	136.27	123.60
1	C	182	GLY	CA-C-O	-9.05	104.31	120.60
1	D	105	PRO	C-N-CA	9.05	141.30	122.30
1	C	83	THR	N-CA-CB	9.05	127.49	110.30
1	C	94	LEU	CA-C-O	-9.05	101.10	120.10
1	B	159	ASP	OD1-CG-OD2	9.04	140.48	123.30
1	F	6	GLY	O-C-N	-9.04	108.23	122.70
1	A	217	PHE	CB-CG-CD2	9.04	127.13	120.80
1	C	10	GLU	N-CA-CB	-9.03	94.34	110.60
1	B	6	GLY	CA-C-N	9.03	137.06	117.20
1	C	67	LEU	CB-CA-C	9.03	127.35	110.20
1	F	20	ALA	CA-C-O	9.02	139.05	120.10
1	A	228	TYR	CG-CD2-CE2	9.02	128.52	121.30
1	F	167	ARG	NE-CZ-NH1	-9.02	115.79	120.30
1	B	24	GLU	CA-CB-CG	9.02	133.24	113.40
1	B	79	TRP	CA-C-O	-9.02	101.16	120.10
1	C	183	CYS	N-CA-CB	-9.02	94.37	110.60
1	B	138	PRO	C-N-CA	-9.01	99.17	121.70
1	C	93	VAL	CA-C-N	9.01	137.03	117.20
1	B	25	LEU	C-N-CA	9.01	144.22	121.70
1	F	29	ARG	CA-C-O	9.01	139.02	120.10
1	D	108	TRP	CH2-CZ2-CE2	9.01	126.41	117.40
1	D	186	VAL	C-N-CA	-9.00	99.19	121.70
1	F	223	ARG	CG-CD-NE	9.00	130.70	111.80
1	C	166	ASP	OD1-CG-OD2	9.00	140.40	123.30
1	E	211	SER	CA-CB-OG	9.00	135.50	111.20
1	B	101	THR	N-CA-C	9.00	135.29	111.00
1	C	206	SER	CA-C-O	9.00	138.99	120.10
1	B	19	ALA	N-CA-CB	-8.99	97.51	110.10
1	E	139	GLN	CG-CD-OE1	-8.99	103.62	121.60
1	C	102	ILE	CA-CB-CG2	8.99	128.88	110.90
1	D	192	ARG	CB-CA-C	8.99	128.37	110.40
1	C	41	PHE	CZ-CE2-CD2	-8.98	109.32	120.10
1	D	190	ASN	N-CA-CB	-8.98	94.43	110.60
1	F	136	ASN	CA-C-N	8.98	136.96	117.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	176	THR	OG1-CB-CG2	-8.98	89.35	110.00
1	D	1	ASN	CA-CB-CG	8.98	133.15	113.40
1	E	165	PHE	CB-CG-CD1	8.98	127.08	120.80
1	A	83	THR	OG1-CB-CG2	8.97	130.64	110.00
1	C	198	ASN	CB-CG-ND2	8.97	138.23	116.70
1	F	151	PRO	C-N-CA	8.97	144.13	121.70
1	C	146	SER	CB-CA-C	-8.97	93.06	110.10
1	C	228	TYR	N-CA-CB	8.97	126.75	110.60
1	B	195	VAL	CA-C-N	8.97	136.93	117.20
1	E	218	VAL	CA-C-O	-8.97	101.27	120.10
1	C	225	LEU	CB-CG-CD2	-8.96	95.76	111.00
1	E	230	GLY	O-C-N	8.96	137.04	122.70
1	B	209	SER	CB-CA-C	-8.96	93.08	110.10
1	B	192	ARG	NH1-CZ-NH2	-8.96	109.55	119.40
1	C	194	ASP	CA-CB-CG	8.95	133.10	113.40
1	D	70	ILE	CB-CG1-CD1	-8.96	88.83	113.90
1	F	187	LEU	N-CA-CB	8.96	128.31	110.40
1	E	48	TRP	CD1-NE1-CE2	8.95	117.06	109.00
1	F	146	SER	N-CA-C	8.95	135.16	111.00
1	A	129	TYR	CE1-CZ-CE2	-8.95	105.49	119.80
1	B	90	TYR	OH-CZ-CE2	-8.95	95.94	120.10
1	B	228	TYR	CB-CG-CD2	-8.95	115.63	121.00
1	E	199	GLN	CB-CA-C	-8.95	92.51	110.40
1	B	28	PHE	CA-CB-CG	8.94	135.36	113.90
1	C	90	TYR	CG-CD1-CE1	8.94	128.45	121.30
1	A	199	GLN	CA-CB-CG	8.94	133.06	113.40
1	E	126	SER	CA-CB-OG	8.94	135.34	111.20
1	C	97	ASP	OD1-CG-OD2	-8.94	106.32	123.30
1	F	39	VAL	CA-CB-CG1	8.94	124.31	110.90
1	A	219	LEU	N-CA-C	-8.93	86.88	111.00
1	F	42	ASP	CB-CG-OD2	8.93	126.34	118.30
1	A	68	LEU	CA-C-N	8.93	136.84	117.20
1	C	182	GLY	CA-C-N	8.92	136.83	117.20
1	C	130	SER	CA-C-N	-8.92	97.58	117.20
1	F	19	ALA	N-CA-CB	8.92	122.59	110.10
1	C	165	PHE	CD1-CG-CD2	-8.92	106.71	118.30
1	E	210	ARG	CD-NE-CZ	-8.92	111.11	123.60
1	B	78	ARG	NE-CZ-NH1	-8.92	115.84	120.30
1	E	192	ARG	CB-CA-C	8.91	128.23	110.40
1	C	10	GLU	CA-C-N	8.91	134.02	116.20
1	A	233	TRP	O-C-N	-8.91	108.45	122.70
1	E	29	ARG	NH1-CZ-NH2	-8.91	109.60	119.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	151	PRO	C-N-CA	8.91	143.97	121.70
1	A	214	ARG	NE-CZ-NH2	8.90	124.75	120.30
1	E	138	PRO	CA-C-N	-8.90	97.61	117.20
1	B	222	ASP	O-C-N	-8.90	108.46	122.70
1	D	39	VAL	CB-CA-C	-8.90	94.49	111.40
1	C	129	TYR	O-C-N	-8.89	108.47	122.70
1	A	29	ARG	NE-CZ-NH2	8.89	124.75	120.30
1	E	3	ILE	CG1-CB-CG2	-8.89	91.84	111.40
1	A	36	CYS	N-CA-CB	8.89	126.60	110.60
1	B	79	TRP	CD1-NE1-CE2	-8.89	101.00	109.00
1	A	48	TRP	CA-C-O	-8.88	101.44	120.10
1	F	95	GLN	CG-CD-NE2	8.88	138.03	116.70
1	E	184	ARG	NH1-CZ-NH2	8.88	129.17	119.40
1	C	49	ALA	CA-C-N	8.88	136.73	117.20
1	A	12	SER	N-CA-C	-8.88	87.03	111.00
1	B	55	ALA	N-CA-CB	-8.87	97.68	110.10
1	E	64	SER	N-CA-CB	8.86	123.79	110.50
1	F	37	ASN	CA-CB-CG	8.86	132.89	113.40
1	C	214	ARG	N-CA-CB	-8.86	94.66	110.60
1	E	28	PHE	CB-CG-CD2	8.86	127.00	120.80
1	A	150	SER	CA-C-O	-8.85	101.52	120.10
1	C	52	THR	CA-CB-CG2	8.85	124.79	112.40
1	A	174	THR	CA-C-O	8.85	138.68	120.10
1	B	22	SER	CA-CB-OG	-8.85	87.31	111.20
1	C	128	LEU	CA-C-O	8.84	138.67	120.10
1	F	35	ASP	N-CA-CB	8.84	126.52	110.60
1	D	177	ALA	O-C-N	8.84	138.23	123.20
1	F	76	THR	CA-CB-CG2	8.84	124.78	112.40
1	A	137	HIS	CB-CG-CD2	-8.84	103.40	130.80
1	E	26	SER	CA-CB-OG	8.84	135.06	111.20
1	D	57	GLY	O-C-N	-8.84	108.56	122.70
1	D	175	ASN	CA-CB-CG	8.84	132.84	113.40
1	F	139	GLN	N-CA-CB	-8.84	94.70	110.60
1	C	224	ASN	OD1-CG-ND2	8.83	142.22	121.90
1	E	29	ARG	CG-CD-NE	8.83	130.34	111.80
1	D	42	ASP	OD1-CG-OD2	8.82	140.06	123.30
1	A	222	ASP	CA-C-O	-8.82	101.58	120.10
1	D	198	ASN	OD1-CG-ND2	8.82	142.18	121.90
1	C	40	LEU	CA-CB-CG	8.81	135.56	115.30
1	D	99	THR	N-CA-C	-8.80	87.24	111.00
1	B	86	SER	CA-CB-OG	8.80	134.96	111.20
1	C	133	GLY	CA-C-O	8.80	136.44	120.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	VAL	CG1-CB-CG2	8.80	124.98	110.90
1	C	168	ASP	CA-C-N	8.79	136.54	117.20
1	C	19	ALA	CA-C-O	-8.79	101.65	120.10
1	C	103	TYR	CA-C-N	8.79	133.78	116.20
1	D	31	THR	N-CA-CB	8.79	126.99	110.30
1	F	153	ARG	CD-NE-CZ	8.78	135.90	123.60
1	B	69	VAL	CA-CB-CG1	8.78	124.07	110.90
1	C	176	THR	N-CA-CB	-8.78	93.61	110.30
1	F	185	ALA	CB-CA-C	8.78	123.27	110.10
1	C	205	THR	N-CA-CB	-8.78	93.62	110.30
1	C	10	GLU	CB-CA-C	8.77	127.94	110.40
1	A	77	ILE	CG1-CB-CG2	-8.77	92.11	111.40
1	A	145	GLN	CG-CD-OE1	-8.77	104.06	121.60
1	A	215	TYR	CA-CB-CG	-8.77	96.74	113.40
1	D	143	ALA	CA-C-N	8.77	136.49	117.20
1	D	163	VAL	CA-CB-CG2	-8.77	97.75	110.90
1	F	64	SER	O-C-N	-8.76	108.69	122.70
1	F	50	SER	N-CA-CB	-8.76	97.37	110.50
1	C	233	TRP	CD1-CG-CD2	-8.75	99.30	106.30
1	E	148	GLN	N-CA-CB	-8.75	94.84	110.60
1	D	125	ASN	N-CA-CB	-8.75	94.85	110.60
1	C	228	TYR	CD1-CE1-CZ	8.75	127.67	119.80
1	E	33	GLN	CB-CG-CD	8.75	134.35	111.60
1	F	87	ILE	N-CA-C	8.74	134.60	111.00
1	D	221	PRO	CB-CA-C	8.74	133.85	112.00
1	B	203	VAL	CB-CA-C	8.74	128.00	111.40
1	C	19	ALA	CB-CA-C	8.74	123.21	110.10
1	A	108	TRP	CE3-CZ3-CH2	8.73	130.81	121.20
1	C	165	PHE	N-CA-CB	-8.73	94.88	110.60
1	E	173	SER	CA-CB-OG	-8.73	87.62	111.20
1	D	214	ARG	O-C-N	-8.73	108.73	122.70
1	D	188	GLN	CA-CB-CG	8.73	132.60	113.40
1	F	202	ALA	O-C-N	-8.73	108.74	122.70
1	A	34	SER	CB-CA-C	8.72	126.67	110.10
1	A	32	MET	N-CA-CB	8.71	126.28	110.60
1	B	22	SER	N-CA-C	8.71	134.53	111.00
1	F	30	PHE	N-CA-CB	-8.71	94.92	110.60
1	C	16	THR	CB-CA-C	-8.71	88.08	111.60
1	E	98	ARG	CG-CD-NE	-8.71	93.50	111.80
1	A	160	CYS	CA-C-O	-8.71	101.82	120.10
1	A	3	ILE	CA-CB-CG2	-8.70	93.49	110.90
1	B	13	HIS	CA-CB-CG	-8.70	98.81	113.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	TYR	CB-CG-CD1	8.70	126.22	121.00
1	D	30	PHE	CB-CG-CD2	-8.70	114.71	120.80
1	D	157	GLU	CG-CD-OE2	-8.70	100.90	118.30
1	E	142	HIS	N-CA-C	8.70	134.48	111.00
1	D	95	GLN	OE1-CD-NE2	-8.69	101.90	121.90
1	E	125	ASN	C-N-CA	8.70	143.44	121.70
1	B	205	THR	CA-CB-OG1	-8.68	90.77	109.00
1	C	137	HIS	CA-C-O	-8.68	101.87	120.10
1	D	64	SER	CA-C-N	-8.68	98.09	117.20
1	F	98	ARG	CB-CA-C	8.68	127.77	110.40
1	D	232	LEU	CA-CB-CG	8.68	135.26	115.30
1	A	228	TYR	CD1-CG-CD2	-8.68	108.35	117.90
1	A	62	LEU	CB-CG-CD1	-8.68	96.25	111.00
1	A	82	GLY	CA-C-N	-8.68	98.11	117.20
1	C	69	VAL	CG1-CB-CG2	-8.68	97.02	110.90
1	D	69	VAL	O-C-N	-8.68	108.82	122.70
1	B	112	THR	O-C-N	-8.67	108.82	122.70
1	F	8	SER	O-C-N	8.67	136.57	122.70
1	A	160	CYS	N-CA-CB	8.67	126.20	110.60
1	E	228	TYR	CB-CG-CD1	-8.67	115.80	121.00
1	C	24	GLU	CA-C-N	8.66	136.26	117.20
1	B	88	GLY	C-N-CA	8.66	143.35	121.70
1	C	158	THR	N-CA-CB	8.66	126.75	110.30
1	E	150	SER	CA-CB-OG	-8.66	87.82	111.20
1	F	146	SER	CA-C-O	-8.66	101.91	120.10
1	C	200	ASN	CB-CG-OD1	-8.66	104.28	121.60
1	F	127	ILE	N-CA-CB	8.65	130.70	110.80
1	B	110	SER	CA-CB-OG	-8.65	87.84	111.20
1	B	229	GLY	CA-C-O	8.65	136.17	120.60
1	F	28	PHE	CB-CA-C	8.65	127.69	110.40
1	D	184	ARG	C-N-CA	8.64	143.31	121.70
1	E	129	TYR	O-C-N	-8.64	108.87	122.70
1	C	107	LEU	O-C-N	8.64	136.53	122.70
1	E	61	VAL	CA-C-O	8.64	138.24	120.10
1	F	225	LEU	CB-CA-C	-8.64	93.79	110.20
1	F	157	GLU	CG-CD-OE1	8.64	135.57	118.30
1	D	210	ARG	NE-CZ-NH2	8.63	124.62	120.30
1	F	141	LEU	CA-C-N	8.63	136.18	117.20
1	D	223	ARG	CD-NE-CZ	-8.62	111.53	123.60
1	D	230	GLY	O-C-N	-8.62	108.90	122.70
1	A	143	ALA	N-CA-C	-8.62	87.73	111.00
1	F	166	ASP	CA-CB-CG	8.62	132.36	113.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	GLY	O-C-N	8.61	137.46	121.10
1	B	169	ASP	CB-CG-OD2	-8.61	110.55	118.30
1	B	83	THR	OG1-CB-CG2	-8.61	90.20	110.00
1	C	139	GLN	CG-CD-NE2	8.61	137.36	116.70
1	A	65	ASP	CB-CG-OD1	-8.61	110.56	118.30
1	B	55	ALA	N-CA-C	8.61	134.24	111.00
1	C	207	GLY	CA-C-N	8.60	136.13	117.20
1	D	10	GLU	C-N-CA	-8.60	104.24	122.30
1	D	208	ASN	CB-CG-ND2	-8.60	96.06	116.70
1	E	168	ASP	OD1-CG-OD2	-8.59	106.97	123.30
1	F	150	SER	CB-CA-C	8.59	126.42	110.10
1	E	87	ILE	N-CA-C	8.59	134.19	111.00
1	F	87	ILE	CG1-CB-CG2	8.59	130.29	111.40
1	A	174	THR	CA-C-N	-8.58	98.32	117.20
1	B	61	VAL	CA-C-N	-8.58	98.32	117.20
1	C	127	ILE	CG1-CB-CG2	-8.58	92.52	111.40
1	E	56	THR	N-CA-CB	8.58	126.61	110.30
1	F	70	ILE	CA-C-O	8.58	138.12	120.10
1	D	46	ARG	N-CA-CB	-8.58	95.16	110.60
1	F	18	HIS	CA-C-O	-8.58	102.08	120.10
1	A	157	GLU	OE1-CD-OE2	-8.57	113.01	123.30
1	C	30	PHE	CB-CA-C	8.57	127.55	110.40
1	B	1	ASN	N-CA-C	-8.57	87.86	111.00
1	B	191	GLY	C-N-CA	-8.57	100.28	121.70
1	B	203	VAL	CG1-CB-CG2	-8.57	97.19	110.90
1	A	46	ARG	CB-CG-CD	8.57	133.87	111.60
1	C	174	THR	CA-CB-OG1	-8.57	91.01	109.00
1	E	129	TYR	CD1-CG-CD2	-8.56	108.48	117.90
1	C	10	GLU	OE1-CD-OE2	-8.56	113.03	123.30
1	B	70	ILE	CA-CB-CG2	8.56	128.02	110.90
1	F	68	LEU	N-CA-CB	8.56	127.52	110.40
1	F	217	PHE	CA-C-O	-8.56	102.13	120.10
1	E	162	LEU	CB-CA-C	8.56	126.46	110.20
1	F	69	VAL	CA-CB-CG1	8.55	123.73	110.90
1	F	129	TYR	CA-C-N	8.55	136.01	117.20
1	B	83	THR	N-CA-CB	-8.55	94.06	110.30
1	E	89	ASN	CB-CG-ND2	8.55	137.22	116.70
1	C	80	SER	N-CA-CB	8.55	123.32	110.50
1	E	142	HIS	N-CA-CB	-8.54	95.23	110.60
1	C	234	THR	CA-C-N	8.54	135.98	117.20
1	E	7	LEU	O-C-N	-8.54	109.04	122.70
1	F	230	GLY	CA-C-N	8.54	135.98	117.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	235	THR	CA-C-O	8.54	138.03	120.10
1	A	1	ASN	CB-CG-OD1	-8.53	104.53	121.60
1	A	63	GLN	N-CA-C	8.53	134.03	111.00
1	A	166	ASP	CA-C-O	-8.53	102.19	120.10
1	F	152	TYR	CA-C-O	-8.53	102.19	120.10
1	C	36	CYS	CB-CA-C	-8.52	93.36	110.40
1	D	45	VAL	C-N-CA	8.52	143.00	121.70
1	A	214	ARG	CA-C-O	8.52	137.98	120.10
1	B	225	LEU	CB-CG-CD1	-8.52	96.52	111.00
1	B	79	TRP	O-C-N	8.51	136.32	122.70
1	A	128	LEU	O-C-N	-8.51	109.08	122.70
1	E	154	LEU	CB-CA-C	-8.51	94.03	110.20
1	F	234	THR	CA-CB-OG1	8.51	126.87	109.00
1	A	78	ARG	CG-CD-NE	8.50	129.66	111.80
1	F	3	ILE	CB-CA-C	-8.50	94.60	111.60
1	A	216	VAL	CA-CB-CG2	8.50	123.65	110.90
1	A	42	ASP	CA-C-N	8.49	135.89	117.20
1	E	38	LEU	C-N-CA	8.49	142.93	121.70
1	A	138	PRO	CA-CB-CG	-8.49	87.87	104.00
1	A	107	LEU	CA-C-N	8.49	135.87	117.20
1	A	152	TYR	CG-CD2-CE2	8.48	128.09	121.30
1	B	28	PHE	N-CA-CB	-8.48	95.33	110.60
1	B	48	TRP	CB-CA-C	-8.48	93.44	110.40
1	A	87	ILE	CA-CB-CG2	-8.48	93.94	110.90
1	A	128	LEU	C-N-CA	8.48	142.90	121.70
1	D	28	PHE	N-CA-CB	-8.47	95.35	110.60
1	E	208	ASN	O-C-N	8.47	136.26	122.70
1	A	235	THR	N-CA-CB	-8.47	94.20	110.30
1	D	69	VAL	CA-C-N	8.47	135.84	117.20
1	D	179	LYS	CA-C-N	8.47	133.14	116.20
1	C	41	PHE	CE1-CZ-CE2	8.47	135.24	120.00
1	D	3	ILE	C-N-CA	8.47	142.87	121.70
1	B	21	GLN	CG-CD-OE1	-8.46	104.67	121.60
1	C	43	SER	CA-CB-OG	8.46	134.06	111.20
1	A	91	VAL	C-N-CA	8.46	142.84	121.70
1	A	225	LEU	CB-CA-C	8.46	126.27	110.20
1	B	145	GLN	CB-CG-CD	8.46	133.59	111.60
1	C	29	ARG	C-N-CA	-8.46	100.56	121.70
1	F	19	ALA	CA-C-O	-8.46	102.34	120.10
1	D	63	GLN	C-N-CA	-8.45	100.57	121.70
1	A	78	ARG	CD-NE-CZ	-8.45	111.77	123.60
1	A	5	PHE	O-C-N	-8.45	108.84	123.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	22	SER	CB-CA-C	-8.45	94.04	110.10
1	E	63	GLN	CB-CA-C	-8.45	93.50	110.40
1	F	203	VAL	CA-C-O	-8.45	102.36	120.10
1	D	232	LEU	CA-C-O	-8.45	102.36	120.10
1	C	195	VAL	CA-CB-CG1	8.44	123.57	110.90
1	C	139	GLN	CA-CB-CG	8.44	131.97	113.40
1	C	10	GLU	C-N-CA	-8.44	104.58	122.30
1	D	233	TRP	CD1-NE1-CE2	-8.44	101.41	109.00
1	B	138	PRO	CA-C-O	8.44	140.45	120.20
1	A	37	ASN	CB-CG-OD1	-8.44	104.73	121.60
1	B	158	THR	C-N-CA	8.44	142.79	121.70
1	D	192	ARG	CA-C-N	8.44	135.76	117.20
1	B	30	PHE	CD1-CE1-CZ	-8.43	109.98	120.10
1	D	172	TRP	CE2-CD2-CG	8.43	114.05	107.30
1	C	65	ASP	CA-C-O	-8.43	102.39	120.10
1	A	135	ASP	OD1-CG-OD2	8.43	139.31	123.30
1	B	194	ASP	N-CA-C	8.43	133.75	111.00
1	C	185	ALA	CB-CA-C	-8.43	97.46	110.10
1	E	59	ARG	CG-CD-NE	-8.43	94.10	111.80
1	F	44	ASP	CA-CB-CG	-8.43	94.86	113.40
1	E	120	VAL	CA-CB-CG1	8.42	123.53	110.90
1	B	10	GLU	CB-CA-C	8.42	127.24	110.40
1	D	30	PHE	CG-CD2-CE2	-8.42	111.54	120.80
1	F	72	THR	O-C-N	8.42	136.17	122.70
1	A	74	GLN	N-CA-CB	-8.41	95.45	110.60
1	C	66	GLY	C-N-CA	-8.41	100.66	121.70
1	D	208	ASN	OD1-CG-ND2	8.41	141.25	121.90
1	F	194	ASP	N-CA-C	8.41	133.72	111.00
1	B	172	TRP	CH2-CZ2-CE2	8.41	125.81	117.40
1	D	145	GLN	C-N-CA	8.41	142.72	121.70
1	F	13	HIS	C-N-CD	-8.41	102.11	120.60
1	E	212	ALA	CB-CA-C	-8.40	97.50	110.10
1	C	42	ASP	N-CA-C	-8.39	88.33	111.00
1	A	137	HIS	N-CA-C	8.39	133.66	111.00
1	A	198	ASN	CB-CA-C	-8.39	93.62	110.40
1	B	109	ASP	CA-CB-CG	-8.38	94.95	113.40
1	B	223	ARG	CB-CG-CD	-8.38	89.80	111.60
1	D	146	SER	N-CA-CB	-8.38	97.92	110.50
1	B	11	GLY	O-C-N	8.38	136.11	122.70
1	D	138	PRO	C-N-CA	-8.38	100.76	121.70
1	B	107	LEU	CA-C-O	-8.38	102.51	120.10
1	B	110	SER	CB-CA-C	-8.37	94.19	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	214	ARG	C-N-CA	8.37	142.64	121.70
1	C	192	ARG	CB-CG-CD	8.37	133.37	111.60
1	D	21	GLN	CB-CA-C	8.37	127.13	110.40
1	E	173	SER	CB-CA-C	-8.36	94.21	110.10
1	B	228	TYR	N-CA-CB	8.36	125.65	110.60
1	E	156	MET	CA-CB-CG	8.36	127.51	113.30
1	A	187	LEU	CB-CA-C	-8.36	94.32	110.20
1	F	235	THR	CA-C-O	8.36	137.66	120.10
1	B	41	PHE	CB-CG-CD1	8.36	126.65	120.80
1	B	201	ILE	C-N-CA	8.35	142.58	121.70
1	E	114	ASN	CB-CG-OD1	-8.35	104.90	121.60
1	C	207	GLY	N-CA-C	8.35	133.97	113.10
1	E	161	ASN	CB-CA-C	8.35	127.10	110.40
1	B	99	THR	N-CA-CB	8.35	126.16	110.30
1	C	197	THR	CA-C-N	-8.35	98.84	117.20
1	D	90	TYR	CA-C-O	-8.35	102.57	120.10
1	E	200	ASN	N-CA-CB	8.35	125.62	110.60
1	A	125	ASN	CA-CB-CG	8.34	131.76	113.40
1	A	38	LEU	CA-CB-CG	-8.34	96.11	115.30
1	A	7	LEU	CB-CG-CD1	8.34	125.18	111.00
1	D	137	HIS	CB-CA-C	-8.34	93.72	110.40
1	E	85	GLY	N-CA-C	-8.34	92.25	113.10
1	C	119	VAL	CA-CB-CG1	8.34	123.41	110.90
1	E	149	LEU	O-C-N	8.34	136.04	122.70
1	A	184	ARG	N-CA-CB	8.33	125.60	110.60
1	F	195	VAL	N-CA-CB	8.33	129.83	111.50
1	D	61	VAL	N-CA-C	8.33	133.49	111.00
1	E	202	ALA	C-N-CA	8.33	142.52	121.70
1	E	152	TYR	CD1-CG-CD2	-8.32	108.75	117.90
1	F	26	SER	O-C-N	-8.32	109.39	122.70
1	D	42	ASP	N-CA-CB	8.32	125.57	110.60
1	C	173	SER	CA-CB-OG	-8.32	88.74	111.20
1	F	125	ASN	N-CA-CB	-8.32	95.63	110.60
1	C	27	SER	CA-C-O	8.31	137.56	120.10
1	F	223	ARG	C-N-CA	8.31	142.49	121.70
1	B	68	LEU	CB-CG-CD2	8.31	125.13	111.00
1	D	136	ASN	CA-C-O	-8.31	102.65	120.10
1	E	73	ALA	C-N-CA	8.31	142.48	121.70
1	B	196	LEU	O-C-N	-8.31	109.41	122.70
1	E	109	ASP	O-C-N	8.31	135.99	122.70
1	F	215	TYR	CD1-CE1-CZ	-8.31	112.32	119.80
1	E	216	VAL	O-C-N	-8.30	109.41	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	228	TYR	CA-C-O	-8.30	102.66	120.10
1	A	188	GLN	N-CA-C	8.30	133.41	111.00
1	A	28	PHE	CB-CG-CD1	8.30	126.61	120.80
1	C	11	GLY	CA-C-N	8.30	135.46	117.20
1	F	169	ASP	CB-CA-C	8.30	127.00	110.40
1	C	25	LEU	CB-CG-CD2	-8.30	96.89	111.00
1	D	28	PHE	CB-CG-CD2	8.30	126.61	120.80
1	E	105	PRO	N-CA-CB	8.29	113.25	103.30
1	E	205	THR	CA-CB-CG2	-8.29	100.79	112.40
1	F	17	LEU	CB-CG-CD2	-8.29	96.90	111.00
1	F	105	PRO	N-CA-C	8.29	133.67	112.10
1	C	2	ASN	O-C-N	-8.29	109.43	122.70
1	F	196	LEU	N-CA-C	8.29	133.39	111.00
1	F	234	THR	CA-CB-CG2	8.29	124.00	112.40
1	B	56	THR	O-C-N	-8.29	109.11	123.20
1	D	183	CYS	CA-CB-SG	8.29	128.92	114.00
1	F	144	THR	N-CA-CB	8.29	126.04	110.30
1	C	50	SER	CA-C-N	8.28	135.42	117.20
1	F	206	SER	O-C-N	-8.29	109.11	123.20
1	D	173	SER	CB-CA-C	-8.28	94.36	110.10
1	A	143	ALA	CA-C-N	8.28	135.42	117.20
1	A	98	ARG	NE-CZ-NH1	-8.28	116.16	120.30
1	A	145	GLN	CB-CA-C	8.28	126.95	110.40
1	D	100	VAL	CA-C-N	8.28	135.41	117.20
1	A	170	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	D	77	ILE	CA-CB-CG1	8.27	126.72	111.00
1	B	38	LEU	O-C-N	8.27	135.93	122.70
1	E	150	SER	N-CA-CB	8.27	122.90	110.50
1	B	108	TRP	C-N-CA	8.26	142.36	121.70
1	C	141	LEU	CA-CB-CG	8.26	134.31	115.30
1	A	17	LEU	CB-CG-CD1	-8.26	96.96	111.00
1	B	124	GLY	CA-C-O	8.26	135.47	120.60
1	C	22	SER	C-N-CA	8.26	142.35	121.70
1	E	229	GLY	C-N-CA	-8.26	104.95	122.30
1	B	131	THR	OG1-CB-CG2	-8.26	91.01	110.00
1	E	30	PHE	C-N-CA	8.26	142.34	121.70
1	B	213	GLY	O-C-N	-8.26	109.49	122.70
1	F	214	ARG	CA-CB-CG	8.26	131.57	113.40
1	D	204	TRP	CB-CG-CD1	-8.26	116.27	127.00
1	F	232	LEU	N-CA-C	8.25	133.28	111.00
1	D	139	GLN	CA-CB-CG	8.25	131.55	113.40
1	F	195	VAL	CA-C-O	-8.25	102.77	120.10

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	149	LEU	CB-CA-C	-8.25	94.53	110.20
1	A	194	ASP	C-N-CA	-8.25	101.09	121.70
1	C	131	THR	OG1-CB-CG2	-8.25	91.03	110.00
1	B	2	ASN	CA-CB-CG	8.24	131.54	113.40
1	E	123	ASN	C-N-CA	8.24	139.61	122.30
1	E	233	TRP	CA-C-O	-8.24	102.78	120.10
1	F	37	ASN	OD1-CG-ND2	8.24	140.86	121.90
1	F	196	LEU	CB-CA-C	-8.24	94.54	110.20
1	A	33	GLN	CA-C-N	-8.24	99.07	117.20
1	A	227	ILE	CG1-CB-CG2	-8.24	93.27	111.40
1	C	206	SER	N-CA-CB	-8.24	98.14	110.50
1	D	155	SER	CA-CB-OG	-8.24	88.96	111.20
1	F	175	ASN	N-CA-CB	8.24	125.42	110.60
1	B	55	ALA	CB-CA-C	8.23	122.44	110.10
1	C	204	TRP	CZ3-CH2-CZ2	-8.23	111.73	121.60
1	B	107	LEU	N-CA-CB	8.22	126.85	110.40
1	B	159	ASP	O-C-N	-8.22	109.54	122.70
1	C	154	LEU	CA-C-N	8.22	135.29	117.20
1	D	194	ASP	CA-CB-CG	-8.22	95.31	113.40
1	A	152	TYR	CB-CG-CD1	-8.22	116.07	121.00
1	E	1	ASN	CB-CA-C	8.22	126.83	110.40
1	B	137	HIS	CB-CA-C	-8.21	93.97	110.40
1	A	219	LEU	CA-CB-CG	8.21	134.19	115.30
1	C	95	GLN	CG-CD-NE2	-8.21	96.99	116.70
1	D	114	ASN	CA-CB-CG	8.21	131.47	113.40
1	E	15	GLN	CB-CA-C	8.21	126.82	110.40
1	C	143	ALA	N-CA-C	-8.21	88.84	111.00
1	D	2	ASN	CB-CA-C	-8.21	93.99	110.40
1	B	129	TYR	N-CA-C	8.20	133.15	111.00
1	B	217	PHE	N-CA-CB	-8.20	95.84	110.60
1	E	233	TRP	CD1-CG-CD2	-8.20	99.74	106.30
1	C	27	SER	CB-CA-C	8.20	125.68	110.10
1	E	198	ASN	N-CA-CB	-8.20	95.85	110.60
1	E	233	TRP	O-C-N	8.20	135.81	122.70
1	F	94	LEU	N-CA-C	-8.19	88.89	111.00
1	F	165	PHE	CA-C-O	-8.19	102.91	120.10
1	F	224	ASN	CB-CA-C	8.19	126.78	110.40
1	A	167	ARG	CA-C-N	8.18	135.20	117.20
1	E	233	TRP	CA-CB-CG	8.18	129.25	113.70
1	F	145	GLN	OE1-CD-NE2	8.18	140.71	121.90
1	D	125	ASN	CB-CA-C	-8.17	94.06	110.40
1	E	136	ASN	O-C-N	-8.17	109.63	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	PHE	N-CA-CB	8.17	125.30	110.60
1	E	113	SER	N-CA-CB	8.17	122.75	110.50
1	C	28	PHE	CB-CA-C	8.16	126.72	110.40
1	C	190	ASN	CB-CG-OD1	-8.16	105.28	121.60
1	B	26	SER	N-CA-CB	-8.16	98.27	110.50
1	C	6	GLY	CA-C-O	-8.15	105.93	120.60
1	D	128	LEU	CB-CG-CD2	8.15	124.86	111.00
1	C	198	ASN	N-CA-CB	-8.15	95.93	110.60
1	E	194	ASP	OD1-CG-OD2	-8.15	107.82	123.30
1	E	71	LEU	CA-C-N	-8.15	99.28	117.20
1	B	55	ALA	C-N-CA	8.14	142.06	121.70
1	D	176	THR	O-C-N	-8.14	109.67	122.70
1	B	209	SER	C-N-CA	-8.14	101.34	121.70
1	B	64	SER	CA-CB-OG	-8.14	89.22	111.20
1	E	5	PHE	CG-CD2-CE2	8.14	129.75	120.80
1	D	16	THR	CB-CA-C	-8.14	89.63	111.60
1	C	48	TRP	CA-C-O	-8.14	103.02	120.10
1	C	150	SER	CA-C-O	-8.14	103.01	120.10
1	F	131	THR	OG1-CB-CG2	8.14	128.71	110.00
1	A	170	ARG	CB-CA-C	8.13	126.67	110.40
1	B	69	VAL	N-CA-CB	8.13	129.39	111.50
1	C	38	LEU	CB-CG-CD1	8.13	124.83	111.00
1	B	175	ASN	C-N-CA	8.13	142.03	121.70
1	D	108	TRP	CD1-CG-CD2	-8.13	99.80	106.30
1	F	63	GLN	CB-CG-CD	8.13	132.74	111.60
1	D	108	TRP	CG-CD1-NE1	8.13	118.23	110.10
1	A	121	ALA	C-N-CA	8.12	142.01	121.70
1	F	214	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	B	57	GLY	O-C-N	-8.12	109.70	122.70
1	B	80	SER	CB-CA-C	-8.12	94.67	110.10
1	E	153	ARG	NE-CZ-NH2	8.12	124.36	120.30
1	B	155	SER	C-N-CA	8.12	141.99	121.70
1	C	138	PRO	CB-CA-C	-8.11	91.72	112.00
1	B	148	GLN	CB-CG-CD	8.11	132.69	111.60
1	C	61	VAL	N-CA-CB	8.11	129.35	111.50
1	A	108	TRP	CD2-CE3-CZ3	-8.11	108.26	118.80
1	E	81	SER	C-N-CA	-8.11	105.27	122.30
1	A	89	ASN	N-CA-CB	-8.11	96.01	110.60
1	B	21	GLN	N-CA-CB	8.11	125.19	110.60
1	C	29	ARG	CD-NE-CZ	8.11	134.95	123.60
1	D	32	MET	C-N-CA	-8.11	101.44	121.70
1	E	87	ILE	CA-CB-CG2	-8.11	94.69	110.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	128	LEU	CA-C-O	8.11	137.12	120.10
1	F	232	LEU	CA-C-N	8.11	135.03	117.20
1	B	29	ARG	CG-CD-NE	8.10	128.82	111.80
1	A	108	TRP	CA-C-N	8.10	135.03	117.20
1	D	61	VAL	C-N-CA	8.10	141.96	121.70
1	B	40	LEU	CB-CG-CD2	-8.10	97.23	111.00
1	B	54	GLY	O-C-N	8.10	135.66	122.70
1	E	31	THR	O-C-N	-8.10	109.74	122.70
1	F	163	VAL	CA-CB-CG2	-8.10	98.75	110.90
1	B	138	PRO	CA-C-N	-8.10	99.39	117.20
1	B	227	ILE	CB-CG1-CD1	-8.10	91.23	113.90
1	A	157	GLU	CA-C-N	8.09	135.00	117.20
1	D	131	THR	N-CA-CB	-8.09	94.93	110.30
1	E	193	MET	CB-CG-SD	-8.09	88.13	112.40
1	B	212	ALA	O-C-N	8.09	136.95	123.20
1	C	84	LYS	CD-CE-NZ	8.09	130.30	111.70
1	D	45	VAL	O-C-N	-8.09	109.76	122.70
1	D	8	SER	CA-C-N	-8.09	99.41	117.20
1	B	189	PRO	C-N-CA	8.08	141.90	121.70
1	A	28	PHE	CZ-CE2-CD2	-8.08	110.41	120.10
1	D	178	GLY	CA-C-O	8.08	135.14	120.60
1	A	166	ASP	CB-CA-C	-8.07	94.26	110.40
1	F	144	THR	CA-C-N	8.07	134.96	117.20
1	D	108	TRP	CD1-NE1-CE2	-8.07	101.74	109.00
1	D	214	ARG	CB-CG-CD	8.07	132.58	111.60
1	D	75	ASN	CB-CG-OD1	-8.06	105.48	121.60
1	A	25	LEU	CD1-CG-CD2	8.06	134.68	110.50
1	C	147	LEU	CB-CA-C	-8.06	94.89	110.20
1	B	129	TYR	CG-CD1-CE1	-8.06	114.85	121.30
1	D	40	LEU	O-C-N	8.05	135.59	122.70
1	A	200	ASN	OD1-CG-ND2	-8.05	103.38	121.90
1	A	70	ILE	O-C-N	-8.05	109.82	122.70
1	A	186	VAL	CG1-CB-CG2	-8.05	98.02	110.90
1	F	155	SER	O-C-N	-8.05	109.82	122.70
1	B	4	LEU	CA-C-O	-8.05	103.20	120.10
1	B	235	THR	N-CA-CB	-8.05	95.01	110.30
1	C	98	ARG	CD-NE-CZ	-8.05	112.33	123.60
1	E	76	THR	N-CA-CB	-8.05	95.01	110.30
1	F	69	VAL	CA-CB-CG2	8.05	122.97	110.90
1	F	234	THR	C-N-CA	8.05	141.82	121.70
1	D	79	TRP	CH2-CZ2-CE2	8.04	125.44	117.40
1	F	204	TRP	CD1-CG-CD2	-8.04	99.86	106.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	THR	CA-C-N	8.04	134.89	117.20
1	F	127	ILE	CA-CB-CG1	8.04	126.27	111.00
1	D	14	PRO	O-C-N	8.04	135.56	122.70
1	E	193	MET	C-N-CA	8.04	141.79	121.70
1	F	98	ARG	O-C-N	-8.04	109.84	122.70
1	C	46	ARG	N-CA-CB	8.03	125.06	110.60
1	A	28	PHE	CG-CD2-CE2	8.03	129.63	120.80
1	C	213	GLY	CA-C-N	8.03	134.86	117.20
1	A	190	ASN	CA-C-O	8.03	136.96	120.10
1	B	98	ARG	NH1-CZ-NH2	-8.03	110.57	119.40
1	E	28	PHE	N-CA-CB	-8.03	96.15	110.60
1	C	77	ILE	CB-CG1-CD1	8.02	136.36	113.90
1	C	196	LEU	C-N-CA	8.02	141.75	121.70
1	A	156	MET	CA-CB-CG	8.02	126.93	113.30
1	E	44	ASP	N-CA-C	-8.02	89.35	111.00
1	F	84	LYS	CA-C-N	8.02	132.23	116.20
1	A	149	LEU	CB-CA-C	-8.01	94.98	110.20
1	A	101	THR	CA-CB-CG2	8.01	123.62	112.40
1	B	201	ILE	CA-C-N	8.00	134.81	117.20
1	F	18	HIS	CA-C-N	8.00	134.81	117.20
1	B	131	THR	N-CA-CB	7.99	125.49	110.30
1	E	214	ARG	CA-CB-CG	7.99	130.98	113.40
1	A	176	THR	CA-CB-OG1	7.99	125.78	109.00
1	F	220	GLN	OE1-CD-NE2	-7.99	103.53	121.90
1	A	114	ASN	CB-CA-C	-7.99	94.43	110.40
1	C	44	ASP	CA-CB-CG	-7.99	95.83	113.40
1	E	157	GLU	CA-CB-CG	-7.98	95.83	113.40
1	F	157	GLU	O-C-N	7.98	135.47	122.70
1	C	157	GLU	CB-CA-C	7.98	126.36	110.40
1	C	43	SER	N-CA-CB	-7.98	98.54	110.50
1	E	60	ALA	O-C-N	-7.98	109.94	122.70
1	A	33	GLN	OE1-CD-NE2	7.97	140.24	121.90
1	B	177	ALA	CA-C-O	7.97	136.83	120.10
1	D	59	ARG	NE-CZ-NH2	7.97	124.28	120.30
1	E	5	PHE	CB-CA-C	7.96	126.33	110.40
1	C	56	THR	CA-C-O	7.96	136.82	120.10
1	D	112	THR	C-N-CA	7.96	141.60	121.70
1	B	101	THR	CA-C-O	-7.96	103.39	120.10
1	E	197	THR	CA-CB-OG1	-7.96	92.29	109.00
1	B	32	MET	CB-CA-C	7.96	126.31	110.40
1	B	218	VAL	CA-CB-CG2	-7.96	98.97	110.90
1	C	58	CYS	CA-C-O	7.96	136.81	120.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	188	GLN	N-CA-C	7.96	132.48	111.00
1	F	107	LEU	CB-CA-C	7.95	125.31	110.20
1	B	16	THR	C-N-CA	-7.95	101.83	121.70
1	D	111	GLY	C-N-CA	7.95	141.57	121.70
1	E	196	LEU	N-CA-CB	-7.94	94.51	110.40
1	D	168	ASP	N-CA-CB	7.94	124.89	110.60
1	F	222	ASP	CB-CG-OD2	-7.94	111.16	118.30
1	B	190	ASN	OD1-CG-ND2	-7.93	103.65	121.90
1	F	83	THR	CA-CB-OG1	7.93	125.66	109.00
1	D	57	GLY	C-N-CA	7.93	141.53	121.70
1	C	51	ASN	CB-CA-C	7.93	126.26	110.40
1	D	42	ASP	CB-CA-C	-7.93	94.54	110.40
1	C	22	SER	O-C-N	-7.93	110.01	122.70
1	A	155	SER	O-C-N	7.93	135.38	122.70
1	C	121	ALA	CB-CA-C	7.93	121.99	110.10
1	F	223	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	B	108	TRP	CG-CD1-NE1	7.92	118.02	110.10
1	C	180	GLY	N-CA-C	7.92	132.91	113.10
1	F	34	SER	C-N-CA	7.92	141.51	121.70
1	B	40	LEU	CB-CG-CD1	7.92	124.47	111.00
1	E	195	VAL	CA-CB-CG1	-7.92	99.02	110.90
1	B	42	ASP	CA-CB-CG	7.92	130.82	113.40
1	D	110	SER	CA-CB-OG	-7.92	89.82	111.20
1	F	87	ILE	CB-CA-C	-7.92	95.77	111.60
1	C	232	LEU	N-CA-CB	-7.91	94.57	110.40
1	D	189	PRO	CA-CB-CG	-7.91	88.97	104.00
1	D	76	THR	OG1-CB-CG2	-7.91	91.80	110.00
1	B	69	VAL	CG1-CB-CG2	-7.91	98.24	110.90
1	F	61	VAL	CA-C-N	-7.90	99.82	117.20
1	F	81	SER	CA-CB-OG	7.90	132.54	111.20
1	E	47	VAL	CB-CA-C	-7.90	96.39	111.40
1	C	233	TRP	CG-CD1-NE1	7.89	117.99	110.10
1	D	187	LEU	CB-CA-C	-7.89	95.20	110.20
1	E	41	PHE	N-CA-CB	-7.89	96.39	110.60
1	D	148	GLN	CB-CA-C	7.89	126.18	110.40
1	A	127	ILE	CA-CB-CG2	-7.89	95.13	110.90
1	F	154	LEU	N-CA-CB	7.88	126.17	110.40
1	F	20	ALA	N-CA-CB	-7.88	99.06	110.10
1	A	3	ILE	CG1-CB-CG2	7.88	128.74	111.40
1	C	90	TYR	CD1-CE1-CZ	-7.88	112.71	119.80
1	A	87	ILE	CB-CG1-CD1	-7.88	91.84	113.90
1	C	39	VAL	CA-C-N	7.88	134.53	117.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	218	VAL	CA-CB-CG2	7.88	122.72	110.90
1	B	128	LEU	CB-CG-CD2	-7.88	97.61	111.00
1	B	227	ILE	CB-CA-C	7.87	127.35	111.60
1	C	211	SER	CA-C-O	-7.87	103.57	120.10
1	D	193	MET	CA-C-O	-7.87	103.57	120.10
1	A	97	ASP	CA-C-N	7.87	134.51	117.20
1	E	26	SER	N-CA-CB	-7.87	98.70	110.50
1	A	102	ILE	CB-CG1-CD1	7.87	135.92	113.90
1	F	206	SER	CB-CA-C	7.87	125.04	110.10
1	B	74	GLN	CB-CA-C	-7.86	94.67	110.40
1	C	46	ARG	CB-CA-C	-7.86	94.67	110.40
1	E	35	ASP	OD1-CG-OD2	-7.86	108.36	123.30
1	B	41	PHE	CA-C-N	7.86	134.49	117.20
1	B	136	ASN	CB-CA-C	-7.86	94.68	110.40
1	E	102	ILE	CA-CB-CG2	7.86	126.62	110.90
1	D	129	TYR	C-N-CA	7.86	141.35	121.70
1	C	16	THR	O-C-N	7.86	135.27	122.70
1	C	166	ASP	CA-C-N	7.86	134.49	117.20
1	D	96	PRO	CA-C-O	-7.86	101.35	120.20
1	F	48	TRP	CD1-NE1-CE2	7.86	116.07	109.00
1	B	47	VAL	N-CA-CB	7.85	128.77	111.50
1	A	86	SER	C-N-CA	-7.85	102.08	121.70
1	B	38	LEU	CA-C-O	-7.85	103.62	120.10
1	D	9	HIS	N-CA-C	7.85	132.19	111.00
1	A	192	ARG	CB-CG-CD	7.85	132.00	111.60
1	A	35	ASP	C-N-CA	7.84	141.31	121.70
1	D	9	HIS	O-C-N	-7.84	110.16	122.70
1	D	216	VAL	CA-CB-CG2	7.84	122.66	110.90
1	E	170	ARG	O-C-N	7.84	135.25	122.70
1	E	223	ARG	CA-CB-CG	7.84	130.65	113.40
1	A	139	GLN	CA-C-N	-7.84	99.96	117.20
1	C	172	TRP	CD1-NE1-CE2	-7.84	101.95	109.00
1	F	130	SER	CA-CB-OG	-7.84	90.04	111.20
1	E	146	SER	N-CA-C	7.83	132.15	111.00
1	A	155	SER	CB-CA-C	7.83	124.98	110.10
1	F	8	SER	CA-CB-OG	7.83	132.35	111.20
1	B	223	ARG	CG-CD-NE	7.83	128.24	111.80
1	D	2	ASN	N-CA-C	7.83	132.13	111.00
1	D	22	SER	O-C-N	7.83	135.23	122.70
1	D	224	ASN	CA-C-N	7.83	134.42	117.20
1	B	226	ALA	CB-CA-C	7.83	121.84	110.10
1	E	125	ASN	O-C-N	-7.82	110.18	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	10	GLU	N-CA-CB	-7.82	96.52	110.60
1	F	101	THR	OG1-CB-CG2	7.82	127.98	110.00
1	A	40	LEU	CB-CA-C	-7.82	95.35	110.20
1	A	65	ASP	N-CA-C	-7.82	89.89	111.00
1	D	87	ILE	CB-CA-C	-7.82	95.96	111.60
1	E	41	PHE	CZ-CE2-CD2	-7.82	110.72	120.10
1	E	71	LEU	CB-CG-CD2	-7.82	97.71	111.00
1	A	118	VAL	C-N-CA	7.81	141.24	121.70
1	D	107	LEU	O-C-N	7.81	135.20	122.70
1	F	85	GLY	CA-C-N	7.81	134.39	117.20
1	A	2	ASN	N-CA-CB	-7.81	96.54	110.60
1	F	89	ASN	CB-CA-C	-7.81	94.79	110.40
1	B	93	VAL	CA-C-O	-7.80	103.72	120.10
1	E	22	SER	N-CA-CB	7.80	122.20	110.50
1	D	1	ASN	CA-C-O	7.80	136.48	120.10
1	F	220	GLN	CA-C-O	7.79	136.47	120.10
1	D	143	ALA	C-N-CA	7.79	141.18	121.70
1	D	149	LEU	CB-CG-CD2	7.79	124.25	111.00
1	A	235	THR	CA-C-O	7.79	136.46	120.10
1	C	149	LEU	C-N-CA	-7.79	102.22	121.70
1	F	201	ILE	CA-CB-CG2	-7.79	95.32	110.90
1	F	152	TYR	CE1-CZ-OH	-7.79	99.08	120.10
1	F	231	ALA	C-N-CA	7.79	141.17	121.70
1	C	10	GLU	CA-C-O	-7.79	103.75	120.10
1	E	192	ARG	NH1-CZ-NH2	7.79	127.97	119.40
1	B	152	TYR	CG-CD2-CE2	7.78	127.53	121.30
1	C	74	GLN	C-N-CA	7.78	141.16	121.70
1	B	38	LEU	CD1-CG-CD2	7.78	133.85	110.50
1	A	109	ASP	OD1-CG-OD2	-7.78	108.52	123.30
1	D	123	ASN	C-N-CA	7.78	138.63	122.30
1	E	228	TYR	CA-C-O	7.78	136.43	120.10
1	B	30	PHE	CA-C-N	7.78	134.30	117.20
1	A	50	SER	CA-C-O	7.77	136.42	120.10
1	E	73	ALA	CB-CA-C	7.77	121.75	110.10
1	A	90	TYR	CD1-CG-CD2	-7.77	109.36	117.90
1	B	164	LEU	CB-CG-CD2	7.77	124.21	111.00
1	B	75	ASN	CA-C-O	-7.76	103.80	120.10
1	F	70	ILE	N-CA-CB	-7.76	92.94	110.80
1	E	190	ASN	C-N-CA	7.76	138.60	122.30
1	B	225	LEU	CA-C-O	-7.76	103.80	120.10
1	E	48	TRP	NE1-CE2-CD2	-7.76	99.54	107.30
1	A	34	SER	CA-CB-OG	7.76	132.15	111.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	34	SER	CB-CA-C	7.76	124.84	110.10
1	C	53	ALA	O-C-N	-7.76	110.01	123.20
1	C	72	THR	OG1-CB-CG2	-7.76	92.16	110.00
1	B	127	ILE	C-N-CA	7.75	141.09	121.70
1	A	170	ARG	CA-CB-CG	7.75	130.46	113.40
1	F	99	THR	N-CA-C	-7.75	90.07	111.00
1	A	166	ASP	CA-CB-CG	7.75	130.45	113.40
1	B	50	SER	CA-C-N	7.75	134.25	117.20
1	C	94	LEU	N-CA-CB	-7.75	94.90	110.40
1	D	234	THR	OG1-CB-CG2	-7.75	92.18	110.00
1	B	142	HIS	ND1-CG-CD2	-7.75	95.16	106.00
1	F	190	ASN	CA-C-O	7.75	136.37	120.10
1	C	41	PHE	CB-CG-CD1	7.74	126.22	120.80
1	C	61	VAL	N-CA-C	7.74	131.91	111.00
1	A	68	LEU	CA-C-O	-7.74	103.84	120.10
1	E	197	THR	C-N-CA	7.74	141.05	121.70
1	E	34	SER	N-CA-CB	-7.74	98.89	110.50
1	D	7	LEU	O-C-N	-7.74	110.32	122.70
1	D	217	PHE	CA-CB-CG	-7.74	95.33	113.90
1	B	67	LEU	O-C-N	-7.74	110.32	122.70
1	A	14	PRO	CA-CB-CG	-7.74	89.30	104.00
1	D	193	MET	N-CA-C	-7.74	90.11	111.00
1	A	75	ASN	OD1-CG-ND2	7.73	139.69	121.90
1	D	107	LEU	CA-CB-CG	7.73	133.08	115.30
1	D	227	ILE	CA-CB-CG2	7.73	126.36	110.90
1	A	48	TRP	CD2-CE3-CZ3	7.73	128.85	118.80
1	D	4	LEU	CB-CA-C	-7.73	95.51	110.20
1	C	193	MET	C-N-CA	7.73	141.02	121.70
1	E	13	HIS	N-CA-CB	-7.73	96.69	110.60
1	B	129	TYR	OH-CZ-CE2	-7.72	99.24	120.10
1	F	50	SER	CB-CA-C	-7.72	95.42	110.10
1	A	28	PHE	O-C-N	7.72	135.06	122.70
1	C	44	ASP	CB-CA-C	-7.72	94.95	110.40
1	D	205	THR	O-C-N	-7.72	110.34	122.70
1	F	182	GLY	CA-C-O	7.72	134.50	120.60
1	E	168	ASP	CB-CA-C	7.72	125.84	110.40
1	F	191	GLY	C-N-CA	-7.72	102.40	121.70
1	A	60	ALA	CB-CA-C	7.71	121.67	110.10
1	B	137	HIS	N-CA-CB	-7.71	96.71	110.60
1	F	75	ASN	OD1-CG-ND2	7.71	139.64	121.90
1	B	130	SER	N-CA-C	-7.71	90.18	111.00
1	D	24	GLU	N-CA-CB	-7.71	96.72	110.60

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	17	LEU	O-C-N	-7.71	110.37	122.70
1	E	189	PRO	CB-CA-C	7.71	131.27	112.00
1	C	227	ILE	CA-C-O	-7.71	103.92	120.10
1	D	160	CYS	C-N-CA	7.70	140.96	121.70
1	E	45	VAL	N-CA-CB	7.70	128.45	111.50
1	B	30	PHE	CG-CD2-CE2	-7.70	112.33	120.80
1	E	168	ASP	N-CA-CB	7.70	124.46	110.60
1	A	13	HIS	CA-CB-CG	7.70	126.69	113.60
1	C	87	ILE	O-C-N	7.70	136.29	123.20
1	C	132	GLN	CB-CA-C	7.70	125.80	110.40
1	E	32	MET	CA-C-N	7.70	134.14	117.20
1	A	2	ASN	CA-CB-CG	-7.70	96.47	113.40
1	A	69	VAL	O-C-N	7.70	135.02	122.70
1	A	74	GLN	CG-CD-OE1	-7.70	106.20	121.60
1	A	223	ARG	O-C-N	-7.70	110.39	122.70
1	E	107	LEU	CB-CG-CD2	-7.70	97.92	111.00
1	F	149	LEU	CA-CB-CG	-7.69	97.61	115.30
1	E	151	PRO	C-N-CA	7.69	140.93	121.70
1	A	119	VAL	N-CA-C	7.69	131.76	111.00
1	F	79	TRP	CB-CG-CD2	7.68	136.59	126.60
1	A	31	THR	CA-CB-CG2	7.68	123.16	112.40
1	E	72	THR	CA-C-N	-7.68	100.30	117.20
1	A	224	ASN	CA-C-O	7.68	136.23	120.10
1	C	122	ASN	C-N-CA	7.68	140.90	121.70
1	C	11	GLY	CA-C-O	-7.68	106.78	120.60
1	E	138	PRO	CB-CA-C	-7.67	92.81	112.00
1	F	47	VAL	CA-CB-CG2	-7.67	99.39	110.90
1	D	74	GLN	CB-CA-C	-7.67	95.06	110.40
1	C	160	CYS	CA-C-O	-7.67	104.00	120.10
1	C	219	LEU	CA-C-O	7.67	136.20	120.10
1	E	156	MET	O-C-N	7.67	134.97	122.70
1	C	30	PHE	CD1-CE1-CZ	7.66	129.30	120.10
1	D	103	TYR	CB-CG-CD2	-7.66	116.40	121.00
1	F	107	LEU	CB-CG-CD2	7.66	124.03	111.00
1	C	85	GLY	CA-C-O	-7.66	106.81	120.60
1	E	92	LEU	CA-CB-CG	7.66	132.92	115.30
1	C	83	THR	N-CA-C	-7.66	90.31	111.00
1	E	97	ASP	CA-CB-CG	7.66	130.25	113.40
1	B	103	TYR	N-CA-CB	7.66	124.38	110.60
1	C	88	GLY	N-CA-C	7.66	132.24	113.10
1	B	221	PRO	N-CD-CG	-7.65	91.72	103.20
1	A	207	GLY	N-CA-C	7.65	132.23	113.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	GLU	CG-CD-OE2	7.65	133.60	118.30
1	A	10	GLU	CG-CD-OE2	-7.65	103.00	118.30
1	A	192	ARG	N-CA-CB	-7.65	96.83	110.60
1	B	36	CYS	CA-C-N	7.65	134.03	117.20
1	D	128	LEU	CB-CG-CD1	7.65	124.00	111.00
1	A	48	TRP	O-C-N	7.64	134.93	122.70
1	C	164	LEU	CA-C-O	-7.64	104.05	120.10
1	B	29	ARG	CA-C-N	-7.64	100.39	117.20
1	E	123	ASN	CA-CB-CG	7.64	130.21	113.40
1	A	102	ILE	CA-CB-CG2	7.64	126.17	110.90
1	D	39	VAL	C-N-CA	7.64	140.79	121.70
1	D	87	ILE	N-CA-C	7.64	131.62	111.00
1	A	129	TYR	N-CA-CB	7.63	124.34	110.60
1	C	233	TRP	CD2-CE3-CZ3	-7.63	108.88	118.80
1	D	173	SER	C-N-CA	7.63	140.78	121.70
1	C	183	CYS	CB-CA-C	7.63	125.66	110.40
1	E	7	LEU	C-N-CA	7.63	140.77	121.70
1	B	192	ARG	C-N-CA	-7.63	102.63	121.70
1	F	49	ALA	CB-CA-C	-7.63	98.66	110.10
1	D	59	ARG	CA-CB-CG	7.63	130.18	113.40
1	E	46	ARG	NE-CZ-NH1	-7.62	116.49	120.30
1	B	98	ARG	NE-CZ-NH1	-7.62	116.49	120.30
1	A	82	GLY	C-N-CA	-7.62	102.65	121.70
1	D	203	VAL	N-CA-CB	7.62	128.27	111.50
1	D	224	ASN	O-C-N	-7.62	110.51	122.70
1	E	103	TYR	CG-CD1-CE1	7.62	127.40	121.30
1	F	78	ARG	CA-C-N	-7.62	100.43	117.20
1	F	43	SER	O-C-N	-7.62	110.51	122.70
1	A	110	SER	CA-C-N	-7.62	100.96	116.20
1	B	50	SER	O-C-N	-7.62	110.51	122.70
1	E	34	SER	N-CA-C	-7.62	90.43	111.00
1	F	131	THR	CA-CB-OG1	-7.62	93.00	109.00
1	F	165	PHE	CD1-CE1-CZ	-7.62	110.96	120.10
1	B	208	ASN	CA-C-N	-7.61	100.45	117.20
1	F	149	LEU	C-N-CA	-7.61	102.67	121.70
1	C	142	HIS	CA-CB-CG	7.61	126.54	113.60
1	C	94	LEU	CA-C-N	7.60	133.93	117.20
1	E	169	ASP	C-N-CA	7.60	140.71	121.70
1	A	32	MET	CB-CA-C	-7.60	95.20	110.40
1	A	40	LEU	CA-C-O	-7.60	104.15	120.10
1	C	172	TRP	CZ3-CH2-CZ2	-7.60	112.48	121.60
1	F	36	CYS	CA-CB-SG	-7.60	100.33	114.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	170	ARG	CA-C-O	-7.60	104.15	120.10
1	A	87	ILE	CG1-CB-CG2	-7.59	94.69	111.40
1	B	128	LEU	CB-CA-C	7.59	124.62	110.20
1	D	79	TRP	CA-C-O	-7.59	104.16	120.10
1	E	19	ALA	O-C-N	-7.59	110.55	122.70
1	C	113	SER	CB-CA-C	7.59	124.52	110.10
1	D	89	ASN	OD1-CG-ND2	7.59	139.36	121.90
1	B	61	VAL	N-CA-C	7.59	131.49	111.00
1	B	149	LEU	CA-CB-CG	-7.58	97.85	115.30
1	C	167	ARG	CG-CD-NE	7.58	127.73	111.80
1	E	99	THR	N-CA-CB	-7.58	95.89	110.30
1	E	148	GLN	CA-CB-CG	7.58	130.08	113.40
1	B	5	PHE	CA-CB-CG	7.58	132.08	113.90
1	E	28	PHE	CD1-CG-CD2	-7.58	108.45	118.30
1	B	224	ASN	CB-CA-C	7.58	125.55	110.40
1	D	217	PHE	CB-CG-CD1	-7.57	115.50	120.80
1	D	91	VAL	CG1-CB-CG2	-7.57	98.79	110.90
1	E	112	THR	O-C-N	-7.57	110.59	122.70
1	F	39	VAL	O-C-N	7.57	134.81	122.70
1	F	190	ASN	N-CA-CB	-7.57	96.98	110.60
1	C	186	VAL	N-CA-CB	-7.56	94.86	111.50
1	F	213	GLY	CA-C-O	-7.56	106.99	120.60
1	D	154	LEU	CD1-CG-CD2	-7.56	87.82	110.50
1	A	176	THR	N-CA-C	-7.56	90.59	111.00
1	D	33	GLN	CA-C-N	7.56	133.83	117.20
1	D	195	VAL	O-C-N	-7.56	110.61	122.70
1	B	142	HIS	ND1-CE1-NE2	-7.55	93.28	109.90
1	F	53	ALA	CA-C-N	7.55	131.30	116.20
1	B	63	GLN	CA-C-N	-7.55	100.59	117.20
1	B	196	LEU	CA-C-N	-7.54	100.61	117.20
1	D	206	SER	CA-C-N	7.54	131.29	116.20
1	E	162	LEU	CB-CG-CD1	-7.54	98.18	111.00
1	B	36	CYS	CA-C-O	-7.54	104.26	120.10
1	E	9	HIS	CA-C-N	-7.54	100.61	117.20
1	B	184	ARG	O-C-N	-7.54	110.64	122.70
1	E	3	ILE	CB-CG1-CD1	-7.54	92.79	113.90
1	E	146	SER	CB-CA-C	-7.54	95.78	110.10
1	D	88	GLY	CA-C-O	-7.54	107.03	120.60
1	D	227	ILE	CA-C-O	-7.54	104.28	120.10
1	F	222	ASP	CB-CG-OD1	-7.54	111.52	118.30
1	B	33	GLN	N-CA-CB	7.53	124.16	110.60
1	E	169	ASP	OD1-CG-OD2	7.53	137.61	123.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	148	GLN	CB-CG-CD	7.53	131.18	111.60
1	D	181	THR	N-CA-CB	-7.53	95.99	110.30
1	A	149	LEU	N-CA-CB	7.53	125.46	110.40
1	A	152	TYR	O-C-N	7.53	134.75	122.70
1	B	68	LEU	CB-CG-CD1	7.53	123.80	111.00
1	D	24	GLU	CA-C-O	-7.53	104.29	120.10
1	D	46	ARG	CA-C-N	7.53	133.76	117.20
1	E	216	VAL	CA-CB-CG1	-7.53	99.61	110.90
1	D	198	ASN	O-C-N	-7.52	110.66	122.70
1	E	138	PRO	CA-CB-CG	-7.52	89.71	104.00
1	C	137	HIS	CG-ND1-CE1	-7.52	95.93	105.70
1	C	118	VAL	CA-C-O	7.52	135.88	120.10
1	D	7	LEU	CB-CG-CD2	-7.51	98.22	111.00
1	D	157	GLU	N-CA-CB	-7.51	97.08	110.60
1	B	149	LEU	C-N-CA	-7.51	102.92	121.70
1	F	222	ASP	CA-C-N	7.51	133.73	117.20
1	A	82	GLY	CA-C-O	7.51	134.12	120.60
1	D	71	LEU	CA-C-O	-7.51	104.33	120.10
1	E	2	ASN	CB-CG-OD1	-7.51	106.58	121.60
1	C	199	GLN	O-C-N	-7.51	110.69	122.70
1	A	53	ALA	C-N-CA	7.51	138.07	122.30
1	E	53	ALA	CB-CA-C	7.51	121.36	110.10
1	C	155	SER	CA-CB-OG	-7.50	90.94	111.20
1	D	79	TRP	CZ3-CH2-CZ2	-7.50	112.59	121.60
1	F	193	MET	CA-C-O	-7.50	104.34	120.10
1	F	195	VAL	N-CA-C	-7.50	90.74	111.00
1	F	217	PHE	CA-CB-CG	-7.50	95.89	113.90
1	A	3	ILE	CB-CG1-CD1	-7.50	92.90	113.90
1	A	70	ILE	CA-CB-CG2	7.50	125.90	110.90
1	B	161	ASN	OD1-CG-ND2	7.50	139.15	121.90
1	B	89	ASN	C-N-CA	7.50	140.45	121.70
1	A	165	PHE	CB-CG-CD2	7.50	126.05	120.80
1	B	63	GLN	CG-CD-OE1	7.50	136.59	121.60
1	C	186	VAL	C-N-CA	7.50	140.44	121.70
1	D	139	GLN	N-CA-CB	7.49	124.09	110.60
1	D	192	ARG	N-CA-CB	-7.49	97.11	110.60
1	E	210	ARG	CB-CA-C	7.49	125.39	110.40
1	D	108	TRP	CE2-CD2-CG	7.49	113.29	107.30
1	D	107	LEU	CD1-CG-CD2	-7.49	88.03	110.50
1	E	54	GLY	CA-C-N	7.49	133.67	117.20
1	F	7	LEU	CA-C-N	-7.49	100.73	117.20
1	C	200	ASN	O-C-N	-7.48	110.73	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	LEU	N-CA-CB	7.48	125.36	110.40
1	C	184	ARG	CA-CB-CG	-7.48	96.95	113.40
1	A	47	VAL	CA-C-N	7.48	133.65	117.20
1	F	5	PHE	C-N-CA	7.48	138.00	122.30
1	E	18	HIS	C-N-CA	-7.47	103.02	121.70
1	D	210	ARG	O-C-N	7.47	134.65	122.70
1	D	75	ASN	CB-CG-ND2	-7.46	98.78	116.70
1	D	169	ASP	CA-C-O	7.46	135.77	120.10
1	B	67	LEU	CA-C-N	7.46	133.62	117.20
1	F	149	LEU	O-C-N	7.46	134.64	122.70
1	E	175	ASN	CA-C-O	7.46	135.77	120.10
1	D	174	THR	N-CA-CB	7.46	124.47	110.30
1	D	217	PHE	O-C-N	-7.46	110.77	122.70
1	E	5	PHE	CA-CB-CG	7.46	131.80	113.90
1	E	128	LEU	CA-CB-CG	7.46	132.46	115.30
1	B	74	GLN	CG-CD-OE1	-7.46	106.69	121.60
1	A	79	TRP	CA-C-O	-7.46	104.44	120.10
1	D	17	LEU	CB-CA-C	7.45	124.36	110.20
1	D	181	THR	CB-CA-C	7.45	131.72	111.60
1	E	166	ASP	CB-CA-C	7.45	125.31	110.40
1	F	25	LEU	CB-CA-C	-7.45	96.04	110.20
1	A	130	SER	N-CA-CB	-7.45	99.32	110.50
1	D	226	ALA	CA-C-O	7.45	135.75	120.10
1	F	149	LEU	CB-CG-CD2	7.45	123.67	111.00
1	D	78	ARG	CA-C-O	7.45	135.74	120.10
1	A	131	THR	CA-C-O	7.45	135.74	120.10
1	E	65	ASP	N-CA-CB	-7.45	97.20	110.60
1	E	84	LYS	CA-CB-CG	7.45	129.78	113.40
1	F	97	ASP	N-CA-CB	-7.45	97.20	110.60
1	D	38	LEU	CA-CB-CG	-7.44	98.18	115.30
1	D	147	LEU	O-C-N	-7.44	110.80	122.70
1	E	68	LEU	CB-CG-CD1	-7.44	98.35	111.00
1	A	83	THR	CA-C-O	-7.44	104.48	120.10
1	A	214	ARG	CB-CG-CD	7.44	130.94	111.60
1	B	5	PHE	O-C-N	-7.44	110.56	123.20
1	B	93	VAL	CA-CB-CG1	7.44	122.06	110.90
1	D	141	LEU	CA-C-O	-7.44	104.48	120.10
1	E	61	VAL	CG1-CB-CG2	-7.44	99.00	110.90
1	F	7	LEU	CA-CB-CG	-7.44	98.19	115.30
1	A	1	ASN	CB-CG-ND2	7.44	134.55	116.70
1	B	41	PHE	N-CA-CB	-7.43	97.22	110.60
1	D	125	ASN	CA-C-O	7.43	135.71	120.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	188	GLN	O-C-N	-7.43	106.98	121.10
1	F	216	VAL	CA-C-O	7.42	135.69	120.10
1	A	91	VAL	CB-CA-C	7.42	125.49	111.40
1	A	105	PRO	O-C-N	7.42	135.81	123.20
1	D	106	GLY	CA-C-O	-7.42	107.25	120.60
1	A	76	THR	CA-C-O	-7.42	104.52	120.10
1	A	126	SER	N-CA-CB	7.42	121.62	110.50
1	F	90	TYR	CG-CD1-CE1	7.42	127.23	121.30
1	C	215	TYR	CZ-CE2-CD2	-7.42	113.13	119.80
1	D	6	GLY	O-C-N	7.42	134.56	122.70
1	B	215	TYR	CB-CA-C	-7.41	95.58	110.40
1	C	152	TYR	CD1-CE1-CZ	7.41	126.47	119.80
1	D	69	VAL	CA-CB-CG2	7.41	122.01	110.90
1	E	28	PHE	CG-CD2-CE2	7.41	128.95	120.80
1	B	221	PRO	C-N-CA	7.40	140.20	121.70
1	C	131	THR	N-CA-C	-7.40	91.01	111.00
1	B	165	PHE	CG-CD1-CE1	7.40	128.94	120.80
1	D	142	HIS	CB-CA-C	-7.40	95.61	110.40
1	D	151	PRO	CA-C-N	7.40	133.47	117.20
1	B	30	PHE	C-N-CA	7.39	140.19	121.70
1	F	137	HIS	CB-CA-C	-7.39	95.61	110.40
1	A	80	SER	CB-CA-C	-7.39	96.05	110.10
1	B	32	MET	C-N-CA	-7.39	103.22	121.70
1	C	140	THR	CA-CB-CG2	7.39	122.75	112.40
1	E	179	LYS	O-C-N	-7.39	110.64	123.20
1	F	228	TYR	CG-CD1-CE1	7.39	127.21	121.30
1	A	155	SER	CA-C-N	-7.38	100.96	117.20
1	B	84	LYS	C-N-CA	7.38	137.81	122.30
1	D	112	THR	N-CA-CB	-7.38	96.27	110.30
1	E	72	THR	CA-C-O	7.38	135.61	120.10
1	F	222	ASP	OD1-CG-OD2	7.38	137.32	123.30
1	E	23	LEU	N-CA-CB	7.37	125.15	110.40
1	E	110	SER	CB-CA-C	-7.37	96.09	110.10
1	C	103	TYR	CE1-CZ-CE2	7.37	131.59	119.80
1	E	222	ASP	CA-C-O	-7.37	104.62	120.10
1	A	137	HIS	CB-CG-ND1	7.37	141.62	123.20
1	C	181	THR	CA-CB-OG1	-7.37	93.53	109.00
1	E	37	ASN	CB-CG-ND2	-7.37	99.02	116.70
1	E	232	LEU	C-N-CA	-7.37	103.28	121.70
1	D	28	PHE	CG-CD1-CE1	7.37	128.90	120.80
1	B	85	GLY	N-CA-C	-7.36	94.69	113.10
1	B	172	TRP	CZ3-CH2-CZ2	-7.36	112.77	121.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	140	THR	N-CA-C	7.36	130.88	111.00
1	E	222	ASP	O-C-N	7.36	134.48	122.70
1	E	114	ASN	OD1-CG-ND2	7.36	138.83	121.90
1	F	108	TRP	CA-C-N	7.36	133.40	117.20
1	B	146	SER	N-CA-C	7.36	130.88	111.00
1	D	75	ASN	CA-CB-CG	-7.36	97.21	113.40
1	A	24	GLU	CG-CD-OE1	7.36	133.02	118.30
1	B	31	THR	CB-CA-C	-7.36	91.73	111.60
1	B	209	SER	N-CA-C	7.36	130.87	111.00
1	D	29	ARG	CB-CA-C	-7.36	95.68	110.40
1	D	112	THR	CA-CB-CG2	-7.36	102.10	112.40
1	E	1	ASN	N-CA-CB	7.36	123.84	110.60
1	A	66	GLY	CA-C-O	-7.35	107.36	120.60
1	B	165	PHE	CA-C-O	-7.35	104.66	120.10
1	D	89	ASN	CA-C-N	7.35	133.37	117.20
1	A	166	ASP	CB-CG-OD1	-7.35	111.68	118.30
1	C	132	GLN	CG-CD-NE2	7.35	134.34	116.70
1	C	59	ARG	CA-CB-CG	7.34	129.56	113.40
1	D	167	ARG	CD-NE-CZ	-7.34	113.32	123.60
1	F	44	ASP	CA-C-O	7.34	135.52	120.10
1	C	48	TRP	CH2-CZ2-CE2	-7.34	110.06	117.40
1	E	58	CYS	O-C-N	-7.34	110.95	122.70
1	F	61	VAL	N-CA-C	7.34	130.82	111.00
1	F	188	GLN	CA-C-O	7.34	135.52	120.10
1	F	193	MET	O-C-N	-7.34	110.95	122.70
1	F	219	LEU	CA-C-O	-7.34	104.68	120.10
1	A	59	ARG	CD-NE-CZ	7.34	133.88	123.60
1	B	163	VAL	CA-C-O	7.34	135.51	120.10
1	B	228	TYR	CD1-CG-CD2	-7.33	109.83	117.90
1	E	122	ASN	O-C-N	-7.33	110.96	122.70
1	E	199	GLN	C-N-CA	7.33	140.03	121.70
1	F	204	TRP	CB-CG-CD1	7.33	136.53	127.00
1	B	167	ARG	NE-CZ-NH1	-7.33	116.64	120.30
1	D	140	THR	CA-C-O	7.33	135.48	120.10
1	E	166	ASP	OD1-CG-OD2	7.33	137.22	123.30
1	F	13	HIS	CB-CA-C	7.33	125.05	110.40
1	A	41	PHE	O-C-N	7.32	134.42	122.70
1	B	30	PHE	CB-CA-C	-7.32	95.76	110.40
1	B	7	LEU	C-N-CA	7.32	140.00	121.70
1	C	193	MET	CB-CA-C	7.32	125.04	110.40
1	F	157	GLU	CA-CB-CG	7.32	129.50	113.40
1	F	224	ASN	CA-CB-CG	-7.32	97.29	113.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	196	LEU	CB-CA-C	-7.32	96.30	110.20
1	F	228	TYR	CB-CG-CD1	7.32	125.39	121.00
1	C	170	ARG	CB-CG-CD	7.31	130.61	111.60
1	A	39	VAL	N-CA-CB	-7.31	95.42	111.50
1	C	13	HIS	O-C-N	-7.31	107.22	121.10
1	D	167	ARG	CB-CA-C	7.31	125.01	110.40
1	C	18	HIS	CA-CB-CG	7.31	126.02	113.60
1	D	85	GLY	CA-C-N	7.31	133.27	117.20
1	F	183	CYS	O-C-N	-7.31	111.01	122.70
1	B	24	GLU	N-CA-CB	-7.30	97.45	110.60
1	D	107	LEU	CA-C-N	7.30	133.27	117.20
1	A	94	LEU	N-CA-C	-7.30	91.28	111.00
1	D	45	VAL	N-CA-CB	7.30	127.56	111.50
1	D	106	GLY	N-CA-C	-7.30	94.85	113.10
1	A	120	VAL	CA-C-N	7.30	133.26	117.20
1	F	129	TYR	CA-CB-CG	7.30	127.27	113.40
1	B	199	GLN	O-C-N	-7.30	111.03	122.70
1	C	132	GLN	CB-CG-CD	7.29	130.57	111.60
1	B	206	SER	CA-CB-OG	7.29	130.89	111.20
1	E	197	THR	CA-CB-CG2	7.29	122.61	112.40
1	F	128	LEU	CB-CG-CD2	7.29	123.40	111.00
1	F	204	TRP	CG-CD2-CE3	-7.29	127.34	133.90
1	E	235	THR	CA-C-O	7.29	135.41	120.10
1	D	37	ASN	CB-CG-OD1	-7.29	107.02	121.60
1	A	59	ARG	O-C-N	7.29	134.36	122.70
1	B	39	VAL	C-N-CA	7.29	139.91	121.70
1	B	131	THR	C-N-CA	-7.29	103.49	121.70
1	B	187	LEU	N-CA-CB	7.29	124.97	110.40
1	C	157	GLU	OE1-CD-OE2	7.29	132.04	123.30
1	B	226	ALA	O-C-N	7.28	134.35	122.70
1	B	18	HIS	O-C-N	-7.28	111.05	122.70
1	C	20	ALA	CA-C-O	7.28	135.39	120.10
1	D	69	VAL	CB-CA-C	7.28	125.23	111.40
1	E	144	THR	N-CA-CB	7.28	124.13	110.30
1	A	83	THR	CA-CB-CG2	-7.28	102.21	112.40
1	B	92	LEU	CA-C-O	-7.28	104.82	120.10
1	C	118	VAL	N-CA-C	7.27	130.64	111.00
1	D	67	LEU	CA-C-N	7.27	133.20	117.20
1	E	12	SER	CA-C-N	-7.27	101.20	117.20
1	E	158	THR	CA-C-O	-7.27	104.83	120.10
1	C	164	LEU	O-C-N	7.27	134.33	122.70
1	E	25	LEU	CD1-CG-CD2	-7.27	88.69	110.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	224	ASN	N-CA-CB	-7.27	97.51	110.60
1	B	13	HIS	N-CA-CB	-7.27	97.52	110.60
1	C	131	THR	CB-CA-C	7.27	131.22	111.60
1	C	229	GLY	N-CA-C	7.27	131.27	113.10
1	C	90	TYR	N-CA-CB	-7.26	97.52	110.60
1	A	84	LYS	CB-CA-C	7.26	124.93	110.40
1	F	14	PRO	N-CA-CB	7.26	112.01	103.30
1	F	100	VAL	CA-C-O	-7.26	104.86	120.10
1	B	230	GLY	CA-C-O	-7.25	107.54	120.60
1	C	121	ALA	C-N-CA	7.25	139.84	121.70
1	F	77	ILE	CA-CB-CG1	7.25	124.78	111.00
1	C	108	TRP	CB-CG-CD2	-7.25	117.17	126.60
1	D	62	LEU	N-CA-CB	7.25	124.90	110.40
1	B	136	ASN	N-CA-CB	7.25	123.65	110.60
1	F	155	SER	CA-CB-OG	-7.25	91.63	111.20
1	E	9	HIS	N-CA-CB	-7.25	97.56	110.60
1	E	173	SER	O-C-N	-7.25	111.11	122.70
1	A	31	THR	C-N-CA	7.24	139.81	121.70
1	E	119	VAL	O-C-N	-7.24	111.11	122.70
1	B	71	LEU	CA-C-O	-7.24	104.90	120.10
1	B	234	THR	CA-CB-CG2	7.24	122.54	112.40
1	C	57	GLY	C-N-CA	-7.24	103.60	121.70
1	D	25	LEU	CB-CG-CD1	-7.24	98.69	111.00
1	B	6	GLY	C-N-CA	7.23	139.78	121.70
1	E	114	ASN	N-CA-C	7.23	130.53	111.00
1	C	147	LEU	CA-C-N	-7.23	101.29	117.20
1	F	145	GLN	CG-CD-OE1	-7.23	107.14	121.60
1	D	211	SER	N-CA-C	7.23	130.51	111.00
1	E	230	GLY	N-CA-C	-7.22	95.04	113.10
1	E	79	TRP	O-C-N	7.22	134.26	122.70
1	C	109	ASP	CA-CB-CG	7.22	129.28	113.40
1	D	91	VAL	CB-CA-C	7.22	125.12	111.40
1	A	81	SER	CB-CA-C	7.22	123.81	110.10
1	C	228	TYR	C-N-CA	7.21	137.45	122.30
1	F	62	LEU	CA-C-N	-7.21	101.33	117.20
1	C	147	LEU	O-C-N	7.21	134.24	122.70
1	A	165	PHE	CD1-CG-CD2	-7.21	108.92	118.30
1	D	167	ARG	CA-C-O	7.21	135.25	120.10
1	A	26	SER	O-C-N	-7.21	111.17	122.70
1	E	195	VAL	CG1-CB-CG2	7.21	122.43	110.90
1	E	215	TYR	CB-CG-CD2	7.21	125.33	121.00
1	B	147	LEU	CB-CA-C	-7.21	96.51	110.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	193	MET	N-CA-CB	7.20	123.57	110.60
1	A	166	ASP	O-C-N	7.20	134.22	122.70
1	A	152	TYR	CD1-CG-CD2	-7.20	109.98	117.90
1	B	69	VAL	O-C-N	7.20	134.22	122.70
1	D	229	GLY	C-N-CA	7.20	137.41	122.30
1	E	220	GLN	CA-CB-CG	-7.20	97.56	113.40
1	B	73	ALA	CA-C-N	7.20	133.03	117.20
1	B	54	GLY	CA-C-N	7.20	133.03	117.20
1	B	224	ASN	CA-C-N	7.20	133.03	117.20
1	D	152	TYR	CZ-CE2-CD2	-7.20	113.32	119.80
1	A	218	VAL	CA-C-O	-7.19	105.00	120.10
1	B	56	THR	CA-C-N	7.19	130.58	116.20
1	F	160	CYS	CA-C-N	-7.18	101.40	117.20
1	A	111	GLY	CA-C-N	7.18	133.00	117.20
1	C	117	SER	CA-C-O	7.18	135.19	120.10
1	D	208	ASN	CA-C-N	-7.18	101.40	117.20
1	E	149	LEU	CA-CB-CG	-7.18	98.78	115.30
1	D	44	ASP	O-C-N	-7.18	111.21	122.70
1	F	59	ARG	CG-CD-NE	7.18	126.87	111.80
1	C	67	LEU	O-C-N	7.18	134.18	122.70
1	C	171	VAL	CA-C-N	7.18	132.99	117.20
1	A	71	LEU	CA-C-O	7.17	135.16	120.10
1	A	81	SER	CA-C-O	-7.17	105.05	120.10
1	C	216	VAL	C-N-CA	7.17	139.62	121.70
1	D	177	ALA	CA-C-N	-7.17	101.87	116.20
1	E	7	LEU	CA-C-O	-7.17	105.05	120.10
1	C	71	LEU	CA-C-N	-7.17	101.44	117.20
1	E	216	VAL	CA-CB-CG2	7.16	121.65	110.90
1	C	64	SER	CA-CB-OG	7.16	130.54	111.20
1	A	33	GLN	CG-CD-NE2	-7.16	99.52	116.70
1	D	137	HIS	N-CA-CB	7.16	123.49	110.60
1	A	72	THR	C-N-CA	7.16	139.60	121.70
1	B	73	ALA	N-CA-C	-7.16	91.67	111.00
1	A	52	THR	CA-CB-CG2	7.16	122.42	112.40
1	A	171	VAL	CA-C-O	-7.16	105.07	120.10
1	C	217	PHE	CB-CG-CD2	-7.16	115.79	120.80
1	F	128	LEU	CB-CG-CD1	7.16	123.17	111.00
1	B	185	ALA	C-N-CA	7.16	139.59	121.70
1	F	210	ARG	CB-CG-CD	-7.16	93.00	111.60
1	C	181	THR	CA-CB-CG2	7.15	122.42	112.40
1	D	147	LEU	CA-CB-CG	7.15	131.75	115.30
1	B	186	VAL	CG1-CB-CG2	-7.15	99.46	110.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	LEU	CA-CB-CG	7.15	131.74	115.30
1	F	101	THR	N-CA-CB	-7.15	96.72	110.30
1	C	66	GLY	CA-C-N	-7.14	101.48	117.20
1	F	139	GLN	CB-CG-CD	7.14	130.17	111.60
1	C	17	LEU	CA-C-N	7.14	132.91	117.20
1	C	152	TYR	CA-CB-CG	7.14	126.97	113.40
1	C	167	ARG	N-CA-CB	7.14	123.45	110.60
1	B	81	SER	CA-C-O	-7.14	105.11	120.10
1	C	131	THR	CA-CB-CG2	7.14	122.39	112.40
1	F	59	ARG	CA-C-N	-7.14	101.49	117.20
1	B	203	VAL	N-CA-C	-7.14	91.73	111.00
1	F	23	LEU	N-CA-CB	-7.14	96.12	110.40
1	A	233	TRP	CB-CG-CD2	7.14	135.88	126.60
1	C	50	SER	O-C-N	-7.13	111.28	122.70
1	C	214	ARG	C-N-CA	7.13	139.54	121.70
1	A	167	ARG	NH1-CZ-NH2	-7.13	111.56	119.40
1	B	128	LEU	CA-C-O	7.13	135.07	120.10
1	A	225	LEU	C-N-CA	-7.13	103.88	121.70
1	C	233	TRP	CE3-CZ3-CH2	7.12	129.04	121.20
1	F	203	VAL	CG1-CB-CG2	-7.12	99.50	110.90
1	F	215	TYR	CG-CD2-CE2	-7.12	115.60	121.30
1	B	160	CYS	CA-CB-SG	-7.12	101.18	114.00
1	B	159	ASP	CB-CG-OD1	-7.12	111.89	118.30
1	E	8	SER	CA-C-O	7.12	135.05	120.10
1	A	145	GLN	CG-CD-NE2	7.12	133.78	116.70
1	C	36	CYS	N-CA-C	7.12	130.22	111.00
1	F	138	PRO	CB-CA-C	-7.11	94.21	112.00
1	C	57	GLY	CA-C-O	-7.11	107.80	120.60
1	C	113	SER	N-CA-CB	-7.11	99.83	110.50
1	D	197	THR	N-CA-C	7.11	130.20	111.00
1	A	59	ARG	CA-CB-CG	7.11	129.03	113.40
1	C	5	PHE	CZ-CE2-CD2	7.11	128.63	120.10
1	C	136	ASN	CA-C-O	7.11	135.02	120.10
1	C	156	MET	CA-C-O	-7.10	105.18	120.10
1	C	224	ASN	CA-CB-CG	-7.10	97.79	113.40
1	F	79	TRP	CD1-NE1-CE2	-7.10	102.61	109.00
1	D	178	GLY	O-C-N	-7.09	111.35	122.70
1	D	222	ASP	CB-CG-OD1	-7.09	111.91	118.30
1	F	52	THR	C-N-CA	7.09	139.44	121.70
1	F	154	LEU	CD1-CG-CD2	-7.09	89.22	110.50
1	C	175	ASN	C-N-CA	7.09	139.43	121.70
1	D	64	SER	N-CA-CB	-7.09	99.86	110.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	144	THR	OG1-CB-CG2	-7.09	93.69	110.00
1	F	30	PHE	CD1-CE1-CZ	-7.09	111.59	120.10
1	A	3	ILE	O-C-N	-7.09	111.36	122.70
1	E	65	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	E	209	SER	N-CA-C	-7.09	91.86	111.00
1	F	234	THR	CA-C-N	7.09	132.80	117.20
1	B	160	CYS	N-CA-CB	7.09	123.36	110.60
1	B	130	SER	O-C-N	-7.09	111.36	122.70
1	B	202	ALA	N-CA-C	-7.09	91.87	111.00
1	D	14	PRO	CA-C-O	-7.09	103.19	120.20
1	C	216	VAL	O-C-N	-7.08	111.36	122.70
1	F	196	LEU	CB-CG-CD1	7.08	123.04	111.00
1	B	233	TRP	CD2-CE2-CZ2	7.08	130.80	122.30
1	C	228	TYR	OH-CZ-CE2	7.08	139.21	120.10
1	A	93	VAL	CG1-CB-CG2	7.08	122.22	110.90
1	C	149	LEU	O-C-N	7.08	134.02	122.70
1	D	209	SER	N-CA-C	7.08	130.11	111.00
1	E	52	THR	CA-C-N	7.08	132.77	117.20
1	F	167	ARG	NE-CZ-NH2	7.08	123.84	120.30
1	A	176	THR	CB-CA-C	7.07	130.70	111.60
1	D	5	PHE	CD1-CE1-CZ	7.07	128.59	120.10
1	D	144	THR	CA-CB-CG2	7.07	122.30	112.40
1	C	207	GLY	CA-C-O	-7.07	107.88	120.60
1	B	175	ASN	CB-CA-C	7.07	124.53	110.40
1	F	108	TRP	CB-CA-C	7.07	124.54	110.40
1	E	221	PRO	O-C-N	7.06	134.00	122.70
1	C	146	SER	N-CA-C	7.06	130.07	111.00
1	D	144	THR	N-CA-C	-7.06	91.93	111.00
1	C	98	ARG	CG-CD-NE	-7.06	96.97	111.80
1	D	91	VAL	CA-C-N	7.06	132.73	117.20
1	B	103	TYR	CG-CD1-CE1	7.06	126.94	121.30
1	A	172	TRP	CD2-CE3-CZ3	7.06	127.97	118.80
1	D	44	ASP	CB-CA-C	7.06	124.51	110.40
1	D	84	LYS	CA-CB-CG	7.05	128.92	113.40
1	C	192	ARG	CA-CB-CG	7.05	128.92	113.40
1	D	199	GLN	CA-C-N	7.05	132.71	117.20
1	D	204	TRP	CA-CB-CG	7.05	127.09	113.70
1	B	196	LEU	CB-CA-C	-7.04	96.82	110.20
1	C	36	CYS	O-C-N	7.04	133.97	122.70
1	B	89	ASN	CA-C-N	7.04	132.69	117.20
1	E	63	GLN	CG-CD-NE2	-7.04	99.81	116.70
1	E	6	GLY	O-C-N	7.03	133.96	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2	ASN	OD1-CG-ND2	-7.03	105.73	121.90
1	C	86	SER	CA-CB-OG	-7.03	92.21	111.20
1	C	216	VAL	CA-C-N	7.03	132.66	117.20
1	E	28	PHE	CG-CD1-CE1	7.03	128.53	120.80
1	E	27	SER	CA-CB-OG	-7.02	92.23	111.20
1	C	48	TRP	CB-CA-C	7.02	124.45	110.40
1	C	126	SER	O-C-N	7.02	133.93	122.70
1	D	154	LEU	O-C-N	-7.02	111.46	122.70
1	E	37	ASN	OD1-CG-ND2	7.02	138.05	121.90
1	F	100	VAL	CA-CB-CG1	-7.02	100.37	110.90
1	A	62	LEU	CB-CG-CD2	7.02	122.94	111.00
1	F	142	HIS	CA-CB-CG	-7.02	101.67	113.60
1	B	61	VAL	CB-CA-C	-7.02	98.06	111.40
1	D	101	THR	OG1-CB-CG2	7.02	126.15	110.00
1	F	141	LEU	CB-CA-C	7.02	123.54	110.20
1	F	142	HIS	CG-ND1-CE1	7.02	118.03	108.20
1	F	159	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	B	147	LEU	O-C-N	7.02	133.93	122.70
1	D	148	GLN	CA-C-O	7.02	134.84	120.10
1	A	164	LEU	C-N-CA	-7.02	104.16	121.70
1	F	87	ILE	CA-CB-CG1	-7.02	97.67	111.00
1	B	59	ARG	NE-CZ-NH1	-7.01	116.79	120.30
1	D	200	ASN	CB-CA-C	7.01	124.42	110.40
1	F	215	TYR	CG-CD1-CE1	7.01	126.91	121.30
1	B	127	ILE	CA-CB-CG2	-7.01	96.88	110.90
1	E	74	GLN	CA-CB-CG	7.01	128.82	113.40
1	E	219	LEU	CB-CA-C	-7.01	96.88	110.20
1	E	5	PHE	CB-CG-CD2	-7.01	115.89	120.80
1	F	151	PRO	O-C-N	-7.01	111.48	122.70
1	A	129	TYR	CZ-CE2-CD2	7.00	126.11	119.80
1	A	172	TRP	CE3-CZ3-CH2	-7.00	113.50	121.20
1	B	50	SER	N-CA-CB	-7.00	100.00	110.50
1	C	79	TRP	N-CA-CB	-7.00	98.00	110.60
1	B	200	ASN	N-CA-C	7.00	129.90	111.00
1	E	43	SER	O-C-N	-7.00	111.51	122.70
1	A	229	GLY	O-C-N	-6.99	111.32	123.20
1	C	116	GLY	C-N-CA	6.99	139.17	121.70
1	E	107	LEU	CA-C-N	6.99	132.57	117.20
1	F	79	TRP	CE3-CZ3-CH2	-6.99	113.51	121.20
1	F	147	LEU	CA-C-N	-6.99	101.83	117.20
1	A	4	LEU	CA-C-O	-6.99	105.43	120.10
1	C	123	ASN	N-CA-C	6.99	129.86	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	188	GLN	CA-C-N	6.98	136.65	117.10
1	F	39	VAL	CA-C-N	-6.98	101.85	117.20
1	D	84	LYS	CB-CA-C	-6.98	96.45	110.40
1	D	101	THR	CA-C-N	6.98	132.55	117.20
1	E	92	LEU	N-CA-CB	6.98	124.36	110.40
1	A	67	LEU	CB-CG-CD2	-6.97	99.14	111.00
1	D	148	GLN	C-N-CA	6.97	139.14	121.70
1	F	77	ILE	O-C-N	-6.97	111.54	122.70
1	A	137	HIS	CG-CD2-NE2	-6.97	95.96	109.20
1	B	110	SER	CA-C-N	6.97	130.14	116.20
1	B	144	THR	OG1-CB-CG2	-6.97	93.97	110.00
1	C	166	ASP	CA-CB-CG	6.97	128.73	113.40
1	A	185	ALA	CA-C-N	-6.96	101.88	117.20
1	D	97	ASP	CA-C-N	6.96	132.52	117.20
1	F	220	GLN	CG-CD-NE2	6.96	133.41	116.70
1	C	159	ASP	OD1-CG-OD2	-6.96	110.08	123.30
1	B	42	ASP	CB-CG-OD1	-6.96	112.04	118.30
1	C	141	LEU	CA-C-O	-6.96	105.49	120.10
1	E	7	LEU	CB-CA-C	-6.96	96.98	110.20
1	E	145	GLN	O-C-N	6.96	133.83	122.70
1	F	43	SER	CA-C-O	6.96	134.71	120.10
1	F	103	TYR	N-CA-CB	6.96	123.12	110.60
1	B	3	ILE	CB-CG1-CD1	-6.96	94.43	113.90
1	B	212	ALA	CA-C-O	-6.96	105.49	120.10
1	B	17	LEU	O-C-N	-6.95	111.58	122.70
1	B	73	ALA	CA-C-O	-6.95	105.50	120.10
1	F	184	ARG	CB-CA-C	-6.95	96.50	110.40
1	D	161	ASN	CB-CA-C	-6.95	96.50	110.40
1	A	93	VAL	O-C-N	6.95	133.81	122.70
1	B	92	LEU	N-CA-C	-6.95	92.25	111.00
1	B	103	TYR	CZ-CE2-CD2	-6.95	113.55	119.80
1	D	37	ASN	CA-C-N	-6.95	101.92	117.20
1	F	194	ASP	OD1-CG-OD2	-6.95	110.10	123.30
1	A	142	HIS	ND1-CG-CD2	-6.94	96.28	106.00
1	B	2	ASN	N-CA-C	6.94	129.75	111.00
1	A	160	CYS	O-C-N	6.94	133.81	122.70
1	E	214	ARG	NH1-CZ-NH2	-6.94	111.76	119.40
1	F	16	THR	N-CA-C	6.94	129.75	111.00
1	B	184	ARG	CB-CA-C	-6.94	96.52	110.40
1	C	64	SER	CA-C-O	6.94	134.67	120.10
1	F	141	LEU	C-N-CA	6.94	139.05	121.70
1	C	29	ARG	NH1-CZ-NH2	-6.94	111.77	119.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	SER	CB-CA-C	6.94	123.28	110.10
1	F	17	LEU	CB-CA-C	-6.94	97.02	110.20
1	F	28	PHE	CD1-CE1-CZ	6.94	128.42	120.10
1	D	137	HIS	CB-CG-ND1	-6.93	105.86	123.20
1	B	21	GLN	CB-CG-CD	6.93	129.62	111.60
1	B	84	LYS	CA-C-N	6.93	130.07	116.20
1	B	225	LEU	CA-CB-CG	-6.93	99.36	115.30
1	E	42	ASP	N-CA-C	-6.93	92.28	111.00
1	F	136	ASN	N-CA-C	6.93	129.72	111.00
1	D	6	GLY	N-CA-C	-6.93	95.78	113.10
1	D	207	GLY	CA-C-O	6.93	133.07	120.60
1	E	123	ASN	N-CA-CB	-6.93	98.13	110.60
1	B	76	THR	CA-C-O	-6.92	105.56	120.10
1	E	47	VAL	CA-C-O	-6.92	105.56	120.10
1	F	129	TYR	CB-CA-C	6.92	124.25	110.40
1	F	158	THR	CA-CB-CG2	-6.92	102.71	112.40
1	E	12	SER	O-C-N	6.92	133.77	122.70
1	F	126	SER	N-CA-CB	-6.92	100.12	110.50
1	E	190	ASN	CA-C-N	6.92	130.03	116.20
1	A	69	VAL	CB-CA-C	-6.91	98.27	111.40
1	A	86	SER	N-CA-C	6.91	129.67	111.00
1	F	2	ASN	N-CA-CB	-6.91	98.16	110.60
1	F	92	LEU	N-CA-CB	6.91	124.23	110.40
1	C	173	SER	N-CA-CB	6.91	120.87	110.50
1	D	233	TRP	CZ3-CH2-CZ2	6.91	129.89	121.60
1	C	160	CYS	CA-C-N	6.91	132.40	117.20
1	B	34	SER	N-CA-CB	6.91	120.86	110.50
1	F	28	PHE	CA-C-O	6.91	134.60	120.10
1	B	72	THR	CA-C-O	-6.90	105.60	120.10
1	B	195	VAL	CA-CB-CG1	6.90	121.25	110.90
1	D	221	PRO	CA-C-N	6.90	132.38	117.20
1	F	80	SER	N-CA-CB	6.90	120.86	110.50
1	A	9	HIS	CA-CB-CG	6.90	125.33	113.60
1	C	49	ALA	CA-C-O	-6.90	105.61	120.10
1	C	1	ASN	N-CA-CB	6.90	123.02	110.60
1	E	66	GLY	C-N-CA	-6.90	104.46	121.70
1	A	63	GLN	CA-C-O	-6.90	105.62	120.10
1	D	138	PRO	O-C-N	-6.89	111.67	122.70
1	D	109	ASP	N-CA-C	6.89	129.61	111.00
1	E	51	ASN	CB-CA-C	-6.89	96.63	110.40
1	D	112	THR	N-CA-C	6.88	129.59	111.00
1	F	208	ASN	CB-CA-C	-6.88	96.63	110.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	91	VAL	C-N-CA	6.88	138.90	121.70
1	B	191	GLY	O-C-N	6.88	133.71	122.70
1	B	1	ASN	CB-CG-OD1	6.87	135.35	121.60
1	B	234	THR	O-C-N	-6.87	111.70	122.70
1	E	227	ILE	O-C-N	-6.87	111.70	122.70
1	D	108	TRP	CE3-CZ3-CH2	6.87	128.76	121.20
1	E	198	ASN	CB-CG-ND2	-6.87	100.21	116.70
1	D	3	ILE	CG1-CB-CG2	-6.87	96.29	111.40
1	C	33	GLN	O-C-N	6.86	133.68	122.70
1	D	2	ASN	O-C-N	-6.86	111.72	122.70
1	C	150	SER	O-C-N	6.86	134.14	121.10
1	D	108	TRP	O-C-N	-6.86	111.72	122.70
1	F	141	LEU	CB-CG-CD2	6.86	122.66	111.00
1	C	152	TYR	OH-CZ-CE2	6.86	138.62	120.10
1	B	141	LEU	C-N-CA	6.85	138.83	121.70
1	B	210	ARG	CG-CD-NE	6.85	126.19	111.80
1	E	204	TRP	O-C-N	6.85	133.66	122.70
1	F	165	PHE	CB-CG-CD1	6.85	125.60	120.80
1	E	161	ASN	O-C-N	6.85	133.66	122.70
1	A	202	ALA	CB-CA-C	6.85	120.38	110.10
1	B	137	HIS	CB-CG-CD2	-6.85	109.57	130.80
1	C	23	LEU	CA-CB-CG	-6.85	99.55	115.30
1	E	201	ILE	N-CA-CB	-6.85	95.05	110.80
1	A	208	ASN	C-N-CA	-6.85	104.58	121.70
1	A	35	ASP	CB-CG-OD2	6.84	124.46	118.30
1	D	178	GLY	C-N-CA	6.84	138.81	121.70
1	A	16	THR	N-CA-C	6.84	129.48	111.00
1	D	88	GLY	CA-C-N	6.84	132.25	117.20
1	A	72	THR	OG1-CB-CG2	-6.84	94.26	110.00
1	A	123	ASN	N-CA-C	6.84	129.47	111.00
1	A	173	SER	N-CA-CB	-6.84	100.24	110.50
1	A	159	ASP	N-CA-CB	6.84	122.91	110.60
1	E	154	LEU	O-C-N	6.84	133.64	122.70
1	F	62	LEU	CA-C-O	6.83	134.45	120.10
1	A	162	LEU	N-CA-CB	-6.83	96.74	110.40
1	C	47	VAL	CA-C-O	-6.83	105.76	120.10
1	B	5	PHE	CA-C-O	6.83	134.44	120.10
1	A	104	GLY	CA-C-N	-6.83	97.99	117.10
1	B	79	TRP	CB-CA-C	-6.83	96.75	110.40
1	A	142	HIS	N-CA-C	6.82	129.42	111.00
1	A	220	GLN	CA-C-O	-6.82	105.77	120.10
1	C	161	ASN	C-N-CA	-6.82	104.66	121.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	201	ILE	N-CA-CB	-6.82	95.12	110.80
1	A	40	LEU	CD1-CG-CD2	-6.81	90.07	110.50
1	B	140	THR	CA-CB-OG1	-6.81	94.70	109.00
1	C	158	THR	CA-CB-OG1	6.81	123.30	109.00
1	D	73	ALA	C-N-CA	6.81	138.72	121.70
1	A	228	TYR	CB-CG-CD1	-6.81	116.92	121.00
1	D	28	PHE	CB-CA-C	6.81	124.02	110.40
1	A	26	SER	CA-C-O	-6.80	105.81	120.10
1	F	211	SER	CB-CA-C	-6.80	97.17	110.10
1	D	46	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	13	HIS	CA-C-O	-6.80	105.82	120.10
1	F	20	ALA	C-N-CA	6.80	138.70	121.70
1	F	166	ASP	CB-CA-C	6.80	124.00	110.40
1	F	193	MET	CB-CG-SD	-6.80	92.00	112.40
1	C	146	SER	C-N-CA	6.80	138.69	121.70
1	B	136	ASN	O-C-N	-6.80	111.83	122.70
1	B	188	GLN	CA-CB-CG	6.80	128.35	113.40
1	B	195	VAL	CG1-CB-CG2	-6.79	100.03	110.90
1	C	190	ASN	CB-CA-C	6.79	123.99	110.40
1	B	105	PRO	N-CA-CB	6.79	111.45	103.30
1	F	67	LEU	CA-C-O	-6.79	105.84	120.10
1	B	2	ASN	CB-CA-C	-6.79	96.83	110.40
1	D	129	TYR	CD1-CG-CD2	6.79	125.36	117.90
1	D	192	ARG	CG-CD-NE	6.79	126.05	111.80
1	C	159	ASP	N-CA-CB	6.78	122.81	110.60
1	D	32	MET	CA-CB-CG	6.78	124.83	113.30
1	D	56	THR	CB-CA-C	-6.78	93.28	111.60
1	E	188	GLN	CA-C-N	6.78	136.09	117.10
1	F	32	MET	CA-C-O	-6.78	105.85	120.10
1	C	187	LEU	CB-CG-CD1	6.78	122.53	111.00
1	A	112	THR	OG1-CB-CG2	-6.78	94.41	110.00
1	A	142	HIS	CA-C-N	6.78	132.11	117.20
1	B	126	SER	CA-C-O	6.78	134.33	120.10
1	D	32	MET	CB-CA-C	-6.78	96.85	110.40
1	A	87	ILE	CA-C-N	6.78	129.75	116.20
1	D	221	PRO	C-N-CA	6.78	138.64	121.70
1	A	62	LEU	N-CA-CB	6.77	123.95	110.40
1	C	130	SER	C-N-CA	6.77	138.63	121.70
1	D	176	THR	CA-C-O	-6.77	105.88	120.10
1	E	234	THR	CA-CB-CG2	6.77	121.88	112.40
1	C	172	TRP	NE1-CE2-CD2	6.77	114.07	107.30
1	A	228	TYR	CD1-CE1-CZ	-6.77	113.71	119.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	141	LEU	CB-CG-CD2	6.77	122.50	111.00
1	D	74	GLN	CG-CD-OE1	-6.76	108.07	121.60
1	D	84	LYS	CA-C-N	6.76	129.73	116.20
1	B	125	ASN	N-CA-C	6.76	129.26	111.00
1	B	158	THR	CA-CB-CG2	-6.76	102.93	112.40
1	D	183	CYS	N-CA-C	6.76	129.26	111.00
1	D	211	SER	N-CA-CB	-6.76	100.36	110.50
1	E	152	TYR	CA-CB-CG	6.76	126.24	113.40
1	F	186	VAL	CA-C-O	-6.76	105.91	120.10
1	F	40	LEU	O-C-N	6.76	133.51	122.70
1	D	84	LYS	N-CA-CB	6.76	122.76	110.60
1	E	78	ARG	CB-CA-C	-6.76	96.89	110.40
1	F	201	ILE	CA-C-N	6.75	132.06	117.20
1	C	46	ARG	CB-CG-CD	6.75	129.16	111.60
1	A	217	PHE	C-N-CA	6.75	138.58	121.70
1	C	72	THR	C-N-CA	-6.75	104.82	121.70
1	B	128	LEU	N-CA-C	-6.75	92.78	111.00
1	D	218	VAL	CA-CB-CG1	-6.75	100.78	110.90
1	E	233	TRP	N-CA-CB	6.75	122.75	110.60
1	C	146	SER	O-C-N	6.75	133.50	122.70
1	E	145	GLN	N-CA-C	-6.74	92.80	111.00
1	F	89	ASN	N-CA-C	6.74	129.20	111.00
1	D	3	ILE	CA-C-O	-6.74	105.95	120.10
1	E	171	VAL	CA-CB-CG1	6.74	121.01	110.90
1	A	44	ASP	N-CA-C	-6.74	92.82	111.00
1	C	214	ARG	CA-C-N	6.74	132.02	117.20
1	D	73	ALA	CB-CA-C	-6.73	100.01	110.10
1	D	87	ILE	C-N-CA	-6.73	108.17	122.30
1	F	125	ASN	CB-CG-ND2	6.72	132.84	116.70
1	A	231	ALA	O-C-N	-6.72	111.94	122.70
1	F	99	THR	CA-CB-CG2	-6.72	102.99	112.40
1	F	232	LEU	CA-CB-CG	6.72	130.76	115.30
1	F	1	ASN	CA-C-O	6.72	134.21	120.10
1	B	15	GLN	CG-CD-NE2	6.72	132.82	116.70
1	C	106	GLY	CA-C-N	-6.72	102.42	117.20
1	A	152	TYR	CG-CD1-CE1	6.71	126.67	121.30
1	C	119	VAL	CB-CA-C	6.71	124.16	111.40
1	C	168	ASP	CA-C-O	-6.71	106.00	120.10
1	E	129	TYR	N-CA-C	6.71	129.12	111.00
1	F	201	ILE	CA-CB-CG1	6.71	123.75	111.00
1	B	44	ASP	CA-CB-CG	6.71	128.16	113.40
1	A	62	LEU	CB-CA-C	-6.71	97.46	110.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	162	LEU	N-CA-CB	-6.70	96.99	110.40
1	B	76	THR	CA-C-N	6.70	131.94	117.20
1	E	209	SER	C-N-CA	6.70	138.45	121.70
1	A	8	SER	N-CA-CB	-6.70	100.45	110.50
1	A	70	ILE	CA-C-O	6.70	134.17	120.10
1	F	204	TRP	CE2-CD2-CG	6.70	112.66	107.30
1	E	119	VAL	N-CA-C	6.70	129.08	111.00
1	E	163	VAL	CA-C-O	-6.70	106.04	120.10
1	C	144	THR	OG1-CB-CG2	6.69	125.40	110.00
1	D	190	ASN	CB-CG-OD1	6.69	134.99	121.60
1	F	181	THR	CA-C-N	6.69	129.59	116.20
1	C	98	ARG	NE-CZ-NH1	-6.69	116.95	120.30
1	E	232	LEU	CD1-CG-CD2	-6.69	90.43	110.50
1	D	139	GLN	CA-C-N	-6.69	102.48	117.20
1	C	37	ASN	CA-C-O	-6.69	106.06	120.10
1	F	165	PHE	N-CA-CB	-6.69	98.56	110.60
1	D	25	LEU	CA-C-O	-6.69	106.06	120.10
1	D	167	ARG	C-N-CA	6.69	138.41	121.70
1	A	21	GLN	O-C-N	6.68	133.39	122.70
1	D	96	PRO	O-C-N	-6.68	112.01	122.70
1	D	222	ASP	CB-CA-C	-6.68	97.03	110.40
1	B	123	ASN	O-C-N	-6.68	111.84	123.20
1	D	92	LEU	CA-C-N	6.68	131.89	117.20
1	A	42	ASP	CA-CB-CG	-6.68	98.71	113.40
1	A	189	PRO	CA-N-CD	-6.68	102.15	111.50
1	D	204	TRP	CA-C-O	-6.68	106.08	120.10
1	D	112	THR	O-C-N	-6.67	112.02	122.70
1	B	212	ALA	N-CA-CB	-6.67	100.76	110.10
1	C	113	SER	C-N-CA	6.67	138.38	121.70
1	C	174	THR	N-CA-CB	6.67	122.98	110.30
1	F	145	GLN	CA-CB-CG	-6.67	98.72	113.40
1	C	228	TYR	CA-C-N	-6.67	102.87	116.20
1	D	177	ALA	N-CA-C	-6.67	93.00	111.00
1	F	155	SER	CA-C-O	6.67	134.10	120.10
1	C	127	ILE	CA-CB-CG2	-6.67	97.57	110.90
1	C	139	GLN	CB-CG-CD	6.67	128.93	111.60
1	A	92	LEU	CA-C-N	6.66	131.86	117.20
1	C	201	ILE	C-N-CA	6.66	138.36	121.70
1	B	11	GLY	CA-C-N	-6.66	102.54	117.20
1	C	26	SER	CA-C-N	6.66	131.86	117.20
1	C	204	TRP	CH2-CZ2-CE2	6.66	124.06	117.40
1	D	188	GLN	CA-C-O	6.66	134.09	120.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	202	ALA	O-C-N	-6.66	112.04	122.70
1	F	25	LEU	CB-CG-CD1	-6.66	99.68	111.00
1	A	102	ILE	C-N-CA	-6.66	105.06	121.70
1	B	6	GLY	N-CA-C	-6.66	96.46	113.10
1	D	164	LEU	CB-CA-C	-6.66	97.56	110.20
1	F	48	TRP	O-C-N	6.66	133.35	122.70
1	F	61	VAL	C-N-CA	-6.66	105.06	121.70
1	F	74	GLN	CB-CA-C	-6.66	97.09	110.40
1	F	110	SER	C-N-CA	-6.66	108.32	122.30
1	A	165	PHE	CG-CD1-CE1	6.65	128.12	120.80
1	C	170	ARG	CA-C-O	-6.65	106.13	120.10
1	D	95	GLN	N-CA-CB	-6.65	98.63	110.60
1	E	194	ASP	CB-CG-OD1	6.65	124.29	118.30
1	A	66	GLY	CA-C-N	6.64	131.82	117.20
1	D	20	ALA	N-CA-CB	-6.64	100.80	110.10
1	A	138	PRO	O-C-N	-6.64	112.07	122.70
1	B	226	ALA	CA-C-N	-6.64	102.59	117.20
1	B	144	THR	O-C-N	-6.64	112.08	122.70
1	D	228	TYR	C-N-CA	6.64	136.24	122.30
1	A	34	SER	O-C-N	-6.64	112.08	122.70
1	A	143	ALA	N-CA-CB	-6.63	100.81	110.10
1	B	40	LEU	CB-CA-C	-6.63	97.60	110.20
1	F	210	ARG	CA-CB-CG	-6.63	98.81	113.40
1	B	219	LEU	CA-CB-CG	6.63	130.54	115.30
1	A	186	VAL	C-N-CA	-6.62	105.14	121.70
1	E	199	GLN	N-CA-CB	-6.62	98.68	110.60
1	E	35	ASP	C-N-CA	6.62	138.26	121.70
1	B	29	ARG	O-C-N	6.62	133.29	122.70
1	C	214	ARG	CG-CD-NE	6.62	125.70	111.80
1	E	16	THR	CB-CA-C	-6.62	93.72	111.60
1	E	67	LEU	C-N-CA	-6.62	105.15	121.70
1	A	195	VAL	CA-C-N	-6.62	102.64	117.20
1	A	227	ILE	CA-C-N	6.62	131.76	117.20
1	B	144	THR	CA-CB-CG2	6.62	121.66	112.40
1	A	97	ASP	CA-C-O	-6.62	106.21	120.10
1	C	46	ARG	CG-CD-NE	6.62	125.69	111.80
1	D	33	GLN	CA-C-O	-6.61	106.21	120.10
1	D	217	PHE	N-CA-CB	-6.61	98.70	110.60
1	E	79	TRP	CD1-NE1-CE2	-6.61	103.05	109.00
1	E	170	ARG	NE-CZ-NH1	-6.61	116.99	120.30
1	E	235	THR	N-CA-CB	-6.61	97.73	110.30
1	E	171	VAL	CA-C-N	6.61	131.75	117.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	GLN	N-CA-C	6.61	128.85	111.00
1	C	119	VAL	C-N-CA	6.61	138.23	121.70
1	A	138	PRO	CA-C-N	6.61	131.74	117.20
1	F	216	VAL	C-N-CA	6.61	138.22	121.70
1	A	156	MET	CG-SD-CE	6.60	110.77	100.20
1	B	1	ASN	C-N-CA	6.60	138.21	121.70
1	B	53	ALA	CA-C-O	-6.60	106.24	120.10
1	F	223	ARG	CA-CB-CG	-6.60	98.88	113.40
1	E	27	SER	CB-CA-C	-6.60	97.57	110.10
1	F	155	SER	C-N-CA	6.60	138.19	121.70
1	F	181	THR	CA-CB-CG2	-6.60	103.16	112.40
1	C	69	VAL	CA-CB-CG2	-6.59	101.01	110.90
1	E	2	ASN	N-CA-CB	-6.59	98.73	110.60
1	C	153	ARG	CB-CG-CD	-6.59	94.46	111.60
1	F	30	PHE	CG-CD2-CE2	-6.59	113.55	120.80
1	D	137	HIS	C-N-CD	-6.59	106.10	120.60
1	B	82	GLY	CA-C-N	-6.59	102.71	117.20
1	C	113	SER	N-CA-C	-6.59	93.22	111.00
1	E	23	LEU	N-CA-C	-6.59	93.22	111.00
1	F	222	ASP	CA-CB-CG	6.59	127.89	113.40
1	B	108	TRP	CE3-CZ3-CH2	6.58	128.44	121.20
1	B	162	LEU	C-N-CA	-6.58	105.24	121.70
1	A	29	ARG	CB-CA-C	-6.58	97.23	110.40
1	F	186	VAL	CA-CB-CG1	6.58	120.77	110.90
1	E	18	HIS	CA-C-O	-6.58	106.28	120.10
1	F	39	VAL	CG1-CB-CG2	-6.58	100.38	110.90
1	B	188	GLN	CA-C-N	6.58	135.51	117.10
1	F	209	SER	CA-C-O	-6.58	106.29	120.10
1	D	152	TYR	CG-CD2-CE2	6.57	126.56	121.30
1	E	192	ARG	CD-NE-CZ	6.57	132.80	123.60
1	E	47	VAL	CG1-CB-CG2	-6.57	100.39	110.90
1	E	154	LEU	CA-CB-CG	6.57	130.40	115.30
1	D	92	LEU	CB-CA-C	-6.57	97.73	110.20
1	E	99	THR	CA-C-O	6.57	133.89	120.10
1	F	235	THR	CA-CB-OG1	6.57	122.79	109.00
1	C	86	SER	CA-C-O	-6.56	106.32	120.10
1	C	109	ASP	CB-CG-OD2	6.56	124.21	118.30
1	C	126	SER	N-CA-CB	6.56	120.34	110.50
1	C	190	ASN	CB-CG-ND2	6.56	132.45	116.70
1	A	130	SER	CA-C-N	6.56	131.63	117.20
1	B	111	GLY	CA-C-N	6.56	131.63	117.20
1	A	30	PHE	CA-CB-CG	6.56	129.64	113.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	103	TYR	N-CA-CB	-6.55	98.80	110.60
1	D	152	TYR	CB-CA-C	-6.55	97.29	110.40
1	B	37	ASN	CA-C-O	-6.55	106.34	120.10
1	A	7	LEU	O-C-N	-6.55	112.22	122.70
1	C	107	LEU	CB-CA-C	6.55	122.65	110.20
1	A	89	ASN	CA-C-O	-6.55	106.35	120.10
1	C	107	LEU	CA-C-N	6.55	131.61	117.20
1	D	198	ASN	CB-CG-OD1	-6.55	108.50	121.60
1	E	30	PHE	CA-CB-CG	6.55	129.62	113.90
1	F	68	LEU	CA-C-N	-6.55	102.79	117.20
1	C	165	PHE	CB-CG-CD2	6.55	125.38	120.80
1	E	184	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	F	1	ASN	N-CA-C	6.54	128.67	111.00
1	F	74	GLN	OE1-CD-NE2	6.54	136.95	121.90
1	A	30	PHE	CB-CG-CD2	6.54	125.38	120.80
1	A	200	ASN	CA-C-O	6.54	133.84	120.10
1	D	168	ASP	CA-C-O	6.54	133.84	120.10
1	F	165	PHE	CA-C-N	6.54	131.60	117.20
1	C	3	ILE	CG1-CB-CG2	-6.54	97.01	111.40
1	C	174	THR	CA-C-O	6.54	133.84	120.10
1	D	141	LEU	N-CA-CB	-6.54	97.32	110.40
1	B	144	THR	CA-CB-OG1	6.54	122.73	109.00
1	A	48	TRP	CH2-CZ2-CE2	-6.54	110.86	117.40
1	C	10	GLU	CB-CG-CD	6.54	131.85	114.20
1	C	163	VAL	CA-CB-CG2	-6.54	101.09	110.90
1	A	63	GLN	CA-CB-CG	-6.54	99.02	113.40
1	A	165	PHE	CZ-CE2-CD2	6.54	127.94	120.10
1	A	130	SER	N-CA-C	6.53	128.63	111.00
1	A	1	ASN	N-CA-C	-6.53	93.38	111.00
1	B	139	GLN	OE1-CD-NE2	-6.53	106.89	121.90
1	E	69	VAL	CB-CA-C	-6.53	99.00	111.40
1	F	44	ASP	CB-CG-OD1	-6.52	112.43	118.30
1	D	188	GLN	CB-CA-C	6.52	123.44	110.40
1	D	206	SER	CA-C-O	-6.52	106.41	120.10
1	A	187	LEU	CB-CG-CD1	6.52	122.08	111.00
1	C	48	TRP	CD2-CE2-CZ2	6.51	130.12	122.30
1	A	219	LEU	CB-CG-CD2	6.51	122.07	111.00
1	B	97	ASP	CA-C-N	6.51	131.53	117.20
1	F	225	LEU	CB-CG-CD2	-6.51	99.93	111.00
1	A	13	HIS	CB-CG-ND1	6.51	139.47	123.20
1	C	195	VAL	N-CA-C	-6.51	93.43	111.00
1	A	78	ARG	O-C-N	-6.51	112.29	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	103	TYR	OH-CZ-CE2	-6.51	102.53	120.10
1	B	132	GLN	N-CA-C	6.50	128.56	111.00
1	D	48	TRP	N-CA-C	-6.50	93.45	111.00
1	A	127	ILE	O-C-N	-6.50	112.31	122.70
1	C	184	ARG	CA-C-O	6.50	133.74	120.10
1	D	131	THR	OG1-CB-CG2	6.50	124.94	110.00
1	C	42	ASP	CA-C-O	-6.49	106.46	120.10
1	A	74	GLN	CB-CA-C	-6.49	97.42	110.40
1	D	59	ARG	CG-CD-NE	-6.49	98.17	111.80
1	E	107	LEU	CB-CG-CD1	6.49	122.03	111.00
1	E	223	ARG	CB-CG-CD	6.49	128.47	111.60
1	C	98	ARG	CA-C-O	6.49	133.72	120.10
1	A	56	THR	CA-CB-CG2	-6.49	103.32	112.40
1	A	225	LEU	CA-C-O	6.49	133.72	120.10
1	D	24	GLU	C-N-CA	6.48	137.91	121.70
1	A	127	ILE	CA-C-N	6.48	131.46	117.20
1	B	16	THR	CB-CA-C	-6.48	94.09	111.60
1	C	40	LEU	CD1-CG-CD2	-6.48	91.05	110.50
1	C	56	THR	C-N-CA	6.48	135.91	122.30
1	C	132	GLN	OE1-CD-NE2	-6.48	106.99	121.90
1	F	21	GLN	O-C-N	6.48	133.07	122.70
1	F	198	ASN	N-CA-CB	-6.48	98.93	110.60
1	A	47	VAL	N-CA-C	6.48	128.50	111.00
1	A	228	TYR	CE1-CZ-OH	-6.48	102.61	120.10
1	C	100	VAL	N-CA-C	-6.48	93.50	111.00
1	C	234	THR	OG1-CB-CG2	-6.48	95.10	110.00
1	F	129	TYR	N-CA-C	6.48	128.49	111.00
1	B	169	ASP	CA-CB-CG	-6.47	99.16	113.40
1	C	48	TRP	CE3-CZ3-CH2	6.47	128.32	121.20
1	C	56	THR	N-CA-CB	6.47	122.60	110.30
1	E	31	THR	CA-C-O	6.47	133.69	120.10
1	F	86	SER	O-C-N	6.47	133.06	122.70
1	F	152	TYR	CE1-CZ-CE2	6.47	130.16	119.80
1	F	154	LEU	CA-C-N	6.47	131.44	117.20
1	C	92	LEU	CA-C-N	6.47	131.44	117.20
1	A	220	GLN	CA-C-N	6.47	135.21	117.10
1	C	206	SER	CA-CB-OG	6.47	128.66	111.20
1	A	231	ALA	CB-CA-C	-6.47	100.40	110.10
1	B	72	THR	OG1-CB-CG2	-6.47	95.13	110.00
1	A	147	LEU	C-N-CA	6.46	137.86	121.70
1	B	97	ASP	CA-CB-CG	6.46	127.62	113.40
1	B	62	LEU	CB-CA-C	-6.46	97.92	110.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	130	SER	N-CA-CB	-6.46	100.81	110.50
1	F	37	ASN	O-C-N	6.46	133.04	122.70
1	D	154	LEU	C-N-CA	6.46	137.85	121.70
1	C	137	HIS	C-N-CA	6.46	149.12	122.00
1	E	181	THR	N-CA-CB	6.46	122.57	110.30
1	E	198	ASN	CB-CG-OD1	6.46	134.51	121.60
1	A	186	VAL	CA-CB-CG2	6.45	120.58	110.90
1	D	172	TRP	CB-CG-CD2	6.45	134.99	126.60
1	E	157	GLU	C-N-CA	-6.45	105.58	121.70
1	E	217	PHE	CA-C-O	-6.45	106.56	120.10
1	D	138	PRO	CA-CB-CG	-6.45	91.75	104.00
1	E	161	ASN	N-CA-CB	-6.45	98.99	110.60
1	D	185	ALA	O-C-N	6.45	133.01	122.70
1	E	232	LEU	CA-C-O	-6.45	106.56	120.10
1	F	68	LEU	CA-C-O	6.45	133.64	120.10
1	D	228	TYR	CA-C-O	-6.44	106.57	120.10
1	D	63	GLN	CG-CD-OE1	-6.44	108.71	121.60
1	F	103	TYR	CG-CD2-CE2	6.44	126.45	121.30
1	B	18	HIS	C-N-CA	-6.44	105.60	121.70
1	F	172	TRP	N-CA-CB	-6.44	99.01	110.60
1	B	111	GLY	C-N-CA	6.44	137.79	121.70
1	B	214	ARG	CB-CG-CD	6.44	128.34	111.60
1	C	47	VAL	CA-C-N	6.44	131.37	117.20
1	F	103	TYR	CB-CG-CD2	6.44	124.86	121.00
1	E	58	CYS	CA-CB-SG	-6.44	102.42	114.00
1	B	181	THR	C-N-CA	-6.43	108.79	122.30
1	A	204	TRP	CA-C-O	6.43	133.60	120.10
1	B	58	CYS	CA-C-O	-6.43	106.60	120.10
1	E	193	MET	N-CA-C	-6.43	93.64	111.00
1	C	44	ASP	CA-C-N	6.43	131.34	117.20
1	E	219	LEU	CB-CG-CD2	6.43	121.93	111.00
1	C	166	ASP	CB-CG-OD2	-6.43	112.52	118.30
1	A	77	ILE	CA-C-N	6.42	131.33	117.20
1	C	46	ARG	CA-CB-CG	6.42	127.53	113.40
1	C	196	LEU	CB-CA-C	-6.42	97.99	110.20
1	A	169	ASP	N-CA-CB	6.42	122.16	110.60
1	A	167	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	D	172	TRP	CD1-NE1-CE2	-6.42	103.22	109.00
1	F	186	VAL	C-N-CA	-6.42	105.65	121.70
1	C	37	ASN	OD1-CG-ND2	6.42	136.66	121.90
1	D	51	ASN	N-CA-CB	-6.42	99.05	110.60
1	F	15	GLN	O-C-N	-6.42	112.43	122.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	GLN	CA-C-O	-6.42	106.63	120.10
1	E	87	ILE	C-N-CA	6.42	135.77	122.30
1	C	117	SER	N-CA-C	6.41	128.32	111.00
1	D	32	MET	CA-C-O	6.41	133.57	120.10
1	D	92	LEU	N-CA-C	-6.41	93.68	111.00
1	D	217	PHE	CG-CD1-CE1	6.41	127.85	120.80
1	E	70	ILE	CA-CB-CG2	-6.41	98.08	110.90
1	B	192	ARG	CA-C-O	-6.41	106.64	120.10
1	C	140	THR	CA-CB-OG1	-6.41	95.54	109.00
1	D	17	LEU	N-CA-CB	6.41	123.22	110.40
1	F	105	PRO	CA-C-N	6.41	129.02	116.20
1	D	39	VAL	CA-CB-CG1	-6.41	101.29	110.90
1	D	143	ALA	CB-CA-C	6.41	119.71	110.10
1	A	205	THR	O-C-N	-6.40	112.46	122.70
1	A	22	SER	CA-CB-OG	6.40	128.48	111.20
1	F	22	SER	O-C-N	-6.40	112.46	122.70
1	B	71	LEU	CB-CG-CD2	-6.40	100.12	111.00
1	A	97	ASP	CA-CB-CG	6.40	127.47	113.40
1	E	36	CYS	CA-C-O	-6.40	106.67	120.10
1	B	142	HIS	N-CA-C	6.40	128.27	111.00
1	A	198	ASN	CB-CG-OD1	-6.39	108.81	121.60
1	B	228	TYR	CA-C-N	6.39	128.99	116.20
1	D	33	GLN	O-C-N	-6.39	112.47	122.70
1	E	94	LEU	CB-CA-C	-6.39	98.05	110.20
1	A	51	ASN	CB-CG-ND2	6.39	132.04	116.70
1	B	232	LEU	CA-C-O	6.39	133.53	120.10
1	D	147	LEU	C-N-CA	6.39	137.68	121.70
1	E	175	ASN	CB-CG-OD1	6.39	134.39	121.60
1	D	104	GLY	CA-C-O	-6.39	109.10	120.60
1	A	45	VAL	CA-C-N	-6.39	103.15	117.20
1	A	103	TYR	O-C-N	-6.39	112.34	123.20
1	E	152	TYR	N-CA-CB	6.38	122.09	110.60
1	E	152	TYR	CD1-CE1-CZ	6.38	125.55	119.80
1	E	137	HIS	CB-CG-CD2	-6.38	111.01	130.80
1	B	58	CYS	N-CA-C	6.38	128.23	111.00
1	B	217	PHE	CA-CB-CG	-6.38	98.58	113.90
1	E	215	TYR	O-C-N	6.38	132.91	122.70
1	F	5	PHE	CG-CD1-CE1	6.38	127.82	120.80
1	F	14	PRO	O-C-N	-6.38	112.49	122.70
1	D	216	VAL	N-CA-CB	-6.38	97.47	111.50
1	C	145	GLN	OE1-CD-NE2	-6.37	107.24	121.90
1	E	28	PHE	O-C-N	-6.37	112.50	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	141	LEU	O-C-N	-6.37	112.50	122.70
1	B	206	SER	O-C-N	-6.37	112.37	123.20
1	C	122	ASN	N-CA-CB	6.37	122.07	110.60
1	F	186	VAL	O-C-N	6.37	132.89	122.70
1	B	21	GLN	OE1-CD-NE2	-6.37	107.26	121.90
1	D	99	THR	CA-C-N	-6.37	103.19	117.20
1	E	147	LEU	CB-CA-C	-6.37	98.11	110.20
1	B	219	LEU	CB-CA-C	-6.36	98.11	110.20
1	E	211	SER	O-C-N	-6.36	112.52	122.70
1	D	58	CYS	CA-C-O	-6.36	106.74	120.10
1	C	59	ARG	NH1-CZ-NH2	6.36	126.39	119.40
1	A	195	VAL	CB-CA-C	6.36	123.47	111.40
1	C	158	THR	O-C-N	-6.36	112.53	122.70
1	E	78	ARG	CB-CG-CD	6.35	128.12	111.60
1	F	92	LEU	O-C-N	6.35	132.87	122.70
1	D	225	LEU	CA-CB-CG	-6.35	100.69	115.30
1	E	159	ASP	OD1-CG-OD2	-6.35	111.23	123.30
1	E	188	GLN	CA-C-O	-6.35	106.76	120.10
1	C	233	TRP	CG-CD2-CE3	-6.35	128.19	133.90
1	F	30	PHE	CA-CB-CG	-6.35	98.66	113.90
1	A	53	ALA	CA-C-O	6.35	133.43	120.10
1	B	219	LEU	CA-C-N	6.35	131.17	117.20
1	E	48	TRP	CA-C-N	6.35	131.17	117.20
1	E	51	ASN	CA-CB-CG	6.35	127.36	113.40
1	F	150	SER	CA-C-O	-6.35	106.77	120.10
1	F	168	ASP	CA-CB-CG	6.35	127.37	113.40
1	A	119	VAL	O-C-N	-6.35	112.55	122.70
1	D	190	ASN	OD1-CG-ND2	-6.35	107.30	121.90
1	A	198	ASN	CA-C-O	6.34	133.42	120.10
1	D	207	GLY	N-CA-C	6.34	128.96	113.10
1	A	163	VAL	N-CA-CB	6.34	125.44	111.50
1	D	200	ASN	CA-CB-CG	-6.34	99.46	113.40
1	B	225	LEU	CB-CG-CD2	6.34	121.77	111.00
1	C	166	ASP	O-C-N	-6.34	112.56	122.70
1	E	169	ASP	CA-CB-CG	6.34	127.34	113.40
1	E	211	SER	CA-C-O	-6.33	106.80	120.10
1	F	10	GLU	CG-CD-OE1	6.33	130.97	118.30
1	A	77	ILE	N-CA-C	6.33	128.10	111.00
1	F	52	THR	CB-CA-C	-6.33	94.51	111.60
1	E	1	ASN	CB-CG-OD1	6.33	134.26	121.60
1	E	46	ARG	NE-CZ-NH2	6.33	123.46	120.30
1	A	56	THR	N-CA-CB	6.33	122.32	110.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	93	VAL	CA-C-O	-6.33	106.81	120.10
1	B	87	ILE	O-C-N	-6.33	112.45	123.20
1	C	205	THR	CB-CA-C	-6.33	94.52	111.60
1	F	108	TRP	CA-C-O	-6.33	106.82	120.10
1	D	165	PHE	N-CA-CB	6.32	121.98	110.60
1	F	50	SER	C-N-CA	6.32	137.49	121.70
1	B	142	HIS	O-C-N	-6.32	112.60	122.70
1	C	167	ARG	CA-C-O	-6.32	106.84	120.10
1	C	201	ILE	CA-CB-CG1	-6.32	99.00	111.00
1	F	33	GLN	CA-C-O	-6.32	106.84	120.10
1	F	189	PRO	CA-C-N	6.32	131.10	117.20
1	A	199	GLN	C-N-CA	6.31	137.48	121.70
1	D	108	TRP	CA-C-N	6.31	131.08	117.20
1	B	17	LEU	CA-C-N	6.31	131.08	117.20
1	C	217	PHE	CG-CD2-CE2	6.31	127.74	120.80
1	F	79	TRP	CB-CA-C	-6.31	97.78	110.40
1	F	151	PRO	CB-CA-C	6.31	127.77	112.00
1	A	175	ASN	OD1-CG-ND2	6.30	136.40	121.90
1	A	219	LEU	CB-CA-C	-6.30	98.22	110.20
1	F	165	PHE	CG-CD1-CE1	6.30	127.73	120.80
1	F	108	TRP	CG-CD2-CE3	-6.30	128.23	133.90
1	A	105	PRO	N-CA-CB	6.30	110.86	103.30
1	C	52	THR	CA-C-N	6.30	131.06	117.20
1	A	107	LEU	CB-CA-C	6.30	122.16	110.20
1	D	83	THR	OG1-CB-CG2	6.30	124.48	110.00
1	E	81	SER	O-C-N	6.29	133.90	123.20
1	F	62	LEU	N-CA-CB	6.29	122.99	110.40
1	B	109	ASP	C-N-CA	6.29	137.43	121.70
1	B	112	THR	CA-C-N	6.29	131.04	117.20
1	D	75	ASN	CB-CA-C	-6.29	97.82	110.40
1	F	56	THR	CB-CA-C	-6.29	94.62	111.60
1	B	108	TRP	CE2-CD2-CG	6.29	112.33	107.30
1	F	129	TYR	CZ-CE2-CD2	-6.29	114.14	119.80
1	C	145	GLN	N-CA-CB	-6.29	99.29	110.60
1	E	149	LEU	N-CA-CB	6.29	122.97	110.40
1	A	97	ASP	N-CA-CB	-6.28	99.29	110.60
1	C	16	THR	C-N-CA	-6.28	105.99	121.70
1	F	235	THR	N-CA-CB	-6.28	98.36	110.30
1	C	5	PHE	CA-C-O	6.28	133.29	120.10
1	D	9	HIS	CA-C-N	6.28	131.02	117.20
1	A	76	THR	CA-C-N	6.28	131.01	117.20
1	A	118	VAL	CA-CB-CG1	6.28	120.32	110.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	ASP	O-C-N	-6.28	112.65	122.70
1	B	137	HIS	C-N-CD	6.28	141.58	128.40
1	F	2	ASN	OD1-CG-ND2	6.28	136.34	121.90
1	B	141	LEU	CD1-CG-CD2	-6.28	91.67	110.50
1	C	176	THR	CA-C-N	6.28	131.00	117.20
1	C	96	PRO	C-N-CA	6.27	137.39	121.70
1	F	192	ARG	CG-CD-NE	6.27	124.97	111.80
1	A	129	TYR	N-CA-C	-6.27	94.06	111.00
1	E	218	VAL	C-N-CA	6.27	137.38	121.70
1	F	206	SER	C-N-CA	6.27	135.47	122.30
1	B	107	LEU	CB-CG-CD1	6.27	121.66	111.00
1	C	232	LEU	CB-CA-C	-6.26	98.30	110.20
1	C	73	ALA	N-CA-CB	6.26	118.87	110.10
1	C	229	GLY	C-N-CA	6.26	135.45	122.30
1	A	104	GLY	CA-C-O	-6.26	109.33	120.60
1	C	62	LEU	CA-C-O	6.26	133.24	120.10
1	C	161	ASN	CB-CG-ND2	6.26	131.72	116.70
1	A	78	ARG	CB-CG-CD	6.26	127.87	111.60
1	B	190	ASN	CB-CG-OD1	-6.26	109.09	121.60
1	E	145	GLN	CG-CD-NE2	6.26	131.71	116.70
1	E	138	PRO	O-C-N	6.25	132.71	122.70
1	B	46	ARG	CG-CD-NE	-6.25	98.68	111.80
1	C	181	THR	C-N-CA	-6.25	109.18	122.30
1	F	105	PRO	C-N-CA	6.25	135.42	122.30
1	E	168	ASP	CB-CG-OD1	6.25	123.92	118.30
1	F	45	VAL	N-CA-C	-6.25	94.14	111.00
1	F	24	GLU	CA-C-O	-6.24	106.99	120.10
1	D	169	ASP	O-C-N	6.24	132.69	122.70
1	A	147	LEU	CA-C-N	6.24	130.93	117.20
1	B	70	ILE	CG1-CB-CG2	-6.24	97.67	111.40
1	C	184	ARG	N-CA-C	-6.24	94.15	111.00
1	C	132	GLN	N-CA-CB	6.24	121.83	110.60
1	B	54	GLY	C-N-CA	-6.24	106.11	121.70
1	D	40	LEU	CA-CB-CG	-6.23	100.96	115.30
1	F	68	LEU	CD1-CG-CD2	6.23	129.20	110.50
1	A	117	SER	N-CA-C	6.23	127.83	111.00
1	B	22	SER	CA-C-N	6.23	130.91	117.20
1	D	204	TRP	N-CA-CB	6.23	121.82	110.60
1	E	74	GLN	CB-CA-C	-6.23	97.94	110.40
1	A	140	THR	CA-C-N	-6.22	103.51	117.20
1	A	206	SER	CA-CB-OG	6.22	128.00	111.20
1	D	33	GLN	OE1-CD-NE2	6.22	136.22	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	67	LEU	N-CA-CB	6.22	122.85	110.40
1	A	194	ASP	CA-C-O	6.22	133.17	120.10
1	D	45	VAL	CA-C-N	-6.22	103.51	117.20
1	A	22	SER	N-CA-CB	-6.22	101.17	110.50
1	C	176	THR	CA-CB-OG1	6.22	122.06	109.00
1	E	35	ASP	CA-C-N	6.22	130.89	117.20
1	B	230	GLY	C-N-CA	6.22	137.25	121.70
1	D	89	ASN	N-CA-C	6.22	127.79	111.00
1	B	79	TRP	CH2-CZ2-CE2	6.22	123.62	117.40
1	E	194	ASP	N-CA-CB	-6.22	99.41	110.60
1	A	185	ALA	CB-CA-C	6.21	119.42	110.10
1	C	192	ARG	CB-CA-C	6.21	122.83	110.40
1	C	185	ALA	N-CA-CB	6.21	118.80	110.10
1	F	74	GLN	N-CA-C	6.21	127.77	111.00
1	D	33	GLN	N-CA-C	6.21	127.77	111.00
1	A	93	VAL	CA-CB-CG1	6.21	120.21	110.90
1	A	188	GLN	OE1-CD-NE2	-6.21	107.62	121.90
1	A	209	SER	N-CA-CB	-6.21	101.19	110.50
1	F	89	ASN	OD1-CG-ND2	6.21	136.17	121.90
1	A	155	SER	C-N-CA	-6.20	106.19	121.70
1	B	164	LEU	N-CA-CB	6.20	122.80	110.40
1	A	109	ASP	CB-CA-C	-6.20	98.00	110.40
1	A	85	GLY	CA-C-N	-6.20	103.56	117.20
1	B	220	GLN	CA-C-O	6.20	133.12	120.10
1	A	18	HIS	N-CA-CB	6.20	121.75	110.60
1	B	16	THR	O-C-N	6.20	132.62	122.70
1	C	25	LEU	N-CA-C	-6.20	94.27	111.00
1	B	165	PHE	C-N-CA	-6.20	106.21	121.70
1	C	25	LEU	C-N-CA	6.20	137.19	121.70
1	C	170	ARG	CA-C-N	6.20	130.83	117.20
1	A	222	ASP	C-N-CA	-6.19	106.22	121.70
1	D	30	PHE	CA-CB-CG	-6.19	99.04	113.90
1	F	51	ASN	OD1-CG-ND2	-6.19	107.67	121.90
1	B	213	GLY	CA-C-O	6.19	131.74	120.60
1	E	235	THR	OG1-CB-CG2	-6.19	95.77	110.00
1	F	74	GLN	C-N-CA	6.19	137.17	121.70
1	A	105	PRO	N-CA-C	-6.19	96.02	112.10
1	C	91	VAL	CA-C-N	6.19	130.81	117.20
1	A	221	PRO	CA-C-N	6.18	130.81	117.20
1	B	15	GLN	O-C-N	6.18	132.60	122.70
1	B	215	TYR	CE1-CZ-OH	6.18	136.80	120.10
1	E	140	THR	C-N-CA	-6.18	106.24	121.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	83	THR	CA-C-N	6.18	130.81	117.20
1	B	13	HIS	CA-C-O	-6.18	107.11	120.10
1	B	63	GLN	CB-CA-C	-6.18	98.03	110.40
1	C	38	LEU	CD1-CG-CD2	-6.18	91.95	110.50
1	A	7	LEU	N-CA-CB	-6.18	98.04	110.40
1	E	10	GLU	CA-C-O	-6.18	107.12	120.10
1	B	217	PHE	CB-CA-C	6.18	122.76	110.40
1	E	114	ASN	CB-CA-C	-6.18	98.04	110.40
1	D	215	TYR	CA-C-O	-6.18	107.13	120.10
1	E	119	VAL	C-N-CA	6.18	137.14	121.70
1	C	28	PHE	CB-CG-CD2	6.17	125.12	120.80
1	B	79	TRP	CB-CG-CD1	-6.17	118.97	127.00
1	A	197	THR	C-N-CA	6.17	137.13	121.70
1	F	206	SER	CA-C-N	6.17	128.54	116.20
1	B	169	ASP	C-N-CA	6.17	137.12	121.70
1	F	7	LEU	CB-CG-CD1	6.17	121.49	111.00
1	A	56	THR	CA-CB-OG1	6.17	121.95	109.00
1	A	195	VAL	N-CA-C	-6.17	94.35	111.00
1	D	97	ASP	CA-CB-CG	6.17	126.96	113.40
1	E	105	PRO	O-C-N	6.17	133.68	123.20
1	C	187	LEU	O-C-N	-6.17	112.84	122.70
1	F	106	GLY	CA-C-N	6.17	130.76	117.20
1	A	228	TYR	OH-CZ-CE2	6.16	136.74	120.10
1	D	87	ILE	CA-C-N	6.16	128.52	116.20
1	F	105	PRO	CB-CG-CD	-6.16	82.47	106.50
1	D	65	ASP	CB-CA-C	6.16	122.72	110.40
1	D	71	LEU	CB-CG-CD2	-6.16	100.53	111.00
1	A	2	ASN	O-C-N	-6.16	112.84	122.70
1	A	162	LEU	CB-CA-C	6.16	121.90	110.20
1	B	79	TRP	CG-CD1-NE1	6.16	116.26	110.10
1	E	34	SER	CA-C-N	6.16	130.75	117.20
1	E	67	LEU	O-C-N	6.16	132.55	122.70
1	F	143	ALA	N-CA-C	-6.16	94.38	111.00
1	D	31	THR	OG1-CB-CG2	-6.16	95.84	110.00
1	F	142	HIS	ND1-CE1-NE2	-6.16	96.36	109.90
1	C	41	PHE	N-CA-CB	-6.15	99.53	110.60
1	B	193	MET	N-CA-C	-6.15	94.40	111.00
1	C	209	SER	O-C-N	-6.15	112.86	122.70
1	A	134	ASN	N-CA-CB	6.15	121.67	110.60
1	B	9	HIS	CA-CB-CG	6.14	124.05	113.60
1	C	222	ASP	CB-CG-OD1	-6.14	112.77	118.30
1	F	229	GLY	CA-C-O	-6.14	109.54	120.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	VAL	CA-CB-CG1	6.14	120.11	110.90
1	A	99	THR	OG1-CB-CG2	6.14	124.13	110.00
1	B	166	ASP	OD1-CG-OD2	-6.14	111.63	123.30
1	F	11	GLY	O-C-N	-6.14	112.88	122.70
1	F	40	LEU	CA-CB-CG	-6.14	101.18	115.30
1	E	70	ILE	CA-C-O	-6.14	107.21	120.10
1	E	129	TYR	CA-C-O	-6.14	107.21	120.10
1	C	82	GLY	CA-C-O	6.14	131.64	120.60
1	F	215	TYR	CA-CB-CG	-6.14	101.74	113.40
1	E	206	SER	N-CA-CB	-6.13	101.30	110.50
1	A	232	LEU	CA-C-O	-6.13	107.23	120.10
1	A	75	ASN	N-CA-CB	6.13	121.63	110.60
1	A	171	VAL	N-CA-C	-6.13	94.45	111.00
1	F	183	CYS	CB-CA-C	6.13	122.66	110.40
1	B	18	HIS	CG-ND1-CE1	-6.13	97.73	105.70
1	F	32	MET	CA-C-N	6.13	130.68	117.20
1	A	31	THR	O-C-N	-6.12	112.90	122.70
1	B	162	LEU	CD1-CG-CD2	-6.12	92.13	110.50
1	B	181	THR	OG1-CB-CG2	-6.12	95.92	110.00
1	A	175	ASN	CB-CG-ND2	-6.12	102.01	116.70
1	B	147	LEU	CD1-CG-CD2	-6.12	92.14	110.50
1	B	222	ASP	CB-CA-C	-6.12	98.16	110.40
1	C	184	ARG	CG-CD-NE	-6.12	98.94	111.80
1	D	145	GLN	CA-C-N	-6.12	103.73	117.20
1	D	184	ARG	CA-C-O	6.12	132.96	120.10
1	D	228	TYR	CG-CD1-CE1	-6.12	116.40	121.30
1	F	196	LEU	O-C-N	-6.12	112.91	122.70
1	A	229	GLY	CA-C-N	-6.12	103.96	116.20
1	B	111	GLY	O-C-N	-6.12	112.91	122.70
1	F	101	THR	CA-C-O	-6.12	107.25	120.10
1	B	194	ASP	CA-C-N	-6.12	103.74	117.20
1	B	216	VAL	CB-CA-C	6.12	123.02	111.40
1	A	144	THR	CA-C-O	-6.11	107.26	120.10
1	C	152	TYR	CB-CG-CD1	-6.11	117.33	121.00
1	D	73	ALA	CA-C-N	6.11	130.65	117.20
1	C	205	THR	CA-CB-OG1	-6.11	96.17	109.00
1	C	104	GLY	N-CA-C	6.11	128.38	113.10
1	E	157	GLU	CG-CD-OE1	-6.11	106.08	118.30
1	F	172	TRP	CA-CB-CG	-6.11	102.09	113.70
1	B	169	ASP	CA-C-N	-6.11	103.76	117.20
1	C	108	TRP	CB-CA-C	-6.11	98.19	110.40
1	D	80	SER	CB-CA-C	-6.11	98.50	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	ILE	CG1-CB-CG2	-6.11	97.97	111.40
1	C	62	LEU	CD1-CG-CD2	-6.11	92.19	110.50
1	E	14	PRO	CA-CB-CG	-6.11	92.40	104.00
1	C	136	ASN	CA-C-N	-6.10	103.78	117.20
1	C	184	ARG	CB-CA-C	-6.10	98.19	110.40
1	D	78	ARG	C-N-CA	-6.10	106.45	121.70
1	A	188	GLN	O-C-N	-6.10	109.52	121.10
1	B	123	ASN	CA-C-O	6.10	132.90	120.10
1	F	9	HIS	CA-C-O	6.10	132.90	120.10
1	A	24	GLU	CB-CA-C	-6.09	98.21	110.40
1	D	7	LEU	CB-CA-C	-6.09	98.62	110.20
1	F	83	THR	OG1-CB-CG2	-6.09	95.98	110.00
1	B	28	PHE	N-CA-C	6.09	127.45	111.00
1	B	174	THR	O-C-N	-6.09	112.95	122.70
1	C	144	THR	CA-CB-CG2	-6.09	103.87	112.40
1	C	42	ASP	CB-CG-OD1	6.09	123.78	118.30
1	F	169	ASP	N-CA-C	-6.08	94.57	111.00
1	C	130	SER	N-CA-C	-6.08	94.58	111.00
1	D	2	ASN	CA-C-N	6.08	130.58	117.20
1	D	26	SER	CA-CB-OG	-6.08	94.78	111.20
1	D	187	LEU	CB-CG-CD2	-6.08	100.67	111.00
1	E	17	LEU	CA-C-N	6.08	130.57	117.20
1	E	229	GLY	N-CA-C	6.08	128.30	113.10
1	E	228	TYR	CZ-CE2-CD2	6.08	125.27	119.80
1	B	139	GLN	O-C-N	6.08	132.42	122.70
1	D	222	ASP	CA-C-N	6.08	130.56	117.20
1	E	147	LEU	CB-CG-CD1	-6.08	100.67	111.00
1	A	136	ASN	O-C-N	-6.07	112.98	122.70
1	F	48	TRP	CB-CA-C	-6.07	98.26	110.40
1	F	233	TRP	CD1-NE1-CE2	-6.07	103.54	109.00
1	B	98	ARG	CB-CA-C	6.07	122.54	110.40
1	B	197	THR	N-CA-CB	-6.07	98.77	110.30
1	F	222	ASP	CA-C-O	-6.07	107.36	120.10
1	F	233	TRP	C-N-CA	6.07	136.87	121.70
1	D	201	ILE	CA-CB-CG1	-6.07	99.48	111.00
1	D	211	SER	C-N-CA	-6.07	106.53	121.70
1	A	122	ASN	C-N-CA	6.06	136.86	121.70
1	F	35	ASP	CB-CA-C	-6.06	98.27	110.40
1	F	147	LEU	CA-CB-CG	6.06	129.25	115.30
1	A	26	SER	N-CA-C	6.06	127.36	111.00
1	B	67	LEU	CD1-CG-CD2	6.06	128.68	110.50
1	E	42	ASP	O-C-N	6.06	132.40	122.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	77	ILE	N-CA-CB	-6.06	96.86	110.80
1	A	192	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	B	105	PRO	CA-C-N	6.06	128.31	116.20
1	B	105	PRO	CA-CB-CG	-6.06	92.49	104.00
1	B	202	ALA	C-N-CA	6.06	136.84	121.70
1	D	217	PHE	N-CA-C	-6.06	94.65	111.00
1	A	46	ARG	N-CA-CB	-6.05	99.70	110.60
1	D	235	THR	N-CA-CB	-6.05	98.80	110.30
1	E	30	PHE	CB-CA-C	-6.05	98.29	110.40
1	E	234	THR	O-C-N	6.05	132.39	122.70
1	B	30	PHE	N-CA-CB	-6.05	99.71	110.60
1	B	215	TYR	N-CA-CB	6.05	121.49	110.60
1	E	231	ALA	O-C-N	6.05	132.38	122.70
1	D	4	LEU	CB-CG-CD1	-6.05	100.72	111.00
1	D	51	ASN	CA-CB-CG	6.05	126.71	113.40
1	D	180	GLY	CA-C-N	-6.05	103.89	117.20
1	F	161	ASN	O-C-N	6.05	132.38	122.70
1	A	10	GLU	N-CA-CB	6.05	121.49	110.60
1	B	108	TRP	CB-CG-CD2	6.05	134.46	126.60
1	C	102	ILE	CA-C-O	-6.05	107.40	120.10
1	C	126	SER	CA-C-O	-6.05	107.40	120.10
1	F	109	ASP	N-CA-CB	6.05	121.48	110.60
1	F	130	SER	N-CA-C	6.04	127.32	111.00
1	A	167	ARG	CA-C-O	-6.04	107.41	120.10
1	C	148	GLN	CA-C-N	6.04	130.50	117.20
1	B	1	ASN	OD1-CG-ND2	-6.04	108.00	121.90
1	F	22	SER	CA-CB-OG	-6.04	94.89	111.20
1	B	165	PHE	O-C-N	6.04	132.36	122.70
1	E	165	PHE	CA-C-O	-6.04	107.42	120.10
1	A	145	GLN	O-C-N	-6.04	113.04	122.70
1	E	177	ALA	N-CA-CB	6.04	118.55	110.10
1	B	162	LEU	CA-CB-CG	6.03	129.18	115.30
1	C	73	ALA	C-N-CA	6.03	136.78	121.70
1	C	210	ARG	CG-CD-NE	-6.03	99.14	111.80
1	B	147	LEU	CA-CB-CG	6.03	129.17	115.30
1	A	90	TYR	CG-CD2-CE2	6.03	126.12	121.30
1	A	136	ASN	CA-C-N	6.03	130.46	117.20
1	F	26	SER	CA-C-O	6.03	132.75	120.10
1	C	87	ILE	N-CA-CB	6.02	124.65	110.80
1	F	201	ILE	CB-CG1-CD1	6.02	130.76	113.90
1	B	91	VAL	C-N-CA	6.02	136.75	121.70
1	C	159	ASP	CA-CB-CG	6.02	126.64	113.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	162	LEU	N-CA-C	-6.02	94.75	111.00
1	C	203	VAL	N-CA-C	-6.02	94.75	111.00
1	E	189	PRO	CA-N-CD	-6.01	103.08	111.50
1	F	153	ARG	NH1-CZ-NH2	6.01	126.02	119.40
1	B	132	GLN	CG-CD-OE1	6.01	133.63	121.60
1	E	158	THR	O-C-N	-6.01	113.08	122.70
1	C	90	TYR	CB-CG-CD1	-6.01	117.39	121.00
1	D	136	ASN	O-C-N	-6.01	113.08	122.70
1	B	102	ILE	CA-CB-CG1	6.01	122.42	111.00
1	A	227	ILE	O-C-N	-6.01	113.09	122.70
1	B	89	ASN	O-C-N	-6.01	113.09	122.70
1	B	102	ILE	O-C-N	-6.01	113.09	122.70
1	E	214	ARG	CA-C-O	6.01	132.71	120.10
1	A	27	SER	CA-C-N	6.00	130.41	117.20
1	A	31	THR	OG1-CB-CG2	-6.00	96.19	110.00
1	A	130	SER	CA-C-O	-6.00	107.49	120.10
1	E	61	VAL	C-N-CA	6.00	136.71	121.70
1	A	74	GLN	OE1-CD-NE2	6.00	135.71	121.90
1	B	201	ILE	N-CA-CB	-6.00	97.00	110.80
1	D	197	THR	CA-CB-CG2	6.00	120.80	112.40
1	F	10	GLU	CA-C-O	-6.00	107.50	120.10
1	F	166	ASP	O-C-N	-6.00	113.10	122.70
1	B	143	ALA	O-C-N	-6.00	113.10	122.70
1	B	197	THR	N-CA-C	6.00	127.20	111.00
1	F	139	GLN	N-CA-C	-6.00	94.80	111.00
1	A	65	ASP	O-C-N	-6.00	113.01	123.20
1	B	189	PRO	O-C-N	6.00	132.29	122.70
1	A	11	GLY	CA-C-N	-6.00	104.01	117.20
1	A	91	VAL	N-CA-C	-6.00	94.81	111.00
1	A	45	VAL	CA-C-O	5.99	132.69	120.10
1	E	234	THR	CA-C-O	-5.99	107.51	120.10
1	D	104	GLY	CA-C-N	-5.99	100.32	117.10
1	B	79	TRP	C-N-CA	5.99	136.67	121.70
1	D	167	ARG	N-CA-C	-5.99	94.83	111.00
1	C	4	LEU	CA-C-N	5.99	130.37	117.20
1	C	207	GLY	C-N-CA	5.99	136.67	121.70
1	C	217	PHE	O-C-N	5.99	132.28	122.70
1	D	157	GLU	CB-CA-C	-5.99	98.43	110.40
1	D	214	ARG	CA-C-N	5.99	130.37	117.20
1	F	38	LEU	N-CA-C	-5.99	94.84	111.00
1	A	138	PRO	C-N-CA	-5.98	106.74	121.70
1	B	226	ALA	N-CA-C	-5.98	94.84	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	146	SER	CA-CB-OG	-5.98	95.04	111.20
1	A	192	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	C	133	GLY	N-CA-C	-5.98	98.14	113.10
1	E	197	THR	CB-CA-C	-5.98	95.45	111.60
1	A	226	ALA	C-N-CA	-5.98	106.75	121.70
1	D	222	ASP	OD1-CG-OD2	-5.98	111.94	123.30
1	A	171	VAL	CA-C-N	5.98	130.35	117.20
1	A	79	TRP	CE3-CZ3-CH2	-5.98	114.62	121.20
1	D	99	THR	CB-CA-C	5.98	127.74	111.60
1	E	102	ILE	CA-C-O	-5.98	107.55	120.10
1	F	1	ASN	CB-CG-OD1	-5.98	109.65	121.60
1	E	61	VAL	O-C-N	-5.98	113.14	122.70
1	D	33	GLN	C-N-CA	5.97	136.63	121.70
1	E	170	ARG	CG-CD-NE	5.97	124.33	111.80
1	B	74	GLN	CB-CG-CD	-5.97	96.08	111.60
1	B	215	TYR	OH-CZ-CE2	-5.97	103.98	120.10
1	B	44	ASP	N-CA-C	-5.97	94.89	111.00
1	C	214	ARG	CA-C-O	5.97	132.63	120.10
1	E	102	ILE	CA-C-N	-5.97	104.07	117.20
1	A	178	GLY	CA-C-N	5.96	130.32	117.20
1	A	223	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	C	172	TRP	CA-C-O	-5.96	107.57	120.10
1	D	179	LYS	CA-C-O	-5.96	107.58	120.10
1	A	38	LEU	CB-CG-CD1	5.96	121.14	111.00
1	B	224	ASN	CB-CG-OD1	5.96	133.52	121.60
1	C	47	VAL	CA-CB-CG1	5.96	119.84	110.90
1	F	67	LEU	C-N-CA	-5.96	106.80	121.70
1	F	126	SER	O-C-N	-5.96	113.16	122.70
1	F	168	ASP	O-C-N	-5.96	113.16	122.70
1	A	68	LEU	O-C-N	-5.96	113.17	122.70
1	C	105	PRO	C-N-CA	-5.96	109.79	122.30
1	A	40	LEU	CB-CG-CD2	-5.96	100.88	111.00
1	C	165	PHE	CA-CB-CG	5.96	128.19	113.90
1	F	164	LEU	CB-CG-CD2	5.96	121.12	111.00
1	B	37	ASN	CA-CB-CG	-5.95	100.30	113.40
1	B	8	SER	N-CA-C	-5.95	94.93	111.00
1	A	111	GLY	O-C-N	-5.95	113.18	122.70
1	D	203	VAL	CA-C-O	-5.95	107.60	120.10
1	F	170	ARG	N-CA-C	5.95	127.07	111.00
1	B	45	VAL	N-CA-C	-5.95	94.94	111.00
1	D	127	ILE	CG1-CB-CG2	5.95	124.48	111.40
1	E	107	LEU	N-CA-CB	-5.95	98.50	110.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	182	GLY	N-CA-C	5.95	127.97	113.10
1	E	16	THR	N-CA-CB	-5.95	99.00	110.30
1	E	196	LEU	O-C-N	5.95	132.22	122.70
1	C	72	THR	CA-C-N	-5.94	104.13	117.20
1	E	36	CYS	CA-C-N	5.94	130.26	117.20
1	E	109	ASP	CB-CG-OD2	-5.94	112.96	118.30
1	C	9	HIS	CB-CG-ND1	-5.93	108.36	123.20
1	A	22	SER	C-N-CA	5.93	136.53	121.70
1	A	165	PHE	CB-CG-CD1	5.93	124.95	120.80
1	B	180	GLY	CA-C-O	-5.93	109.92	120.60
1	C	217	PHE	CA-C-O	-5.93	107.64	120.10
1	D	23	LEU	CB-CG-CD2	-5.93	100.92	111.00
1	B	74	GLN	CA-C-O	5.93	132.55	120.10
1	A	233	TRP	CB-CG-CD1	-5.93	119.29	127.00
1	F	17	LEU	N-CA-CB	5.93	122.26	110.40
1	D	169	ASP	C-N-CA	5.93	136.52	121.70
1	E	144	THR	O-C-N	5.93	132.18	122.70
1	B	74	GLN	CA-C-N	-5.92	104.17	117.20
1	C	51	ASN	CA-C-N	5.92	130.24	117.20
1	E	44	ASP	CA-CB-CG	5.92	126.43	113.40
1	E	78	ARG	CA-C-O	-5.92	107.66	120.10
1	B	23	LEU	N-CA-C	-5.92	95.02	111.00
1	A	15	GLN	C-N-CA	5.92	136.50	121.70
1	C	26	SER	O-C-N	-5.92	113.23	122.70
1	E	152	TYR	CA-C-N	-5.92	104.18	117.20
1	C	225	LEU	CA-C-O	-5.92	107.68	120.10
1	D	14	PRO	CB-CA-C	-5.92	97.21	112.00
1	B	184	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	A	25	LEU	N-CA-C	-5.91	95.05	111.00
1	B	126	SER	CA-CB-OG	-5.91	95.25	111.20
1	D	205	THR	CA-C-O	5.91	132.51	120.10
1	B	26	SER	CA-C-O	5.91	132.50	120.10
1	E	29	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	B	41	PHE	O-C-N	-5.90	113.25	122.70
1	C	2	ASN	CB-CA-C	5.90	122.20	110.40
1	F	181	THR	N-CA-C	5.90	126.93	111.00
1	E	210	ARG	O-C-N	-5.90	113.26	122.70
1	F	56	THR	N-CA-CB	5.90	121.51	110.30
1	C	51	ASN	CA-C-O	-5.90	107.72	120.10
1	A	37	ASN	CB-CA-C	5.90	122.19	110.40
1	A	58	CYS	O-C-N	-5.90	113.27	122.70
1	D	159	ASP	O-C-N	-5.90	113.27	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	12	SER	CA-C-O	-5.89	107.72	120.10
1	C	37	ASN	N-CA-CB	-5.89	99.99	110.60
1	E	90	TYR	CG-CD1-CE1	5.89	126.02	121.30
1	E	143	ALA	CB-CA-C	5.89	118.94	110.10
1	F	40	LEU	CA-C-N	-5.89	104.23	117.20
1	C	21	GLN	CB-CA-C	5.89	122.18	110.40
1	C	108	TRP	CB-CG-CD1	5.89	134.66	127.00
1	A	151	PRO	C-N-CA	5.89	136.43	121.70
1	B	83	THR	C-N-CA	5.89	136.42	121.70
1	B	112	THR	N-CA-C	5.89	126.90	111.00
1	D	230	GLY	C-N-CA	5.89	136.42	121.70
1	B	35	ASP	O-C-N	-5.89	113.28	122.70
1	C	58	CYS	O-C-N	-5.89	113.28	122.70
1	D	233	TRP	CG-CD2-CE3	-5.89	128.60	133.90
1	E	156	MET	CB-CG-SD	5.89	130.06	112.40
1	B	85	GLY	O-C-N	-5.88	113.28	122.70
1	B	164	LEU	CD1-CG-CD2	-5.88	92.85	110.50
1	C	72	THR	CA-CB-CG2	-5.88	104.16	112.40
1	E	4	LEU	CA-C-O	-5.88	107.74	120.10
1	E	126	SER	C-N-CA	5.88	136.41	121.70
1	E	165	PHE	N-CA-C	5.88	126.89	111.00
1	B	1	ASN	CB-CA-C	5.88	122.17	110.40
1	B	57	GLY	C-N-CA	5.88	136.41	121.70
1	D	161	ASN	O-C-N	5.88	132.11	122.70
1	F	11	GLY	N-CA-C	-5.88	98.39	113.10
1	A	9	HIS	ND1-CG-CD2	-5.88	97.77	106.00
1	F	233	TRP	N-CA-C	-5.88	95.13	111.00
1	A	141	LEU	CA-C-N	-5.88	104.27	117.20
1	B	193	MET	CB-CA-C	5.88	122.15	110.40
1	E	117	SER	N-CA-C	5.88	126.87	111.00
1	B	226	ALA	C-N-CA	-5.88	107.01	121.70
1	E	141	LEU	CA-CB-CG	5.88	128.81	115.30
1	A	168	ASP	CA-CB-CG	-5.87	100.48	113.40
1	A	173	SER	O-C-N	-5.87	113.30	122.70
1	B	63	GLN	C-N-CA	-5.87	107.02	121.70
1	E	9	HIS	O-C-N	5.87	132.09	122.70
1	A	204	TRP	O-C-N	-5.87	113.31	122.70
1	D	164	LEU	CA-CB-CG	-5.87	101.81	115.30
1	E	184	ARG	CB-CG-CD	5.87	126.85	111.60
1	F	212	ALA	N-CA-CB	-5.87	101.89	110.10
1	D	215	TYR	CE1-CZ-OH	5.86	135.93	120.10
1	F	32	MET	N-CA-CB	-5.86	100.05	110.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	69	VAL	C-N-CA	5.86	136.36	121.70
1	A	203	VAL	CG1-CB-CG2	-5.86	101.52	110.90
1	C	120	VAL	CB-CA-C	-5.86	100.26	111.40
1	C	166	ASP	CA-C-O	-5.86	107.79	120.10
1	F	97	ASP	CA-CB-CG	5.86	126.29	113.40
1	E	62	LEU	N-CA-CB	5.86	122.12	110.40
1	A	36	CYS	CA-C-O	-5.86	107.80	120.10
1	D	32	MET	N-CA-C	-5.86	95.18	111.00
1	D	179	LYS	N-CA-CB	5.86	121.14	110.60
1	A	192	ARG	O-C-N	-5.86	113.33	122.70
1	D	233	TRP	CB-CA-C	-5.86	98.69	110.40
1	F	141	LEU	CA-C-O	-5.86	107.80	120.10
1	B	78	ARG	CB-CA-C	5.85	122.11	110.40
1	E	172	TRP	CB-CG-CD2	5.85	134.21	126.60
1	A	188	GLN	CA-CB-CG	-5.85	100.53	113.40
1	B	87	ILE	CA-C-O	5.85	132.39	120.10
1	B	198	ASN	N-CA-C	5.85	126.80	111.00
1	F	48	TRP	CG-CD1-NE1	-5.85	104.25	110.10
1	A	201	ILE	CA-CB-CG1	5.85	122.11	111.00
1	D	9	HIS	N-CA-CB	-5.85	100.07	110.60
1	D	63	GLN	N-CA-C	5.85	126.79	111.00
1	C	202	ALA	C-N-CA	5.84	136.31	121.70
1	E	16	THR	C-N-CA	-5.84	107.09	121.70
1	B	95	GLN	O-C-N	-5.84	110.00	121.10
1	B	153	ARG	NH1-CZ-NH2	5.84	125.83	119.40
1	F	159	ASP	O-C-N	-5.84	113.35	122.70
1	B	90	TYR	CA-CB-CG	5.84	124.50	113.40
1	F	56	THR	OG1-CB-CG2	-5.84	96.56	110.00
1	F	110	SER	O-C-N	5.84	133.13	123.20
1	C	40	LEU	CB-CG-CD2	5.84	120.93	111.00
1	C	112	THR	CA-CB-OG1	-5.84	96.74	109.00
1	B	166	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	F	41	PHE	CZ-CE2-CD2	5.84	127.11	120.10
1	A	7	LEU	CB-CG-CD2	5.84	120.92	111.00
1	A	97	ASP	CB-CG-OD1	5.84	123.55	118.30
1	D	126	SER	N-CA-CB	-5.84	101.75	110.50
1	B	25	LEU	CA-C-N	-5.83	104.36	117.20
1	D	7	LEU	CA-CB-CG	-5.83	101.89	115.30
1	B	10	GLU	CG-CD-OE1	-5.83	106.64	118.30
1	D	174	THR	CB-CA-C	-5.83	95.85	111.60
1	D	201	ILE	CA-C-O	-5.83	107.86	120.10
1	D	5	PHE	CA-C-N	5.83	127.86	116.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	17	LEU	CA-C-O	-5.83	107.86	120.10
1	E	51	ASN	O-C-N	5.83	132.03	122.70
1	A	119	VAL	N-CA-CB	-5.83	98.68	111.50
1	E	121	ALA	CA-C-O	5.83	132.34	120.10
1	B	128	LEU	C-N-CA	5.83	136.26	121.70
1	B	146	SER	CA-C-O	-5.83	107.87	120.10
1	C	192	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	D	149	LEU	CA-CB-CG	-5.83	101.90	115.30
1	F	185	ALA	C-N-CA	-5.82	107.14	121.70
1	C	233	TRP	CD1-NE1-CE2	-5.82	103.76	109.00
1	F	76	THR	O-C-N	-5.82	113.38	122.70
1	E	90	TYR	CD1-CG-CD2	-5.82	111.50	117.90
1	F	47	VAL	CA-C-N	5.82	130.00	117.20
1	B	22	SER	CA-C-O	5.82	132.32	120.10
1	B	37	ASN	C-N-CA	-5.82	107.16	121.70
1	D	46	ARG	O-C-N	-5.82	113.39	122.70
1	B	92	LEU	CB-CG-CD2	5.82	120.89	111.00
1	C	120	VAL	CA-C-N	5.81	129.99	117.20
1	E	119	VAL	N-CA-CB	-5.81	98.71	111.50
1	B	205	THR	OG1-CB-CG2	-5.81	96.64	110.00
1	F	194	ASP	CB-CA-C	-5.81	98.78	110.40
1	C	26	SER	CA-C-O	-5.81	107.90	120.10
1	C	140	THR	CA-C-O	5.81	132.29	120.10
1	F	79	TRP	CZ3-CH2-CZ2	5.81	128.57	121.60
1	B	36	CYS	C-N-CA	-5.80	107.19	121.70
1	B	203	VAL	O-C-N	-5.80	113.42	122.70
1	C	224	ASN	CB-CG-ND2	-5.80	102.77	116.70
1	C	62	LEU	CA-C-N	-5.80	104.44	117.20
1	D	110	SER	CB-CA-C	5.80	121.12	110.10
1	F	175	ASN	CB-CA-C	-5.80	98.80	110.40
1	A	134	ASN	C-N-CA	5.80	136.20	121.70
1	B	136	ASN	CA-C-O	-5.80	107.92	120.10
1	C	200	ASN	C-N-CA	5.80	136.20	121.70
1	F	105	PRO	CB-CA-C	-5.80	97.50	112.00
1	A	24	GLU	OE1-CD-OE2	-5.79	116.35	123.30
1	A	232	LEU	CA-C-N	5.79	129.95	117.20
1	F	29	ARG	CA-C-N	-5.79	104.45	117.20
1	F	169	ASP	C-N-CA	5.79	136.19	121.70
1	B	163	VAL	CA-CB-CG2	-5.79	102.21	110.90
1	E	77	ILE	O-C-N	-5.79	113.43	122.70
1	E	26	SER	CA-C-O	-5.79	107.94	120.10
1	E	192	ARG	CG-CD-NE	5.79	123.96	111.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	25	LEU	CA-CB-CG	5.79	128.62	115.30
1	C	139	GLN	CA-C-O	5.79	132.25	120.10
1	F	64	SER	N-CA-C	5.79	126.63	111.00
1	A	51	ASN	CB-CG-OD1	-5.79	110.03	121.60
1	A	193	MET	N-CA-C	-5.79	95.38	111.00
1	F	100	VAL	O-C-N	-5.79	113.44	122.70
1	B	12	SER	CA-C-N	-5.78	104.48	117.20
1	F	6	GLY	C-N-CA	5.78	136.15	121.70
1	F	84	LYS	O-C-N	-5.78	113.37	123.20
1	B	72	THR	N-CA-CB	-5.78	99.32	110.30
1	E	144	THR	OG1-CB-CG2	5.78	123.29	110.00
1	B	78	ARG	CD-NE-CZ	5.78	131.69	123.60
1	F	52	THR	CA-CB-CG2	-5.78	104.31	112.40
1	A	201	ILE	CG1-CB-CG2	-5.77	98.70	111.40
1	E	48	TRP	CA-CB-CG	-5.77	102.73	113.70
1	E	61	VAL	CA-CB-CG1	5.77	119.56	110.90
1	A	5	PHE	C-N-CA	-5.77	110.18	122.30
1	C	223	ARG	O-C-N	-5.77	113.47	122.70
1	A	30	PHE	N-CA-CB	5.77	120.98	110.60
1	B	101	THR	CB-CA-C	-5.77	96.03	111.60
1	B	123	ASN	CB-CA-C	5.77	121.94	110.40
1	C	177	ALA	C-N-CA	5.77	134.41	122.30
1	D	89	ASN	CB-CG-ND2	5.77	130.54	116.70
1	E	83	THR	C-N-CA	5.77	136.12	121.70
1	F	16	THR	C-N-CA	-5.77	107.28	121.70
1	A	90	TYR	N-CA-CB	5.77	120.98	110.60
1	B	24	GLU	CG-CD-OE2	-5.76	106.77	118.30
1	C	176	THR	CA-CB-CG2	-5.76	104.33	112.40
1	D	184	ARG	CB-CA-C	-5.76	98.87	110.40
1	A	233	TRP	N-CA-CB	-5.76	100.23	110.60
1	F	107	LEU	O-C-N	-5.76	113.48	122.70
1	A	69	VAL	N-CA-CB	5.76	124.17	111.50
1	A	102	ILE	CB-CA-C	5.76	123.11	111.60
1	E	46	ARG	O-C-N	-5.76	113.49	122.70
1	F	75	ASN	CB-CG-OD1	-5.76	110.09	121.60
1	F	165	PHE	CB-CG-CD2	-5.76	116.77	120.80
1	A	102	ILE	CA-C-O	-5.75	108.02	120.10
1	E	102	ILE	CG1-CB-CG2	-5.75	98.74	111.40
1	C	46	ARG	CA-C-O	-5.75	108.02	120.10
1	E	79	TRP	CG-CD1-NE1	5.75	115.85	110.10
1	B	166	ASP	N-CA-CB	5.75	120.95	110.60
1	B	233	TRP	NE1-CE2-CZ2	-5.75	124.08	130.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	172	TRP	CE2-CD2-CE3	-5.75	111.80	118.70
1	A	84	LYS	N-CA-CB	-5.75	100.26	110.60
1	C	33	GLN	CG-CD-NE2	-5.75	102.91	116.70
1	C	41	PHE	CA-C-O	-5.75	108.03	120.10
1	B	233	TRP	C-N-CA	5.74	136.06	121.70
1	D	88	GLY	N-CA-C	5.74	127.46	113.10
1	E	169	ASP	CB-CG-OD1	-5.74	113.13	118.30
1	F	155	SER	N-CA-CB	5.74	119.12	110.50
1	A	129	TYR	CA-CB-CG	-5.74	102.50	113.40
1	B	91	VAL	CA-C-N	5.74	129.82	117.20
1	C	164	LEU	CD1-CG-CD2	5.74	127.71	110.50
1	A	147	LEU	N-CA-CB	5.74	121.87	110.40
1	B	163	VAL	N-CA-CB	-5.74	98.88	111.50
1	D	79	TRP	CG-CD1-NE1	-5.74	104.36	110.10
1	A	6	GLY	N-CA-C	-5.73	98.77	113.10
1	B	26	SER	CA-C-N	-5.73	104.58	117.20
1	A	41	PHE	CE1-CZ-CE2	5.73	130.31	120.00
1	B	41	PHE	N-CA-C	5.73	126.47	111.00
1	C	45	VAL	C-N-CA	5.73	136.02	121.70
1	D	87	ILE	O-C-N	5.73	132.94	123.20
1	C	99	THR	CA-C-N	5.73	129.80	117.20
1	E	183	CYS	O-C-N	5.73	131.86	122.70
1	A	233	TRP	CD2-CE3-CZ3	-5.72	111.36	118.80
1	F	233	TRP	CB-CG-CD2	-5.72	119.16	126.60
1	A	70	ILE	CA-CB-CG1	-5.72	100.13	111.00
1	F	223	ARG	O-C-N	-5.72	113.55	122.70
1	D	93	VAL	CA-CB-CG1	5.72	119.48	110.90
1	C	15	GLN	CG-CD-NE2	-5.72	102.98	116.70
1	A	147	LEU	O-C-N	-5.71	113.56	122.70
1	B	9	HIS	CA-C-N	-5.71	104.63	117.20
1	B	221	PRO	N-CA-CB	-5.71	96.31	102.60
1	C	36	CYS	CA-C-O	-5.71	108.10	120.10
1	E	198	ASN	CB-CA-C	-5.71	98.97	110.40
1	A	5	PHE	CG-CD2-CE2	5.71	127.08	120.80
1	C	226	ALA	N-CA-CB	5.71	118.10	110.10
1	B	10	GLU	CB-CG-CD	-5.71	98.78	114.20
1	D	157	GLU	CG-CD-OE1	5.71	129.72	118.30
1	E	47	VAL	N-CA-CB	5.71	124.06	111.50
1	D	1	ASN	CB-CA-C	5.71	121.82	110.40
1	D	45	VAL	CA-C-O	5.71	132.09	120.10
1	D	29	ARG	CB-CG-CD	5.71	126.43	111.60
1	D	108	TRP	CG-CD2-CE3	5.71	139.03	133.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	18	HIS	O-C-N	5.71	131.83	122.70
1	B	141	LEU	CA-C-N	5.70	129.75	117.20
1	B	145	GLN	OE1-CD-NE2	-5.70	108.78	121.90
1	A	215	TYR	CB-CA-C	-5.70	99.00	110.40
1	D	127	ILE	CA-CB-CG2	-5.70	99.50	110.90
1	F	216	VAL	CA-CB-CG2	5.70	119.45	110.90
1	A	138	PRO	CB-CA-C	-5.70	97.76	112.00
1	B	99	THR	CA-CB-CG2	5.70	120.38	112.40
1	E	54	GLY	CA-C-O	-5.70	110.35	120.60
1	F	110	SER	CA-C-N	5.70	127.59	116.20
1	A	224	ASN	CA-CB-CG	-5.69	100.87	113.40
1	D	129	TYR	O-C-N	-5.69	113.59	122.70
1	F	95	GLN	CG-CD-OE1	-5.69	110.22	121.60
1	A	197	THR	CA-CB-CG2	5.69	120.37	112.40
1	E	30	PHE	CA-C-O	-5.69	108.15	120.10
1	E	79	TRP	CD1-CG-CD2	-5.69	101.75	106.30
1	A	217	PHE	CG-CD1-CE1	5.69	127.06	120.80
1	E	65	ASP	CA-C-O	5.69	132.05	120.10
1	A	215	TYR	CD1-CG-CD2	-5.69	111.64	117.90
1	B	26	SER	C-N-CA	5.69	135.92	121.70
1	C	29	ARG	CB-CA-C	-5.69	99.02	110.40
1	D	102	ILE	CA-CB-CG2	5.69	122.27	110.90
1	A	151	PRO	N-CA-CB	-5.69	96.35	102.60
1	C	89	ASN	CA-C-O	-5.69	108.16	120.10
1	B	59	ARG	CA-C-O	5.68	132.04	120.10
1	E	137	HIS	CE1-NE2-CD2	-5.68	92.39	106.60
1	F	152	TYR	CG-CD1-CE1	-5.68	116.75	121.30
1	E	59	ARG	CA-C-N	-5.68	104.70	117.20
1	E	41	PHE	CA-CB-CG	5.68	127.53	113.90
1	A	42	ASP	CB-CG-OD2	5.68	123.41	118.30
1	D	37	ASN	CB-CA-C	5.68	121.75	110.40
1	B	91	VAL	CB-CA-C	5.68	122.18	111.40
1	C	226	ALA	CB-CA-C	-5.68	101.59	110.10
1	E	105	PRO	N-CA-C	-5.68	97.34	112.10
1	D	109	ASP	CA-CB-CG	-5.67	100.91	113.40
1	C	40	LEU	CA-C-N	5.67	129.68	117.20
1	D	153	ARG	CA-C-N	-5.67	104.72	117.20
1	B	89	ASN	N-CA-C	5.67	126.31	111.00
1	B	181	THR	CA-C-N	5.67	127.54	116.20
1	E	24	GLU	C-N-CA	5.67	135.88	121.70
1	E	141	LEU	CB-CA-C	5.67	120.97	110.20
1	E	112	THR	CA-C-O	-5.67	108.19	120.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ASN	CA-CB-CG	5.67	125.87	113.40
1	A	109	ASP	CB-CG-OD2	5.67	123.40	118.30
1	F	99	THR	N-CA-CB	5.67	121.06	110.30
1	C	16	THR	CA-CB-CG2	-5.66	104.47	112.40
1	F	203	VAL	CA-C-N	5.66	129.66	117.20
1	C	5	PHE	CA-C-N	-5.66	104.88	116.20
1	F	16	THR	CB-CA-C	-5.66	96.33	111.60
1	B	200	ASN	CB-CA-C	-5.66	99.09	110.40
1	A	192	ARG	NH1-CZ-NH2	-5.65	113.18	119.40
1	A	210	ARG	CA-C-O	5.65	131.97	120.10
1	C	91	VAL	CG1-CB-CG2	-5.65	101.86	110.90
1	D	20	ALA	N-CA-C	-5.65	95.74	111.00
1	E	52	THR	N-CA-C	-5.65	95.74	111.00
1	B	208	ASN	CB-CA-C	-5.65	99.10	110.40
1	E	166	ASP	O-C-N	-5.65	113.66	122.70
1	B	35	ASP	CA-C-O	5.65	131.96	120.10
1	D	16	THR	CA-CB-OG1	5.65	120.86	109.00
1	E	127	ILE	N-CA-C	5.65	126.25	111.00
1	E	127	ILE	N-CA-CB	-5.65	97.81	110.80
1	C	156	MET	C-N-CA	-5.65	107.58	121.70
1	C	215	TYR	CB-CA-C	-5.64	99.11	110.40
1	D	10	GLU	OE1-CD-OE2	5.64	130.07	123.30
1	E	105	PRO	CB-CA-C	-5.64	97.89	112.00
1	C	37	ASN	CB-CG-ND2	5.64	130.24	116.70
1	D	87	ILE	CA-CB-CG2	5.64	122.18	110.90
1	D	156	MET	O-C-N	-5.64	113.67	122.70
1	D	168	ASP	CA-C-N	-5.64	104.79	117.20
1	D	62	LEU	O-C-N	-5.64	113.68	122.70
1	D	191	GLY	N-CA-C	5.64	127.20	113.10
1	F	108	TRP	N-CA-CB	-5.64	100.45	110.60
1	A	161	ASN	CA-CB-CG	5.64	125.80	113.40
1	E	206	SER	CB-CA-C	5.64	120.81	110.10
1	A	203	VAL	N-CA-CB	-5.63	99.11	111.50
1	C	120	VAL	CA-C-O	-5.63	108.27	120.10
1	D	129	TYR	CG-CD2-CE2	5.63	125.81	121.30
1	B	20	ALA	N-CA-C	-5.63	95.80	111.00
1	B	79	TRP	CE2-CD2-CG	5.63	111.81	107.30
1	B	148	GLN	CG-CD-NE2	-5.63	103.18	116.70
1	F	29	ARG	CB-CA-C	5.63	121.66	110.40
1	E	62	LEU	C-N-CA	-5.63	107.63	121.70
1	E	73	ALA	N-CA-CB	-5.63	102.22	110.10
1	E	189	PRO	N-CD-CG	-5.63	94.76	103.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	137	HIS	CA-CB-CG	-5.63	104.03	113.60
1	B	104	GLY	CA-C-O	5.63	130.73	120.60
1	C	76	THR	CA-C-N	5.62	129.57	117.20
1	C	162	LEU	C-N-CA	-5.62	107.64	121.70
1	A	110	SER	N-CA-CB	-5.62	102.07	110.50
1	E	103	TYR	CA-C-N	5.62	127.44	116.20
1	A	23	LEU	CA-CB-CG	5.62	128.22	115.30
1	D	209	SER	CB-CA-C	-5.62	99.42	110.10
1	E	56	THR	CA-CB-OG1	5.62	120.80	109.00
1	D	195	VAL	C-N-CA	5.62	135.74	121.70
1	D	185	ALA	CB-CA-C	-5.62	101.68	110.10
1	D	190	ASN	CB-CA-C	5.62	121.63	110.40
1	A	205	THR	CA-C-O	5.61	131.89	120.10
1	F	40	LEU	CB-CG-CD1	-5.61	101.46	111.00
1	A	230	GLY	CA-C-N	5.61	129.54	117.20
1	A	5	PHE	CB-CG-CD1	-5.61	116.88	120.80
1	A	129	TYR	OH-CZ-CE2	5.61	135.24	120.10
1	B	160	CYS	CA-C-O	-5.61	108.33	120.10
1	D	58	CYS	CB-CA-C	5.61	121.61	110.40
1	F	24	GLU	C-N-CA	5.61	135.71	121.70
1	B	70	ILE	O-C-N	-5.60	113.73	122.70
1	A	180	GLY	C-N-CA	-5.60	107.69	121.70
1	A	205	THR	C-N-CA	5.60	135.71	121.70
1	B	161	ASN	N-CA-CB	-5.60	100.52	110.60
1	D	218	VAL	CA-C-O	-5.60	108.34	120.10
1	E	188	GLN	CG-CD-OE1	-5.60	110.40	121.60
1	C	172	TRP	CB-CG-CD1	5.60	134.28	127.00
1	C	188	GLN	CG-CD-NE2	-5.60	103.27	116.70
1	D	153	ARG	O-C-N	5.60	131.65	122.70
1	C	13	HIS	ND1-CG-CD2	-5.59	98.17	106.00
1	E	5	PHE	CD1-CG-CD2	-5.59	111.03	118.30
1	E	6	GLY	CA-C-O	-5.59	110.53	120.60
1	B	47	VAL	CB-CA-C	-5.59	100.78	111.40
1	B	68	LEU	CA-C-N	-5.59	104.90	117.20
1	B	145	GLN	N-CA-CB	5.59	120.66	110.60
1	F	89	ASN	CA-CB-CG	5.59	125.69	113.40
1	A	9	HIS	O-C-N	-5.59	113.76	122.70
1	B	106	GLY	N-CA-C	-5.58	99.14	113.10
1	A	105	PRO	CA-C-O	-5.58	106.80	120.20
1	D	113	SER	N-CA-C	5.58	126.08	111.00
1	E	210	ARG	CA-CB-CG	5.58	125.68	113.40
1	F	158	THR	CA-C-N	5.58	129.48	117.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	ARG	O-C-N	5.58	131.63	122.70
1	E	157	GLU	N-CA-CB	-5.58	100.56	110.60
1	A	90	TYR	CD1-CE1-CZ	-5.57	114.78	119.80
1	A	196	LEU	CB-CA-C	-5.57	99.61	110.20
1	D	8	SER	O-C-N	5.57	131.62	122.70
1	F	62	LEU	CB-CA-C	-5.57	99.61	110.20
1	E	146	SER	N-CA-CB	-5.57	102.14	110.50
1	A	66	GLY	C-N-CA	-5.57	107.77	121.70
1	B	103	TYR	CE1-CZ-CE2	5.57	128.71	119.80
1	B	169	ASP	CB-CA-C	5.57	121.53	110.40
1	F	34	SER	CA-C-O	-5.57	108.41	120.10
1	A	102	ILE	CG1-CB-CG2	-5.57	99.15	111.40
1	C	39	VAL	CB-CA-C	-5.57	100.83	111.40
1	D	105	PRO	O-C-N	5.56	132.66	123.20
1	D	50	SER	CB-CA-C	5.56	120.67	110.10
1	E	91	VAL	O-C-N	-5.56	113.80	122.70
1	E	24	GLU	CA-C-N	5.56	129.43	117.20
1	E	155	SER	N-CA-C	5.56	126.01	111.00
1	E	180	GLY	O-C-N	5.56	131.60	122.70
1	C	81	SER	CB-CA-C	5.56	120.66	110.10
1	F	79	TRP	NE1-CE2-CZ2	-5.56	124.29	130.40
1	D	153	ARG	NH1-CZ-NH2	5.55	125.51	119.40
1	B	234	THR	OG1-CB-CG2	-5.55	97.23	110.00
1	A	134	ASN	CB-CG-ND2	5.55	130.02	116.70
1	D	197	THR	CB-CA-C	-5.55	96.62	111.60
1	E	91	VAL	CA-C-N	5.55	129.41	117.20
1	F	46	ARG	N-CA-C	-5.55	96.02	111.00
1	C	14	PRO	CA-N-CD	-5.55	103.74	111.50
1	E	151	PRO	O-C-N	-5.55	113.83	122.70
1	A	192	ARG	CB-CA-C	5.54	121.49	110.40
1	B	20	ALA	N-CA-CB	-5.54	102.34	110.10
1	B	172	TRP	CB-CG-CD2	5.54	133.81	126.60
1	E	109	ASP	OD1-CG-OD2	-5.54	112.77	123.30
1	D	79	TRP	CA-C-N	5.54	129.39	117.20
1	E	78	ARG	CA-C-N	5.54	129.39	117.20
1	A	79	TRP	CH2-CZ2-CE2	5.54	122.94	117.40
1	E	29	ARG	CB-CA-C	5.54	121.47	110.40
1	E	74	GLN	OE1-CD-NE2	-5.54	109.17	121.90
1	C	46	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	E	48	TRP	CZ3-CH2-CZ2	-5.53	114.97	121.60
1	B	177	ALA	N-CA-CB	-5.53	102.36	110.10
1	D	92	LEU	CB-CG-CD2	5.53	120.40	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	157	GLU	N-CA-C	5.53	125.92	111.00
1	E	144	THR	CA-C-O	-5.53	108.49	120.10
1	A	119	VAL	CA-C-N	5.53	129.35	117.20
1	B	15	GLN	CA-C-O	-5.53	108.50	120.10
1	B	38	LEU	N-CA-C	-5.53	96.08	111.00
1	B	136	ASN	N-CA-C	5.53	125.92	111.00
1	C	231	ALA	N-CA-C	5.53	125.92	111.00
1	A	4	LEU	CB-CG-CD2	5.52	120.39	111.00
1	B	195	VAL	N-CA-CB	5.52	123.65	111.50
1	D	91	VAL	CA-CB-CG2	-5.52	102.61	110.90
1	E	155	SER	O-C-N	-5.52	113.86	122.70
1	E	176	THR	CA-CB-OG1	5.52	120.60	109.00
1	F	110	SER	N-CA-C	-5.52	96.09	111.00
1	A	115	LYS	CB-CA-C	5.52	121.44	110.40
1	C	72	THR	N-CA-CB	-5.52	99.81	110.30
1	E	161	ASN	OD1-CG-ND2	5.52	134.60	121.90
1	A	166	ASP	N-CA-C	-5.52	96.10	111.00
1	E	78	ARG	N-CA-CB	5.52	120.53	110.60
1	A	24	GLU	CA-CB-CG	5.52	125.54	113.40
1	A	70	ILE	CB-CA-C	-5.52	100.57	111.60
1	C	207	GLY	O-C-N	-5.51	113.88	122.70
1	E	225	LEU	CA-CB-CG	5.51	127.98	115.30
1	E	103	TYR	CA-C-O	-5.51	108.52	120.10
1	C	108	TRP	CA-C-O	-5.51	108.53	120.10
1	C	172	TRP	CA-C-N	5.51	129.32	117.20
1	D	209	SER	CA-CB-OG	-5.51	96.32	111.20
1	F	233	TRP	CB-CG-CD1	5.51	134.16	127.00
1	E	197	THR	N-CA-CB	-5.51	99.83	110.30
1	D	141	LEU	CA-C-N	5.51	129.32	117.20
1	D	164	LEU	CA-C-N	5.51	129.32	117.20
1	F	79	TRP	CB-CG-CD1	-5.51	119.84	127.00
1	F	91	VAL	O-C-N	-5.50	113.89	122.70
1	A	41	PHE	CD1-CG-CD2	5.50	125.45	118.30
1	B	99	THR	CA-CB-OG1	5.50	120.55	109.00
1	B	43	SER	CA-CB-OG	5.50	126.05	111.20
1	F	158	THR	OG1-CB-CG2	5.50	122.65	110.00
1	C	124	GLY	CA-C-N	5.50	129.29	117.20
1	C	187	LEU	CA-C-O	5.50	131.64	120.10
1	B	35	ASP	N-CA-C	-5.49	96.17	111.00
1	E	90	TYR	OH-CZ-CE2	5.49	134.92	120.10
1	E	96	PRO	N-CA-CB	-5.49	96.56	102.60
1	C	222	ASP	CB-CG-OD2	5.49	123.24	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	LEU	CA-CB-CG	5.49	127.92	115.30
1	D	139	GLN	CG-CD-NE2	-5.49	103.53	116.70
1	D	48	TRP	CA-C-O	-5.49	108.58	120.10
1	A	187	LEU	C-N-CA	-5.48	107.99	121.70
1	A	78	ARG	C-N-CA	5.48	135.41	121.70
1	E	41	PHE	O-C-N	5.48	131.47	122.70
1	F	197	THR	OG1-CB-CG2	5.48	122.61	110.00
1	A	11	GLY	C-N-CA	-5.48	108.00	121.70
1	B	99	THR	C-N-CA	-5.48	108.00	121.70
1	D	186	VAL	CA-CB-CG2	5.48	119.12	110.90
1	E	137	HIS	CG-CD2-NE2	5.48	119.61	109.20
1	C	30	PHE	N-CA-CB	5.48	120.46	110.60
1	C	106	GLY	O-C-N	-5.48	113.93	122.70
1	F	109	ASP	N-CA-C	-5.48	96.21	111.00
1	F	215	TYR	CB-CA-C	-5.48	99.44	110.40
1	E	152	TYR	N-CA-C	-5.48	96.22	111.00
1	B	190	ASN	CA-CB-CG	5.47	125.44	113.40
1	D	177	ALA	CB-CA-C	-5.47	101.89	110.10
1	F	168	ASP	OD1-CG-OD2	-5.47	112.90	123.30
1	A	185	ALA	CA-C-O	5.47	131.59	120.10
1	C	83	THR	CA-C-O	-5.47	108.61	120.10
1	F	59	ARG	CA-C-O	5.47	131.59	120.10
1	C	8	SER	CA-CB-OG	-5.47	96.43	111.20
1	C	76	THR	O-C-N	-5.47	113.95	122.70
1	E	10	GLU	N-CA-C	-5.47	96.23	111.00
1	E	109	ASP	N-CA-CB	5.47	120.45	110.60
1	E	196	LEU	CB-CA-C	-5.47	99.81	110.20
1	E	89	ASN	CB-CA-C	5.47	121.33	110.40
1	B	8	SER	CB-CA-C	-5.47	99.71	110.10
1	D	16	THR	N-CA-CB	5.47	120.69	110.30
1	D	227	ILE	CA-C-N	5.47	129.23	117.20
1	F	65	ASP	CA-C-N	5.46	127.13	116.20
1	A	85	GLY	O-C-N	5.46	131.44	122.70
1	D	90	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	F	167	ARG	N-CA-CB	-5.46	100.77	110.60
1	D	86	SER	CA-C-O	-5.46	108.63	120.10
1	F	210	ARG	CB-CA-C	5.46	121.32	110.40
1	C	187	LEU	CB-CA-C	-5.46	99.83	110.20
1	D	14	PRO	N-CA-CB	5.46	109.85	103.30
1	F	202	ALA	CA-C-O	5.46	131.56	120.10
1	B	227	ILE	O-C-N	-5.45	113.97	122.70
1	E	27	SER	CA-C-O	5.45	131.55	120.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	LYS	CG-CD-CE	-5.45	95.55	111.90
1	A	103	TYR	CD1-CE1-CZ	-5.45	114.90	119.80
1	B	167	ARG	N-CA-C	-5.45	96.29	111.00
1	C	30	PHE	O-C-N	5.45	131.42	122.70
1	C	175	ASN	CB-CG-OD1	5.45	132.50	121.60
1	A	18	HIS	N-CA-C	-5.44	96.31	111.00
1	A	120	VAL	CA-C-O	-5.44	108.68	120.10
1	A	228	TYR	CA-C-O	5.44	131.52	120.10
1	C	162	LEU	CB-CA-C	5.44	120.53	110.20
1	C	194	ASP	O-C-N	-5.44	114.00	122.70
1	D	201	ILE	CB-CA-C	-5.44	100.72	111.60
1	E	137	HIS	ND1-CE1-NE2	5.44	121.87	109.90
1	A	35	ASP	OD1-CG-OD2	-5.44	112.97	123.30
1	B	232	LEU	CA-CB-CG	5.44	127.81	115.30
1	D	22	SER	N-CA-CB	-5.44	102.34	110.50
1	B	23	LEU	O-C-N	5.44	131.40	122.70
1	E	192	ARG	CB-CG-CD	5.44	125.74	111.60
1	F	164	LEU	O-C-N	5.44	131.40	122.70
1	A	98	ARG	CD-NE-CZ	-5.43	115.99	123.60
1	A	222	ASP	O-C-N	5.43	131.40	122.70
1	C	50	SER	CA-CB-OG	5.43	125.87	111.20
1	F	10	GLU	CA-CB-CG	-5.43	101.44	113.40
1	F	102	ILE	N-CA-C	5.43	125.67	111.00
1	A	226	ALA	CA-C-O	-5.43	108.69	120.10
1	C	39	VAL	C-N-CA	5.43	135.28	121.70
1	E	105	PRO	C-N-CA	-5.43	110.89	122.30
1	C	5	PHE	CE1-CZ-CE2	-5.43	110.22	120.00
1	C	68	LEU	CA-CB-CG	5.43	127.79	115.30
1	E	139	GLN	N-CA-CB	-5.43	100.82	110.60
1	B	210	ARG	CA-CB-CG	5.43	125.35	113.40
1	C	24	GLU	C-N-CA	5.43	135.27	121.70
1	B	158	THR	CA-C-O	-5.43	108.70	120.10
1	E	39	VAL	CB-CA-C	-5.43	101.09	111.40
1	B	129	TYR	CE1-CZ-OH	5.42	134.75	120.10
1	B	32	MET	CG-SD-CE	5.42	108.88	100.20
1	D	5	PHE	CA-C-O	-5.42	108.71	120.10
1	E	217	PHE	CZ-CE2-CD2	5.42	126.61	120.10
1	A	59	ARG	N-CA-C	-5.42	96.36	111.00
1	B	207	GLY	O-C-N	-5.42	114.03	122.70
1	C	71	LEU	CA-C-O	5.42	131.49	120.10
1	C	111	GLY	CA-C-O	-5.42	110.84	120.60
1	E	64	SER	CA-C-O	5.42	131.48	120.10

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	96	PRO	CB-CA-C	5.42	125.55	112.00
1	F	142	HIS	CB-CA-C	-5.42	99.56	110.40
1	A	221	PRO	CA-C-O	5.42	133.20	120.20
1	B	62	LEU	CD1-CG-CD2	-5.42	94.25	110.50
1	B	216	VAL	CA-C-O	5.42	131.47	120.10
1	A	100	VAL	CA-C-N	5.42	129.11	117.20
1	D	158	THR	CA-CB-OG1	-5.41	97.63	109.00
1	E	216	VAL	CA-C-N	5.41	129.11	117.20
1	F	74	GLN	O-C-N	-5.41	114.04	122.70
1	A	131	THR	CA-CB-CG2	-5.41	104.83	112.40
1	B	59	ARG	CA-C-N	-5.41	105.30	117.20
1	D	141	LEU	CB-CA-C	-5.41	99.92	110.20
1	E	42	ASP	CA-C-O	-5.41	108.74	120.10
1	A	168	ASP	O-C-N	-5.41	114.05	122.70
1	E	48	TRP	CG-CD1-NE1	-5.41	104.69	110.10
1	A	183	CYS	CA-CB-SG	5.40	123.73	114.00
1	A	45	VAL	CG1-CB-CG2	-5.40	102.26	110.90
1	A	184	ARG	CA-C-N	-5.40	105.32	117.20
1	C	203	VAL	N-CA-CB	-5.40	99.62	111.50
1	C	27	SER	C-N-CA	-5.40	108.21	121.70
1	C	82	GLY	O-C-N	-5.40	114.06	122.70
1	D	5	PHE	CD1-CG-CD2	-5.40	111.28	118.30
1	D	180	GLY	CA-C-O	5.40	130.32	120.60
1	D	207	GLY	CA-C-N	-5.40	105.32	117.20
1	E	192	ARG	N-CA-CB	-5.40	100.89	110.60
1	C	174	THR	CA-CB-CG2	5.39	119.95	112.40
1	F	139	GLN	CA-CB-CG	-5.39	101.53	113.40
1	B	187	LEU	CB-CG-CD2	5.39	120.17	111.00
1	E	92	LEU	CB-CG-CD1	5.39	120.17	111.00
1	A	79	TRP	N-CA-CB	-5.39	100.90	110.60
1	E	129	TYR	C-N-CA	5.39	135.17	121.70
1	F	7	LEU	N-CA-C	5.39	125.55	111.00
1	C	69	VAL	CB-CA-C	-5.39	101.16	111.40
1	E	143	ALA	N-CA-C	-5.39	96.45	111.00
1	A	228	TYR	C-N-CA	5.39	133.61	122.30
1	B	198	ASN	O-C-N	-5.39	114.08	122.70
1	C	2	ASN	CA-C-O	5.39	131.41	120.10
1	C	125	ASN	C-N-CA	5.39	135.17	121.70
1	F	159	ASP	CB-CA-C	5.39	121.17	110.40
1	F	228	TYR	CA-C-N	5.39	126.97	116.20
1	B	164	LEU	CA-C-O	-5.38	108.79	120.10
1	C	165	PHE	O-C-N	5.38	131.31	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	19	ALA	CA-C-N	5.38	129.04	117.20
1	F	219	LEU	C-N-CA	-5.38	108.24	121.70
1	B	125	ASN	CA-CB-CG	5.38	125.24	113.40
1	E	210	ARG	C-N-CA	5.38	135.15	121.70
1	F	175	ASN	OD1-CG-ND2	5.38	134.28	121.90
1	F	191	GLY	O-C-N	5.38	131.31	122.70
1	E	71	LEU	C-N-CA	-5.38	108.25	121.70
1	D	87	ILE	CA-CB-CG1	-5.38	100.78	111.00
1	D	157	GLU	CB-CG-CD	5.38	128.72	114.20
1	F	45	VAL	CB-CA-C	5.38	121.62	111.40
1	F	80	SER	CA-C-N	-5.38	105.37	117.20
1	D	103	TYR	CZ-CE2-CD2	-5.38	114.96	119.80
1	F	96	PRO	O-C-N	-5.38	114.10	122.70
1	E	113	SER	CA-C-O	5.38	131.39	120.10
1	E	221	PRO	CA-C-O	-5.38	107.30	120.20
1	A	12	SER	O-C-N	5.37	131.30	122.70
1	C	64	SER	CB-CA-C	-5.37	99.89	110.10
1	D	140	THR	C-N-CA	5.37	135.13	121.70
1	A	234	THR	CA-C-O	-5.37	108.82	120.10
1	B	52	THR	OG1-CB-CG2	-5.37	97.65	110.00
1	E	148	GLN	CB-CG-CD	5.37	125.56	111.60
1	A	214	ARG	NH1-CZ-NH2	-5.37	113.50	119.40
1	B	163	VAL	C-N-CA	5.37	135.12	121.70
1	F	41	PHE	CG-CD1-CE1	5.37	126.70	120.80
1	D	78	ARG	N-CA-CB	-5.36	100.95	110.60
1	D	114	ASN	CB-CG-OD1	5.36	132.33	121.60
1	D	184	ARG	N-CA-CB	5.36	120.25	110.60
1	B	77	ILE	N-CA-CB	-5.36	98.47	110.80
1	E	75	ASN	C-N-CA	-5.36	108.30	121.70
1	F	57	GLY	C-N-CA	5.36	135.10	121.70
1	F	139	GLN	CG-CD-NE2	-5.36	103.83	116.70
1	C	204	TRP	C-N-CA	5.36	135.10	121.70
1	F	233	TRP	N-CA-CB	-5.36	100.95	110.60
1	A	14	PRO	N-CA-CB	5.36	109.73	103.30
1	C	204	TRP	CE3-CZ3-CH2	5.36	127.09	121.20
1	F	164	LEU	C-N-CA	-5.36	108.31	121.70
1	A	79	TRP	CD2-CE3-CZ3	5.35	125.76	118.80
1	E	12	SER	N-CA-CB	5.35	118.53	110.50
1	E	117	SER	C-N-CA	5.35	135.07	121.70
1	F	19	ALA	CA-C-N	5.35	128.97	117.20
1	F	196	LEU	CD1-CG-CD2	-5.35	94.45	110.50
1	A	208	ASN	CB-CG-ND2	5.35	129.53	116.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	GLN	CA-CB-CG	-5.35	101.64	113.40
1	B	103	TYR	CB-CG-CD1	-5.35	117.79	121.00
1	B	175	ASN	CA-C-N	5.35	128.97	117.20
1	C	116	GLY	CA-C-N	5.35	128.97	117.20
1	E	139	GLN	N-CA-C	-5.35	96.56	111.00
1	F	193	MET	N-CA-C	-5.35	96.57	111.00
1	A	34	SER	C-N-CA	5.34	135.06	121.70
1	E	35	ASP	CA-C-O	5.34	131.32	120.10
1	E	71	LEU	CB-CA-C	-5.34	100.05	110.20
1	B	221	PRO	O-C-N	-5.34	114.16	122.70
1	D	41	PHE	CA-C-O	5.34	131.31	120.10
1	E	35	ASP	CB-CA-C	-5.34	99.73	110.40
1	F	70	ILE	CA-C-N	-5.34	105.46	117.20
1	F	86	SER	CA-CB-OG	5.34	125.61	111.20
1	C	17	LEU	CB-CG-CD1	-5.33	101.93	111.00
1	C	74	GLN	CG-CD-OE1	-5.33	110.93	121.60
1	A	12	SER	CA-C-N	-5.33	105.47	117.20
1	C	4	LEU	O-C-N	5.33	131.23	122.70
1	D	55	ALA	O-C-N	-5.33	114.17	122.70
1	F	189	PRO	CA-N-CD	-5.33	104.04	111.50
1	B	2	ASN	O-C-N	-5.33	114.17	122.70
1	D	75	ASN	C-N-CA	-5.33	108.38	121.70
1	D	146	SER	CA-CB-OG	-5.33	96.81	111.20
1	B	201	ILE	CA-CB-CG2	5.33	121.55	110.90
1	C	179	LYS	CA-CB-CG	-5.33	101.68	113.40
1	D	28	PHE	N-CA-C	-5.33	96.62	111.00
1	D	42	ASP	CB-CG-OD1	-5.33	113.51	118.30
1	F	152	TYR	CA-C-N	5.33	128.92	117.20
1	E	231	ALA	CA-C-O	-5.32	108.92	120.10
1	B	208	ASN	CA-C-O	5.32	131.27	120.10
1	C	37	ASN	O-C-N	5.32	131.21	122.70
1	F	189	PRO	N-CD-CG	5.32	111.18	103.20
1	A	97	ASP	OD1-CG-OD2	5.32	133.40	123.30
1	E	111	GLY	CA-C-N	-5.32	105.50	117.20
1	E	231	ALA	N-CA-C	-5.32	96.64	111.00
1	C	114	ASN	CA-CB-CG	5.32	125.09	113.40
1	D	200	ASN	N-CA-C	5.32	125.35	111.00
1	A	94	LEU	CA-C-O	5.31	131.26	120.10
1	C	163	VAL	CB-CA-C	5.31	121.49	111.40
1	C	225	LEU	CA-C-N	5.31	128.89	117.20
1	D	234	THR	N-CA-CB	-5.31	100.21	110.30
1	C	87	ILE	CA-CB-CG1	-5.31	100.91	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	158	THR	N-CA-CB	5.31	120.39	110.30
1	C	30	PHE	CE1-CZ-CE2	-5.31	110.44	120.00
1	E	18	HIS	CG-ND1-CE1	5.31	115.63	108.20
1	F	170	ARG	CD-NE-CZ	5.31	131.03	123.60
1	F	225	LEU	CB-CG-CD1	-5.31	101.97	111.00
1	E	37	ASN	CA-C-O	-5.31	108.95	120.10
1	A	28	PHE	CA-C-N	-5.30	105.53	117.20
1	B	142	HIS	CA-C-O	-5.30	108.96	120.10
1	D	90	TYR	O-C-N	5.30	131.19	122.70
1	F	213	GLY	CA-C-N	5.30	128.87	117.20
1	C	132	GLN	CA-C-N	5.30	126.81	116.20
1	D	170	ARG	CG-CD-NE	5.30	122.94	111.80
1	F	62	LEU	CA-CB-CG	5.30	127.50	115.30
1	D	70	ILE	O-C-N	-5.30	114.22	122.70
1	E	79	TRP	CA-C-O	-5.30	108.97	120.10
1	A	157	GLU	N-CA-C	5.30	125.31	111.00
1	B	21	GLN	O-C-N	-5.30	114.22	122.70
1	B	162	LEU	CB-CG-CD2	-5.30	101.99	111.00
1	C	93	VAL	CA-CB-CG1	5.30	118.85	110.90
1	C	148	GLN	CA-C-O	-5.30	108.97	120.10
1	C	204	TRP	O-C-N	-5.30	114.22	122.70
1	C	154	LEU	C-N-CA	-5.29	108.46	121.70
1	C	102	ILE	CG1-CB-CG2	-5.29	99.75	111.40
1	E	104	GLY	N-CA-C	5.29	126.34	113.10
1	B	211	SER	CA-C-N	5.29	128.84	117.20
1	C	199	GLN	C-N-CA	5.29	134.93	121.70
1	D	153	ARG	CB-CG-CD	-5.29	97.84	111.60
1	A	40	LEU	N-CA-CB	5.29	120.98	110.40
1	A	73	ALA	CB-CA-C	-5.29	102.17	110.10
1	B	144	THR	N-CA-CB	5.29	120.35	110.30
1	A	49	ALA	CA-C-N	5.29	128.83	117.20
1	B	200	ASN	CB-CG-ND2	-5.29	104.01	116.70
1	C	5	PHE	N-CA-CB	5.29	120.12	110.60
1	C	199	GLN	CG-CD-OE1	5.29	132.18	121.60
1	E	21	GLN	OE1-CD-NE2	5.29	134.06	121.90
1	F	103	TYR	CZ-CE2-CD2	-5.29	115.04	119.80
1	E	9	HIS	N-CA-C	5.29	125.27	111.00
1	F	218	VAL	CA-C-O	-5.29	109.00	120.10
1	C	25	LEU	CA-C-N	5.29	128.83	117.20
1	C	148	GLN	N-CA-C	5.29	125.27	111.00
1	F	23	LEU	C-N-CA	-5.29	108.49	121.70
1	A	3	ILE	CA-C-O	5.28	131.19	120.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	ARG	CA-CB-CG	-5.28	101.77	113.40
1	E	143	ALA	O-C-N	5.28	131.15	122.70
1	A	101	THR	CA-C-O	-5.28	109.01	120.10
1	A	56	THR	C-N-CA	5.28	133.39	122.30
1	D	153	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	38	LEU	CB-CA-C	-5.28	100.17	110.20
1	C	91	VAL	O-C-N	-5.28	114.26	122.70
1	B	139	GLN	CA-C-O	-5.28	109.02	120.10
1	B	158	THR	CB-CA-C	-5.28	97.35	111.60
1	C	103	TYR	O-C-N	-5.28	114.23	123.20
1	E	86	SER	CA-C-O	-5.28	109.02	120.10
1	C	149	LEU	CB-CG-CD2	5.27	119.97	111.00
1	B	196	LEU	N-CA-C	5.27	125.23	111.00
1	B	148	GLN	CA-C-O	-5.27	109.03	120.10
1	D	16	THR	N-CA-C	5.27	125.23	111.00
1	D	215	TYR	CB-CA-C	-5.27	99.86	110.40
1	E	103	TYR	CD1-CG-CD2	-5.27	112.10	117.90
1	E	108	TRP	CD1-NE1-CE2	-5.27	104.26	109.00
1	C	169	ASP	C-N-CA	5.27	134.87	121.70
1	F	145	GLN	N-CA-C	5.27	125.22	111.00
1	A	4	LEU	N-CA-CB	-5.27	99.87	110.40
1	E	111	GLY	CA-C-O	-5.26	111.12	120.60
1	F	33	GLN	CG-CD-NE2	-5.26	104.06	116.70
1	B	189	PRO	N-CA-CB	5.26	109.62	103.30
1	B	83	THR	CA-C-N	5.26	128.78	117.20
1	E	73	ALA	CA-C-O	5.26	131.15	120.10
1	F	163	VAL	CB-CA-C	5.26	121.40	111.40
1	C	198	ASN	CA-CB-CG	-5.26	101.83	113.40
1	E	43	SER	N-CA-CB	-5.26	102.61	110.50
1	F	45	VAL	C-N-CA	-5.26	108.55	121.70
1	A	123	ASN	CB-CA-C	-5.26	99.88	110.40
1	A	201	ILE	CA-C-O	5.26	131.14	120.10
1	D	175	ASN	C-N-CA	5.25	134.84	121.70
1	F	170	ARG	O-C-N	-5.25	114.29	122.70
1	C	49	ALA	N-CA-C	5.25	125.18	111.00
1	C	77	ILE	N-CA-C	5.25	125.18	111.00
1	D	100	VAL	C-N-CA	5.25	134.83	121.70
1	F	87	ILE	CA-C-O	-5.25	109.07	120.10
1	C	193	MET	N-CA-C	-5.25	96.83	111.00
1	B	206	SER	CA-C-N	5.25	126.69	116.20
1	F	78	ARG	CD-NE-CZ	-5.25	116.25	123.60
1	A	181	THR	CA-C-O	-5.25	109.09	120.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	215	TYR	N-CA-CB	5.25	120.04	110.60
1	E	214	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	E	107	LEU	CA-CB-CG	5.24	127.36	115.30
1	E	223	ARG	O-C-N	-5.24	114.31	122.70
1	B	128	LEU	CD1-CG-CD2	-5.24	94.77	110.50
1	E	57	GLY	CA-C-O	5.24	130.04	120.60
1	A	89	ASN	CA-C-N	5.24	128.73	117.20
1	B	14	PRO	CA-N-CD	-5.24	104.16	111.50
1	B	153	ARG	CB-CA-C	-5.24	99.92	110.40
1	B	5	PHE	C-N-CA	5.24	133.30	122.30
1	F	217	PHE	CZ-CE2-CD2	-5.24	113.81	120.10
1	C	154	LEU	CB-CG-CD1	5.24	119.90	111.00
1	F	69	VAL	CB-CA-C	5.24	121.35	111.40
1	D	219	LEU	CB-CG-CD1	5.24	119.90	111.00
1	E	70	ILE	N-CA-CB	-5.24	98.76	110.80
1	E	82	GLY	CA-C-O	-5.24	111.17	120.60
1	F	139	GLN	O-C-N	5.24	131.08	122.70
1	A	163	VAL	O-C-N	5.23	131.07	122.70
1	C	23	LEU	O-C-N	5.23	131.07	122.70
1	F	10	GLU	OE1-CD-OE2	-5.23	117.02	123.30
1	D	167	ARG	N-CA-CB	5.23	120.02	110.60
1	E	127	ILE	CA-CB-CG2	-5.23	100.44	110.90
1	E	157	GLU	N-CA-C	5.23	125.12	111.00
1	F	21	GLN	CA-CB-CG	5.22	124.89	113.40
1	A	217	PHE	O-C-N	5.22	131.05	122.70
1	F	125	ASN	N-CA-C	5.22	125.10	111.00
1	B	208	ASN	OD1-CG-ND2	5.22	133.90	121.90
1	C	175	ASN	CA-C-O	-5.22	109.14	120.10
1	E	64	SER	CA-CB-OG	5.22	125.29	111.20
1	E	172	TRP	CE2-CD2-CG	5.22	111.47	107.30
1	A	157	GLU	CB-CG-CD	5.21	128.28	114.20
1	D	59	ARG	CD-NE-CZ	5.21	130.90	123.60
1	E	89	ASN	OD1-CG-ND2	5.21	133.89	121.90
1	E	153	ARG	CG-CD-NE	-5.21	100.85	111.80
1	F	37	ASN	C-N-CA	-5.21	108.66	121.70
1	F	144	THR	N-CA-C	-5.21	96.92	111.00
1	B	105	PRO	O-C-N	5.21	132.06	123.20
1	C	63	GLN	OE1-CD-NE2	-5.21	109.92	121.90
1	D	145	GLN	CA-C-O	5.21	131.04	120.10
1	F	44	ASP	OD1-CG-OD2	5.21	133.20	123.30
1	B	197	THR	CA-C-O	5.21	131.04	120.10
1	C	139	GLN	CG-CD-OE1	-5.21	111.18	121.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	169	ASP	CB-CG-OD1	5.21	122.99	118.30
1	F	182	GLY	CA-C-N	-5.21	105.74	117.20
1	C	199	GLN	CB-CG-CD	-5.21	98.06	111.60
1	D	127	ILE	CA-CB-CG1	5.21	120.89	111.00
1	E	232	LEU	CA-C-N	5.21	128.65	117.20
1	A	118	VAL	CG1-CB-CG2	-5.20	102.57	110.90
1	A	172	TRP	CD1-CG-CD2	-5.20	102.14	106.30
1	B	224	ASN	C-N-CA	5.20	134.70	121.70
1	C	116	GLY	O-C-N	-5.20	114.38	122.70
1	C	140	THR	CB-CA-C	-5.20	97.56	111.60
1	D	66	GLY	O-C-N	-5.20	114.38	122.70
1	D	90	TYR	CG-CD2-CE2	5.20	125.46	121.30
1	E	129	TYR	N-CA-CB	-5.20	101.24	110.60
1	A	141	LEU	CB-CA-C	-5.20	100.32	110.20
1	B	100	VAL	CG1-CB-CG2	-5.20	102.58	110.90
1	C	129	TYR	CA-C-N	5.20	128.64	117.20
1	E	108	TRP	CA-C-O	-5.20	109.19	120.10
1	A	217	PHE	CA-C-N	5.20	128.63	117.20
1	E	226	ALA	CA-C-O	-5.20	109.19	120.10
1	F	103	TYR	CD1-CG-CD2	-5.20	112.19	117.90
1	F	215	TYR	CZ-CE2-CD2	5.20	124.47	119.80
1	B	175	ASN	CA-C-O	-5.19	109.19	120.10
1	E	189	PRO	CB-CG-CD	-5.19	86.25	106.50
1	C	72	THR	N-CA-C	5.19	125.02	111.00
1	F	30	PHE	CB-CA-C	-5.19	100.02	110.40
1	A	39	VAL	N-CA-C	5.19	125.02	111.00
1	D	108	TRP	CB-CG-CD2	5.19	133.35	126.60
1	E	118	VAL	CA-CB-CG1	5.19	118.68	110.90
1	A	53	ALA	O-C-N	-5.19	114.38	123.20
1	C	19	ALA	O-C-N	-5.19	114.40	122.70
1	D	107	LEU	N-CA-C	-5.19	96.99	111.00
1	C	19	ALA	N-CA-C	5.18	125.00	111.00
1	E	48	TRP	CA-C-O	-5.18	109.21	120.10
1	A	79	TRP	CB-CG-CD2	5.18	133.34	126.60
1	C	136	ASN	CB-CG-OD1	-5.18	111.23	121.60
1	F	36	CYS	CA-C-N	5.18	128.60	117.20
1	F	159	ASP	CA-CB-CG	5.18	124.80	113.40
1	A	114	ASN	OD1-CG-ND2	5.18	133.81	121.90
1	B	63	GLN	OE1-CD-NE2	-5.18	109.99	121.90
1	C	118	VAL	CA-CB-CG1	5.18	118.67	110.90
1	E	145	GLN	C-N-CA	5.18	134.65	121.70
1	F	207	GLY	O-C-N	-5.18	114.41	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	202	ALA	CB-CA-C	5.18	117.87	110.10
1	F	85	GLY	C-N-CA	5.18	134.65	121.70
1	C	13	HIS	CG-CD2-NE2	5.17	119.03	109.20
1	C	21	GLN	CA-CB-CG	-5.17	102.01	113.40
1	E	121	ALA	C-N-CA	5.17	134.63	121.70
1	A	115	LYS	C-N-CA	5.17	133.16	122.30
1	C	137	HIS	ND1-CE1-NE2	5.17	121.28	109.90
1	C	193	MET	CA-CB-CG	-5.17	104.51	113.30
1	D	69	VAL	CA-C-O	-5.17	109.24	120.10
1	A	59	ARG	CG-CD-NE	5.17	122.65	111.80
1	B	39	VAL	O-C-N	-5.17	114.43	122.70
1	E	233	TRP	C-N-CA	-5.17	108.78	121.70
1	A	128	LEU	CB-CG-CD2	5.17	119.78	111.00
1	C	180	GLY	CA-C-O	-5.17	111.30	120.60
1	C	156	MET	CA-C-N	-5.17	105.84	117.20
1	C	3	ILE	CB-CG1-CD1	-5.16	99.44	113.90
1	E	137	HIS	C-N-CA	5.16	143.69	122.00
1	F	95	GLN	CA-C-O	-5.16	109.25	120.10
1	A	173	SER	CB-CA-C	5.16	119.91	110.10
1	D	213	GLY	C-N-CA	-5.16	108.80	121.70
1	F	30	PHE	CA-C-O	5.16	130.94	120.10
1	C	153	ARG	C-N-CA	-5.16	108.80	121.70
1	A	33	GLN	O-C-N	-5.16	114.45	122.70
1	B	97	ASP	CB-CA-C	5.16	120.71	110.40
1	E	164	LEU	C-N-CA	-5.16	108.81	121.70
1	E	28	PHE	CB-CG-CD1	5.16	124.41	120.80
1	C	30	PHE	CG-CD1-CE1	-5.15	115.13	120.80
1	E	32	MET	CA-CB-CG	5.15	122.06	113.30
1	B	204	TRP	CB-CG-CD1	5.15	133.70	127.00
1	F	159	ASP	OD1-CG-OD2	5.15	133.09	123.30
1	D	3	ILE	CA-CB-CG1	-5.15	101.22	111.00
1	E	31	THR	CA-CB-CG2	-5.15	105.19	112.40
1	D	217	PHE	CE1-CZ-CE2	5.15	129.26	120.00
1	A	192	ARG	N-CA-C	5.15	124.89	111.00
1	A	198	ASN	O-C-N	-5.15	114.47	122.70
1	B	109	ASP	CA-C-N	-5.15	105.88	117.20
1	D	85	GLY	O-C-N	-5.14	114.47	122.70
1	D	103	TYR	CD1-CG-CD2	-5.14	112.24	117.90
1	F	78	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	F	232	LEU	O-C-N	5.14	130.93	122.70
1	B	30	PHE	CG-CD1-CE1	5.14	126.45	120.80
1	C	66	GLY	CA-C-O	5.14	129.85	120.60

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	89	ASN	CA-C-O	-5.14	109.31	120.10
1	B	193	MET	CB-CG-SD	-5.14	96.99	112.40
1	D	130	SER	CA-C-N	-5.14	105.90	117.20
1	E	47	VAL	CA-C-N	5.14	128.50	117.20
1	B	138	PRO	CB-CA-C	-5.13	99.16	112.00
1	C	45	VAL	CA-C-O	5.13	130.88	120.10
1	D	196	LEU	CD1-CG-CD2	-5.13	95.10	110.50
1	F	81	SER	C-N-CA	-5.13	111.53	122.30
1	F	183	CYS	CA-C-O	5.13	130.87	120.10
1	D	11	GLY	N-CA-C	-5.13	100.28	113.10
1	D	84	LYS	C-N-CA	-5.13	111.53	122.30
1	E	63	GLN	CG-CD-OE1	5.12	131.85	121.60
1	E	155	SER	CA-C-N	5.12	128.47	117.20
1	F	21	GLN	CB-CA-C	5.12	120.65	110.40
1	C	3	ILE	CA-C-O	-5.12	109.34	120.10
1	D	212	ALA	CA-C-N	5.12	126.44	116.20
1	A	152	TYR	CA-C-O	-5.12	109.35	120.10
1	A	190	ASN	CB-CA-C	5.12	120.64	110.40
1	B	48	TRP	C-N-CA	-5.12	108.91	121.70
1	E	97	ASP	CA-C-O	-5.12	109.36	120.10
1	B	157	GLU	O-C-N	5.11	130.88	122.70
1	A	96	PRO	CA-N-CD	-5.11	104.34	111.50
1	C	40	LEU	CA-C-O	5.11	130.83	120.10
1	F	49	ALA	CA-C-O	-5.11	109.36	120.10
1	A	50	SER	N-CA-C	-5.11	97.20	111.00
1	C	65	ASP	CB-CA-C	5.11	120.62	110.40
1	F	161	ASN	CA-C-N	-5.11	105.96	117.20
1	C	7	LEU	CB-CA-C	5.11	119.91	110.20
1	C	49	ALA	O-C-N	-5.11	114.53	122.70
1	D	2	ASN	C-N-CA	5.11	134.47	121.70
1	E	172	TRP	O-C-N	5.11	130.87	122.70
1	F	15	GLN	N-CA-C	-5.10	97.22	111.00
1	A	164	LEU	CD1-CG-CD2	-5.10	95.19	110.50
1	C	145	GLN	N-CA-C	-5.10	97.22	111.00
1	D	156	MET	N-CA-CB	-5.10	101.42	110.60
1	A	164	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	B	166	ASP	N-CA-C	-5.10	97.23	111.00
1	E	98	ARG	C-N-CA	5.10	134.45	121.70
1	A	221	PRO	N-CA-C	-5.10	98.85	112.10
1	E	4	LEU	CB-CA-C	5.10	119.89	110.20
1	F	18	HIS	N-CA-CB	-5.10	101.43	110.60
1	D	233	TRP	CB-CG-CD2	5.10	133.22	126.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	30	PHE	CZ-CE2-CD2	-5.10	113.98	120.10
1	B	69	VAL	CA-C-O	-5.09	109.40	120.10
1	D	52	THR	CA-C-O	-5.09	109.40	120.10
1	C	14	PRO	C-N-CA	-5.09	108.97	121.70
1	E	145	GLN	N-CA-CB	5.09	119.77	110.60
1	C	78	ARG	CB-CG-CD	-5.09	98.38	111.60
1	C	201	ILE	CA-C-O	5.09	130.78	120.10
1	A	114	ASN	CB-CG-ND2	5.08	128.91	116.70
1	B	175	ASN	CB-CG-OD1	-5.08	111.43	121.60
1	B	231	ALA	N-CA-C	-5.08	97.27	111.00
1	C	36	CYS	N-CA-CB	-5.08	101.45	110.60
1	A	76	THR	CA-CB-OG1	5.08	119.67	109.00
1	D	77	ILE	O-C-N	-5.08	114.57	122.70
1	E	159	ASP	CA-C-O	5.08	130.77	120.10
1	C	28	PHE	C-N-CA	5.08	134.39	121.70
1	C	208	ASN	N-CA-C	-5.08	97.29	111.00
1	E	48	TRP	CE3-CZ3-CH2	5.08	126.79	121.20
1	E	89	ASN	CA-C-N	5.08	128.37	117.20
1	F	153	ARG	N-CA-C	5.08	124.71	111.00
1	B	161	ASN	O-C-N	5.08	130.82	122.70
1	A	2	ASN	CA-C-N	5.08	128.36	117.20
1	B	81	SER	O-C-N	-5.07	114.58	123.20
1	B	234	THR	CA-C-N	5.07	128.36	117.20
1	D	156	MET	CA-C-N	5.07	128.36	117.20
1	F	76	THR	OG1-CB-CG2	-5.07	98.33	110.00
1	E	88	GLY	C-N-CA	-5.07	109.02	121.70
1	A	13	HIS	CB-CA-C	5.07	120.54	110.40
1	B	127	ILE	CG1-CB-CG2	5.07	122.56	111.40
1	B	208	ASN	C-N-CA	-5.07	109.03	121.70
1	C	59	ARG	N-CA-CB	-5.07	101.47	110.60
1	C	79	TRP	C-N-CA	5.07	134.38	121.70
1	C	93	VAL	C-N-CA	5.07	134.38	121.70
1	B	31	THR	CA-C-N	-5.07	106.05	117.20
1	C	225	LEU	N-CA-CB	-5.07	100.27	110.40
1	F	161	ASN	CB-CG-OD1	-5.07	111.47	121.60
1	B	51	ASN	CA-CB-CG	5.07	124.54	113.40
1	D	74	GLN	CG-CD-NE2	5.07	128.85	116.70
1	F	53	ALA	CA-C-O	-5.07	109.46	120.10
1	A	196	LEU	CA-C-N	-5.06	106.06	117.20
1	E	82	GLY	O-C-N	5.06	130.80	122.70
1	A	71	LEU	C-N-CA	-5.06	109.04	121.70
1	A	192	ARG	CD-NE-CZ	5.06	130.69	123.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	113	SER	CA-C-O	5.06	130.73	120.10
1	A	99	THR	CA-C-N	5.06	128.34	117.20
1	B	152	TYR	CZ-CE2-CD2	-5.06	115.25	119.80
1	C	212	ALA	N-CA-C	5.06	124.67	111.00
1	F	50	SER	CA-CB-OG	-5.06	97.54	111.20
1	B	210	ARG	CB-CG-CD	5.06	124.75	111.60
1	E	206	SER	CA-C-N	5.06	126.32	116.20
1	D	39	VAL	N-CA-CB	5.06	122.62	111.50
1	D	190	ASN	C-N-CA	5.06	132.92	122.30
1	F	99	THR	OG1-CB-CG2	5.06	121.63	110.00
1	A	143	ALA	CA-C-O	-5.06	109.48	120.10
1	C	144	THR	CA-CB-OG1	5.05	119.61	109.00
1	B	170	ARG	CA-C-O	5.05	130.71	120.10
1	B	10	GLU	N-CA-CB	-5.05	101.51	110.60
1	B	125	ASN	C-N-CA	5.05	134.33	121.70
1	E	177	ALA	CA-C-O	5.05	130.71	120.10
1	C	62	LEU	C-N-CA	5.05	134.32	121.70
1	D	24	GLU	N-CA-C	5.05	124.63	111.00
1	F	192	ARG	CA-C-O	5.05	130.70	120.10
1	C	180	GLY	O-C-N	5.05	130.77	122.70
1	D	191	GLY	O-C-N	5.05	130.77	122.70
1	B	111	GLY	N-CA-C	5.04	125.71	113.10
1	A	77	ILE	CB-CG1-CD1	5.04	128.02	113.90
1	D	32	MET	CA-C-N	-5.04	106.11	117.20
1	D	141	LEU	CA-CB-CG	-5.04	103.70	115.30
1	E	128	LEU	N-CA-CB	-5.04	100.31	110.40
1	F	181	THR	C-N-CA	-5.04	111.71	122.30
1	C	9	HIS	CB-CG-CD2	5.04	146.43	130.80
1	E	227	ILE	CA-CB-CG2	5.04	120.98	110.90
1	A	25	LEU	CA-C-O	-5.04	109.52	120.10
1	F	30	PHE	O-C-N	-5.04	114.64	122.70
1	E	20	ALA	N-CA-CB	5.04	117.15	110.10
1	B	28	PHE	CD1-CE1-CZ	5.04	126.14	120.10
1	B	30	PHE	CD1-CG-CD2	5.04	124.85	118.30
1	C	48	TRP	NE1-CE2-CZ2	-5.04	124.86	130.40
1	D	69	VAL	C-N-CA	5.04	134.29	121.70
1	D	230	GLY	CA-C-O	-5.04	111.54	120.60
1	E	164	LEU	N-CA-CB	-5.04	100.33	110.40
1	D	62	LEU	CB-CA-C	-5.03	100.64	110.20
1	D	68	LEU	CD1-CG-CD2	-5.03	95.40	110.50
1	F	49	ALA	C-N-CA	5.03	134.28	121.70
1	A	217	PHE	CD1-CE1-CZ	-5.03	114.06	120.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	101	THR	CA-C-N	5.03	128.27	117.20
1	D	67	LEU	CB-CA-C	5.03	119.76	110.20
1	A	10	GLU	CG-CD-OE1	5.03	128.36	118.30
1	E	6	GLY	C-N-CA	-5.03	109.13	121.70
1	A	69	VAL	C-N-CA	5.03	134.27	121.70
1	A	172	TRP	CA-C-O	-5.03	109.54	120.10
1	C	14	PRO	CB-CA-C	-5.03	99.43	112.00
1	C	185	ALA	C-N-CA	5.03	134.26	121.70
1	D	114	ASN	N-CA-CB	-5.03	101.56	110.60
1	D	202	ALA	CA-C-O	-5.03	109.55	120.10
1	F	75	ASN	C-N-CA	-5.03	109.14	121.70
1	F	107	LEU	CB-CG-CD1	-5.03	102.45	111.00
1	D	41	PHE	CG-CD2-CE2	5.02	126.33	120.80
1	B	34	SER	CA-C-O	-5.02	109.55	120.10
1	D	105	PRO	CB-CA-C	-5.02	99.44	112.00
1	E	94	LEU	C-N-CA	5.02	134.26	121.70
1	E	225	LEU	N-CA-C	-5.02	97.44	111.00
1	F	9	HIS	CG-ND1-CE1	5.02	115.23	108.20
1	F	99	THR	CA-CB-OG1	5.02	119.55	109.00
1	C	109	ASP	C-N-CA	5.02	134.25	121.70
1	F	231	ALA	N-CA-C	-5.02	97.45	111.00
1	C	236	GLY	CA-C-O	5.02	129.63	120.60
1	D	17	LEU	CB-CG-CD2	5.01	119.53	111.00
1	D	55	ALA	CB-CA-C	-5.01	102.58	110.10
1	D	63	GLN	O-C-N	5.01	130.72	122.70
1	B	94	LEU	CA-CB-CG	5.01	126.83	115.30
1	E	8	SER	CA-CB-OG	-5.01	97.67	111.20
1	C	235	THR	CA-C-N	5.01	126.22	116.20
1	E	187	LEU	CB-CG-CD2	-5.01	102.48	111.00
1	E	192	ARG	CA-CB-CG	5.00	124.41	113.40
1	E	210	ARG	NE-CZ-NH2	5.00	122.80	120.30
1	F	42	ASP	CA-CB-CG	5.00	124.41	113.40
1	F	224	ASN	CA-C-O	-5.00	109.59	120.10
1	D	79	TRP	NE1-CE2-CD2	-5.00	102.30	107.30

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	9	HIS	CA
1	A	87	ILE	CA
1	B	60	ALA	CA
1	B	168	ASP	CA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
1	F	60	ALA	CA
1	F	195	VAL	CA

All (342) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	TYR	Mainchain
1	A	104	GLY	Mainchain,Peptide
1	A	108	TRP	Mainchain
1	A	111	GLY	Mainchain
1	A	119	VAL	Mainchain
1	A	128	LEU	Mainchain
1	A	13	HIS	Mainchain
1	A	136	ASN	Mainchain
1	A	137	HIS	Mainchain,Peptide
1	A	138	PRO	Mainchain
1	A	139	GLN	Mainchain
1	A	146	SER	Mainchain
1	A	157	GLU	Mainchain
1	A	158	THR	Mainchain
1	A	166	ASP	Mainchain
1	A	170	ARG	Mainchain
1	A	171	VAL	Mainchain
1	A	173	SER	Mainchain
1	A	181	THR	Mainchain
1	A	185	ALA	Mainchain
1	A	188	GLN	Mainchain
1	A	189	PRO	Mainchain
1	A	19	ALA	Mainchain
1	A	192	ARG	Mainchain
1	A	199	GLN	Mainchain
1	A	2	ASN	Peptide
1	A	214	ARG	Mainchain
1	A	215	TYR	Mainchain
1	A	219	LEU	Mainchain
1	A	220	GLN	Mainchain
1	A	221	PRO	Mainchain
1	A	222	ASP	Mainchain
1	A	228	TYR	Mainchain
1	A	231	ALA	Mainchain
1	A	25	LEU	Mainchain
1	A	30	PHE	Mainchain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	A	34	SER	Mainchain
1	A	37	ASN	Mainchain
1	A	38	LEU	Mainchain
1	A	44	ASP	Mainchain
1	A	49	ALA	Mainchain
1	A	5	PHE	Mainchain
1	A	53	ALA	Mainchain
1	A	55	ALA	Mainchain
1	A	60	ALA	Mainchain
1	A	62	LEU	Mainchain
1	A	63	GLN	Mainchain
1	A	68	LEU	Mainchain
1	A	72	THR	Mainchain,Peptide
1	A	75	ASN	Mainchain
1	A	76	THR	Mainchain
1	A	78	ARG	Mainchain
1	A	81	SER	Mainchain
1	A	87	ILE	Mainchain
1	A	89	ASN	Mainchain
1	A	90	TYR	Mainchain
1	A	98	ARG	Mainchain
1	B	104	GLY	Peptide
1	B	105	PRO	Mainchain
1	B	107	LEU	Mainchain,Peptide
1	B	108	TRP	Mainchain,Peptide
1	B	11	GLY	Mainchain,Peptide
1	B	12	SER	Mainchain
1	B	127	ILE	Mainchain
1	B	129	TYR	Mainchain
1	B	13	HIS	Mainchain,Peptide
1	B	130	SER	Mainchain
1	B	131	THR	Mainchain
1	B	136	ASN	Mainchain
1	B	137	HIS	Mainchain,Peptide
1	B	143	ALA	Mainchain
1	B	150	SER	Mainchain
1	B	151	PRO	Mainchain
1	B	156	MET	Mainchain
1	B	158	THR	Mainchain
1	B	159	ASP	Mainchain
1	B	162	LEU	Mainchain
1	B	164	LEU	Mainchain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	B	175	ASN	Mainchain
1	B	18	HIS	Peptide
1	B	189	PRO	Mainchain
1	B	194	ASP	Mainchain
1	B	195	VAL	Mainchain
1	B	198	ASN	Mainchain
1	B	20	ALA	Mainchain
1	B	209	SER	Mainchain
1	B	21	GLN	Peptide
1	B	210	ARG	Mainchain
1	B	214	ARG	Mainchain
1	B	222	ASP	Mainchain
1	B	225	LEU	Mainchain
1	B	226	ALA	Mainchain
1	B	228	TYR	Peptide
1	B	229	GLY	Mainchain
1	B	234	THR	Mainchain
1	B	24	GLU	Mainchain
1	B	27	SER	Mainchain
1	B	30	PHE	Mainchain
1	B	31	THR	Mainchain
1	B	32	MET	Mainchain
1	B	41	PHE	Mainchain
1	B	42	ASP	Mainchain
1	B	46	ARG	Mainchain
1	B	48	TRP	Mainchain
1	B	53	ALA	Peptide
1	B	55	ALA	Mainchain
1	B	56	THR	Mainchain
1	B	57	GLY	Mainchain
1	B	6	GLY	Peptide
1	B	60	ALA	Mainchain
1	B	62	LEU	Mainchain
1	B	7	LEU	Mainchain
1	B	70	ILE	Peptide
1	B	72	THR	Mainchain
1	B	73	ALA	Mainchain
1	B	76	THR	Peptide
1	B	86	SER	Mainchain
1	B	88	GLY	Mainchain
1	B	90	TYR	Sidechain,Mainchain
1	B	91	VAL	Mainchain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	B	92	LEU	Mainchain
1	B	94	LEU	Mainchain
1	B	95	GLN	Mainchain
1	B	97	ASP	Mainchain
1	C	102	ILE	Mainchain
1	C	104	GLY	Mainchain,Peptide
1	C	111	GLY	Mainchain
1	C	117	SER	Peptide
1	C	12	SER	Mainchain
1	C	124	GLY	Mainchain,Peptide
1	C	126	SER	Mainchain
1	C	128	LEU	Mainchain
1	C	13	HIS	Mainchain,Peptide
1	C	132	GLN	Mainchain
1	C	137	HIS	Mainchain,Peptide
1	C	138	PRO	Mainchain
1	C	142	HIS	Mainchain
1	C	145	GLN	Mainchain
1	C	154	LEU	Mainchain
1	C	155	SER	Mainchain
1	C	156	MET	Mainchain
1	C	157	GLU	Mainchain
1	C	16	THR	Mainchain
1	C	166	ASP	Mainchain
1	C	167	ARG	Mainchain
1	C	168	ASP	Sidechain,Mainchain
1	C	175	ASN	Peptide
1	C	180	GLY	Mainchain
1	C	189	PRO	Mainchain
1	C	193	MET	Mainchain
1	C	195	VAL	Mainchain
1	C	199	GLN	Mainchain
1	C	2	ASN	Mainchain
1	C	200	ASN	Mainchain
1	C	201	ILE	Mainchain
1	C	206	SER	Peptide
1	C	207	GLY	Mainchain
1	C	21	GLN	Mainchain
1	C	215	TYR	Mainchain
1	C	216	VAL	Mainchain
1	C	22	SER	Mainchain
1	C	227	ILE	Mainchain

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	C	229	GLY	Mainchain
1	C	230	GLY	Mainchain,Peptide
1	C	231	ALA	Mainchain
1	C	233	TRP	Mainchain
1	C	234	THR	Mainchain
1	C	24	GLU	Mainchain
1	C	26	SER	Mainchain
1	C	30	PHE	Sidechain
1	C	38	LEU	Mainchain
1	C	46	ARG	Mainchain
1	C	48	TRP	Mainchain
1	C	49	ALA	Mainchain
1	C	51	ASN	Mainchain
1	C	60	ALA	Mainchain
1	C	65	ASP	Mainchain
1	C	7	LEU	Mainchain
1	C	73	ALA	Mainchain
1	C	74	GLN	Mainchain
1	C	76	THR	Mainchain
1	C	8	SER	Mainchain,Peptide
1	C	90	TYR	Mainchain
1	D	100	VAL	Mainchain
1	D	104	GLY	Peptide
1	D	105	PRO	Mainchain
1	D	124	GLY	Mainchain
1	D	129	TYR	Mainchain
1	D	13	HIS	Mainchain,Peptide
1	D	130	SER	Mainchain
1	D	137	HIS	Mainchain,Peptide
1	D	141	LEU	Mainchain
1	D	143	ALA	Mainchain
1	D	146	SER	Mainchain
1	D	148	GLN	Mainchain
1	D	150	SER	Peptide
1	D	158	THR	Mainchain
1	D	16	THR	Mainchain
1	D	167	ARG	Sidechain,Mainchain
1	D	187	LEU	Mainchain
1	D	192	ARG	Mainchain
1	D	193	MET	Mainchain
1	D	20	ALA	Mainchain
1	D	206	SER	Mainchain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	D	209	SER	Mainchain
1	D	21	GLN	Mainchain
1	D	210	ARG	Mainchain
1	D	215	TYR	Mainchain
1	D	217	PHE	Mainchain
1	D	227	ILE	Mainchain
1	D	228	TYR	Mainchain
1	D	229	GLY	Mainchain,Peptide
1	D	230	GLY	Mainchain
1	D	24	GLU	Mainchain
1	D	33	GLN	Mainchain
1	D	34	SER	Mainchain
1	D	35	ASP	Mainchain
1	D	45	VAL	Mainchain
1	D	5	PHE	Mainchain
1	D	56	THR	Mainchain
1	D	6	GLY	Mainchain,Peptide
1	D	60	ALA	Mainchain,Peptide
1	D	61	VAL	Mainchain
1	D	64	SER	Mainchain
1	D	69	VAL	Mainchain
1	D	81	SER	Mainchain
1	D	86	SER	Mainchain
1	D	89	ASN	Mainchain
1	E	104	GLY	Mainchain,Peptide
1	E	11	GLY	Mainchain
1	E	110	SER	Mainchain
1	E	128	LEU	Mainchain,Peptide
1	E	13	HIS	Mainchain,Peptide
1	E	130	SER	Mainchain
1	E	136	ASN	Mainchain
1	E	137	HIS	Mainchain,Peptide
1	E	138	PRO	Mainchain
1	E	147	LEU	Mainchain
1	E	151	PRO	Mainchain
1	E	158	THR	Mainchain
1	E	162	LEU	Mainchain
1	E	165	PHE	Mainchain
1	E	173	SER	Mainchain
1	E	177	ALA	Mainchain
1	E	188	GLN	Mainchain
1	E	206	SER	Mainchain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	E	22	SER	Mainchain
1	E	227	ILE	Mainchain
1	E	231	ALA	Mainchain
1	E	25	LEU	Mainchain
1	E	30	PHE	Mainchain
1	E	33	GLN	Mainchain
1	E	34	SER	Mainchain
1	E	38	LEU	Mainchain
1	E	63	GLN	Mainchain
1	E	66	GLY	Mainchain
1	E	70	ILE	Mainchain
1	E	78	ARG	Mainchain
1	E	86	SER	Mainchain
1	E	9	HIS	Peptide
1	E	90	TYR	Mainchain
1	E	91	VAL	Mainchain
1	E	97	ASP	Mainchain
1	F	103	TYR	Mainchain
1	F	105	PRO	Mainchain
1	F	107	LEU	Mainchain
1	F	124	GLY	Peptide
1	F	128	LEU	Mainchain
1	F	13	HIS	Mainchain,Peptide
1	F	130	SER	Peptide
1	F	137	HIS	Mainchain,Peptide
1	F	14	PRO	Mainchain
1	F	140	THR	Mainchain
1	F	141	LEU	Mainchain
1	F	146	SER	Mainchain
1	F	149	LEU	Mainchain
1	F	15	GLN	Mainchain
1	F	150	SER	Mainchain
1	F	152	TYR	Mainchain
1	F	158	THR	Mainchain
1	F	184	ARG	Mainchain
1	F	185	ALA	Mainchain
1	F	189	PRO	Mainchain
1	F	193	MET	Mainchain,Peptide
1	F	195	VAL	Mainchain
1	F	197	THR	Mainchain
1	F	205	THR	Mainchain
1	F	208	ASN	Mainchain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	F	210	ARG	Mainchain
1	F	214	ARG	Mainchain
1	F	219	LEU	Mainchain
1	F	222	ASP	Mainchain
1	F	23	LEU	Mainchain
1	F	230	GLY	Mainchain
1	F	231	ALA	Peptide
1	F	45	VAL	Mainchain
1	F	52	THR	Mainchain
1	F	54	GLY	Mainchain
1	F	55	ALA	Mainchain
1	F	56	THR	Mainchain
1	F	60	ALA	Mainchain
1	F	63	GLN	Mainchain
1	F	76	THR	Mainchain,Peptide
1	F	78	ARG	Sidechain
1	F	83	THR	Mainchain
1	F	85	GLY	Peptide
1	F	86	SER	Mainchain
1	F	89	ASN	Mainchain
1	F	9	HIS	Mainchain,Peptide
1	F	91	VAL	Mainchain
1	F	95	GLN	Mainchain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1778	0	1700	282	0
1	B	1694	0	1600	265	0
1	C	1772	0	1695	270	0
1	D	1702	0	1613	321	0
1	E	1759	0	1684	310	0
1	F	1659	0	1579	305	0
2	A	19	0	0	1	0
2	B	15	0	0	0	0
2	C	6	0	0	0	0
2	D	8	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	8	0	0	0	0
2	F	11	0	0	0	0
All	All	10431	0	9871	1677	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 84.

All (1677) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:ILE:CD1	1:D:77:ILE:CG1	1.80	1.57
1:E:131:THR:CA	1:E:131:THR:C	1.75	1.50
1:E:136:ASN:CA	1:E:136:ASN:CB	1.88	1.49
1:A:131:THR:CB	1:A:131:THR:OG1	1.64	1.46
1:D:64:SER:OG	1:D:64:SER:CB	1.67	1.43
1:E:158:THR:CB	1:F:151:PRO:HG2	1.55	1.32
1:C:72:THR:CG2	1:C:76:THR:H	1.49	1.25
1:C:73:ALA:CA	1:F:189:PRO:HG2	1.70	1.21
1:E:158:THR:CB	1:F:151:PRO:CG	2.22	1.16
1:B:37:ASN:HB2	1:B:53:ALA:HB2	1.23	1.16
1:F:159:ASP:O	1:F:160:CYS:HB3	1.41	1.16
1:B:151:PRO:CD	1:D:34:SER:HB2	1.76	1.16
1:D:7:LEU:O	1:D:9:HIS:N	1.80	1.15
1:B:72:THR:HG22	1:B:74:GLN:HB2	1.17	1.14
1:C:73:ALA:C	1:F:189:PRO:HG2	1.68	1.13
1:E:87:ILE:HG23	1:E:88:GLY:H	1.03	1.12
1:B:3:ILE:HG22	1:B:93:VAL:HB	1.30	1.11
1:E:6:GLY:HA2	1:E:62:LEU:HD23	1.27	1.11
1:E:26:SER:O	1:E:27:SER:HB2	1.46	1.10
1:D:217:PHE:CE2	1:D:225:LEU:HD22	1.86	1.10
1:A:72:THR:HG22	1:A:76:THR:H	0.99	1.10
1:C:7:LEU:HD11	1:C:61:VAL:HG11	1.29	1.09
1:D:16:THR:HG22	1:D:61:VAL:H	1.07	1.09
1:A:131:THR:O	1:A:131:THR:HG22	1.42	1.08
1:C:72:THR:HG21	1:C:76:THR:H	1.09	1.07
1:F:7:LEU:O	1:F:9:HIS:N	1.88	1.07
1:E:131:THR:C	1:E:131:THR:CB	2.24	1.06
1:C:26:SER:O	1:C:27:SER:HB3	1.43	1.06
1:B:197:THR:HG21	1:B:201:ILE:HB	1.08	1.06
1:E:32:MET:HE2	1:E:60:ALA:HB2	1.31	1.06
1:C:74:GLN:N	1:F:189:PRO:HG2	1.71	1.05

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:SER:OG	1:F:33:GLN:HG3	1.54	1.05
1:E:158:THR:N	1:F:151:PRO:HG3	1.72	1.04
1:F:126:SER:O	1:F:147:LEU:HD11	1.54	1.04
1:C:146:SER:OG	1:C:147:LEU:N	1.84	1.04
1:E:4:LEU:HD12	1:E:5:PHE:N	1.69	1.04
1:E:64:SER:O	1:E:65:ASP:HB3	1.55	1.04
1:D:77:ILE:O	1:D:77:ILE:HG22	1.56	1.03
1:F:161:ASN:ND2	1:F:176:THR:H	1.54	1.03
1:C:74:GLN:HG3	1:F:189:PRO:HB2	1.40	1.03
1:E:158:THR:CA	1:F:151:PRO:HG3	1.89	1.02
1:B:151:PRO:HD2	1:D:34:SER:HB2	1.04	1.02
1:B:217:PHE:CE1	1:B:225:LEU:HB3	1.94	1.02
1:E:158:THR:HB	1:F:151:PRO:HG2	1.38	1.01
1:A:12:SER:HB3	1:A:221:PRO:HD2	1.41	1.01
1:B:154:LEU:HG	1:B:225:LEU:HD11	1.40	1.01
1:B:222:ASP:HB2	1:B:224:ASN:OD1	1.61	1.01
1:D:170:ARG:HH11	1:D:170:ARG:HG2	1.25	1.01
1:E:97:ASP:OD1	1:E:99:THR:HB	1.59	1.00
1:A:12:SER:HB3	1:A:221:PRO:CD	1.89	1.00
1:E:9:HIS:HB2	1:E:10:GLU:HG3	1.43	1.00
1:B:68:LEU:HD13	1:B:92:LEU:HD13	1.44	1.00
1:B:197:THR:HG21	1:B:201:ILE:CB	1.91	0.99
1:D:127:ILE:HG22	1:D:147:LEU:HD21	1.44	0.99
1:B:217:PHE:HE1	1:B:225:LEU:HB3	1.22	0.98
1:A:72:THR:HG22	1:A:76:THR:N	1.78	0.98
1:E:6:GLY:CA	1:E:62:LEU:HD23	1.94	0.98
1:C:97:ASP:HB3	1:C:136:ASN:HD22	1.27	0.97
1:E:127:ILE:O	1:E:127:ILE:HG23	1.64	0.97
1:D:64:SER:OG	1:D:64:SER:CA	2.10	0.97
1:C:4:LEU:HD22	1:C:17:LEU:HD23	1.45	0.96
1:D:83:THR:O	1:D:84:LYS:HB3	1.62	0.96
1:B:146:SER:O	1:B:147:LEU:HB2	1.63	0.96
1:A:72:THR:HG23	1:A:74:GLN:H	1.24	0.96
1:D:220:GLN:NE2	1:D:228:TYR:OH	1.98	0.95
1:A:62:LEU:HD21	1:A:90:TYR:HB2	1.47	0.95
1:B:151:PRO:HD2	1:D:34:SER:CB	1.95	0.95
1:C:73:ALA:O	1:C:75:ASN:N	2.00	0.95
1:E:158:THR:O	1:E:160:CYS:N	1.99	0.95
1:C:73:ALA:CA	1:F:189:PRO:CG	2.46	0.94
1:E:87:ILE:HG23	1:E:88:GLY:N	1.68	0.94
1:F:230:GLY:O	1:F:231:ALA:HB2	1.66	0.94

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:PHE:CZ	1:D:220:GLN:HG2	2.03	0.94
1:A:151:PRO:HD2	1:A:152:TYR:H	1.30	0.93
1:B:28:PHE:CE2	1:B:98:ARG:HG3	2.03	0.93
1:C:72:THR:O	1:C:73:ALA:HB3	1.67	0.93
1:D:184:ARG:HH22	1:D:200:ASN:HD21	0.94	0.93
1:B:154:LEU:CG	1:B:225:LEU:HD11	1.97	0.93
1:F:100:VAL:HG23	1:F:235:THR:HG21	1.50	0.93
1:D:178:GLY:O	1:D:180:GLY:N	2.00	0.92
1:F:131:THR:HG22	1:F:131:THR:O	1.70	0.92
1:A:110:SER:HB2	1:A:112:THR:HG23	1.50	0.92
1:E:22:SER:HB3	1:E:31:THR:HG22	1.51	0.92
1:C:72:THR:CG2	1:C:76:THR:N	2.32	0.92
1:D:16:THR:CG2	1:D:61:VAL:H	1.82	0.92
1:A:77:ILE:O	1:A:77:ILE:HG22	1.65	0.92
1:F:224:ASN:O	1:F:225:LEU:HD12	1.68	0.92
1:D:217:PHE:HE2	1:D:225:LEU:HD22	1.29	0.92
1:A:179:LYS:HB3	1:A:179:LYS:NZ	1.83	0.92
1:A:200:ASN:H	1:A:200:ASN:HD22	1.10	0.92
1:E:158:THR:CA	1:F:151:PRO:CG	2.47	0.92
1:F:25:LEU:HB2	1:F:94:LEU:HD21	1.52	0.91
1:C:18:HIS:HB2	1:C:21:GLN:NE2	1.83	0.91
1:C:72:THR:HG21	1:C:76:THR:N	1.84	0.91
1:E:105:PRO:HD2	1:E:210:ARG:NH2	1.86	0.90
1:A:86:SER:O	1:A:87:ILE:HG13	1.71	0.90
1:A:108:TRP:HB2	1:A:208:ASN:ND2	1.86	0.90
1:A:32:MET:HE2	1:A:60:ALA:HB2	1.51	0.90
1:D:131:THR:HG21	1:D:214:ARG:CZ	2.01	0.90
1:C:176:THR:O	1:C:177:ALA:HB3	1.70	0.90
1:F:2:ASN:HA	1:F:23:LEU:HD22	1.54	0.90
1:A:127:ILE:O	1:A:127:ILE:HG23	1.69	0.90
1:A:22:SER:HB3	1:A:31:THR:HG22	1.55	0.89
1:C:7:LEU:HD11	1:C:61:VAL:CG1	2.01	0.89
1:E:22:SER:CB	1:E:31:THR:HG22	2.03	0.89
1:C:29:ARG:HH21	1:C:31:THR:CG2	1.86	0.89
1:B:47:VAL:HG12	1:B:47:VAL:O	1.70	0.89
1:D:217:PHE:O	1:D:217:PHE:HD2	1.55	0.89
1:A:56:THR:O	1:A:73:ALA:HB2	1.72	0.89
1:F:129:TYR:HD1	1:F:130:SER:N	1.68	0.89
1:A:131:THR:CG2	1:A:131:THR:OG1	2.21	0.89
1:B:188:GLN:HG3	1:B:189:PRO:HD3	1.53	0.88
1:D:37:ASN:HD22	1:D:38:LEU:H	1.21	0.88

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:SER:O	1:E:27:SER:CB	2.13	0.88
1:D:3:ILE:HG22	1:D:93:VAL:HB	1.54	0.88
1:E:101:THR:OG1	1:E:234:THR:HB	1.72	0.88
1:D:184:ARG:HH22	1:D:200:ASN:ND2	1.70	0.88
1:D:176:THR:O	1:D:177:ALA:HB2	1.74	0.88
1:D:100:VAL:HB	1:D:235:THR:OG1	1.74	0.87
1:C:73:ALA:HA	1:F:189:PRO:CG	2.02	0.87
1:D:161:ASN:HA	1:D:176:THR:CG2	2.04	0.87
1:C:217:PHE:HA	1:C:227:ILE:CG2	2.03	0.87
1:C:97:ASP:HB3	1:C:136:ASN:ND2	1.88	0.87
1:D:161:ASN:HA	1:D:176:THR:HG22	1.57	0.87
1:D:150:SER:HB3	1:D:151:PRO:CD	2.05	0.86
1:F:159:ASP:O	1:F:160:CYS:CB	2.19	0.86
1:B:197:THR:OG1	1:B:201:ILE:HD12	1.73	0.86
1:C:140:THR:OG1	1:C:141:LEU:N	2.05	0.86
1:F:87:ILE:HG23	1:F:88:GLY:N	1.87	0.86
1:D:25:LEU:O	1:D:28:PHE:HB2	1.75	0.86
1:E:12:SER:HB3	1:E:221:PRO:HD2	1.57	0.86
1:B:217:PHE:HZ	1:B:225:LEU:HD13	1.39	0.86
1:E:4:LEU:HD12	1:E:5:PHE:H	1.37	0.86
1:A:215:TYR:HD2	1:A:215:TYR:N	1.74	0.86
1:E:129:TYR:O	1:E:130:SER:HB2	1.74	0.86
1:D:176:THR:O	1:D:177:ALA:CB	2.09	0.86
1:B:143:ALA:O	1:B:145:GLN:N	2.09	0.86
1:E:87:ILE:CG2	1:E:88:GLY:H	1.88	0.85
1:C:72:THR:HG22	1:C:76:THR:H	1.41	0.85
1:E:101:THR:HG22	1:E:103:TYR:CE1	2.10	0.85
1:B:37:ASN:ND2	1:B:52:THR:H	1.74	0.85
1:B:90:TYR:CD2	1:B:104:GLY:HA3	2.12	0.85
1:B:22:SER:HA	1:B:31:THR:HA	1.59	0.85
1:C:56:THR:HG22	1:C:57:GLY:H	1.42	0.85
1:D:208:ASN:N	1:D:208:ASN:OD1	2.09	0.85
1:C:49:ALA:O	1:C:50:SER:C	2.13	0.84
1:C:74:GLN:CG	1:F:189:PRO:HB2	2.05	0.84
1:C:90:TYR:CD2	1:C:104:GLY:HA3	2.12	0.84
1:C:110:SER:OG	1:C:225:LEU:HB2	1.77	0.84
1:C:205:THR:HG23	1:C:205:THR:O	1.74	0.84
1:F:16:THR:HG22	1:F:17:LEU:N	1.91	0.84
1:D:39:VAL:HG12	1:D:40:LEU:N	1.92	0.84
1:C:73:ALA:HA	1:F:189:PRO:HG2	1.58	0.84
1:B:3:ILE:HG22	1:B:93:VAL:CB	2.08	0.84

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:VAL:O	1:A:120:VAL:HB	1.77	0.84
1:E:92:LEU:HG	1:E:100:VAL:CG1	2.07	0.84
1:B:18:HIS:HB2	1:B:21:GLN:OE1	1.77	0.84
1:E:72:THR:HG22	1:E:76:THR:H	1.42	0.84
1:F:30:PHE:HZ	1:F:38:LEU:HD21	1.43	0.84
1:A:129:TYR:HD2	1:A:130:SER:N	1.76	0.84
1:B:197:THR:O	1:B:197:THR:HG23	1.78	0.83
1:E:127:ILE:CG2	1:E:217:PHE:HB3	2.07	0.83
1:B:35:ASP:O	1:B:36:CYS:HB2	1.77	0.83
1:D:7:LEU:O	1:D:8:SER:C	2.14	0.83
1:A:129:TYR:CD2	1:A:130:SER:N	2.46	0.83
1:B:189:PRO:HG3	1:E:74:GLN:HG2	1.60	0.83
1:A:195:VAL:CG1	1:A:204:TRP:HB3	2.08	0.83
1:A:161:ASN:ND2	1:A:176:THR:H	1.77	0.83
1:D:150:SER:HB3	1:D:151:PRO:HD3	1.59	0.83
1:B:157:GLU:HG3	1:B:161:ASN:HB3	1.58	0.83
1:C:67:LEU:HD21	1:C:82:GLY:HA2	1.60	0.83
1:C:2:ASN:OD1	1:C:3:ILE:HG22	1.76	0.83
1:D:166:ASP:O	1:D:167:ARG:O	1.97	0.82
1:B:188:GLN:CG	1:B:189:PRO:HD3	2.10	0.82
1:B:163:VAL:HG21	1:B:165:PHE:CE1	2.13	0.82
1:F:74:GLN:O	1:F:76:THR:HG22	1.79	0.82
1:A:56:THR:HG22	1:A:57:GLY:H	1.44	0.82
1:D:217:PHE:CZ	1:D:225:LEU:HD13	2.15	0.82
1:D:184:ARG:NH2	1:D:200:ASN:HD21	1.77	0.82
1:D:63:GLN:NE2	1:D:69:VAL:HG22	1.95	0.81
1:F:195:VAL:HG13	1:F:204:TRP:HB3	1.61	0.81
1:E:72:THR:HB	1:E:76:THR:HG22	1.62	0.81
1:A:105:PRO:HB2	1:A:210:ARG:HH22	1.45	0.81
1:D:63:GLN:HE22	1:D:69:VAL:CG2	1.92	0.81
1:B:67:LEU:HD11	1:B:84:LYS:HG3	1.60	0.81
1:C:18:HIS:HB2	1:C:21:GLN:HE21	1.43	0.81
1:A:22:SER:HB3	1:A:31:THR:CG2	2.09	0.81
1:C:74:GLN:N	1:F:189:PRO:CG	2.43	0.81
1:E:32:MET:CE	1:E:60:ALA:HB2	2.08	0.81
1:D:127:ILE:CG2	1:D:147:LEU:HD21	2.10	0.81
1:E:150:SER:HB3	1:E:151:PRO:HD3	1.63	0.81
1:E:17:LEU:HB2	1:E:60:ALA:HB3	1.59	0.81
1:E:72:THR:CB	1:E:76:THR:HG22	2.11	0.81
1:D:16:THR:HG22	1:D:61:VAL:N	1.92	0.80
1:F:41:PHE:CE2	1:F:46:ARG:HG2	2.16	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:ILE:O	1:F:77:ILE:HG22	1.78	0.80
1:D:63:GLN:HB2	1:D:67:LEU:O	1.81	0.80
1:D:142:HIS:O	1:D:143:ALA:CB	2.26	0.80
1:D:16:THR:HG21	1:D:61:VAL:HG22	1.63	0.80
1:A:131:THR:CG2	1:A:131:THR:O	2.28	0.80
1:B:129:TYR:O	1:B:130:SER:HB2	1.81	0.80
1:E:61:VAL:HG22	1:E:62:LEU:N	1.96	0.80
1:E:129:TYR:O	1:E:130:SER:CB	2.28	0.80
1:C:61:VAL:HG12	1:C:62:LEU:N	1.96	0.80
1:A:22:SER:HA	1:A:31:THR:HA	1.61	0.80
1:C:152:TYR:CE2	1:C:223:ARG:HG3	2.16	0.80
1:B:217:PHE:CZ	1:B:225:LEU:HD13	2.17	0.80
1:D:158:THR:O	1:D:160:CYS:N	2.14	0.80
1:D:142:HIS:O	1:D:143:ALA:HB3	1.81	0.80
1:E:115:LYS:HD2	1:E:115:LYS:H	1.46	0.80
1:C:127:ILE:CG2	1:C:217:PHE:HB3	2.11	0.79
1:A:200:ASN:HD22	1:A:200:ASN:N	1.75	0.79
1:A:157:GLU:HG3	1:C:26:SER:OG	1.81	0.79
1:C:89:ASN:H	1:C:89:ASN:ND2	1.80	0.79
1:C:29:ARG:HH21	1:C:31:THR:HG21	1.47	0.79
1:E:158:THR:H	1:F:151:PRO:HG3	1.47	0.79
1:A:37:ASN:HD21	1:A:51:ASN:H	1.30	0.79
1:B:197:THR:CG2	1:B:201:ILE:HB	2.03	0.78
1:D:70:ILE:HG22	1:D:70:ILE:O	1.82	0.78
1:E:72:THR:HB	1:E:76:THR:O	1.84	0.78
1:B:109:ASP:HB2	1:B:111:GLY:H	1.49	0.78
1:A:75:ASN:ND2	1:D:196:LEU:HD11	1.98	0.78
1:A:129:TYR:HD2	1:A:129:TYR:C	1.87	0.78
1:E:69:VAL:HG21	1:E:71:LEU:HG	1.65	0.78
1:D:217:PHE:HZ	1:D:225:LEU:HD13	1.47	0.78
1:D:140:THR:OG1	1:D:141:LEU:N	2.16	0.78
1:D:39:VAL:HG12	1:D:40:LEU:H	1.49	0.78
1:E:158:THR:N	1:F:151:PRO:CG	2.47	0.78
1:B:55:ALA:HB1	1:B:56:THR:HG23	1.64	0.78
1:E:192:ARG:NH2	1:E:194:ASP:OD2	2.17	0.78
1:B:151:PRO:CD	1:D:34:SER:CB	2.58	0.77
1:C:97:ASP:CB	1:C:136:ASN:HD22	1.97	0.77
1:C:176:THR:O	1:C:177:ALA:CB	2.31	0.77
1:F:197:THR:HG21	1:F:201:ILE:HD12	1.64	0.77
1:D:170:ARG:NH1	1:D:170:ARG:HG2	1.98	0.77
1:D:77:ILE:O	1:D:77:ILE:CG2	2.32	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:THR:HG21	1:F:203:VAL:HG13	1.65	0.77
1:C:146:SER:HG	1:C:147:LEU:H	1.33	0.77
1:F:197:THR:HB	1:F:201:ILE:HB	1.66	0.77
1:C:74:GLN:HA	1:F:189:PRO:HD2	1.67	0.77
1:A:112:THR:O	1:A:223:ARG:NH1	2.18	0.77
1:C:167:ARG:O	1:C:169:ASP:N	2.17	0.77
1:A:47:VAL:O	1:A:47:VAL:HG12	1.83	0.77
1:D:56:THR:HG22	1:D:57:GLY:N	2.00	0.77
1:C:73:ALA:HB1	1:F:189:PRO:CG	2.15	0.76
1:D:229:GLY:C	1:D:230:GLY:O	2.22	0.76
1:A:223:ARG:HH11	1:A:223:ARG:HB3	1.50	0.76
1:A:5:PHE:HE2	1:A:220:GLN:HE21	1.31	0.76
1:E:70:ILE:HG13	1:E:79:TRP:CE3	2.21	0.76
1:E:177:ALA:O	1:E:179:LYS:HG3	1.85	0.76
1:F:217:PHE:CD2	1:F:217:PHE:C	2.56	0.76
1:B:63:GLN:CG	1:B:64:SER:H	1.98	0.76
1:E:12:SER:HB3	1:E:221:PRO:CD	2.15	0.76
1:A:129:TYR:C	1:A:129:TYR:CD2	2.57	0.76
1:B:35:ASP:O	1:B:36:CYS:CB	2.32	0.76
1:F:29:ARG:O	1:F:40:LEU:HD12	1.86	0.76
1:A:37:ASN:ND2	1:A:52:THR:H	1.83	0.76
1:C:92:LEU:HD21	1:C:100:VAL:HG13	1.68	0.76
1:C:83:THR:HG22	1:C:84:LYS:H	1.50	0.76
1:B:94:LEU:HB2	1:B:100:VAL:HG12	1.66	0.76
1:F:42:ASP:O	1:F:43:SER:HB2	1.86	0.76
1:B:72:THR:CG2	1:B:74:GLN:HB2	2.10	0.76
1:F:41:PHE:HE2	1:F:46:ARG:HG2	1.51	0.75
1:A:39:VAL:HG22	1:A:49:ALA:HB1	1.68	0.75
1:E:72:THR:HG21	1:E:76:THR:HG22	1.67	0.75
1:A:161:ASN:HD22	1:A:176:THR:H	1.34	0.75
1:B:21:GLN:O	1:B:32:MET:N	2.14	0.75
1:D:217:PHE:O	1:D:217:PHE:CD2	2.38	0.75
1:D:43:SER:O	1:D:44:ASP:HB3	1.86	0.75
1:E:56:THR:HG22	1:E:57:GLY:H	1.51	0.75
1:F:87:ILE:CG2	1:F:88:GLY:N	2.50	0.75
1:B:63:GLN:HG3	1:B:64:SER:H	1.51	0.75
1:D:150:SER:H	1:D:152:TYR:H	1.35	0.75
1:F:101:THR:HG23	1:F:102:ILE:N	2.02	0.74
1:A:119:VAL:HG23	1:A:151:PRO:HD3	1.69	0.74
1:E:136:ASN:HA	1:E:136:ASN:CB	2.14	0.74
1:E:61:VAL:HG22	1:E:62:LEU:H	1.50	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:GLU:O	1:A:12:SER:N	2.19	0.74
1:F:67:LEU:N	1:F:67:LEU:HD13	2.01	0.74
1:E:18:HIS:H	1:E:21:GLN:CG	2.00	0.74
1:F:161:ASN:HD21	1:F:175:ASN:N	1.86	0.74
1:E:150:SER:HB3	1:E:151:PRO:CD	2.16	0.74
1:C:146:SER:O	1:C:154:LEU:O	2.05	0.74
1:E:161:ASN:HB2	1:E:176:THR:O	1.87	0.74
1:E:110:SER:OG	1:E:225:LEU:HB3	1.87	0.74
1:E:220:GLN:HB3	1:E:222:ASP:OD1	1.88	0.74
1:E:170:ARG:CG	1:E:170:ARG:HH11	1.99	0.74
1:D:63:GLN:HE22	1:D:69:VAL:HG22	1.49	0.74
1:A:32:MET:CE	1:A:60:ALA:HB2	2.17	0.74
1:B:37:ASN:HD21	1:B:51:ASN:N	1.86	0.74
1:A:151:PRO:CD	1:A:152:TYR:H	2.00	0.74
1:B:63:GLN:CG	1:B:64:SER:N	2.51	0.74
1:B:44:ASP:OD1	1:B:45:VAL:N	2.21	0.74
1:F:28:PHE:HB3	1:F:94:LEU:HD11	1.70	0.73
1:E:143:ALA:HA	1:E:156:MET:O	1.88	0.73
1:B:25:LEU:O	1:B:28:PHE:N	2.21	0.73
1:A:18:HIS:O	1:A:20:ALA:N	2.21	0.73
1:E:129:TYR:HD1	1:E:130:SER:N	1.86	0.73
1:D:217:PHE:HD2	1:D:217:PHE:C	1.90	0.73
1:C:217:PHE:HA	1:C:227:ILE:HG22	1.69	0.73
1:A:154:LEU:HD22	1:A:162:LEU:HD22	1.69	0.73
1:E:87:ILE:CG2	1:E:88:GLY:N	2.50	0.73
1:E:72:THR:CG2	1:E:76:THR:HG22	2.19	0.73
1:C:166:ASP:OD1	1:C:166:ASP:O	2.07	0.73
1:F:67:LEU:H	1:F:67:LEU:HD13	1.53	0.73
1:E:19:ALA:O	1:E:20:ALA:HB2	1.89	0.73
1:D:77:ILE:CD1	1:D:77:ILE:CB	2.66	0.73
1:C:97:ASP:CB	1:C:136:ASN:ND2	2.52	0.73
1:A:196:LEU:CD1	1:A:202:ALA:HB2	2.18	0.73
1:E:142:HIS:O	1:E:143:ALA:CB	2.37	0.73
1:F:129:TYR:CD1	1:F:130:SER:N	2.55	0.73
1:C:73:ALA:HA	1:F:189:PRO:HG3	1.71	0.72
1:F:204:TRP:CE3	1:F:205:THR:N	2.57	0.72
1:A:127:ILE:CG2	1:A:217:PHE:HB3	2.19	0.72
1:D:37:ASN:ND2	1:D:38:LEU:H	1.86	0.72
1:A:210:ARG:HB3	1:A:215:TYR:OH	1.90	0.72
1:E:72:THR:HG23	1:E:73:ALA:N	2.03	0.72
1:B:30:PHE:HE1	1:B:38:LEU:HG	1.54	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:TYR:N	1:A:215:TYR:CD2	2.41	0.72
1:B:220:GLN:CB	1:B:221:PRO:CD	2.66	0.72
1:B:78:ARG:NE	1:B:78:ARG:HA	1.91	0.72
1:B:199:GLN:O	1:B:200:ASN:HB2	1.89	0.72
1:C:48:TRP:O	1:C:49:ALA:HB2	1.90	0.72
1:F:67:LEU:N	1:F:67:LEU:CD1	2.52	0.72
1:F:90:TYR:CD2	1:F:104:GLY:HA3	2.24	0.72
1:A:179:LYS:HB3	1:A:179:LYS:HZ1	1.53	0.72
1:B:30:PHE:CE1	1:B:38:LEU:HG	2.25	0.72
1:D:197:THR:HG21	1:D:201:ILE:HB	1.71	0.72
1:A:18:HIS:O	1:A:21:GLN:HB2	1.90	0.72
1:A:22:SER:HB3	1:A:31:THR:CB	2.20	0.71
1:B:90:TYR:HD2	1:B:104:GLY:HA3	1.54	0.71
1:C:48:TRP:O	1:C:49:ALA:CB	2.38	0.71
1:D:131:THR:HG21	1:D:214:ARG:NE	2.05	0.71
1:E:111:GLY:H	1:E:224:ASN:HD21	1.36	0.71
1:F:31:THR:O	1:F:31:THR:HG23	1.90	0.71
1:E:163:VAL:HG21	1:E:170:ARG:HG2	1.71	0.71
1:B:77:ILE:HG22	1:B:77:ILE:O	1.90	0.71
1:F:127:ILE:HG22	1:F:147:LEU:HD11	1.73	0.71
1:C:182:GLY:H	1:C:198:ASN:HB2	1.55	0.71
1:D:64:SER:OG	1:D:64:SER:HA	1.90	0.71
1:B:189:PRO:CG	1:E:74:GLN:HG2	2.21	0.71
1:F:197:THR:CB	1:F:201:ILE:HB	2.20	0.71
1:B:95:GLN:HB3	1:B:96:PRO:CD	2.20	0.71
1:A:26:SER:OG	1:C:157:GLU:OE1	2.08	0.71
1:E:154:LEU:HD12	1:E:154:LEU:O	1.91	0.71
1:D:217:PHE:C	1:D:217:PHE:CD2	2.58	0.70
1:A:63:GLN:HE22	1:A:67:LEU:HD13	1.56	0.70
1:D:8:SER:HA	1:D:9:HIS:ND1	2.06	0.70
1:A:157:GLU:HG3	1:C:26:SER:HG	1.54	0.70
1:E:129:TYR:CD1	1:E:130:SER:N	2.59	0.70
1:D:168:ASP:O	1:D:169:ASP:HB3	1.89	0.70
1:C:72:THR:O	1:C:73:ALA:CB	2.34	0.70
1:A:69:VAL:O	1:A:69:VAL:HG23	1.91	0.70
1:D:109:ASP:HB2	1:D:225:LEU:O	1.91	0.70
1:C:26:SER:O	1:C:27:SER:CB	2.25	0.70
1:E:117:SER:O	1:E:119:VAL:HG13	1.91	0.70
1:A:37:ASN:HD21	1:A:51:ASN:N	1.89	0.70
1:E:220:GLN:OE1	1:E:224:ASN:HB3	1.92	0.70
1:C:77:ILE:HG22	1:C:77:ILE:O	1.92	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LEU:HD11	1:A:221:PRO:HB3	1.72	0.70
1:A:223:ARG:CG	1:A:223:ARG:HH11	2.03	0.70
1:E:97:ASP:OD1	1:E:99:THR:CB	2.39	0.70
1:C:89:ASN:N	1:C:89:ASN:ND2	2.40	0.70
1:A:146:SER:O	1:A:147:LEU:HB2	1.92	0.69
1:A:95:GLN:OE1	1:A:103:TYR:OH	2.08	0.69
1:F:141:LEU:HD12	1:F:145:GLN:HB3	1.73	0.69
1:E:72:THR:HG21	1:E:76:THR:CG2	2.22	0.69
1:F:7:LEU:O	1:F:9:HIS:CA	2.41	0.69
1:F:155:SER:O	1:F:162:LEU:HD23	1.92	0.69
1:A:10:GLU:O	1:A:11:GLY:C	2.28	0.69
1:B:78:ARG:HE	1:B:78:ARG:HA	1.56	0.69
1:B:48:TRP:O	1:B:49:ALA:HB2	1.93	0.69
1:D:170:ARG:HH11	1:D:170:ARG:CG	1.97	0.69
1:B:185:ALA:HA	1:B:194:ASP:O	1.93	0.69
1:A:222:ASP:N	1:A:222:ASP:OD1	2.21	0.69
1:E:195:VAL:HG12	1:E:204:TRP:O	1.92	0.69
1:D:77:ILE:CD1	1:D:77:ILE:HB	2.21	0.69
1:C:75:ASN:ND2	1:F:188:GLN:HE22	1.91	0.69
1:E:131:THR:C	1:E:131:THR:CG2	2.60	0.69
1:A:9:HIS:O	1:A:11:GLY:N	2.26	0.69
1:D:93:VAL:HG23	1:D:94:LEU:N	2.07	0.69
1:E:18:HIS:H	1:E:21:GLN:HG2	1.58	0.68
1:F:211:SER:OG	1:F:212:ALA:N	2.22	0.68
1:B:85:GLY:O	1:B:86:SER:O	2.10	0.68
1:E:26:SER:HG	1:F:33:GLN:HG3	1.57	0.68
1:D:5:PHE:CE2	1:D:220:GLN:HG2	2.29	0.68
1:E:101:THR:CG2	1:E:103:TYR:CE1	2.76	0.68
1:C:73:ALA:CB	1:F:189:PRO:CG	2.71	0.68
1:B:203:VAL:O	1:B:204:TRP:HB2	1.94	0.68
1:D:152:TYR:CB	1:D:219:LEU:HD21	2.24	0.68
1:E:158:THR:OG1	1:F:151:PRO:CD	2.41	0.68
1:E:158:THR:H	1:F:151:PRO:CG	2.04	0.68
1:C:52:THR:CG2	1:C:79:TRP:HB2	2.23	0.68
1:A:142:HIS:N	1:A:145:GLN:OE1	2.20	0.68
1:C:193:MET:H	1:C:206:SER:HB3	1.57	0.68
1:F:30:PHE:CZ	1:F:38:LEU:HD21	2.28	0.68
1:C:53:ALA:O	1:C:78:ARG:NH2	2.25	0.68
1:F:137:HIS:HB3	1:F:138:PRO:HA	1.75	0.68
1:E:131:THR:C	1:E:131:THR:HG22	2.15	0.68
1:D:129:TYR:CE1	1:D:131:THR:HB	2.28	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:PHE:HB2	1:C:40:LEU:HB2	1.75	0.68
1:D:137:HIS:HB2	1:D:138:PRO:CA	2.23	0.68
1:B:107:LEU:HD12	1:B:107:LEU:O	1.94	0.68
1:B:158:THR:OG1	1:B:159:ASP:N	2.22	0.68
1:A:113:SER:HB2	1:A:222:ASP:HB2	1.75	0.68
1:B:95:GLN:HB3	1:B:96:PRO:HD3	1.75	0.68
1:D:105:PRO:C	1:D:106:GLY:O	2.32	0.68
1:D:52:THR:CG2	1:D:79:TRP:HB2	2.25	0.67
1:E:106:GLY:HA2	1:E:228:TYR:HA	1.74	0.67
1:D:37:ASN:HD22	1:D:38:LEU:N	1.90	0.67
1:D:224:ASN:N	1:D:224:ASN:HD22	1.90	0.67
1:A:223:ARG:CB	1:A:223:ARG:HH11	2.08	0.67
1:A:62:LEU:HD21	1:A:90:TYR:CB	2.24	0.67
1:F:94:LEU:HG	1:F:94:LEU:O	1.94	0.67
1:A:229:GLY:HA2	1:A:230:GLY:O	1.93	0.67
1:F:184:ARG:O	1:F:185:ALA:HB2	1.95	0.67
1:B:195:VAL:O	1:B:195:VAL:HG12	1.94	0.67
1:E:115:LYS:CD	1:E:115:LYS:H	2.07	0.67
1:B:109:ASP:OD1	1:B:224:ASN:ND2	2.28	0.67
1:E:25:LEU:O	1:E:26:SER:C	2.30	0.67
1:D:169:ASP:OD2	1:D:169:ASP:O	2.13	0.67
1:C:16:THR:HG22	1:C:17:LEU:N	2.10	0.67
1:B:71:LEU:HD22	1:B:77:ILE:H	1.59	0.67
1:F:176:THR:HG21	1:F:203:VAL:CG1	2.25	0.67
1:B:129:TYR:HD1	1:B:131:THR:H	1.42	0.67
1:A:72:THR:OG1	1:A:73:ALA:N	2.27	0.67
1:F:215:TYR:CD1	1:F:227:ILE:HD11	2.30	0.67
1:D:37:ASN:HD21	1:D:51:ASN:H	1.43	0.67
1:C:72:THR:HG21	1:C:76:THR:OG1	1.95	0.67
1:F:161:ASN:HD21	1:F:175:ASN:H	1.42	0.67
1:A:18:HIS:HB2	1:A:21:GLN:OE1	1.94	0.67
1:B:70:ILE:O	1:B:70:ILE:HG22	1.92	0.67
1:D:197:THR:HG22	1:D:199:GLN:H	1.60	0.67
1:A:75:ASN:HD21	1:D:196:LEU:HD21	1.60	0.67
1:B:195:VAL:O	1:B:195:VAL:CG1	2.42	0.67
1:F:28:PHE:O	1:F:29:ARG:HB2	1.95	0.67
1:C:56:THR:CG2	1:C:57:GLY:H	2.04	0.67
1:B:222:ASP:CB	1:B:224:ASN:OD1	2.41	0.66
1:C:137:HIS:N	1:C:137:HIS:CD2	2.59	0.66
1:B:146:SER:OG	1:B:155:SER:HB2	1.95	0.66
1:D:70:ILE:CG2	1:D:70:ILE:O	2.43	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:MET:HE2	1:A:60:ALA:CB	2.23	0.66
1:F:23:LEU:HB2	1:F:30:PHE:O	1.96	0.66
1:D:72:THR:HG22	1:D:74:GLN:HB2	1.77	0.66
1:B:154:LEU:HG	1:B:225:LEU:CD1	2.24	0.66
1:E:39:VAL:HG12	1:E:40:LEU:N	2.08	0.66
1:D:141:LEU:O	1:D:185:ALA:HB3	1.94	0.66
1:F:158:THR:O	1:F:159:ASP:C	2.34	0.66
1:A:179:LYS:NZ	1:A:179:LYS:CB	2.56	0.66
1:E:58:CYS:HA	1:E:71:LEU:O	1.95	0.66
1:A:7:LEU:HD11	1:A:61:VAL:HG13	1.78	0.66
1:B:9:HIS:CD2	1:B:10:GLU:HB2	2.31	0.66
1:E:26:SER:OG	1:F:33:GLN:CG	2.37	0.66
1:A:72:THR:O	1:A:75:ASN:N	2.23	0.66
1:D:201:ILE:O	1:D:201:ILE:HG22	1.94	0.66
1:C:155:SER:N	1:C:163:VAL:O	2.25	0.66
1:E:100:VAL:O	1:E:235:THR:HG22	1.96	0.66
1:D:162:LEU:HB2	1:D:174:THR:OG1	1.96	0.66
1:C:220:GLN:OE1	1:C:224:ASN:HB3	1.95	0.66
1:C:2:ASN:HD21	1:C:125:ASN:ND2	1.93	0.66
1:D:42:ASP:O	1:D:43:SER:HB2	1.95	0.66
1:E:72:THR:CG2	1:E:76:THR:H	2.09	0.66
1:F:143:ALA:HA	1:F:156:MET:O	1.95	0.66
1:B:216:VAL:HG22	1:B:217:PHE:H	1.61	0.66
1:A:22:SER:HB3	1:A:31:THR:HB	1.78	0.66
1:A:63:GLN:NE2	1:A:67:LEU:HD13	2.10	0.66
1:C:72:THR:HG23	1:C:73:ALA:C	2.17	0.65
1:C:130:SER:HA	1:C:139:GLN:HG3	1.79	0.65
1:F:149:LEU:O	1:F:150:SER:CB	2.43	0.65
1:B:202:ALA:O	1:B:203:VAL:HB	1.96	0.65
1:F:129:TYR:HE1	1:F:131:THR:N	1.94	0.65
1:E:158:THR:C	1:F:151:PRO:HG3	2.15	0.65
1:E:194:ASP:HB3	1:E:196:LEU:HD13	1.78	0.65
1:D:150:SER:CB	1:D:151:PRO:CD	2.74	0.65
1:D:165:PHE:HB3	1:D:169:ASP:H	1.62	0.65
1:A:62:LEU:CD2	1:A:90:TYR:HB2	2.25	0.65
1:A:86:SER:O	1:A:87:ILE:CG1	2.45	0.65
1:C:110:SER:HB2	1:C:112:THR:HG23	1.78	0.65
1:E:219:LEU:HD13	1:E:225:LEU:CD2	2.27	0.65
1:B:95:GLN:CB	1:B:96:PRO:CD	2.73	0.65
1:D:137:HIS:ND1	1:D:137:HIS:N	2.42	0.65
1:F:161:ASN:HD21	1:F:176:THR:H	1.42	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:129:TYR:C	1:F:129:TYR:HD1	1.94	0.65
1:C:72:THR:HG22	1:C:76:THR:N	2.05	0.65
1:E:61:VAL:HG12	1:E:69:VAL:HG22	1.78	0.65
1:E:22:SER:HA	1:E:31:THR:HA	1.78	0.65
1:B:92:LEU:HB2	1:B:102:ILE:HG13	1.78	0.65
1:E:100:VAL:H	1:E:235:THR:HG21	1.61	0.65
1:C:197:THR:HG21	1:C:199:GLN:OE1	1.97	0.65
1:C:65:ASP:C	1:C:65:ASP:OD1	2.33	0.65
1:B:100:VAL:O	1:B:101:THR:OG1	2.12	0.65
1:F:129:TYR:OH	1:F:131:THR:CB	2.44	0.65
1:B:142:HIS:O	1:B:143:ALA:CB	2.43	0.65
1:C:52:THR:O	1:C:78:ARG:NH1	2.29	0.65
1:E:219:LEU:HD13	1:E:225:LEU:HD23	1.79	0.65
1:A:12:SER:CB	1:A:221:PRO:HD2	2.22	0.65
1:D:44:ASP:O	1:D:45:VAL:CB	2.43	0.65
1:D:97:ASP:N	1:D:97:ASP:OD1	2.30	0.65
1:B:217:PHE:CG	1:B:217:PHE:O	2.45	0.64
1:F:154:LEU:CD2	1:F:225:LEU:HD21	2.27	0.64
1:A:37:ASN:HB2	1:A:53:ALA:HB2	1.78	0.64
1:D:42:ASP:O	1:D:44:ASP:N	2.30	0.64
1:E:165:PHE:HE2	1:E:170:ARG:HG3	1.62	0.64
1:A:195:VAL:HG11	1:A:204:TRP:HB3	1.78	0.64
1:E:181:THR:O	1:E:182:GLY:C	2.34	0.64
1:C:210:ARG:HB2	1:C:215:TYR:OH	1.96	0.64
1:F:185:ALA:HA	1:F:194:ASP:O	1.96	0.64
1:E:72:THR:HG23	1:E:73:ALA:HB3	1.79	0.64
1:F:204:TRP:CD2	1:F:205:THR:N	2.66	0.64
1:A:26:SER:O	1:A:27:SER:CB	2.41	0.64
1:B:148:GLN:HA	1:B:153:ARG:HA	1.79	0.64
1:B:228:TYR:N	1:B:228:TYR:CD2	2.66	0.64
1:B:82:GLY:O	1:B:83:THR:C	2.36	0.64
1:D:32:MET:HE2	1:D:38:LEU:HB2	1.78	0.64
1:C:59:ARG:HH12	1:F:184:ARG:NH2	1.95	0.64
1:B:154:LEU:CD2	1:B:225:LEU:HD11	2.28	0.64
1:F:190:ASN:OD1	1:F:190:ASN:O	2.15	0.64
1:F:193:MET:HB3	1:F:206:SER:HB3	1.78	0.64
1:C:127:ILE:HG22	1:C:217:PHE:HB3	1.80	0.64
1:D:150:SER:CB	1:D:151:PRO:HD3	2.28	0.64
1:E:127:ILE:HG21	1:E:217:PHE:HB3	1.79	0.64
1:C:152:TYR:CD2	1:C:223:ARG:HG3	2.32	0.64
1:B:163:VAL:HG21	1:B:165:PHE:CZ	2.32	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:HIS:HA	1:D:15:GLN:HE22	1.62	0.64
1:A:110:SER:OG	1:A:225:LEU:HB2	1.97	0.64
1:D:153:ARG:HG3	1:D:153:ARG:O	1.95	0.64
1:C:162:LEU:O	1:C:173:SER:OG	2.16	0.64
1:E:119:VAL:HG21	1:E:151:PRO:HD3	1.78	0.64
1:A:39:VAL:HG12	1:A:41:PHE:CE1	2.31	0.64
1:E:142:HIS:O	1:E:143:ALA:HB3	1.97	0.64
1:B:26:SER:O	1:B:27:SER:CB	2.46	0.64
1:C:4:LEU:CD1	1:C:14:PRO:HB2	2.28	0.64
1:F:40:LEU:HB3	1:F:48:TRP:H	1.61	0.64
1:E:77:ILE:HG22	1:E:77:ILE:O	1.97	0.64
1:D:217:PHE:CZ	1:D:225:LEU:HD22	2.33	0.64
1:C:7:LEU:CD1	1:C:61:VAL:CG1	2.76	0.64
1:F:7:LEU:HA	1:F:15:GLN:HG2	1.79	0.64
1:A:17:LEU:O	1:A:59:ARG:HB2	1.98	0.64
1:D:101:THR:OG1	1:D:234:THR:HA	1.98	0.64
1:A:26:SER:O	1:A:27:SER:HB3	1.96	0.64
1:C:222:ASP:N	1:C:222:ASP:OD1	2.29	0.64
1:F:58:CYS:HA	1:F:71:LEU:O	1.97	0.64
1:D:6:GLY:HA3	1:D:62:LEU:HD23	1.80	0.63
1:C:4:LEU:CD2	1:C:17:LEU:HD23	2.24	0.63
1:D:233:TRP:CH2	1:D:235:THR:HG23	2.33	0.63
1:E:32:MET:HG2	1:E:60:ALA:CB	2.28	0.63
1:E:195:VAL:HG11	1:E:204:TRP:HB3	1.79	0.63
1:E:195:VAL:HG13	1:E:195:VAL:O	1.97	0.63
1:E:4:LEU:HD12	1:E:4:LEU:C	2.15	0.63
1:F:31:THR:HG22	1:F:39:VAL:O	1.99	0.63
1:F:30:PHE:HA	1:F:39:VAL:O	1.98	0.63
1:C:188:GLN:O	1:C:191:GLY:N	2.31	0.63
1:F:188:GLN:HE21	1:F:189:PRO:HD2	1.62	0.63
1:B:109:ASP:CB	1:B:111:GLY:H	2.10	0.63
1:A:191:GLY:HA3	1:A:215:TYR:CD1	2.33	0.63
1:F:229:GLY:C	1:F:230:GLY:O	2.31	0.63
1:D:157:GLU:HB2	1:D:161:ASN:O	1.99	0.63
1:E:150:SER:CB	1:E:151:PRO:CD	2.73	0.63
1:B:143:ALA:O	1:B:144:THR:C	2.36	0.63
1:A:44:ASP:O	1:A:45:VAL:O	2.17	0.63
1:C:97:ASP:CG	1:C:136:ASN:ND2	2.52	0.63
1:D:143:ALA:C	1:D:145:GLN:H	2.02	0.63
1:F:169:ASP:C	1:F:169:ASP:OD2	2.37	0.63
1:B:217:PHE:C	1:B:217:PHE:CD1	2.67	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:TYR:CE1	1:F:229:GLY:HA3	2.34	0.63
1:C:47:VAL:O	1:C:47:VAL:HG12	1.99	0.63
1:F:223:ARG:HB3	1:F:223:ARG:HH11	1.63	0.63
1:B:30:PHE:C	1:B:30:PHE:CD1	2.65	0.63
1:F:223:ARG:HH11	1:F:223:ARG:CB	2.12	0.63
1:E:69:VAL:HG23	1:E:71:LEU:N	2.14	0.62
1:A:74:GLN:HE21	1:D:189:PRO:HG3	1.64	0.62
1:C:156:MET:O	1:C:157:GLU:O	2.17	0.62
1:D:152:TYR:HB3	1:D:219:LEU:HD21	1.79	0.62
1:F:137:HIS:HB3	1:F:138:PRO:CA	2.28	0.62
1:F:127:ILE:HG22	1:F:147:LEU:CD1	2.29	0.62
1:C:162:LEU:HB3	1:C:174:THR:HG23	1.80	0.62
1:D:27:SER:HB2	1:D:28:PHE:CD2	2.34	0.62
1:E:37:ASN:OD1	1:E:51:ASN:N	2.30	0.62
1:B:34:SER:OG	1:D:151:PRO:CD	2.48	0.62
1:B:28:PHE:HE2	1:B:98:ARG:HG3	1.63	0.62
1:A:29:ARG:HE	1:A:31:THR:CG2	2.13	0.62
1:E:188:GLN:HG3	1:E:189:PRO:HD2	1.82	0.62
1:B:12:SER:OG	1:B:222:ASP:OD1	2.08	0.62
1:A:157:GLU:CG	1:C:26:SER:OG	2.47	0.62
1:B:146:SER:O	1:B:147:LEU:CB	2.29	0.62
1:F:217:PHE:HZ	1:F:225:LEU:CD2	2.13	0.62
1:A:127:ILE:HG21	1:A:217:PHE:HB3	1.81	0.62
1:D:70:ILE:HG21	1:D:79:TRP:HB3	1.82	0.62
1:B:37:ASN:OD1	1:B:49:ALA:HB1	2.00	0.62
1:C:7:LEU:CD1	1:C:61:VAL:HG11	2.19	0.62
1:D:226:ALA:HB3	1:D:228:TYR:CE2	2.35	0.62
1:E:101:THR:HG22	1:E:103:TYR:CD1	2.34	0.62
1:D:38:LEU:O	1:D:49:ALA:HA	2.00	0.62
1:C:157:GLU:HB3	1:C:159:ASP:OD1	2.00	0.62
1:B:18:HIS:O	1:B:32:MET:HB3	1.99	0.62
1:F:91:VAL:O	1:F:102:ILE:HG23	2.00	0.62
1:F:102:ILE:HG22	1:F:103:TYR:N	2.16	0.61
1:D:128:LEU:O	1:D:129:TYR:CB	2.47	0.61
1:F:156:MET:SD	1:F:185:ALA:HB2	2.41	0.61
1:D:129:TYR:HD1	1:D:130:SER:N	1.98	0.61
1:C:216:VAL:O	1:C:227:ILE:HG22	2.01	0.61
1:C:90:TYR:CE2	1:C:104:GLY:HA3	2.35	0.61
1:E:112:THR:OG1	1:E:223:ARG:O	2.13	0.61
1:E:195:VAL:CG1	1:E:204:TRP:HB3	2.30	0.61
1:D:130:SER:O	1:D:131:THR:OG1	2.15	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:GLN:HE22	1:D:69:VAL:HG21	1.66	0.61
1:D:16:THR:CG2	1:D:61:VAL:N	2.57	0.61
1:D:161:ASN:HA	1:D:176:THR:HG21	1.79	0.61
1:E:92:LEU:CG	1:E:100:VAL:HG11	2.31	0.61
1:A:56:THR:CG2	1:A:57:GLY:H	2.12	0.61
1:A:75:ASN:HD22	1:D:196:LEU:HD11	1.64	0.61
1:F:154:LEU:HD23	1:F:225:LEU:HD21	1.81	0.61
1:E:234:THR:OG1	1:E:235:THR:N	2.33	0.61
1:A:131:THR:CB	1:A:131:THR:HG1	2.07	0.61
1:E:158:THR:H	1:F:151:PRO:HD3	1.65	0.61
1:C:127:ILE:O	1:C:127:ILE:HG23	2.00	0.61
1:A:4:LEU:C	1:A:4:LEU:CD2	2.68	0.61
1:B:30:PHE:C	1:B:30:PHE:HD1	2.02	0.61
1:F:142:HIS:O	1:F:156:MET:HB3	2.00	0.61
1:B:129:TYR:O	1:B:130:SER:CB	2.49	0.61
1:E:162:LEU:HB3	1:E:174:THR:CG2	2.31	0.61
1:C:193:MET:H	1:C:206:SER:CB	2.14	0.61
1:B:35:ASP:OD2	1:B:53:ALA:HB1	2.00	0.60
1:B:217:PHE:HZ	1:B:225:LEU:CD1	2.10	0.60
1:D:92:LEU:HA	1:D:102:ILE:HG13	1.82	0.60
1:B:186:VAL:O	1:B:194:ASP:HB2	2.01	0.60
1:A:163:VAL:HG23	1:A:164:LEU:N	2.16	0.60
1:E:109:ASP:HA	1:E:225:LEU:O	2.00	0.60
1:D:32:MET:CE	1:D:38:LEU:HB2	2.32	0.60
1:B:109:ASP:N	1:B:109:ASP:OD2	2.33	0.60
1:D:101:THR:HG23	1:D:102:ILE:N	2.16	0.60
1:F:67:LEU:HD11	1:F:84:LYS:HB3	1.82	0.60
1:E:215:TYR:CE1	1:E:229:GLY:HA2	2.36	0.60
1:F:220:GLN:NE2	1:F:228:TYR:OH	2.33	0.60
1:D:147:LEU:O	1:D:153:ARG:HA	2.00	0.60
1:D:100:VAL:O	1:D:101:THR:OG1	2.15	0.60
1:F:166:ASP:O	1:F:167:ARG:C	2.35	0.60
1:A:110:SER:HG	1:A:225:LEU:HB2	1.66	0.60
1:D:159:ASP:O	1:D:177:ALA:HA	2.02	0.60
1:D:107:LEU:HD11	1:D:209:SER:HA	1.84	0.60
1:A:154:LEU:HD23	1:A:163:VAL:O	2.01	0.60
1:D:153:ARG:NH2	1:D:165:PHE:CE1	2.70	0.60
1:D:36:CYS:SG	1:D:55:ALA:HB3	2.42	0.60
1:D:42:ASP:O	1:D:43:SER:CB	2.49	0.60
1:D:187:LEU:HD13	1:D:227:ILE:HD12	1.84	0.60
1:E:193:MET:H	1:E:206:SER:HB3	1.66	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:MET:HE3	1:A:156:MET:HA	1.82	0.60
1:D:64:SER:HG	1:D:64:SER:CB	2.10	0.60
1:E:27:SER:HB2	1:F:34:SER:OG	2.01	0.60
1:E:119:VAL:CG2	1:E:151:PRO:HD3	2.32	0.60
1:C:33:GLN:NE2	1:C:35:ASP:OD1	2.34	0.60
1:B:192:ARG:HA	1:B:206:SER:OG	2.02	0.60
1:F:129:TYR:HE1	1:F:131:THR:H	1.48	0.60
1:F:63:GLN:HE21	1:F:69:VAL:HG21	1.65	0.60
1:F:188:GLN:HB3	1:F:192:ARG:H	1.66	0.60
1:F:141:LEU:CD1	1:F:145:GLN:HB3	2.31	0.60
1:E:72:THR:CG2	1:E:73:ALA:N	2.64	0.60
1:D:167:ARG:O	1:D:168:ASP:C	2.38	0.60
1:A:200:ASN:ND2	1:A:200:ASN:N	2.48	0.60
1:C:195:VAL:HG13	1:C:204:TRP:HB3	1.83	0.60
1:E:116:GLY:O	1:E:118:VAL:HG23	2.02	0.60
1:D:197:THR:HB	1:D:201:ILE:HB	1.83	0.60
1:B:9:HIS:HD2	1:B:10:GLU:HB2	1.65	0.59
1:B:148:GLN:HB3	1:B:153:ARG:HB3	1.85	0.59
1:E:162:LEU:HB3	1:E:174:THR:HG21	1.84	0.59
1:E:158:THR:H	1:F:151:PRO:CD	2.15	0.59
1:C:72:THR:HG23	1:C:73:ALA:O	2.02	0.59
1:D:128:LEU:O	1:D:129:TYR:CG	2.55	0.59
1:B:183:CYS:HA	1:B:196:LEU:O	2.02	0.59
1:D:112:THR:O	1:D:223:ARG:NH1	2.30	0.59
1:F:187:LEU:HD11	1:F:227:ILE:HD12	1.82	0.59
1:D:44:ASP:O	1:D:45:VAL:HB	2.02	0.59
1:E:63:GLN:HB2	1:E:67:LEU:H	1.66	0.59
1:A:104:GLY:C	1:A:105:PRO:O	2.39	0.59
1:C:56:THR:HG22	1:C:57:GLY:N	2.17	0.59
1:B:60:ALA:HB2	1:B:70:ILE:CD1	2.32	0.59
1:D:153:ARG:NH2	1:D:165:PHE:HE1	2.00	0.59
1:F:59:ARG:O	1:F:70:ILE:HA	2.01	0.59
1:F:63:GLN:HB2	1:F:67:LEU:O	2.03	0.59
1:D:197:THR:HG22	1:D:199:GLN:O	2.03	0.59
1:D:137:HIS:HB2	1:D:138:PRO:HA	1.82	0.59
1:D:71:LEU:HD21	1:D:77:ILE:HG13	1.83	0.59
1:E:9:HIS:HB2	1:E:10:GLU:CG	2.26	0.59
1:F:217:PHE:CZ	1:F:225:LEU:HD23	2.37	0.59
1:B:70:ILE:O	1:B:78:ARG:N	2.35	0.59
1:D:84:LYS:HG3	1:D:84:LYS:O	2.02	0.59
1:B:37:ASN:HD21	1:B:51:ASN:H	1.48	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:GLN:HB2	1:D:99:THR:O	2.03	0.59
1:D:174:THR:O	1:D:174:THR:HG22	2.02	0.59
1:A:161:ASN:HD21	1:A:175:ASN:H	1.50	0.59
1:F:2:ASN:O	1:F:93:VAL:HG23	2.03	0.59
1:C:215:TYR:CD1	1:C:229:GLY:HA2	2.38	0.59
1:D:165:PHE:HD2	1:D:170:ARG:HA	1.66	0.59
1:A:90:TYR:CD1	1:A:90:TYR:N	2.69	0.59
1:D:182:GLY:HA3	1:D:198:ASN:H	1.67	0.59
1:C:188:GLN:O	1:C:190:ASN:N	2.36	0.59
1:B:168:ASP:O	1:B:169:ASP:HB3	2.03	0.59
1:A:120:VAL:HG22	1:A:122:ASN:O	2.03	0.59
1:E:92:LEU:CG	1:E:100:VAL:CG1	2.81	0.59
1:A:52:THR:HG21	1:A:79:TRP:HB2	1.83	0.59
1:B:3:ILE:HG22	1:B:93:VAL:CG1	2.32	0.58
1:F:2:ASN:HA	1:F:23:LEU:CD2	2.32	0.58
1:F:126:SER:O	1:F:147:LEU:CD1	2.42	0.58
1:E:39:VAL:CG1	1:E:40:LEU:N	2.66	0.58
1:D:32:MET:HE1	1:D:70:ILE:HD11	1.85	0.58
1:A:210:ARG:O	1:A:211:SER:C	2.40	0.58
1:E:92:LEU:HG	1:E:100:VAL:HG11	1.83	0.58
1:B:171:VAL:HB	1:B:223:ARG:HH12	1.69	0.58
1:A:101:THR:HG22	1:A:103:TYR:CZ	2.39	0.58
1:B:106:GLY:O	1:B:107:LEU:HB3	2.02	0.58
1:E:70:ILE:HG13	1:E:79:TRP:HE3	1.64	0.58
1:F:25:LEU:O	1:F:28:PHE:HB2	2.04	0.58
1:B:48:TRP:CG	1:B:49:ALA:N	2.69	0.58
1:D:16:THR:HG22	1:D:17:LEU:N	2.17	0.58
1:A:104:GLY:HA2	1:A:105:PRO:O	2.04	0.58
1:E:92:LEU:HD11	1:E:100:VAL:HG11	1.84	0.58
1:C:30:PHE:HB2	1:C:40:LEU:HA	1.85	0.58
1:A:58:CYS:HA	1:A:71:LEU:O	2.03	0.58
1:D:129:TYR:HD2	1:D:215:TYR:O	1.86	0.58
1:A:108:TRP:HB2	1:A:208:ASN:HD21	1.63	0.58
1:E:163:VAL:CG2	1:E:170:ARG:HG2	2.33	0.58
1:B:183:CYS:HB3	1:B:196:LEU:O	2.04	0.58
1:C:64:SER:O	1:C:87:ILE:O	2.21	0.58
1:A:64:SER:O	1:A:87:ILE:O	2.22	0.58
1:E:170:ARG:CB	1:E:170:ARG:HH11	2.17	0.58
1:B:42:ASP:O	1:B:43:SER:HB2	2.03	0.58
1:F:162:LEU:HD11	1:F:193:MET:CE	2.34	0.58
1:F:142:HIS:CD2	1:F:145:GLN:OE1	2.56	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:MET:HG2	1:E:60:ALA:HB3	1.85	0.58
1:A:220:GLN:HG2	1:A:221:PRO:HD3	1.86	0.58
1:C:4:LEU:HD12	1:C:5:PHE:N	2.17	0.58
1:E:219:LEU:CD1	1:E:225:LEU:HD23	2.34	0.58
1:E:59:ARG:O	1:E:71:LEU:N	2.36	0.58
1:E:69:VAL:CG2	1:E:69:VAL:O	2.52	0.58
1:D:5:PHE:HZ	1:D:220:GLN:HG2	1.63	0.58
1:B:192:ARG:C	1:B:193:MET:O	2.41	0.57
1:D:204:TRP:CG	1:D:205:THR:N	2.70	0.57
1:D:37:ASN:ND2	1:D:38:LEU:N	2.51	0.57
1:F:128:LEU:HB3	1:F:129:TYR:CD2	2.39	0.57
1:A:161:ASN:HD21	1:A:175:ASN:N	2.02	0.57
1:E:119:VAL:O	1:E:120:VAL:HB	2.03	0.57
1:E:157:GLU:HG2	1:F:150:SER:OG	2.04	0.57
1:D:204:TRP:CE3	1:D:205:THR:HA	2.39	0.57
1:A:167:ARG:O	1:A:169:ASP:N	2.37	0.57
1:F:197:THR:O	1:F:199:GLN:N	2.38	0.57
1:E:161:ASN:ND2	1:E:176:THR:H	2.01	0.57
1:C:4:LEU:HD22	1:C:17:LEU:CD2	2.27	0.57
1:D:3:ILE:CG2	1:D:93:VAL:HB	2.31	0.57
1:E:92:LEU:CD1	1:E:100:VAL:HG11	2.34	0.57
1:E:128:LEU:O	1:E:129:TYR:C	2.38	0.57
1:D:154:LEU:CG	1:D:225:LEU:HD11	2.35	0.57
1:D:156:MET:O	1:D:157:GLU:O	2.22	0.57
1:C:41:PHE:HA	1:C:45:VAL:O	2.05	0.57
1:A:220:GLN:HB2	1:A:224:ASN:HB3	1.86	0.57
1:A:127:ILE:O	1:A:127:ILE:CG2	2.47	0.57
1:C:80:SER:OG	1:C:81:SER:N	2.37	0.57
1:C:89:ASN:HD22	1:C:89:ASN:H	1.51	0.57
1:D:137:HIS:CB	1:D:138:PRO:CA	2.83	0.57
1:A:152:TYR:CD2	1:A:223:ARG:HG3	2.40	0.57
1:C:67:LEU:HD21	1:C:82:GLY:CA	2.31	0.57
1:F:142:HIS:N	1:F:142:HIS:CD2	2.70	0.57
1:E:64:SER:O	1:E:65:ASP:CB	2.30	0.57
1:A:4:LEU:C	1:A:4:LEU:HD23	2.25	0.57
1:E:152:TYR:O	1:E:153:ARG:HB3	2.04	0.57
1:C:120:VAL:HG13	1:C:122:ASN:O	2.05	0.57
1:A:160:CYS:O	1:A:176:THR:HG23	2.05	0.57
1:E:188:GLN:HG3	1:E:189:PRO:CD	2.34	0.57
1:D:62:LEU:HA	1:D:68:LEU:HA	1.85	0.57
1:D:160:CYS:SG	1:D:180:GLY:HA3	2.44	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:30:PHE:HA	1:F:31:THR:HG22	1.87	0.57
1:A:22:SER:CB	1:A:31:THR:HG22	2.33	0.57
1:E:148:GLN:HA	1:E:153:ARG:HA	1.87	0.57
1:D:39:VAL:CG1	1:D:40:LEU:N	2.67	0.56
1:A:119:VAL:CG2	1:A:151:PRO:HD3	2.35	0.56
1:D:156:MET:O	1:D:157:GLU:C	2.41	0.56
1:C:74:GLN:HG3	1:F:189:PRO:CB	2.26	0.56
1:C:74:GLN:H	1:F:189:PRO:CG	2.17	0.56
1:B:35:ASP:OD1	1:B:35:ASP:N	2.33	0.56
1:E:29:ARG:NH2	1:E:41:PHE:CE1	2.73	0.56
1:E:149:LEU:HD13	1:E:221:PRO:HA	1.87	0.56
1:A:13:HIS:HA	1:A:14:PRO:O	2.04	0.56
1:E:159:ASP:OD1	1:E:159:ASP:N	2.36	0.56
1:E:158:THR:CG2	1:F:151:PRO:HG2	2.32	0.56
1:F:167:ARG:O	1:F:168:ASP:C	2.43	0.56
1:F:146:SER:OG	1:F:155:SER:HB3	2.05	0.56
1:D:166:ASP:C	1:D:167:ARG:O	2.43	0.56
1:C:211:SER:O	1:C:212:ALA:C	2.44	0.56
1:B:29:ARG:O	1:B:41:PHE:N	2.38	0.56
1:E:177:ALA:O	1:E:179:LYS:N	2.39	0.56
1:C:114:ASN:ND2	1:C:223:ARG:HD3	2.21	0.56
1:F:72:THR:HG22	1:F:74:GLN:HB2	1.87	0.56
1:D:215:TYR:O	1:D:216:VAL:HB	2.04	0.56
1:F:227:ILE:HG12	1:F:227:ILE:O	2.04	0.56
1:C:163:VAL:HG23	1:C:164:LEU:N	2.20	0.56
1:C:87:ILE:O	1:C:88:GLY:O	2.24	0.56
1:C:69:VAL:O	1:C:69:VAL:HG23	2.06	0.56
1:E:159:ASP:O	1:E:160:CYS:HB3	2.05	0.56
1:B:100:VAL:O	1:B:234:THR:HA	2.05	0.56
1:F:215:TYR:HD1	1:F:227:ILE:HD11	1.70	0.56
1:D:137:HIS:HB3	1:D:138:PRO:C	2.26	0.56
1:A:69:VAL:CG2	1:A:69:VAL:O	2.51	0.56
1:A:52:THR:O	1:A:78:ARG:NH1	2.38	0.56
1:E:111:GLY:H	1:E:224:ASN:ND2	2.03	0.56
1:D:104:GLY:HA2	1:D:105:PRO:O	2.06	0.56
1:E:80:SER:OG	1:E:81:SER:N	2.35	0.56
1:D:31:THR:N	1:D:39:VAL:O	2.32	0.56
1:B:132:GLN:HG2	1:B:214:ARG:HH12	1.71	0.56
1:A:74:GLN:HE21	1:D:189:PRO:CG	2.18	0.56
1:A:54:GLY:O	1:A:55:ALA:HB2	2.05	0.56
1:A:75:ASN:ND2	1:D:196:LEU:HD21	2.21	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:TYR:CB	1:C:131:THR:HG22	2.36	0.56
1:A:154:LEU:O	1:A:155:SER:CB	2.46	0.56
1:B:17:LEU:H	1:B:61:VAL:H	1.53	0.56
1:F:90:TYR:CD1	1:F:90:TYR:N	2.72	0.56
1:B:37:ASN:HD21	1:B:52:THR:H	1.52	0.56
1:B:188:GLN:CG	1:B:189:PRO:CD	2.83	0.56
1:D:103:TYR:HB3	1:D:228:TYR:O	2.06	0.56
1:A:134:ASN:N	1:A:214:ARG:HH22	2.03	0.56
1:B:37:ASN:HD22	1:B:52:THR:H	1.49	0.55
1:B:146:SER:O	1:B:147:LEU:O	2.23	0.55
1:C:113:SER:HA	1:C:222:ASP:O	2.06	0.55
1:A:131:THR:HG21	1:A:131:THR:OG1	2.03	0.55
1:E:141:LEU:CD2	1:E:185:ALA:HB3	2.36	0.55
1:A:72:THR:HG21	1:A:76:THR:OG1	2.07	0.55
1:A:5:PHE:HE2	1:A:220:GLN:NE2	2.03	0.55
1:C:166:ASP:HB2	1:C:171:VAL:HG11	1.87	0.55
1:E:176:THR:HG23	1:E:179:LYS:HD3	1.87	0.55
1:A:152:TYR:CE2	1:A:223:ARG:HG3	2.41	0.55
1:D:152:TYR:HB2	1:D:219:LEU:HD21	1.88	0.55
1:F:71:LEU:CD2	1:F:77:ILE:H	2.19	0.55
1:D:163:VAL:HG21	1:D:165:PHE:CZ	2.42	0.55
1:F:76:THR:HA	1:F:77:ILE:HG13	1.89	0.55
1:B:59:ARG:NH2	1:B:71:LEU:HD12	2.21	0.55
1:A:232:LEU:HG	1:A:232:LEU:O	2.05	0.55
1:F:211:SER:OG	1:F:212:ALA:O	2.24	0.55
1:A:225:LEU:O	1:A:226:ALA:HB2	2.06	0.55
1:A:37:ASN:HD22	1:A:52:THR:H	1.52	0.55
1:F:67:LEU:CD1	1:F:84:LYS:HB3	2.36	0.55
1:C:217:PHE:HA	1:C:227:ILE:HG23	1.88	0.55
1:F:77:ILE:O	1:F:77:ILE:CG2	2.49	0.55
1:C:161:ASN:HD21	1:C:175:ASN:CA	2.20	0.55
1:F:16:THR:HG23	1:F:61:VAL:H	1.72	0.55
1:E:56:THR:HG22	1:E:57:GLY:N	2.20	0.55
1:D:18:HIS:H	1:D:21:GLN:HG3	1.72	0.55
1:C:95:GLN:HE21	1:C:99:THR:HG22	1.72	0.55
1:F:87:ILE:CG2	1:F:88:GLY:H	2.18	0.55
1:A:43:SER:C	1:A:44:ASP:O	2.43	0.55
1:A:110:SER:OG	1:A:225:LEU:N	2.39	0.54
1:D:101:THR:HG21	1:D:103:TYR:OH	2.08	0.54
1:F:110:SER:OG	1:F:225:LEU:HD13	2.07	0.54
1:F:193:MET:O	1:F:204:TRP:HZ3	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ASP:O	1:A:167:ARG:O	2.25	0.54
1:C:167:ARG:O	1:C:168:ASP:C	2.44	0.54
1:A:4:LEU:HD12	1:A:17:LEU:HD21	1.89	0.54
1:A:174:THR:O	1:A:175:ASN:OD1	2.26	0.54
1:C:163:VAL:HG23	1:C:164:LEU:H	1.73	0.54
1:A:150:SER:OG	1:A:151:PRO:N	2.40	0.54
1:D:223:ARG:CB	1:D:223:ARG:HH11	2.21	0.54
1:C:93:VAL:CG2	1:C:95:GLN:HG3	2.37	0.54
1:A:77:ILE:CG2	1:A:77:ILE:O	2.40	0.54
1:F:75:ASN:O	1:F:76:THR:HB	2.06	0.54
1:E:152:TYR:HA	1:E:165:PHE:O	2.07	0.54
1:F:142:HIS:H	1:F:145:GLN:HB2	1.73	0.54
1:A:222:ASP:O	1:A:223:ARG:C	2.44	0.54
1:C:95:GLN:NE2	1:C:99:THR:CG2	2.71	0.54
1:C:163:VAL:CG2	1:C:164:LEU:N	2.69	0.54
1:B:220:GLN:HB2	1:B:221:PRO:CD	2.38	0.54
1:B:214:ARG:O	1:B:215:TYR:HD2	1.91	0.54
1:C:52:THR:HG21	1:C:79:TRP:HB2	1.89	0.54
1:B:28:PHE:CE2	1:B:98:ARG:CG	2.87	0.54
1:B:228:TYR:N	1:B:228:TYR:HD2	2.06	0.54
1:F:95:GLN:HE21	1:F:99:THR:CG2	2.20	0.54
1:D:95:GLN:HG2	1:D:128:LEU:CD2	2.37	0.54
1:D:161:ASN:ND2	1:D:175:ASN:H	2.06	0.54
1:D:197:THR:CG2	1:D:201:ILE:HB	2.36	0.54
1:C:74:GLN:H	1:F:189:PRO:CB	2.20	0.54
1:A:151:PRO:HD2	1:A:152:TYR:N	2.13	0.54
1:F:63:GLN:NE2	1:F:69:VAL:CG2	2.71	0.54
1:E:110:SER:N	1:E:225:LEU:O	2.40	0.54
1:B:176:THR:O	1:B:176:THR:HG22	2.06	0.54
1:B:65:ASP:OD1	1:B:65:ASP:N	2.40	0.54
1:E:37:ASN:OD1	1:E:51:ASN:HA	2.08	0.54
1:D:101:THR:CG2	1:D:102:ILE:N	2.70	0.54
1:F:70:ILE:O	1:F:70:ILE:HG22	2.08	0.54
1:A:101:THR:HA	1:A:233:TRP:O	2.08	0.54
1:C:119:VAL:O	1:C:120:VAL:HG23	2.08	0.54
1:A:220:GLN:HB2	1:A:224:ASN:CB	2.38	0.53
1:C:2:ASN:OD1	1:C:2:ASN:C	2.45	0.53
1:A:143:ALA:O	1:A:144:THR:CB	2.51	0.53
1:E:5:PHE:O	1:E:6:GLY:C	2.44	0.53
1:E:62:LEU:HG	1:E:62:LEU:O	2.04	0.53
1:B:189:PRO:CD	1:B:190:ASN:N	2.72	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:GLY:HA2	1:E:62:LEU:CD2	2.18	0.53
1:B:197:THR:O	1:B:199:GLN:N	2.41	0.53
1:C:220:GLN:O	1:C:221:PRO:C	2.46	0.53
1:C:63:GLN:OE1	1:F:200:ASN:ND2	2.41	0.53
1:E:166:ASP:O	1:E:168:ASP:N	2.41	0.53
1:B:90:TYR:CD2	1:B:104:GLY:CA	2.89	0.53
1:A:63:GLN:HG2	1:D:199:GLN:HA	1.90	0.53
1:A:185:ALA:HA	1:A:194:ASP:O	2.07	0.53
1:D:197:THR:CB	1:D:201:ILE:HB	2.39	0.53
1:C:101:THR:CG2	1:C:103:TYR:CE1	2.92	0.53
1:F:146:SER:HG	1:F:155:SER:HB3	1.74	0.53
1:C:73:ALA:HB1	1:F:189:PRO:HG3	1.88	0.53
1:F:142:HIS:HD2	1:F:145:GLN:OE1	1.92	0.53
1:F:2:ASN:OD1	1:F:3:ILE:N	2.41	0.53
1:E:101:THR:HG1	1:E:234:THR:HB	1.73	0.53
1:D:44:ASP:C	1:D:44:ASP:OD1	2.47	0.53
1:C:235:THR:O	1:C:236:GLY:C	2.47	0.53
1:E:83:THR:HG22	1:E:84:LYS:N	2.24	0.53
1:F:148:GLN:HG3	1:F:153:ARG:HB3	1.90	0.53
1:A:56:THR:HG22	1:A:57:GLY:N	2.18	0.53
1:D:16:THR:CG2	1:D:61:VAL:HG22	2.38	0.53
1:B:220:GLN:NE2	1:B:228:TYR:OH	2.41	0.53
1:F:156:MET:SD	1:F:184:ARG:O	2.66	0.53
1:E:63:GLN:HB2	1:E:67:LEU:N	2.24	0.53
1:D:152:TYR:CD2	1:D:152:TYR:N	2.76	0.53
1:D:166:ASP:O	1:D:167:ARG:C	2.46	0.53
1:B:67:LEU:O	1:B:68:LEU:C	2.45	0.53
1:A:157:GLU:CD	1:C:26:SER:OG	2.48	0.53
1:B:67:LEU:CD1	1:B:84:LYS:HG3	2.34	0.53
1:F:230:GLY:O	1:F:231:ALA:CB	2.29	0.53
1:C:33:GLN:HG3	1:C:37:ASN:O	2.08	0.53
1:A:193:MET:CG	1:A:204:TRP:HZ3	2.21	0.53
1:A:7:LEU:CD1	1:A:61:VAL:HG13	2.39	0.53
1:F:220:GLN:CB	1:F:221:PRO:CD	2.86	0.53
1:D:187:LEU:CD2	1:D:217:PHE:HB2	2.39	0.52
1:B:199:GLN:O	1:B:200:ASN:CB	2.56	0.52
1:E:29:ARG:HH21	1:E:31:THR:CG2	2.22	0.52
1:F:71:LEU:HD23	1:F:77:ILE:H	1.73	0.52
1:D:197:THR:O	1:D:198:ASN:C	2.46	0.52
1:C:32:MET:HE3	1:C:59:ARG:HA	1.91	0.52
1:F:140:THR:OG1	1:F:141:LEU:N	2.40	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:THR:O	1:A:74:GLN:N	2.42	0.52
1:A:127:ILE:HG22	1:A:217:PHE:O	2.09	0.52
1:C:112:THR:O	1:C:113:SER:C	2.42	0.52
1:C:12:SER:HB3	1:C:221:PRO:HB2	1.92	0.52
1:E:162:LEU:HD12	1:E:174:THR:HG21	1.91	0.52
1:E:72:THR:HG22	1:E:75:ASN:N	2.24	0.52
1:A:18:HIS:O	1:A:19:ALA:C	2.47	0.52
1:C:197:THR:CG2	1:C:199:GLN:OE1	2.56	0.52
1:E:38:LEU:N	1:E:50:SER:OG	2.37	0.52
1:D:109:ASP:CB	1:D:225:LEU:O	2.57	0.52
1:C:162:LEU:CB	1:C:174:THR:HG23	2.40	0.52
1:F:18:HIS:HB2	1:F:21:GLN:CD	2.30	0.52
1:C:92:LEU:HD21	1:C:100:VAL:CG1	2.37	0.52
1:B:110:SER:HB3	1:B:112:THR:HG22	1.91	0.52
1:D:37:ASN:HD21	1:D:51:ASN:N	2.08	0.52
1:F:167:ARG:O	1:F:169:ASP:N	2.43	0.52
1:C:147:LEU:O	1:C:154:LEU:N	2.25	0.52
1:A:134:ASN:N	1:A:214:ARG:NH2	2.58	0.52
1:A:142:HIS:O	1:A:156:MET:HB3	2.10	0.52
1:F:220:GLN:HB3	1:F:221:PRO:CD	2.40	0.52
1:D:63:GLN:NE2	1:D:69:VAL:CG2	2.61	0.52
1:E:69:VAL:CG2	1:E:71:LEU:HG	2.39	0.52
1:E:27:SER:HB3	1:E:28:PHE:CD2	2.43	0.52
1:D:108:TRP:O	1:D:109:ASP:HB3	2.10	0.52
1:D:101:THR:HG23	1:D:102:ILE:H	1.75	0.52
1:C:18:HIS:CB	1:C:21:GLN:NE2	2.66	0.52
1:D:93:VAL:CG2	1:D:94:LEU:N	2.69	0.52
1:B:61:VAL:HG22	1:B:62:LEU:N	2.25	0.52
1:B:224:ASN:O	1:B:225:LEU:HD23	2.10	0.52
1:F:129:TYR:HH	1:F:131:THR:CB	2.23	0.52
1:C:36:CYS:HB3	1:C:78:ARG:NH1	2.25	0.52
1:F:67:LEU:HD12	1:F:67:LEU:N	2.23	0.52
1:C:58:CYS:HA	1:C:71:LEU:O	2.10	0.52
1:C:58:CYS:HB2	1:C:71:LEU:O	2.09	0.52
1:B:143:ALA:HA	1:B:156:MET:O	2.09	0.52
1:B:157:GLU:CG	1:B:161:ASN:HB3	2.34	0.52
1:E:141:LEU:HD22	1:E:185:ALA:HB3	1.91	0.52
1:A:48:TRP:CD1	1:A:235:THR:HG22	2.45	0.52
1:B:188:GLN:CB	1:B:189:PRO:CD	2.88	0.52
1:D:129:TYR:CE1	1:D:131:THR:CB	2.92	0.52
1:C:130:SER:C	1:C:131:THR:O	2.43	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ASN:HD21	1:D:175:ASN:H	1.58	0.52
1:D:161:ASN:HD22	1:D:176:THR:HB	1.75	0.52
1:D:161:ASN:ND2	1:D:176:THR:H	2.08	0.52
1:E:210:ARG:HG3	1:E:211:SER:H	1.74	0.52
1:C:195:VAL:CG2	1:C:203:VAL:HG12	2.40	0.52
1:C:72:THR:HG21	1:C:76:THR:CA	2.39	0.51
1:D:224:ASN:O	1:D:225:LEU:HD23	2.10	0.51
1:A:12:SER:HB3	1:A:221:PRO:CG	2.39	0.51
1:E:127:ILE:HG12	1:E:138:PRO:O	2.09	0.51
1:C:4:LEU:HD12	1:C:4:LEU:C	2.29	0.51
1:B:216:VAL:HG22	1:B:217:PHE:N	2.22	0.51
1:F:128:LEU:HA	1:F:129:TYR:HB3	1.91	0.51
1:D:28:PHE:CZ	1:D:98:ARG:HG3	2.45	0.51
1:B:220:GLN:HB3	1:B:221:PRO:CD	2.40	0.51
1:C:137:HIS:HB3	1:C:138:PRO:CA	2.40	0.51
1:D:178:GLY:O	1:D:179:LYS:C	2.48	0.51
1:B:142:HIS:O	1:B:143:ALA:HB2	2.11	0.51
1:F:201:ILE:HG22	1:F:202:ALA:N	2.24	0.51
1:A:39:VAL:CG1	1:A:41:PHE:CE1	2.92	0.51
1:B:44:ASP:O	1:B:45:VAL:HB	2.10	0.51
1:D:211:SER:O	1:D:212:ALA:C	2.46	0.51
1:E:93:VAL:HG23	1:E:94:LEU:N	2.25	0.51
1:A:90:TYR:CD2	1:A:104:GLY:HA3	2.46	0.51
1:A:161:ASN:ND2	1:A:176:THR:N	2.54	0.51
1:A:179:LYS:HZ2	1:A:179:LYS:HB3	1.68	0.51
1:A:179:LYS:HZ1	1:A:179:LYS:CB	2.22	0.51
1:E:185:ALA:HA	1:E:194:ASP:O	2.10	0.51
1:E:109:ASP:HA	1:E:226:ALA:HA	1.92	0.51
1:D:87:ILE:O	1:D:88:GLY:O	2.28	0.51
1:F:161:ASN:ND2	1:F:176:THR:N	2.39	0.51
1:B:188:GLN:HG3	1:E:74:GLN:HA	1.92	0.51
1:A:119:VAL:HG21	1:A:151:PRO:CG	2.40	0.51
1:A:104:GLY:CA	1:A:105:PRO:O	2.59	0.51
1:C:155:SER:O	1:C:162:LEU:HD23	2.11	0.51
1:C:34:SER:O	1:C:56:THR:HG23	2.09	0.51
1:E:125:ASN:HA	1:E:147:LEU:CD1	2.40	0.51
1:A:156:MET:CE	1:A:156:MET:HA	2.40	0.51
1:F:220:GLN:HB3	1:F:221:PRO:HD2	1.92	0.51
1:C:44:ASP:O	1:C:45:VAL:CG2	2.58	0.51
1:D:23:LEU:H	1:D:30:PHE:HB3	1.76	0.51
1:D:39:VAL:CG1	1:D:40:LEU:H	2.20	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:ASP:H	1:F:151:PRO:HB3	1.75	0.51
1:B:94:LEU:CB	1:B:100:VAL:HG12	2.40	0.51
1:B:225:LEU:O	1:B:226:ALA:HB2	2.10	0.51
1:D:154:LEU:CD2	1:D:225:LEU:HD11	2.40	0.51
1:E:117:SER:O	1:E:119:VAL:HG22	2.10	0.51
1:A:42:ASP:O	1:A:43:SER:CB	2.58	0.51
1:C:161:ASN:HD21	1:C:175:ASN:HA	1.75	0.51
1:A:30:PHE:CD1	1:A:100:VAL:HG21	2.45	0.51
1:B:101:THR:HG21	1:B:103:TYR:CZ	2.45	0.51
1:A:159:ASP:HB2	1:A:177:ALA:HB1	1.92	0.51
1:B:94:LEU:HA	1:B:100:VAL:HG12	1.93	0.51
1:E:26:SER:CB	1:F:33:GLN:HG3	2.39	0.51
1:F:30:PHE:CZ	1:F:38:LEU:HD11	2.46	0.51
1:B:142:HIS:H	1:B:145:GLN:HB3	1.76	0.51
1:B:71:LEU:HD22	1:B:77:ILE:N	2.25	0.51
1:E:107:LEU:HD12	1:E:208:ASN:HB2	1.91	0.51
1:D:89:ASN:O	1:D:90:TYR:CD1	2.64	0.51
1:E:48:TRP:CD2	1:E:49:ALA:N	2.78	0.51
1:D:100:VAL:HB	1:D:235:THR:HG1	1.73	0.51
1:C:143:ALA:O	1:C:144:THR:CB	2.58	0.51
1:C:159:ASP:HB2	1:C:177:ALA:HA	1.93	0.51
1:D:56:THR:CG2	1:D:57:GLY:N	2.65	0.51
1:C:101:THR:HG22	1:C:103:TYR:CE1	2.46	0.51
1:F:50:SER:O	1:F:52:THR:N	2.44	0.51
1:A:97:ASP:O	1:A:98:ARG:C	2.48	0.51
1:B:103:TYR:CD1	1:B:216:VAL:HB	2.46	0.51
1:E:4:LEU:CD1	1:E:5:PHE:H	2.15	0.51
1:D:189:PRO:CD	1:D:190:ASN:H	2.19	0.51
1:E:105:PRO:HD2	1:E:210:ARG:HH22	1.70	0.51
1:B:71:LEU:CD2	1:B:77:ILE:H	2.22	0.51
1:A:150:SER:OG	1:A:151:PRO:CD	2.59	0.50
1:C:112:THR:OG1	1:C:223:ARG:O	2.27	0.50
1:E:18:HIS:HB2	1:E:21:GLN:NE2	2.26	0.50
1:C:141:LEU:HD11	1:C:147:LEU:HD13	1.92	0.50
1:E:12:SER:HB3	1:E:221:PRO:CG	2.40	0.50
1:E:19:ALA:O	1:E:20:ALA:CB	2.50	0.50
1:C:42:ASP:O	1:C:43:SER:C	2.50	0.50
1:D:9:HIS:HA	1:D:15:GLN:NE2	2.26	0.50
1:B:217:PHE:O	1:B:217:PHE:CD1	2.64	0.50
1:A:117:SER:O	1:A:119:VAL:HG13	2.11	0.50
1:C:97:ASP:OD1	1:C:99:THR:HB	2.12	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:HIS:HB2	1:D:145:GLN:HB2	1.93	0.50
1:C:166:ASP:C	1:C:167:ARG:O	2.42	0.50
1:F:153:ARG:HE	1:F:165:PHE:HD1	1.56	0.50
1:A:28:PHE:CZ	1:A:98:ARG:HG3	2.46	0.50
1:D:4:LEU:HD22	1:D:17:LEU:CD2	2.41	0.50
1:C:74:GLN:H	1:F:189:PRO:HB2	1.76	0.50
1:B:216:VAL:O	1:B:217:PHE:HB2	2.12	0.50
1:D:168:ASP:O	1:D:169:ASP:CB	2.54	0.50
1:C:97:ASP:C	1:C:97:ASP:OD1	2.49	0.50
1:E:30:PHE:CE1	1:E:100:VAL:HG21	2.46	0.50
1:B:215:TYR:CD2	1:B:229:GLY:HA2	2.47	0.50
1:D:108:TRP:C	1:D:108:TRP:CD2	2.83	0.50
1:D:25:LEU:O	1:D:26:SER:C	2.50	0.50
1:F:16:THR:HG22	1:F:17:LEU:H	1.75	0.50
1:C:2:ASN:HD21	1:C:125:ASN:HD22	1.60	0.50
1:B:163:VAL:CG2	1:B:165:PHE:CE1	2.92	0.50
1:B:63:GLN:O	1:B:64:SER:C	2.47	0.50
1:F:101:THR:OG1	1:F:234:THR:HA	2.11	0.50
1:B:107:LEU:HD12	1:B:107:LEU:C	2.32	0.50
1:E:36:CYS:SG	1:E:55:ALA:HB3	2.52	0.50
1:B:90:TYR:HB3	1:B:103:TYR:O	2.12	0.50
1:E:69:VAL:HG22	1:E:69:VAL:O	2.11	0.50
1:C:97:ASP:CG	1:C:136:ASN:HD21	2.14	0.50
1:D:181:THR:O	1:D:182:GLY:C	2.50	0.50
1:A:159:ASP:HB2	1:A:178:GLY:H	1.75	0.50
1:E:159:ASP:O	1:E:177:ALA:HA	2.12	0.50
1:E:69:VAL:HG21	1:E:71:LEU:CG	2.39	0.50
1:E:9:HIS:CB	1:E:10:GLU:HG3	2.29	0.50
1:B:142:HIS:HB2	1:B:145:GLN:OE1	2.11	0.50
1:B:156:MET:O	1:B:157:GLU:C	2.49	0.50
1:F:220:GLN:HG2	1:F:221:PRO:HD3	1.94	0.50
1:A:72:THR:HG23	1:A:74:GLN:N	2.08	0.50
1:C:137:HIS:CB	1:C:138:PRO:CA	2.86	0.50
1:D:169:ASP:O	1:D:171:VAL:HG12	2.12	0.50
1:F:7:LEU:O	1:F:9:HIS:HA	2.09	0.49
1:B:68:LEU:CD1	1:B:92:LEU:HD13	2.30	0.49
1:C:50:SER:HB2	1:C:79:TRP:CD1	2.47	0.49
1:C:152:TYR:CZ	1:C:223:ARG:HG3	2.47	0.49
1:A:199:GLN:CG	1:A:199:GLN:O	2.59	0.49
1:C:137:HIS:H	1:C:137:HIS:CD2	2.30	0.49
1:E:22:SER:OG	1:E:31:THR:HG22	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:VAL:HG12	1:A:204:TRP:HE3	1.77	0.49
1:F:106:GLY:O	1:F:107:LEU:CB	2.57	0.49
1:F:188:GLN:HE21	1:F:189:PRO:CD	2.25	0.49
1:B:213:GLY:O	1:B:214:ARG:C	2.51	0.49
1:E:63:GLN:HB2	1:E:67:LEU:O	2.11	0.49
1:B:34:SER:OG	1:D:151:PRO:HD3	2.12	0.49
1:D:151:PRO:HB3	1:D:167:ARG:HG2	1.93	0.49
1:D:161:ASN:CA	1:D:176:THR:HG22	2.36	0.49
1:E:9:HIS:HD2	1:E:10:GLU:HB2	1.76	0.49
1:C:4:LEU:HD13	1:C:14:PRO:HB2	1.94	0.49
1:F:217:PHE:HZ	1:F:225:LEU:HD22	1.77	0.49
1:E:136:ASN:C	1:E:136:ASN:CB	2.76	0.49
1:D:70:ILE:HG22	1:D:79:TRP:N	2.27	0.49
1:F:63:GLN:HE21	1:F:69:VAL:CG2	2.25	0.49
1:D:197:THR:O	1:D:199:GLN:O	2.30	0.49
1:C:190:ASN:OD1	1:C:209:SER:HB2	2.13	0.49
1:D:204:TRP:CD2	1:D:205:THR:N	2.81	0.49
1:B:110:SER:HB3	1:B:112:THR:CG2	2.43	0.49
1:B:132:GLN:HE21	1:B:214:ARG:NH1	2.09	0.49
1:A:4:LEU:HD23	1:A:5:PHE:N	2.27	0.49
1:A:160:CYS:SG	1:A:203:VAL:HG11	2.52	0.49
1:D:50:SER:O	1:D:51:ASN:CB	2.57	0.49
1:D:63:GLN:CG	1:D:64:SER:N	2.75	0.49
1:D:189:PRO:CD	1:D:190:ASN:N	2.70	0.49
1:A:195:VAL:HG13	1:A:204:TRP:HB3	1.91	0.49
1:D:29:ARG:O	1:D:40:LEU:HD12	2.11	0.49
1:A:170:ARG:NH1	1:A:173:SER:HB3	2.28	0.49
1:A:220:GLN:HB3	1:A:222:ASP:H	1.76	0.49
1:A:90:TYR:HB3	1:A:91:VAL:O	2.12	0.49
1:E:12:SER:HB3	1:E:221:PRO:HG2	1.92	0.49
1:B:77:ILE:CG2	1:B:78:ARG:N	2.72	0.49
1:F:142:HIS:N	1:F:145:GLN:HB2	2.28	0.49
1:E:72:THR:HG23	1:E:73:ALA:CB	2.43	0.49
1:E:62:LEU:HD21	1:E:90:TYR:HB3	1.95	0.49
1:C:217:PHE:CA	1:C:227:ILE:CG2	2.85	0.49
1:A:164:LEU:HD11	1:A:225:LEU:HD21	1.93	0.49
1:B:23:LEU:H	1:B:30:PHE:HB3	1.77	0.49
1:A:39:VAL:HG22	1:A:49:ALA:CB	2.40	0.49
1:D:67:LEU:HD22	1:D:80:SER:OG	2.12	0.49
1:D:87:ILE:HG22	1:D:88:GLY:N	2.27	0.49
1:D:110:SER:HB2	1:D:112:THR:OG1	2.13	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:SER:HB3	1:E:9:HIS:ND1	2.28	0.49
1:C:47:VAL:O	1:C:48:TRP:HB2	2.12	0.49
1:A:19:ALA:O	1:A:20:ALA:CB	2.61	0.49
1:E:161:ASN:HD21	1:E:175:ASN:H	1.61	0.48
1:B:194:ASP:OD1	1:B:194:ASP:C	2.50	0.48
1:C:185:ALA:HA	1:C:195:VAL:HA	1.93	0.48
1:E:92:LEU:HG	1:E:100:VAL:HG13	1.93	0.48
1:F:50:SER:HB3	1:F:52:THR:OG1	2.11	0.48
1:E:232:LEU:O	1:E:233:TRP:CB	2.60	0.48
1:E:161:ASN:HD22	1:E:176:THR:H	1.60	0.48
1:B:132:GLN:O	1:B:132:GLN:HG3	2.12	0.48
1:B:187:LEU:C	1:B:188:GLN:O	2.52	0.48
1:A:75:ASN:HB2	1:D:188:GLN:NE2	2.28	0.48
1:A:151:PRO:CD	1:A:152:TYR:N	2.73	0.48
1:C:30:PHE:CB	1:C:40:LEU:HB2	2.42	0.48
1:D:107:LEU:CD1	1:D:209:SER:HA	2.43	0.48
1:E:102:ILE:HD12	1:E:233:TRP:CE3	2.47	0.48
1:C:150:SER:HB3	1:C:151:PRO:HD3	1.94	0.48
1:B:94:LEU:HB2	1:B:100:VAL:CG1	2.41	0.48
1:F:225:LEU:HD12	1:F:225:LEU:N	2.28	0.48
1:A:52:THR:CG2	1:A:79:TRP:HB2	2.43	0.48
1:A:18:HIS:HB3	1:A:19:ALA:HB3	1.95	0.48
1:B:3:ILE:HD12	1:B:3:ILE:HG21	1.57	0.48
1:E:32:MET:HG2	1:E:60:ALA:HB2	1.95	0.48
1:A:190:ASN:HB2	1:A:210:ARG:O	2.13	0.48
1:A:217:PHE:HD1	1:A:227:ILE:HG22	1.78	0.48
1:C:22:SER:OG	1:C:31:THR:HB	2.14	0.48
1:D:197:THR:HG22	1:D:199:GLN:N	2.26	0.48
1:A:142:HIS:O	1:A:156:MET:HG3	2.13	0.48
1:E:107:LEU:CD1	1:E:208:ASN:HB2	2.43	0.48
1:B:129:TYR:HD2	1:B:215:TYR:O	1.96	0.48
1:F:129:TYR:O	1:F:130:SER:OG	2.28	0.48
1:A:167:ARG:O	1:A:168:ASP:C	2.51	0.48
1:F:87:ILE:O	1:F:88:GLY:C	2.51	0.48
1:F:61:VAL:HG12	1:F:62:LEU:N	2.28	0.48
1:B:62:LEU:HG	1:B:63:GLN:N	2.25	0.48
1:B:186:VAL:O	1:B:194:ASP:CB	2.61	0.48
1:B:194:ASP:OD1	1:B:195:VAL:N	2.47	0.48
1:B:193:MET:HG3	1:B:204:TRP:CZ3	2.49	0.48
1:D:165:PHE:HD2	1:D:170:ARG:CA	2.25	0.48
1:F:224:ASN:O	1:F:225:LEU:CD1	2.52	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:ARG:NH2	1:C:31:THR:HG21	2.24	0.48
1:E:81:SER:OG	1:E:82:GLY:N	2.46	0.48
1:F:162:LEU:HD11	1:F:193:MET:HE2	1.96	0.48
1:D:215:TYR:CE1	1:D:229:GLY:HA3	2.49	0.48
1:A:5:PHE:CE2	1:A:220:GLN:NE2	2.81	0.48
1:F:105:PRO:O	1:F:228:TYR:HA	2.14	0.48
1:F:217:PHE:CZ	1:F:225:LEU:CD2	2.94	0.48
1:E:39:VAL:HG11	1:E:41:PHE:CE1	2.49	0.48
1:C:176:THR:HG22	1:C:203:VAL:HG13	1.95	0.48
1:C:221:PRO:O	1:C:222:ASP:C	2.52	0.48
1:C:102:ILE:HD13	1:C:102:ILE:N	2.28	0.48
1:E:163:VAL:HG22	1:E:165:PHE:CE2	2.48	0.48
1:D:82:GLY:O	1:D:83:THR:O	2.31	0.48
1:D:187:LEU:HD22	1:D:217:PHE:HB2	1.95	0.48
1:D:217:PHE:HZ	1:D:225:LEU:CD1	2.20	0.48
1:F:199:GLN:O	1:F:200:ASN:HB2	2.14	0.48
1:B:40:LEU:HG	1:B:40:LEU:O	2.13	0.48
1:B:200:ASN:N	1:B:200:ASN:HD22	1.99	0.48
1:F:70:ILE:HG22	1:F:78:ARG:HB2	1.96	0.48
1:A:102:ILE:O	1:A:231:ALA:HA	2.13	0.48
1:F:193:MET:O	1:F:204:TRP:CZ3	2.66	0.47
1:B:72:THR:HG21	1:B:76:THR:HG23	1.94	0.47
1:D:188:GLN:NE2	1:D:194:ASP:OD2	2.47	0.47
1:B:197:THR:O	1:B:198:ASN:C	2.52	0.47
1:A:176:THR:CG2	1:A:176:THR:O	2.61	0.47
1:B:163:VAL:HG13	1:B:163:VAL:H	1.37	0.47
1:F:188:GLN:HG3	1:F:189:PRO:HD2	1.96	0.47
1:D:162:LEU:CB	1:D:174:THR:OG1	2.62	0.47
1:E:110:SER:OG	1:E:225:LEU:CB	2.60	0.47
1:B:60:ALA:HB2	1:B:70:ILE:HD11	1.96	0.47
1:C:119:VAL:HG12	1:C:120:VAL:H	1.78	0.47
1:F:195:VAL:CG1	1:F:204:TRP:HB3	2.40	0.47
1:F:161:ASN:HA	1:F:161:ASN:HD22	1.35	0.47
1:A:220:GLN:HG2	1:A:221:PRO:CD	2.44	0.47
1:D:2:ASN:HD22	1:D:2:ASN:N	2.12	0.47
1:F:16:THR:CG2	1:F:61:VAL:H	2.27	0.47
1:A:48:TRP:CE2	1:A:235:THR:HG22	2.50	0.47
1:F:106:GLY:O	1:F:107:LEU:HB2	2.13	0.47
1:C:8:SER:HB2	1:C:9:HIS:HB2	1.95	0.47
1:A:192:ARG:HD2	1:A:205:THR:OG1	2.13	0.47
1:D:129:TYR:HE1	1:D:131:THR:CB	2.26	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:VAL:HG12	1:B:203:VAL:CG1	2.44	0.47
1:B:192:ARG:HB3	1:B:206:SER:OG	2.14	0.47
1:C:203:VAL:HG12	1:C:204:TRP:N	2.29	0.47
1:F:95:GLN:O	1:F:97:ASP:N	2.48	0.47
1:A:97:ASP:OD1	1:A:99:THR:HB	2.15	0.47
1:E:37:ASN:OD1	1:E:51:ASN:CA	2.63	0.47
1:E:17:LEU:H	1:E:61:VAL:H	1.62	0.47
1:A:193:MET:HG3	1:A:204:TRP:HZ3	1.79	0.47
1:D:182:GLY:HA3	1:D:198:ASN:N	2.30	0.47
1:D:70:ILE:HG22	1:D:79:TRP:H	1.79	0.47
1:A:161:ASN:ND2	1:A:175:ASN:N	2.62	0.47
1:D:55:ALA:HB1	1:D:56:THR:H	1.56	0.47
1:E:142:HIS:HB2	1:E:145:GLN:OE1	2.14	0.47
1:E:182:GLY:HA3	1:E:198:ASN:CA	2.45	0.47
1:E:159:ASP:N	1:F:151:PRO:HG3	2.29	0.47
1:E:158:THR:HB	1:F:152:TYR:CZ	2.49	0.47
1:F:172:TRP:CH2	1:F:174:THR:HG23	2.49	0.47
1:F:186:VAL:HG22	1:F:194:ASP:CB	2.45	0.47
1:B:90:TYR:N	1:B:90:TYR:CD1	2.82	0.47
1:F:125:ASN:HA	1:F:147:LEU:HG	1.95	0.47
1:A:163:VAL:HB	1:A:173:SER:OG	2.14	0.47
1:A:119:VAL:HG21	1:A:151:PRO:HG3	1.96	0.47
1:F:187:LEU:HD22	1:F:217:PHE:HB2	1.97	0.47
1:C:157:GLU:HG2	1:C:163:VAL:HG13	1.97	0.47
1:B:30:PHE:HD1	1:B:31:THR:N	2.12	0.47
1:C:23:LEU:O	1:C:30:PHE:N	2.48	0.47
1:C:210:ARG:HB3	1:C:211:SER:H	1.37	0.47
1:A:192:ARG:HG3	1:A:209:SER:HB3	1.97	0.47
1:F:56:THR:HG23	1:F:57:GLY:N	2.28	0.47
1:B:151:PRO:HD3	1:D:34:SER:HB2	1.86	0.47
1:A:109:ASP:HB3	1:A:226:ALA:HB2	1.97	0.47
1:A:163:VAL:HG21	1:A:165:PHE:CZ	2.48	0.47
1:B:163:VAL:HG23	1:B:164:LEU:N	2.30	0.47
1:B:220:GLN:HB3	1:B:221:PRO:HD3	1.97	0.47
1:A:25:LEU:HA	1:A:25:LEU:HD13	1.81	0.47
1:C:139:GLN:O	1:C:140:THR:HB	2.15	0.47
1:C:217:PHE:CA	1:C:227:ILE:HG22	2.42	0.47
1:A:146:SER:HA	1:A:154:LEU:O	2.14	0.47
1:E:97:ASP:O	1:E:98:ARG:CB	2.63	0.47
1:F:60:ALA:HB2	1:F:70:ILE:HD11	1.96	0.47
1:D:146:SER:OG	1:D:155:SER:HB2	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:SER:O	1:D:81:SER:C	2.51	0.47
1:B:86:SER:HB2	1:B:90:TYR:OH	2.15	0.47
1:F:25:LEU:N	1:F:94:LEU:HD21	2.30	0.47
1:C:142:HIS:CD2	1:C:145:GLN:OE1	2.68	0.47
1:F:30:PHE:CD1	1:F:39:VAL:O	2.68	0.47
1:E:30:PHE:CE2	1:E:92:LEU:HD11	2.50	0.47
1:C:38:LEU:HD22	1:C:60:ALA:HB2	1.97	0.47
1:F:180:GLY:O	1:F:181:THR:HB	2.14	0.47
1:E:87:ILE:O	1:E:88:GLY:O	2.33	0.46
1:B:225:LEU:O	1:B:226:ALA:CB	2.56	0.46
1:A:60:ALA:O	1:A:69:VAL:O	2.33	0.46
1:D:72:THR:HG22	1:D:74:GLN:CB	2.45	0.46
1:E:107:LEU:O	1:E:208:ASN:ND2	2.48	0.46
1:E:216:VAL:CG1	1:E:216:VAL:O	2.59	0.46
1:D:64:SER:O	1:D:87:ILE:O	2.33	0.46
1:E:32:MET:O	1:E:32:MET:SD	2.73	0.46
1:A:72:THR:HG22	1:A:76:THR:CA	2.44	0.46
1:A:119:VAL:CG2	1:A:150:SER:OG	2.63	0.46
1:D:169:ASP:OD2	1:D:169:ASP:C	2.54	0.46
1:D:102:ILE:HD12	1:D:233:TRP:CE3	2.50	0.46
1:D:184:ARG:HG2	1:D:184:ARG:NH1	2.30	0.46
1:B:152:TYR:OH	1:B:221:PRO:O	2.33	0.46
1:A:101:THR:CG2	1:A:103:TYR:CZ	2.97	0.46
1:E:104:GLY:HA2	1:E:105:PRO:O	2.15	0.46
1:F:63:GLN:O	1:F:64:SER:C	2.52	0.46
1:F:63:GLN:O	1:F:65:ASP:N	2.48	0.46
1:E:170:ARG:NH1	1:E:170:ARG:CG	2.66	0.46
1:E:193:MET:CG	1:E:204:TRP:HZ3	2.28	0.46
1:C:8:SER:CB	1:C:9:HIS:HB2	2.44	0.46
1:B:37:ASN:HD22	1:B:53:ALA:N	2.13	0.46
1:B:188:GLN:CB	1:B:189:PRO:HD3	2.43	0.46
1:E:29:ARG:NH2	1:E:31:THR:HG21	2.30	0.46
1:C:48:TRP:CD2	1:C:49:ALA:N	2.83	0.46
1:F:6:GLY:HA2	1:F:62:LEU:O	2.15	0.46
1:C:40:LEU:HD22	1:C:100:VAL:HG23	1.98	0.46
1:D:195:VAL:HG13	1:D:204:TRP:HB3	1.97	0.46
1:F:204:TRP:CE3	1:F:204:TRP:C	2.89	0.46
1:F:128:LEU:HA	1:F:129:TYR:CG	2.51	0.46
1:A:146:SER:O	1:A:147:LEU:O	2.34	0.46
1:C:36:CYS:HB3	1:C:78:ARG:HH11	1.80	0.46
1:B:164:LEU:CD1	1:B:171:VAL:HG22	2.45	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:SER:HB2	1:E:112:THR:HG23	1.97	0.46
1:E:171:VAL:HG22	1:E:172:TRP:N	2.31	0.46
1:E:215:TYR:HE1	1:E:229:GLY:HA2	1.77	0.46
1:D:110:SER:CB	1:D:112:THR:OG1	2.64	0.46
1:E:118:VAL:HG13	1:E:221:PRO:HB2	1.98	0.46
1:B:6:GLY:HA2	1:B:62:LEU:HD23	1.97	0.46
1:D:45:VAL:CA	1:D:46:ARG:HG3	2.46	0.46
1:F:137:HIS:N	1:F:137:HIS:CD2	2.83	0.46
1:D:71:LEU:CD2	1:D:77:ILE:HG13	2.46	0.46
1:E:52:THR:HB	1:E:78:ARG:HD3	1.97	0.46
1:E:4:LEU:CD1	1:E:5:PHE:N	2.61	0.46
1:C:29:ARG:HH21	1:C:31:THR:HG23	1.74	0.46
1:E:194:ASP:HB3	1:E:196:LEU:CD1	2.45	0.46
1:B:17:LEU:H	1:B:61:VAL:N	2.13	0.46
1:F:90:TYR:CE2	1:F:104:GLY:HA3	2.51	0.46
1:D:90:TYR:HE2	1:D:232:LEU:HD22	1.80	0.46
1:C:74:GLN:HG2	1:F:189:PRO:HB2	1.95	0.46
1:A:119:VAL:HB	1:A:150:SER:OG	2.16	0.46
1:D:161:ASN:HD21	1:D:175:ASN:CA	2.29	0.46
1:E:224:ASN:HA	1:E:224:ASN:HD22	1.41	0.46
1:A:106:GLY:HA2	1:A:228:TYR:HA	1.98	0.46
1:B:93:VAL:HG23	1:B:94:LEU:N	2.31	0.46
1:F:28:PHE:HB3	1:F:94:LEU:CD1	2.43	0.46
1:C:215:TYR:N	1:C:215:TYR:CD2	2.77	0.46
1:F:163:VAL:HG21	1:F:165:PHE:CZ	2.51	0.46
1:A:72:THR:CG2	1:A:76:THR:OG1	2.64	0.46
1:F:17:LEU:O	1:F:60:ALA:N	2.43	0.46
1:A:95:GLN:HA	1:A:96:PRO:HD3	1.85	0.46
1:E:71:LEU:HD23	1:E:71:LEU:HA	1.75	0.45
1:F:217:PHE:HZ	1:F:225:LEU:HD23	1.74	0.45
1:F:23:LEU:HA	1:F:23:LEU:HD23	1.57	0.45
1:C:33:GLN:HB2	1:C:33:GLN:HE21	1.17	0.45
1:D:181:THR:O	1:D:183:CYS:N	2.49	0.45
1:E:193:MET:H	1:E:206:SER:CB	2.29	0.45
1:E:113:SER:HB3	1:E:114:ASN:H	1.65	0.45
1:D:67:LEU:HD13	1:D:69:VAL:HG13	1.98	0.45
1:D:68:LEU:HD23	1:D:79:TRP:HZ3	1.81	0.45
1:B:103:TYR:CE1	1:B:216:VAL:HB	2.51	0.45
1:B:18:HIS:HB2	1:B:21:GLN:HG3	1.98	0.45
1:F:99:THR:HG23	1:F:99:THR:O	2.16	0.45
1:D:62:LEU:O	1:D:63:GLN:O	2.34	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:MET:N	1:B:206:SER:HB3	2.31	0.45
1:A:112:THR:H	1:A:224:ASN:ND2	2.14	0.45
1:A:187:LEU:HD12	1:A:191:GLY:HA2	1.98	0.45
1:E:172:TRP:CG	1:E:173:SER:N	2.84	0.45
1:D:84:LYS:CG	1:D:84:LYS:O	2.64	0.45
1:F:192:ARG:HA	1:F:206:SER:OG	2.16	0.45
1:B:216:VAL:O	1:B:217:PHE:CB	2.58	0.45
1:D:4:LEU:HD22	1:D:17:LEU:HD21	1.98	0.45
1:E:23:LEU:O	1:E:29:ARG:HA	2.17	0.45
1:F:17:LEU:HD23	1:F:17:LEU:HA	1.74	0.45
1:F:184:ARG:HB2	1:F:185:ALA:H	1.20	0.45
1:B:132:GLN:CG	1:B:214:ARG:HH12	2.28	0.45
1:D:129:TYR:CD2	1:D:215:TYR:O	2.68	0.45
1:A:150:SER:OG	1:A:151:PRO:HD3	2.17	0.45
1:F:28:PHE:HE2	1:F:42:ASP:OD2	1.99	0.45
1:D:166:ASP:HB2	1:D:171:VAL:HG11	1.99	0.45
1:F:217:PHE:HD2	1:F:217:PHE:C	2.13	0.45
1:C:143:ALA:HA	1:C:156:MET:O	2.16	0.45
1:B:60:ALA:HB2	1:B:70:ILE:HD12	1.98	0.45
1:A:223:ARG:NH1	1:A:223:ARG:HB3	2.25	0.45
1:F:31:THR:CG2	1:F:39:VAL:O	2.64	0.45
1:E:149:LEU:CD1	1:E:221:PRO:HA	2.47	0.45
1:C:78:ARG:HD2	1:C:78:ARG:HH11	1.39	0.45
1:B:48:TRP:CE2	1:B:235:THR:HG21	2.50	0.45
1:C:92:LEU:CD2	1:C:100:VAL:HG13	2.44	0.45
1:D:23:LEU:HD12	1:D:30:PHE:HD2	1.81	0.45
1:E:78:ARG:O	1:E:79:TRP:HB2	2.16	0.45
1:E:63:GLN:O	1:E:65:ASP:N	2.50	0.45
1:E:119:VAL:CG2	1:E:151:PRO:CD	2.95	0.45
1:E:95:GLN:HB2	1:E:95:GLN:HE21	1.45	0.45
1:F:176:THR:CG2	1:F:203:VAL:HG22	2.47	0.45
1:B:161:ASN:HA	1:B:161:ASN:HD22	1.46	0.45
1:E:162:LEU:HD12	1:E:174:THR:CG2	2.47	0.45
1:D:201:ILE:HD13	1:D:201:ILE:HG23	1.73	0.45
1:C:9:HIS:HB3	1:C:10:GLU:H	1.58	0.45
1:F:44:ASP:O	1:F:45:VAL:HG23	2.17	0.45
1:D:19:ALA:O	1:D:32:MET:O	2.35	0.44
1:D:31:THR:O	1:D:38:LEU:HD12	2.16	0.44
1:F:18:HIS:O	1:F:32:MET:CB	2.65	0.44
1:F:197:THR:HG21	1:F:201:ILE:CD1	2.42	0.44
1:E:153:ARG:NH2	1:E:165:PHE:CE1	2.82	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:GLY:O	1:B:107:LEU:CB	2.61	0.44
1:B:208:ASN:HB2	1:B:209:SER:H	1.40	0.44
1:D:52:THR:HG21	1:D:79:TRP:HB2	1.99	0.44
1:D:112:THR:HG21	1:D:172:TRP:HB2	1.99	0.44
1:F:215:TYR:N	1:F:215:TYR:CD2	2.84	0.44
1:B:63:GLN:HE22	1:B:69:VAL:HG22	1.82	0.44
1:A:48:TRP:CE3	1:A:49:ALA:HA	2.53	0.44
1:B:5:PHE:HE2	1:B:220:GLN:NE2	2.15	0.44
1:D:81:SER:OG	1:D:82:GLY:N	2.50	0.44
1:B:9:HIS:HB2	1:B:10:GLU:HB2	1.99	0.44
1:E:29:ARG:HH21	1:E:31:THR:HG23	1.82	0.44
1:F:42:ASP:OD2	1:F:98:ARG:NH1	2.43	0.44
1:E:30:PHE:CD1	1:E:100:VAL:HG21	2.52	0.44
1:B:220:GLN:O	1:B:221:PRO:C	2.54	0.44
1:B:162:LEU:HD23	1:B:162:LEU:HA	1.73	0.44
1:F:159:ASP:OD2	1:F:161:ASN:HB2	2.17	0.44
1:D:217:PHE:CZ	1:D:225:LEU:CD1	2.96	0.44
1:D:150:SER:HB3	1:D:151:PRO:HD2	1.97	0.44
1:A:232:LEU:O	1:A:233:TRP:HB2	2.17	0.44
1:B:65:ASP:O	1:B:66:GLY:C	2.56	0.44
1:A:3:ILE:H	1:A:3:ILE:HG22	1.22	0.44
1:D:193:MET:CE	1:D:193:MET:HA	2.47	0.44
1:C:137:HIS:H	1:C:137:HIS:HD2	1.63	0.44
1:C:92:LEU:HA	1:C:102:ILE:HA	1.99	0.44
1:A:116:GLY:O	1:A:118:VAL:HG23	2.18	0.44
1:B:139:GLN:HE21	1:B:139:GLN:HB2	1.48	0.44
1:C:74:GLN:H	1:F:189:PRO:HG2	1.67	0.44
1:B:10:GLU:OE2	1:B:222:ASP:OD2	2.36	0.44
1:E:61:VAL:CG2	1:E:62:LEU:H	2.25	0.44
1:A:150:SER:H	1:A:152:TYR:HB2	1.83	0.44
1:D:2:ASN:HB2	1:D:94:LEU:HB3	1.99	0.44
1:A:96:PRO:HG2	1:A:136:ASN:HA	1.99	0.44
1:C:38:LEU:O	1:C:39:VAL:HG23	2.18	0.44
1:F:180:GLY:O	1:F:181:THR:CB	2.60	0.44
1:C:25:LEU:O	1:C:28:PHE:N	2.47	0.44
1:F:208:ASN:N	1:F:208:ASN:OD1	2.50	0.44
1:B:86:SER:HB3	1:B:87:ILE:H	1.06	0.44
1:D:150:SER:N	1:D:152:TYR:H	2.10	0.44
1:F:217:PHE:CD2	1:F:218:VAL:N	2.86	0.44
1:A:101:THR:HG22	1:A:103:TYR:CE1	2.52	0.44
1:E:130:SER:HA	1:E:139:GLN:OE1	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:GLN:HE21	1:E:21:GLN:HB2	1.18	0.44
1:C:193:MET:N	1:C:206:SER:HB3	2.28	0.44
1:A:112:THR:OG1	1:A:223:ARG:O	2.36	0.44
1:D:162:LEU:HD23	1:D:162:LEU:HA	1.72	0.44
1:A:176:THR:O	1:A:176:THR:HG23	2.18	0.44
1:B:63:GLN:HE21	1:B:63:GLN:HB2	1.26	0.44
1:A:199:GLN:HG2	1:A:201:ILE:HD12	1.99	0.44
1:E:200:ASN:N	1:E:200:ASN:ND2	2.64	0.44
1:D:33:GLN:HB2	1:D:37:ASN:O	2.18	0.43
1:E:179:LYS:NZ	1:E:203:VAL:HG13	2.32	0.43
1:F:174:THR:HG22	1:F:204:TRP:NE1	2.33	0.43
1:E:37:ASN:HA	1:E:52:THR:HG1	1.83	0.43
1:E:29:ARG:NH2	1:E:41:PHE:CD1	2.86	0.43
1:E:223:ARG:CG	1:E:223:ARG:HH11	2.29	0.43
1:E:163:VAL:HB	1:E:173:SER:OG	2.17	0.43
1:E:172:TRP:CH2	1:E:174:THR:HG22	2.53	0.43
1:F:152:TYR:HD2	1:F:166:ASP:HB2	1.83	0.43
1:F:127:ILE:HD13	1:F:127:ILE:HG21	1.74	0.43
1:A:147:LEU:HA	1:A:147:LEU:HD12	1.79	0.43
1:D:50:SER:O	1:D:51:ASN:HB3	2.18	0.43
1:F:166:ASP:O	1:F:167:ARG:O	2.36	0.43
1:F:142:HIS:HD2	1:F:145:GLN:CD	2.22	0.43
1:E:72:THR:CG2	1:E:74:GLN:H	2.31	0.43
1:A:75:ASN:HD22	1:D:196:LEU:CD1	2.31	0.43
1:C:140:THR:HG1	1:C:141:LEU:H	1.63	0.43
1:C:155:SER:O	1:C:163:VAL:N	2.45	0.43
1:C:48:TRP:CG	1:C:49:ALA:N	2.86	0.43
1:C:205:THR:O	1:C:205:THR:CG2	2.53	0.43
1:A:193:MET:H	1:A:206:SER:HB3	1.83	0.43
1:E:141:LEU:CD1	1:E:147:LEU:HD23	2.48	0.43
1:C:83:THR:HG22	1:C:84:LYS:N	2.25	0.43
1:C:188:GLN:HA	1:C:189:PRO:HD3	1.77	0.43
1:A:65:ASP:OD1	1:A:65:ASP:N	2.51	0.43
1:D:63:GLN:HB3	1:D:67:LEU:H	1.83	0.43
1:F:156:MET:CE	1:F:161:ASN:O	2.67	0.43
1:F:185:ALA:O	1:F:186:VAL:CG1	2.66	0.43
1:C:138:PRO:C	1:C:140:THR:H	2.20	0.43
1:D:161:ASN:HD21	1:D:175:ASN:N	2.17	0.43
1:B:153:ARG:HG3	1:B:165:PHE:HB2	2.01	0.43
1:A:50:SER:O	1:A:51:ASN:CB	2.64	0.43
1:B:210:ARG:HG3	1:B:211:SER:H	1.84	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:SER:OG	1:D:114:ASN:N	2.50	0.43
1:C:74:GLN:H	1:C:74:GLN:HG3	1.47	0.43
1:B:129:TYR:CD1	1:B:131:THR:N	2.87	0.43
1:D:164:LEU:HA	1:D:164:LEU:HD23	1.71	0.43
1:E:9:HIS:CD2	1:E:10:GLU:HB2	2.52	0.43
1:C:113:SER:HA	1:C:222:ASP:HB2	2.01	0.43
1:E:166:ASP:O	1:E:167:ARG:C	2.57	0.43
1:B:35:ASP:O	1:B:53:ALA:HA	2.19	0.43
1:D:187:LEU:CD2	1:D:217:PHE:CB	2.96	0.43
1:B:193:MET:HG3	1:B:204:TRP:HZ3	1.83	0.43
1:A:224:ASN:HA	1:A:224:ASN:HD22	1.37	0.43
1:C:35:ASP:O	1:C:36:CYS:HB2	2.18	0.43
1:C:67:LEU:HD22	1:C:80:SER:OG	2.18	0.43
1:B:164:LEU:HD12	1:B:172:TRP:HB3	2.01	0.43
1:E:91:VAL:HG21	1:E:228:TYR:CD2	2.53	0.43
1:F:186:VAL:HG22	1:F:194:ASP:HB3	2.00	0.43
1:B:193:MET:CG	1:B:204:TRP:CZ3	3.02	0.43
1:C:95:GLN:NE2	1:C:99:THR:HG22	2.33	0.43
1:B:157:GLU:HG3	1:B:161:ASN:CB	2.40	0.43
1:F:44:ASP:O	1:F:45:VAL:CB	2.66	0.43
1:F:190:ASN:C	1:F:190:ASN:OD1	2.57	0.43
1:B:168:ASP:O	1:B:169:ASP:CB	2.64	0.43
1:E:87:ILE:HD12	1:E:87:ILE:HA	1.82	0.43
1:F:154:LEU:CG	1:F:225:LEU:HD21	2.49	0.43
1:F:77:ILE:HD13	1:F:77:ILE:HG21	1.73	0.43
1:A:44:ASP:O	1:A:45:VAL:C	2.56	0.43
1:E:189:PRO:O	1:E:213:GLY:O	2.37	0.43
1:D:30:PHE:CD1	1:D:30:PHE:C	2.84	0.43
1:D:64:SER:C	1:D:64:SER:OG	2.56	0.43
1:E:158:THR:OG1	1:F:151:PRO:CG	2.56	0.43
1:E:159:ASP:HB2	1:E:177:ALA:HB1	2.01	0.43
1:D:153:ARG:HH21	1:D:165:PHE:HE1	1.67	0.43
1:B:92:LEU:HA	1:B:102:ILE:HG13	2.01	0.43
1:A:217:PHE:CD1	1:A:227:ILE:HG22	2.53	0.43
1:A:19:ALA:O	1:A:20:ALA:HB2	2.19	0.43
1:E:232:LEU:O	1:E:233:TRP:HB2	2.19	0.43
1:D:83:THR:O	1:D:84:LYS:CB	2.38	0.42
1:B:201:ILE:O	1:B:202:ALA:HB2	2.19	0.42
1:F:18:HIS:O	1:F:32:MET:HB3	2.18	0.42
1:C:68:LEU:O	1:C:79:TRP:HZ3	2.02	0.42
1:D:46:ARG:O	1:D:47:VAL:HG13	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ARG:NH2	1:B:41:PHE:CE1	2.87	0.42
1:C:107:LEU:HD12	1:C:107:LEU:O	2.19	0.42
1:E:154:LEU:HD23	1:E:225:LEU:HD11	2.00	0.42
1:B:110:SER:O	1:B:112:THR:HG22	2.18	0.42
1:B:129:TYR:O	1:B:187:LEU:O	2.37	0.42
1:D:217:PHE:CD2	1:D:218:VAL:N	2.88	0.42
1:C:174:THR:HB	1:C:204:TRP:CG	2.55	0.42
1:C:49:ALA:O	1:C:50:SER:O	2.38	0.42
1:C:52:THR:HG21	1:C:79:TRP:CB	2.48	0.42
1:F:16:THR:CG2	1:F:17:LEU:N	2.70	0.42
1:A:128:LEU:O	1:A:129:TYR:CD2	2.72	0.42
1:B:220:GLN:CB	1:B:221:PRO:HD2	2.49	0.42
1:B:174:THR:OG1	1:B:176:THR:HB	2.19	0.42
1:C:101:THR:HG21	1:C:103:TYR:CE1	2.54	0.42
1:C:71:LEU:HA	1:C:71:LEU:HD23	1.71	0.42
1:C:73:ALA:HB1	1:F:189:PRO:CB	2.47	0.42
1:C:61:VAL:HG12	1:C:62:LEU:H	1.78	0.42
1:E:211:SER:O	1:E:212:ALA:C	2.57	0.42
1:D:94:LEU:HD12	1:D:94:LEU:C	2.31	0.42
1:F:199:GLN:O	1:F:200:ASN:CB	2.67	0.42
1:B:152:TYR:HE1	1:B:220:GLN:O	2.03	0.42
1:D:204:TRP:C	1:D:205:THR:HG22	2.40	0.42
1:B:210:ARG:CG	1:B:211:SER:H	2.32	0.42
1:E:158:THR:OG1	1:F:151:PRO:HD3	2.17	0.42
1:F:7:LEU:H	1:F:7:LEU:HG	1.37	0.42
1:F:30:PHE:CE1	1:F:38:LEU:HG	2.54	0.42
1:C:221:PRO:O	1:C:223:ARG:N	2.52	0.42
1:F:16:THR:HG23	1:F:61:VAL:N	2.34	0.42
1:B:163:VAL:HG12	1:B:173:SER:OG	2.19	0.42
1:A:50:SER:O	1:A:51:ASN:HB2	2.20	0.42
1:D:137:HIS:CB	1:D:138:PRO:C	2.88	0.42
1:C:41:PHE:HD2	1:C:45:VAL:H	1.67	0.42
1:C:127:ILE:HA	1:C:138:PRO:HG2	2.00	0.42
1:A:151:PRO:HD2	1:A:152:TYR:CG	2.55	0.42
1:B:172:TRP:CE3	1:B:172:TRP:C	2.93	0.42
1:E:142:HIS:HB2	1:E:145:GLN:CG	2.50	0.42
1:B:77:ILE:O	1:B:78:ARG:HD2	2.20	0.42
1:B:208:ASN:OD1	1:B:208:ASN:N	2.52	0.42
1:F:68:LEU:C	1:F:68:LEU:HD23	2.38	0.42
1:D:153:ARG:O	1:D:164:LEU:HD23	2.19	0.42
1:E:217:PHE:HA	1:E:227:ILE:HB	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:TRP:CG	1:A:235:THR:HG22	2.55	0.42
1:E:207:GLY:C	1:E:208:ASN:O	2.50	0.42
1:F:143:ALA:CA	1:F:156:MET:O	2.65	0.42
1:A:109:ASP:HB2	1:A:110:SER:H	1.66	0.42
1:F:32:MET:HE2	1:F:38:LEU:HB2	2.01	0.42
1:E:100:VAL:N	1:E:235:THR:HG21	2.31	0.42
1:A:70:ILE:O	1:A:78:ARG:N	2.48	0.42
1:D:56:THR:HG22	1:D:57:GLY:CA	2.49	0.42
1:D:11:GLY:O	1:D:13:HIS:N	2.52	0.42
1:B:154:LEU:HD21	1:B:225:LEU:HD11	2.02	0.42
1:A:74:GLN:HA	1:D:189:PRO:HD3	2.02	0.42
1:D:223:ARG:CG	1:D:223:ARG:HH11	2.27	0.42
1:F:29:ARG:O	1:F:41:PHE:N	2.40	0.42
1:E:219:LEU:HA	1:E:219:LEU:HD12	1.65	0.42
1:E:199:GLN:CA	1:E:199:GLN:HE21	2.33	0.42
1:D:67:LEU:HD13	1:D:69:VAL:CG1	2.50	0.42
1:B:190:ASN:OD1	1:B:190:ASN:C	2.58	0.42
1:D:166:ASP:OD2	1:D:223:ARG:HD2	2.19	0.42
1:A:128:LEU:HD11	2:A:244:HOH:O	2.19	0.42
1:D:160:CYS:O	1:D:176:THR:CG2	2.67	0.41
1:E:24:GLU:HG2	1:E:29:ARG:HB3	2.01	0.41
1:A:160:CYS:O	1:A:160:CYS:SG	2.77	0.41
1:C:195:VAL:HG22	1:C:203:VAL:HG12	2.02	0.41
1:C:81:SER:O	1:C:82:GLY:C	2.58	0.41
1:C:171:VAL:HG23	1:C:171:VAL:O	2.19	0.41
1:B:220:GLN:HB2	1:B:221:PRO:HD2	2.02	0.41
1:B:59:ARG:NH2	1:B:71:LEU:CD1	2.83	0.41
1:D:197:THR:O	1:D:199:GLN:N	2.53	0.41
1:E:102:ILE:HD12	1:E:233:TRP:HE3	1.85	0.41
1:C:183:CYS:HB3	1:C:196:LEU:O	2.20	0.41
1:F:97:ASP:OD1	1:F:97:ASP:N	2.52	0.41
1:D:85:GLY:O	1:D:86:SER:O	2.38	0.41
1:E:158:THR:C	1:F:151:PRO:CG	2.82	0.41
1:D:95:GLN:HG2	1:D:128:LEU:HD23	2.03	0.41
1:C:130:SER:H	1:C:131:THR:HG23	1.85	0.41
1:A:161:ASN:HD21	1:A:175:ASN:CA	2.34	0.41
1:C:142:HIS:O	1:C:156:MET:HG3	2.20	0.41
1:A:101:THR:C	1:A:102:ILE:HG13	2.32	0.41
1:C:210:ARG:NH1	1:C:229:GLY:O	2.54	0.41
1:F:95:GLN:HE21	1:F:99:THR:HG21	1.83	0.41
1:A:92:LEU:HG	1:A:100:VAL:HG12	2.01	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:CYS:HA	1:F:196:LEU:O	2.20	0.41
1:B:48:TRP:CZ2	1:B:235:THR:HG21	2.55	0.41
1:F:87:ILE:HG23	1:F:88:GLY:H	1.68	0.41
1:F:76:THR:OG1	1:F:76:THR:O	2.29	0.41
1:F:65:ASP:OD1	1:F:67:LEU:HD13	2.20	0.41
1:E:165:PHE:CE2	1:E:170:ARG:HG3	2.50	0.41
1:D:205:THR:O	1:D:206:SER:C	2.59	0.41
1:F:95:GLN:HE21	1:F:99:THR:HG23	1.85	0.41
1:F:85:GLY:O	1:F:86:SER:O	2.39	0.41
1:C:73:ALA:HB1	1:F:189:PRO:HB3	2.02	0.41
1:F:142:HIS:H	1:F:142:HIS:CD2	2.39	0.41
1:E:35:ASP:O	1:E:37:ASN:N	2.54	0.41
1:C:23:LEU:HD23	1:C:23:LEU:HA	1.37	0.41
1:F:47:VAL:HG12	1:F:47:VAL:O	2.20	0.41
1:F:156:MET:HE3	1:F:161:ASN:O	2.21	0.41
1:D:189:PRO:HD2	1:D:190:ASN:H	1.86	0.41
1:F:217:PHE:CE2	1:F:225:LEU:HB3	2.56	0.41
1:D:162:LEU:N	1:D:174:THR:OG1	2.37	0.41
1:D:174:THR:HB	1:D:176:THR:HB	2.03	0.41
1:A:161:ASN:HA	1:A:176:THR:HG22	2.03	0.41
1:F:40:LEU:HA	1:F:40:LEU:HD12	1.44	0.41
1:D:142:HIS:HB2	1:D:145:GLN:CB	2.51	0.41
1:E:18:HIS:H	1:E:21:GLN:CB	2.34	0.41
1:B:16:THR:HG22	1:B:59:ARG:HG3	2.01	0.41
1:B:39:VAL:CG1	1:B:40:LEU:N	2.81	0.41
1:A:25:LEU:N	1:A:94:LEU:HD23	2.35	0.41
1:C:137:HIS:HB2	1:C:138:PRO:HA	2.03	0.41
1:E:120:VAL:HG22	1:E:122:ASN:O	2.20	0.41
1:E:196:LEU:HD12	1:E:202:ALA:HB2	2.02	0.41
1:C:25:LEU:HD13	1:C:25:LEU:HA	1.75	0.41
1:F:204:TRP:CH2	1:F:206:SER:N	2.89	0.41
1:E:52:THR:HB	1:E:78:ARG:HH11	1.86	0.41
1:E:26:SER:O	1:E:26:SER:OG	2.32	0.41
1:D:187:LEU:HD11	1:D:215:TYR:HB3	2.03	0.41
1:C:195:VAL:HG13	1:C:204:TRP:HE3	1.85	0.41
1:E:119:VAL:HG21	1:E:151:PRO:CD	2.47	0.41
1:E:120:VAL:HG23	1:E:149:LEU:CD2	2.50	0.41
1:F:161:ASN:HD21	1:F:176:THR:N	2.14	0.41
1:B:197:THR:H	1:B:197:THR:HG22	1.66	0.41
1:A:172:TRP:O	1:A:173:SER:HB2	2.17	0.41
1:F:19:ALA:O	1:F:32:MET:O	2.39	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:76:THR:O	1:F:77:ILE:HB	2.08	0.41
1:A:102:ILE:HB	1:A:232:LEU:HB3	2.03	0.41
1:A:156:MET:CA	1:A:156:MET:CE	2.99	0.41
1:E:182:GLY:HA3	1:E:198:ASN:N	2.35	0.41
1:F:47:VAL:CG1	1:F:47:VAL:O	2.68	0.41
1:A:188:GLN:CG	1:A:189:PRO:CD	2.99	0.41
1:A:124:GLY:HA2	1:A:125:ASN:HD22	1.86	0.41
1:A:124:GLY:HA2	1:A:125:ASN:ND2	2.35	0.41
1:C:72:THR:H	1:C:72:THR:HG22	1.51	0.41
1:E:17:LEU:HD23	1:E:17:LEU:HA	1.66	0.41
1:D:215:TYR:O	1:D:216:VAL:CB	2.69	0.41
1:A:72:THR:CG2	1:A:76:THR:H	1.94	0.41
1:F:127:ILE:C	1:F:128:LEU:O	2.54	0.41
1:A:179:LYS:HE3	1:A:203:VAL:HG22	2.03	0.41
1:C:104:GLY:HA2	1:C:105:PRO:O	2.21	0.41
1:C:210:ARG:HH11	1:C:210:ARG:HD2	1.61	0.41
1:C:69:VAL:HG22	1:C:69:VAL:H	1.69	0.41
1:E:158:THR:O	1:E:159:ASP:C	2.40	0.40
1:D:187:LEU:CD1	1:D:227:ILE:HD12	2.51	0.40
1:C:127:ILE:HG23	1:C:217:PHE:HB3	1.96	0.40
1:A:166:ASP:OD2	1:A:223:ARG:HD2	2.20	0.40
1:B:22:SER:CA	1:B:31:THR:HA	2.40	0.40
1:C:87:ILE:CG2	1:C:88:GLY:N	2.84	0.40
1:A:3:ILE:CD1	1:A:218:VAL:HG11	2.50	0.40
1:E:129:TYR:HE1	1:E:131:THR:N	2.18	0.40
1:D:78:ARG:O	1:D:79:TRP:HB2	2.21	0.40
1:E:32:MET:HE1	1:E:70:ILE:HG23	2.02	0.40
1:D:233:TRP:CG	1:D:234:THR:N	2.85	0.40
1:C:35:ASP:O	1:C:36:CYS:CB	2.69	0.40
1:A:196:LEU:CD1	1:A:202:ALA:CB	2.95	0.40
1:A:28:PHE:N	1:A:28:PHE:CD2	2.88	0.40
1:F:44:ASP:OD1	1:F:45:VAL:N	2.54	0.40
1:D:128:LEU:O	1:D:129:TYR:CD2	2.75	0.40
1:A:153:ARG:NH1	1:A:165:PHE:CD1	2.89	0.40
1:A:4:LEU:CD1	1:A:17:LEU:HD21	2.51	0.40
1:A:214:ARG:C	1:A:215:TYR:HD2	2.21	0.40
1:B:39:VAL:HG12	1:B:40:LEU:N	2.33	0.40
1:B:149:LEU:HD12	1:B:219:LEU:HG	2.04	0.40
1:E:129:TYR:C	1:E:129:TYR:CD1	2.95	0.40
1:F:143:ALA:O	1:F:144:THR:HG22	2.22	0.40
1:B:187:LEU:HD22	1:B:217:PHE:HB2	2.04	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:LEU:HA	1:D:225:LEU:HD23	1.60	0.40
1:C:137:HIS:HB3	1:C:138:PRO:C	2.42	0.40
1:E:156:MET:CE	1:E:183:CYS:HB3	2.52	0.40
1:F:191:GLY:HA2	1:F:227:ILE:CD1	2.51	0.40
1:B:220:GLN:HA	1:B:221:PRO:HD3	1.76	0.40
1:C:193:MET:O	1:C:206:SER:N	2.38	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	229/236 (97%)	158 (69%)	41 (18%)	30 (13%)	0	2
1	B	213/236 (90%)	132 (62%)	42 (20%)	39 (18%)	0	1
1	C	230/236 (98%)	150 (65%)	42 (18%)	38 (16%)	0	1
1	D	217/236 (92%)	148 (68%)	30 (14%)	39 (18%)	0	1
1	E	227/236 (96%)	150 (66%)	39 (17%)	38 (17%)	0	1
1	F	208/236 (88%)	138 (66%)	37 (18%)	33 (16%)	0	1
All	All	1324/1416 (94%)	876 (66%)	231 (17%)	217 (16%)	0	1

All (217) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	11	GLY
1	A	14	PRO
1	A	19	ALA
1	A	20	ALA
1	A	34	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	45	VAL
1	A	61	VAL
1	A	73	ALA
1	A	77	ILE
1	A	88	GLY
1	A	105	PRO
1	A	119	VAL
1	A	120	VAL
1	A	122	ASN
1	A	138	PRO
1	A	198	ASN
1	A	206	SER
1	A	207	GLY
1	A	231	ALA
1	B	7	LEU
1	B	12	SER
1	B	43	SER
1	B	45	VAL
1	B	56	THR
1	B	77	ILE
1	B	81	SER
1	B	86	SER
1	B	87	ILE
1	B	105	PRO
1	B	130	SER
1	B	143	ALA
1	B	144	THR
1	B	147	LEU
1	B	150	SER
1	B	167	ARG
1	B	189	PRO
1	B	196	LEU
1	B	198	ASN
1	B	200	ASN
1	B	201	ILE
1	B	203	VAL
1	C	9	HIS
1	C	26	SER
1	C	36	CYS
1	C	52	THR
1	C	74	GLN
1	C	77	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	88	GLY
1	C	105	PRO
1	C	117	SER
1	C	119	VAL
1	C	120	VAL
1	C	122	ASN
1	C	130	SER
1	C	146	SER
1	C	150	SER
1	C	157	GLU
1	C	167	ARG
1	C	168	ASP
1	C	176	THR
1	C	200	ASN
1	C	207	GLY
1	C	222	ASP
1	D	7	LEU
1	D	9	HIS
1	D	27	SER
1	D	43	SER
1	D	45	VAL
1	D	61	VAL
1	D	63	GLN
1	D	83	THR
1	D	84	LYS
1	D	88	GLY
1	D	125	ASN
1	D	129	TYR
1	D	130	SER
1	D	143	ALA
1	D	147	LEU
1	D	157	GLU
1	D	159	ASP
1	D	169	ASP
1	D	170	ARG
1	D	177	ALA
1	D	179	LYS
1	D	188	GLN
1	D	230	GLY
1	E	7	LEU
1	E	9	HIS
1	E	10	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	E	12	SER
1	E	13	HIS
1	E	14	PRO
1	E	33	GLN
1	E	36	CYS
1	E	45	VAL
1	E	65	ASP
1	E	86	SER
1	E	88	GLY
1	E	117	SER
1	E	118	VAL
1	E	120	VAL
1	E	129	TYR
1	E	130	SER
1	E	143	ALA
1	E	159	ASP
1	E	160	CYS
1	E	167	ARG
1	E	168	ASP
1	E	183	CYS
1	E	231	ALA
1	F	8	SER
1	F	9	HIS
1	F	14	PRO
1	F	27	SER
1	F	45	VAL
1	F	87	ILE
1	F	125	ASN
1	F	130	SER
1	F	147	LEU
1	F	160	CYS
1	F	194	ASP
1	F	196	LEU
1	F	198	ASN
1	F	200	ASN
1	F	231	ALA
1	A	26	SER
1	A	191	GLY
1	A	232	LEU
1	B	27	SER
1	B	49	ALA
1	B	61	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	83	THR
1	B	107	LEU
1	B	111	GLY
1	B	159	ASP
1	B	188	GLN
1	B	223	ARG
1	B	231	ALA
1	C	27	SER
1	C	45	VAL
1	C	49	ALA
1	C	50	SER
1	C	61	VAL
1	C	73	ALA
1	C	125	ASN
1	D	8	SER
1	D	13	HIS
1	D	77	ILE
1	D	107	LEU
1	D	167	ARG
1	D	168	ASP
1	D	202	ALA
1	E	27	SER
1	E	61	VAL
1	E	147	LEU
1	E	150	SER
1	E	209	SER
1	E	229	GLY
1	E	232	LEU
1	F	7	LEU
1	F	26	SER
1	F	43	SER
1	F	61	VAL
1	F	75	ASN
1	F	81	SER
1	F	88	GLY
1	F	107	LEU
1	F	150	SER
1	F	168	ASP
1	F	190	ASN
1	F	224	ASN
1	A	129	TYR
1	A	150	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	167	ARG
1	B	168	ASP
1	C	140	THR
1	C	170	ARG
1	C	177	ALA
1	C	221	PRO
1	D	44	ASP
1	D	86	SER
1	D	150	SER
1	D	189	PRO
1	E	107	LEU
1	E	138	PRO
1	E	181	THR
1	F	129	TYR
1	F	225	LEU
1	A	9	HIS
1	A	220	GLN
1	B	11	GLY
1	B	36	CYS
1	B	95	GLN
1	B	229	GLY
1	C	10	GLU
1	C	87	ILE
1	C	147	LEU
1	D	144	THR
1	E	79	TRP
1	E	114	ASN
1	F	189	PRO
1	F	211	SER
1	A	168	ASP
1	B	170	ARG
1	B	191	GLY
1	D	28	PHE
1	D	97	ASP
1	D	182	GLY
1	E	211	SER
1	F	64	SER
1	C	189	PRO
1	E	43	SER
1	A	178	GLY
1	D	14	PRO
1	C	118	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	96	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/198 (100%)	99 (50%)	98 (50%)	0	0
1	B	187/198 (94%)	96 (51%)	91 (49%)	0	0
1	C	195/198 (98%)	111 (57%)	84 (43%)	0	0
1	D	187/198 (94%)	101 (54%)	86 (46%)	0	0
1	E	194/198 (98%)	112 (58%)	82 (42%)	0	0
1	F	183/198 (92%)	108 (59%)	75 (41%)	0	0
All	All	1143/1188 (96%)	627 (55%)	516 (45%)	0	0

All (516) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	5	PHE
1	A	8	SER
1	A	10	GLU
1	A	12	SER
1	A	14	PRO
1	A	17	LEU
1	A	22	SER
1	A	24	GLU
1	A	25	LEU
1	A	27	SER
1	A	30	PHE
1	A	31	THR
1	A	32	MET
1	A	33	GLN
1	A	34	SER
1	A	37	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	38	LEU
1	A	43	SER
1	A	47	VAL
1	A	50	SER
1	A	52	THR
1	A	56	THR
1	A	58	CYS
1	A	59	ARG
1	A	68	LEU
1	A	71	LEU
1	A	74	GLN
1	A	78	ARG
1	A	84	LYS
1	A	87	ILE
1	A	92	LEU
1	A	93	VAL
1	A	94	LEU
1	A	99	THR
1	A	100	VAL
1	A	103	TYR
1	A	105	PRO
1	A	107	LEU
1	A	108	TRP
1	A	109	ASP
1	A	110	SER
1	A	115	LYS
1	A	119	VAL
1	A	120	VAL
1	A	122	ASN
1	A	125	ASN
1	A	129	TYR
1	A	136	ASN
1	A	138	PRO
1	A	141	LEU
1	A	144	THR
1	A	147	LEU
1	A	154	LEU
1	A	155	SER
1	A	156	MET
1	A	157	GLU
1	A	158	THR
1	A	162	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	163	VAL
1	A	164	LEU
1	A	167	ARG
1	A	168	ASP
1	A	169	ASP
1	A	170	ARG
1	A	171	VAL
1	A	173	SER
1	A	174	THR
1	A	175	ASN
1	A	176	THR
1	A	179	LYS
1	A	181	THR
1	A	183	CYS
1	A	184	ARG
1	A	186	VAL
1	A	187	LEU
1	A	188	GLN
1	A	192	ARG
1	A	195	VAL
1	A	196	LEU
1	A	200	ASN
1	A	201	ILE
1	A	203	VAL
1	A	205	THR
1	A	206	SER
1	A	208	ASN
1	A	210	ARG
1	A	215	TYR
1	A	216	VAL
1	A	217	PHE
1	A	218	VAL
1	A	221	PRO
1	A	222	ASP
1	A	223	ARG
1	A	224	ASN
1	A	227	ILE
1	A	232	LEU
1	A	234	THR
1	B	1	ASN
1	B	2	ASN
1	B	3	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	8	SER
1	B	9	HIS
1	B	10	GLU
1	B	12	SER
1	B	16	THR
1	B	21	GLN
1	B	22	SER
1	B	23	LEU
1	B	29	ARG
1	B	30	PHE
1	B	31	THR
1	B	32	MET
1	B	33	GLN
1	B	36	CYS
1	B	45	VAL
1	B	47	VAL
1	B	56	THR
1	B	58	CYS
1	B	59	ARG
1	B	63	GLN
1	B	64	SER
1	B	67	LEU
1	B	68	LEU
1	B	69	VAL
1	B	71	LEU
1	B	76	THR
1	B	78	ARG
1	B	83	THR
1	B	84	LYS
1	B	86	SER
1	B	87	ILE
1	B	90	TYR
1	B	92	LEU
1	B	93	VAL
1	B	94	LEU
1	B	97	ASP
1	B	98	ARG
1	B	105	PRO
1	B	107	LEU
1	B	112	THR
1	B	125	ASN
1	B	126	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	127	ILE
1	B	129	TYR
1	B	130	SER
1	B	132	GLN
1	B	140	THR
1	B	144	THR
1	B	146	SER
1	B	147	LEU
1	B	148	GLN
1	B	149	LEU
1	B	151	PRO
1	B	153	ARG
1	B	155	SER
1	B	156	MET
1	B	158	THR
1	B	159	ASP
1	B	161	ASN
1	B	162	LEU
1	B	163	VAL
1	B	167	ARG
1	B	169	ASP
1	B	170	ARG
1	B	171	VAL
1	B	172	TRP
1	B	173	SER
1	B	181	THR
1	B	184	ARG
1	B	186	VAL
1	B	187	LEU
1	B	188	GLN
1	B	192	ARG
1	B	194	ASP
1	B	196	LEU
1	B	197	THR
1	B	205	THR
1	B	206	SER
1	B	209	SER
1	B	216	VAL
1	B	220	GLN
1	B	222	ASP
1	B	227	ILE
1	B	228	TYR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	232	LEU
1	B	233	TRP
1	B	234	THR
1	B	235	THR
1	C	3	ILE
1	C	4	LEU
1	C	5	PHE
1	C	8	SER
1	C	9	HIS
1	C	10	GLU
1	C	12	SER
1	C	16	THR
1	C	22	SER
1	C	24	GLU
1	C	25	LEU
1	C	27	SER
1	C	30	PHE
1	C	31	THR
1	C	32	MET
1	C	33	GLN
1	C	40	LEU
1	C	43	SER
1	C	46	ARG
1	C	51	ASN
1	C	56	THR
1	C	59	ARG
1	C	61	VAL
1	C	62	LEU
1	C	63	GLN
1	C	67	LEU
1	C	72	THR
1	C	78	ARG
1	C	79	TRP
1	C	86	SER
1	C	87	ILE
1	C	89	ASN
1	C	92	LEU
1	C	93	VAL
1	C	96	PRO
1	C	110	SER
1	C	112	THR
1	C	113	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	118	VAL
1	C	122	ASN
1	C	127	ILE
1	C	130	SER
1	C	131	THR
1	C	136	ASN
1	C	137	HIS
1	C	139	GLN
1	C	144	THR
1	C	145	GLN
1	C	146	SER
1	C	147	LEU
1	C	149	LEU
1	C	150	SER
1	C	154	LEU
1	C	156	MET
1	C	159	ASP
1	C	160	CYS
1	C	162	LEU
1	C	163	VAL
1	C	164	LEU
1	C	167	ARG
1	C	171	VAL
1	C	173	SER
1	C	175	ASN
1	C	176	THR
1	C	183	CYS
1	C	184	ARG
1	C	192	ARG
1	C	193	MET
1	C	195	VAL
1	C	196	LEU
1	C	199	GLN
1	C	200	ASN
1	C	201	ILE
1	C	203	VAL
1	C	206	SER
1	C	211	SER
1	C	216	VAL
1	C	218	VAL
1	C	219	LEU
1	C	221	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	224	ASN
1	C	227	ILE
1	C	233	TRP
1	C	234	THR
1	D	2	ASN
1	D	3	ILE
1	D	4	LEU
1	D	12	SER
1	D	16	THR
1	D	17	LEU
1	D	25	LEU
1	D	29	ARG
1	D	30	PHE
1	D	32	MET
1	D	37	ASN
1	D	43	SER
1	D	44	ASP
1	D	46	ARG
1	D	47	VAL
1	D	48	TRP
1	D	50	SER
1	D	56	THR
1	D	58	CYS
1	D	59	ARG
1	D	61	VAL
1	D	63	GLN
1	D	65	ASP
1	D	67	LEU
1	D	68	LEU
1	D	70	ILE
1	D	71	LEU
1	D	72	THR
1	D	76	THR
1	D	78	ARG
1	D	81	SER
1	D	83	THR
1	D	84	LYS
1	D	86	SER
1	D	87	ILE
1	D	92	LEU
1	D	93	VAL
1	D	95	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	102	ILE
1	D	105	PRO
1	D	107	LEU
1	D	108	TRP
1	D	109	ASP
1	D	126	SER
1	D	127	ILE
1	D	128	LEU
1	D	129	TYR
1	D	137	HIS
1	D	138	PRO
1	D	147	LEU
1	D	148	GLN
1	D	149	LEU
1	D	153	ARG
1	D	154	LEU
1	D	155	SER
1	D	156	MET
1	D	158	THR
1	D	161	ASN
1	D	162	LEU
1	D	164	LEU
1	D	167	ARG
1	D	169	ASP
1	D	170	ARG
1	D	171	VAL
1	D	176	THR
1	D	181	THR
1	D	186	VAL
1	D	187	LEU
1	D	193	MET
1	D	195	VAL
1	D	196	LEU
1	D	200	ASN
1	D	201	ILE
1	D	204	TRP
1	D	205	THR
1	D	211	SER
1	D	214	ARG
1	D	216	VAL
1	D	217	PHE
1	D	219	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	222	ASP
1	D	223	ARG
1	D	224	ASN
1	D	227	ILE
1	D	233	TRP
1	D	234	THR
1	E	1	ASN
1	E	2	ASN
1	E	3	ILE
1	E	4	LEU
1	E	14	PRO
1	E	21	GLN
1	E	22	SER
1	E	23	LEU
1	E	25	LEU
1	E	27	SER
1	E	29	ARG
1	E	32	MET
1	E	34	SER
1	E	40	LEU
1	E	45	VAL
1	E	51	ASN
1	E	52	THR
1	E	56	THR
1	E	59	ARG
1	E	67	LEU
1	E	70	ILE
1	E	72	THR
1	E	78	ARG
1	E	86	SER
1	E	87	ILE
1	E	89	ASN
1	E	91	VAL
1	E	92	LEU
1	E	96	PRO
1	E	101	THR
1	E	105	PRO
1	E	108	TRP
1	E	110	SER
1	E	115	LYS
1	E	119	VAL
1	E	123	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	125	ASN
1	E	127	ILE
1	E	128	LEU
1	E	129	TYR
1	E	131	THR
1	E	141	LEU
1	E	144	THR
1	E	146	SER
1	E	147	LEU
1	E	148	GLN
1	E	149	LEU
1	E	151	PRO
1	E	154	LEU
1	E	156	MET
1	E	158	THR
1	E	162	LEU
1	E	163	VAL
1	E	164	LEU
1	E	167	ARG
1	E	169	ASP
1	E	170	ARG
1	E	171	VAL
1	E	173	SER
1	E	175	ASN
1	E	189	PRO
1	E	192	ARG
1	E	193	MET
1	E	199	GLN
1	E	200	ASN
1	E	201	ILE
1	E	206	SER
1	E	208	ASN
1	E	210	ARG
1	E	211	SER
1	E	214	ARG
1	E	216	VAL
1	E	217	PHE
1	E	223	ARG
1	E	224	ASN
1	E	225	LEU
1	E	227	ILE
1	E	228	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	232	LEU
1	E	233	TRP
1	E	234	THR
1	E	235	THR
1	F	1	ASN
1	F	3	ILE
1	F	8	SER
1	F	10	GLU
1	F	12	SER
1	F	16	THR
1	F	23	LEU
1	F	25	LEU
1	F	26	SER
1	F	29	ARG
1	F	32	MET
1	F	33	GLN
1	F	37	ASN
1	F	38	LEU
1	F	43	SER
1	F	51	ASN
1	F	52	THR
1	F	61	VAL
1	F	65	ASP
1	F	67	LEU
1	F	68	LEU
1	F	70	ILE
1	F	76	THR
1	F	78	ARG
1	F	81	SER
1	F	84	LYS
1	F	86	SER
1	F	87	ILE
1	F	90	TYR
1	F	92	LEU
1	F	94	LEU
1	F	100	VAL
1	F	101	THR
1	F	109	ASP
1	F	125	ASN
1	F	127	ILE
1	F	128	LEU
1	F	129	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	131	THR
1	F	138	PRO
1	F	140	THR
1	F	142	HIS
1	F	145	GLN
1	F	146	SER
1	F	148	GLN
1	F	150	SER
1	F	152	TYR
1	F	153	ARG
1	F	154	LEU
1	F	155	SER
1	F	157	GLU
1	F	160	CYS
1	F	161	ASN
1	F	162	LEU
1	F	163	VAL
1	F	164	LEU
1	F	166	ASP
1	F	169	ASP
1	F	171	VAL
1	F	174	THR
1	F	181	THR
1	F	183	CYS
1	F	184	ARG
1	F	188	GLN
1	F	192	ARG
1	F	193	MET
1	F	204	TRP
1	F	208	ASN
1	F	210	ARG
1	F	211	SER
1	F	222	ASP
1	F	223	ARG
1	F	224	ASN
1	F	225	LEU
1	F	227	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	37	ASN
1	A	63	GLN
1	A	74	GLN
1	A	125	ASN
1	A	137	HIS
1	A	161	ASN
1	A	199	GLN
1	A	200	ASN
1	A	208	ASN
1	A	220	GLN
1	A	224	ASN
1	B	2	ASN
1	B	9	HIS
1	B	13	HIS
1	B	37	ASN
1	B	63	GLN
1	B	132	GLN
1	B	139	GLN
1	B	142	HIS
1	B	161	ASN
1	B	188	GLN
1	B	200	ASN
1	B	220	GLN
1	C	21	GLN
1	C	33	GLN
1	C	75	ASN
1	C	89	ASN
1	C	114	ASN
1	C	125	ASN
1	C	136	ASN
1	C	137	HIS
1	C	142	HIS
1	C	161	ASN
1	C	224	ASN
1	D	2	ASN
1	D	18	HIS
1	D	37	ASN
1	D	63	GLN
1	D	161	ASN
1	D	188	GLN
1	D	200	ASN
1	D	220	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	224	ASN
1	E	21	GLN
1	E	63	GLN
1	E	95	GLN
1	E	142	HIS
1	E	161	ASN
1	E	199	GLN
1	E	200	ASN
1	E	208	ASN
1	E	224	ASN
1	F	13	HIS
1	F	21	GLN
1	F	33	GLN
1	F	63	GLN
1	F	95	GLN
1	F	142	HIS
1	F	148	GLN
1	F	161	ASN
1	F	175	ASN
1	F	188	GLN
1	F	200	ASN
1	F	220	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.