



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:50 PM GMT

PDB ID : 1HCY
Title : CRYSTAL STRUCTURE OF HEXAMERIC HAEMOCYANIN FROM PAN-
ULIRUS INTERRUPTUS REFINED AT 3.2 ANGSTROMS RESOLUTION
Authors : Volbeda, A.; Hol, W.G.J.
Deposited on : 1991-05-15
Resolution : 3.20 Å(reported)

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

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

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

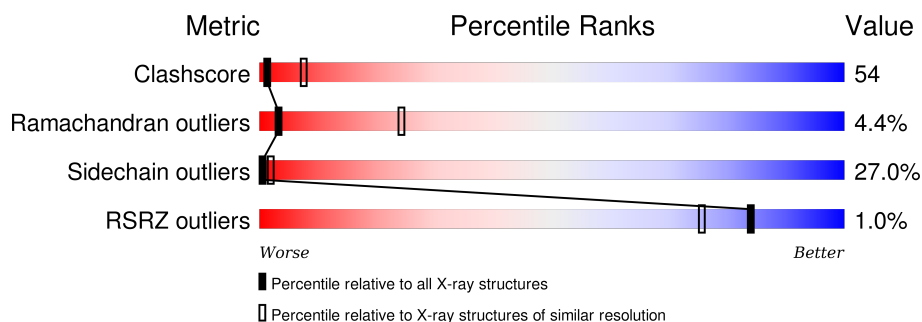
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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

Mol	Chain	Length	Quality of chain
1	A	657	 6% 29% 47% 16% .
1	B	657	 6% 29% 46% 16% .
1	C	657	 6% 30% 47% 16% .
1	D	657	 6% 29% 47% 16% .
1	E	657	 6% 28% 47% 16% .
1	F	657	 6% 30% 46% 15% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31790 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 ARTHROPODAN HEMOCYANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	644	Total	C	N	O	S	0	0	0
			5239	3322	904	992	21			
1	B	644	Total	C	N	O	S	0	0	0
			5239	3322	904	992	21			
1	C	644	Total	C	N	O	S	0	0	0
			5239	3322	904	992	21			
1	D	644	Total	C	N	O	S	0	0	0
			5239	3322	904	992	21			
1	E	644	Total	C	N	O	S	0	0	0
			5239	3322	904	992	21			
1	F	644	Total	C	N	O	S	0	0	0
			5239	3322	904	992	21			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ASP	GLU	CONFLICT	UNP P04254
A	163	PRO	GLN	CONFLICT	UNP P04254
A	458	ASN	LYS	CONFLICT	UNP P04254
A	514	SER	LYS	CONFLICT	UNP P04254
B	32	ASP	GLU	CONFLICT	UNP P04254
B	163	PRO	GLN	CONFLICT	UNP P04254
B	458	ASN	LYS	CONFLICT	UNP P04254
B	514	SER	LYS	CONFLICT	UNP P04254
C	32	ASP	GLU	CONFLICT	UNP P04254
C	163	PRO	GLN	CONFLICT	UNP P04254
C	458	ASN	LYS	CONFLICT	UNP P04254
C	514	SER	LYS	CONFLICT	UNP P04254
D	32	ASP	GLU	CONFLICT	UNP P04254
D	163	PRO	GLN	CONFLICT	UNP P04254
D	458	ASN	LYS	CONFLICT	UNP P04254
D	514	SER	LYS	CONFLICT	UNP P04254
E	32	ASP	GLU	CONFLICT	UNP P04254

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	163	PRO	GLN	CONFLICT	UNP P04254
E	458	ASN	LYS	CONFLICT	UNP P04254
E	514	SER	LYS	CONFLICT	UNP P04254
F	32	ASP	GLU	CONFLICT	UNP P04254
F	163	PRO	GLN	CONFLICT	UNP P04254
F	458	ASN	LYS	CONFLICT	UNP P04254
F	514	SER	LYS	CONFLICT	UNP P04254

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	C	2	Total	C	N	O	0	0
			28	16	2	10		
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cu	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	176	Total	O	0	0
			176	176		
4	B	4	Total	O	0	0
			4	4		
4	C	2	Total	O	0	0
			2	2		
4	E	3	Total	O	0	0
			3	3		

Continued on next page...

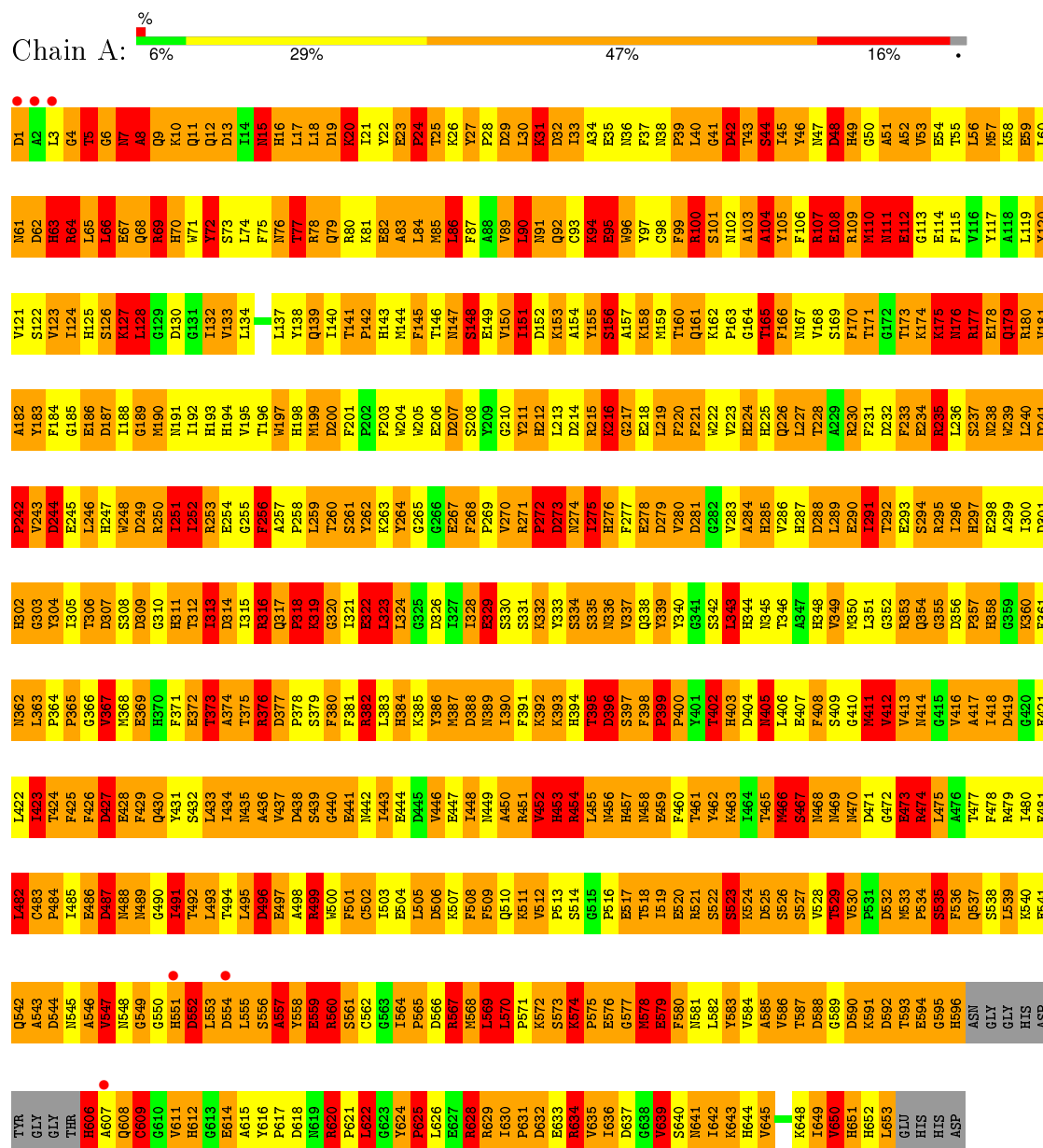
Continued from previous page...

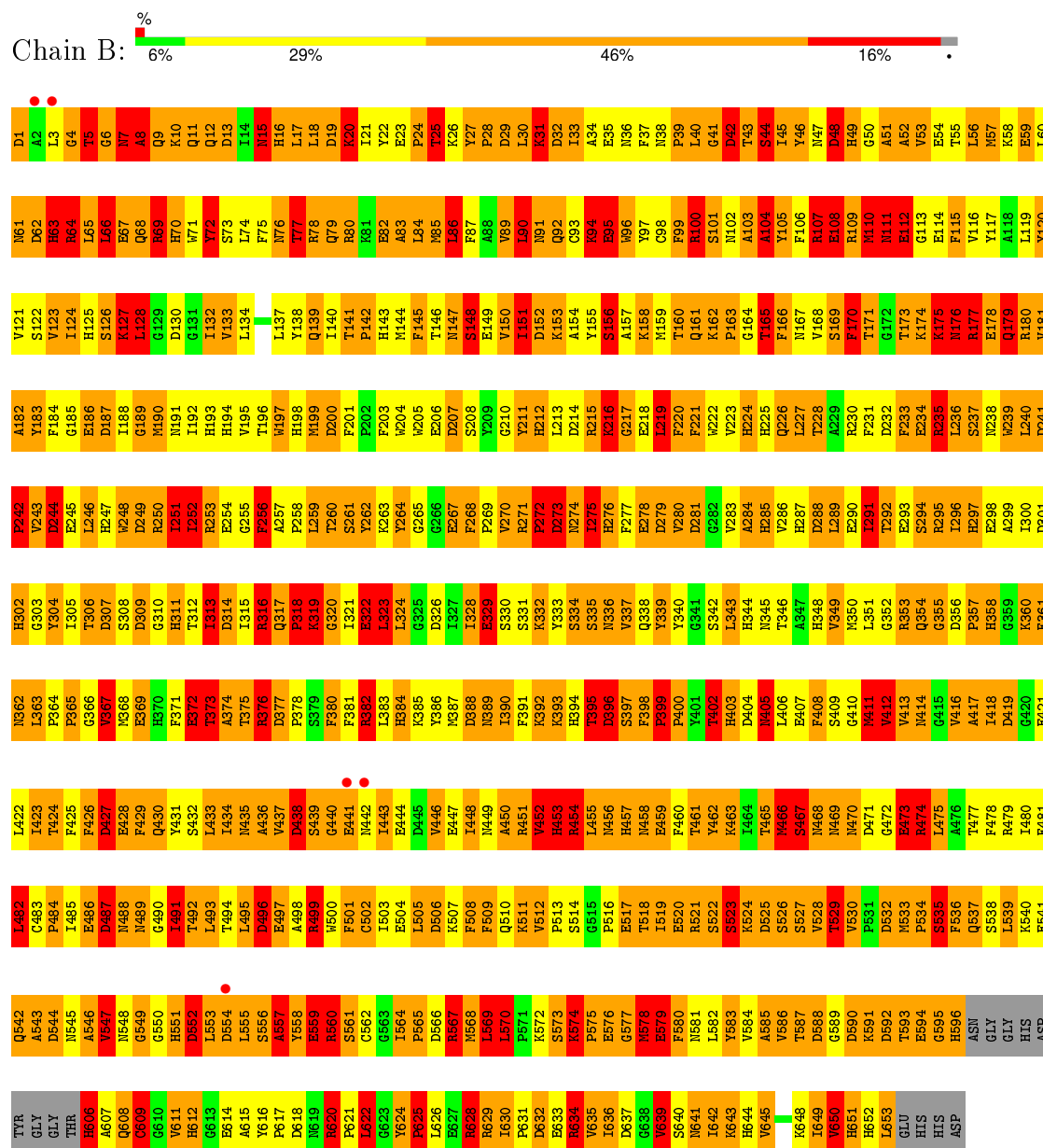
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	1	Total	O	0	0
			1	1		

3 Residue-property plots

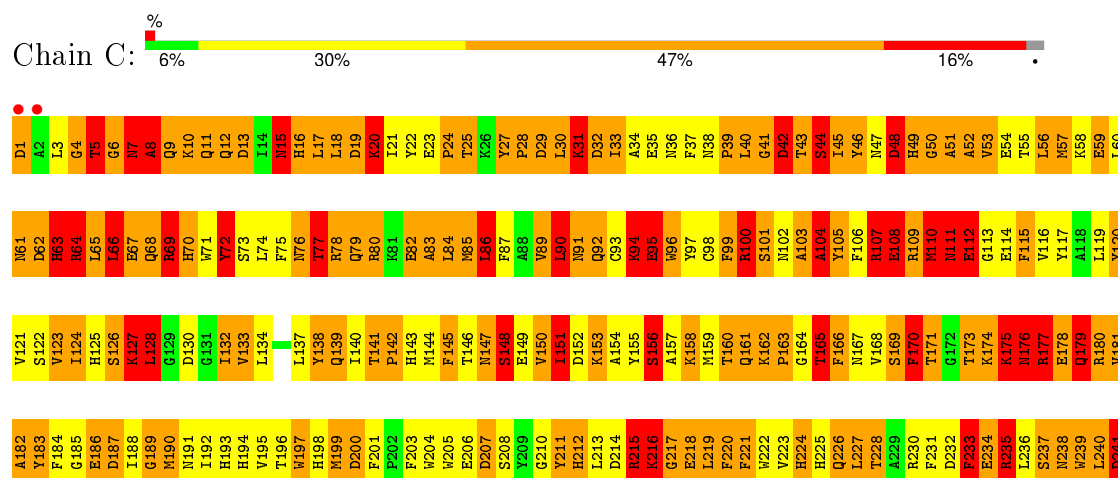
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ARTHROPODAN HEMOCYANIN

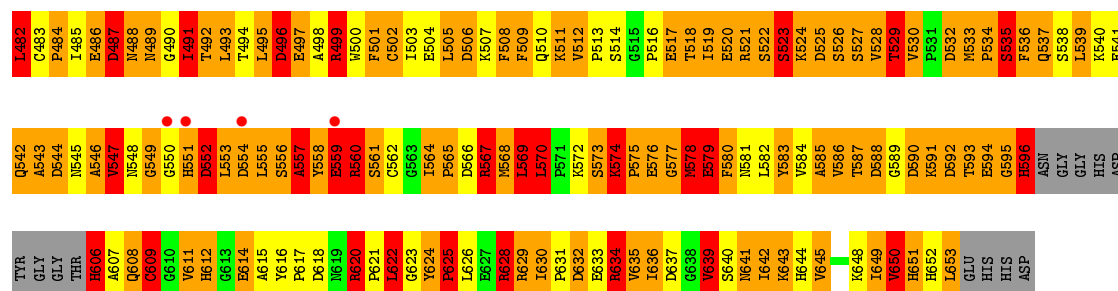




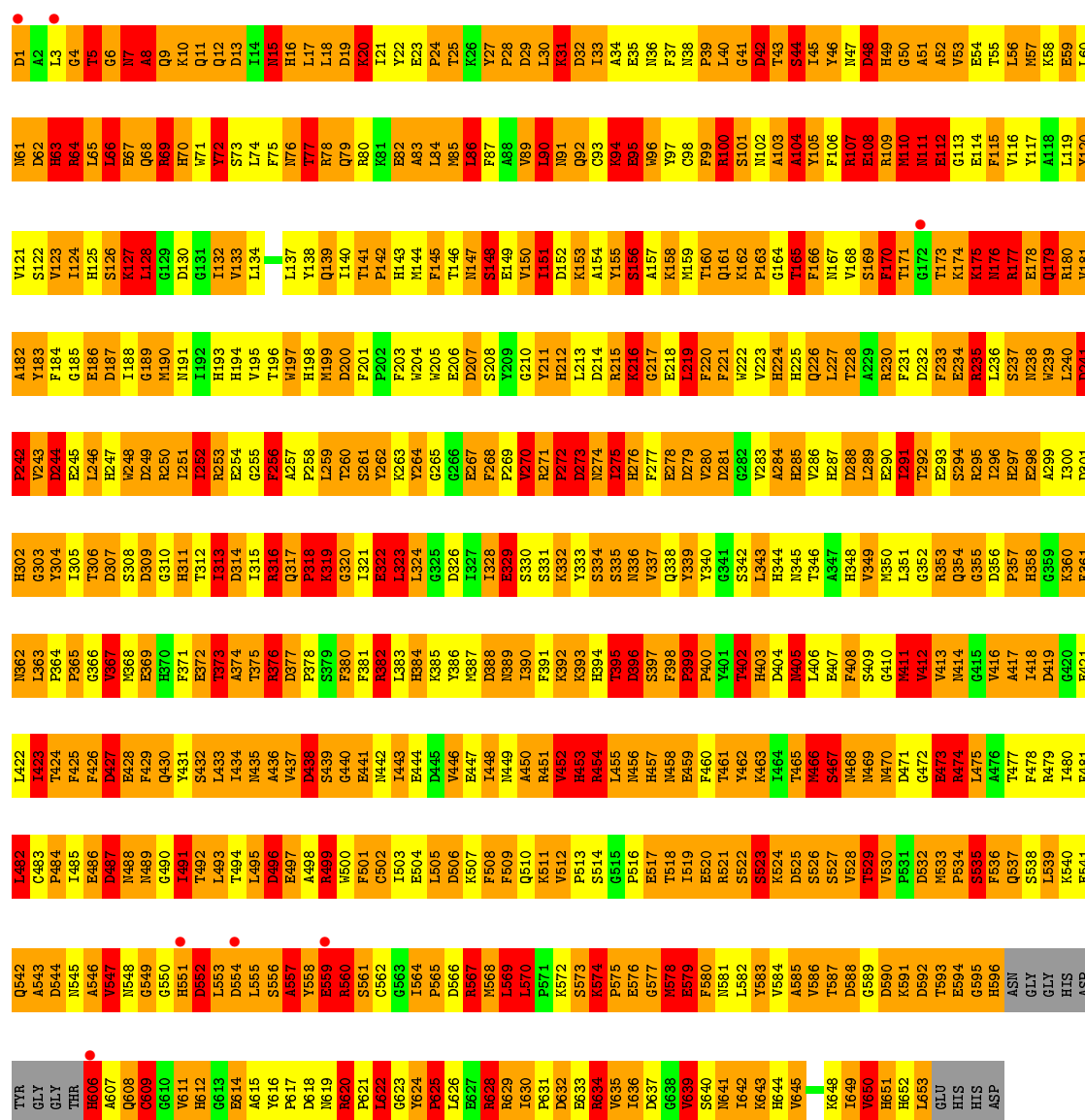
- Molecule 1: ARTHROPODAN HEMOCYANIN







- Molecule 1: ARTHROPODAN HEMOCYANIN



- Molecule 1: ARTHROPODAN HEMOCYANIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.80Å 193.10Å 122.20Å 90.00° 118.10° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20 8.00 – 3.16	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.20) 75.6 (8.00-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	CORELS, PROLSQ	Depositor
R, R_{free}	0.221 , (Not available) 0.216 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 41.1	EDS
Estimated twinning fraction	0.095 for -h-l,k,h 0.095 for l,k,-h-l 0.105 for h,-k,-h-l 0.097 for -h-l,-k,l 0.104 for l,-k,h	Xtriage
L-test for twinning ¹	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 59193 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	31790	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NDG, NAG, CU

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	1.67	39/5385 (0.7%)	3.87	1158/7301 (15.9%)
1	B	1.67	40/5385 (0.7%)	3.87	1154/7301 (15.8%)
1	C	1.67	38/5385 (0.7%)	3.87	1154/7301 (15.8%)
1	D	1.67	38/5385 (0.7%)	3.87	1151/7301 (15.8%)
1	E	1.67	39/5385 (0.7%)	3.87	1156/7301 (15.8%)
1	F	1.67	39/5385 (0.7%)	3.87	1154/7301 (15.8%)
All	All	1.67	233/32310 (0.7%)	3.87	6927/43806 (15.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	7
1	C	0	7
1	D	0	7
1	E	0	7
1	F	0	7
All	All	0	42

All (233) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	217	GLY	N-CA	9.44	1.60	1.46
1	D	217	GLY	N-CA	9.44	1.60	1.46
1	C	217	GLY	N-CA	9.42	1.60	1.46
1	B	217	GLY	N-CA	9.42	1.60	1.46
1	A	217	GLY	N-CA	9.41	1.60	1.46
1	E	217	GLY	N-CA	9.35	1.60	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	330	SER	CB-OG	-8.43	1.31	1.42
1	E	330	SER	CB-OG	-8.42	1.31	1.42
1	F	330	SER	CB-OG	-8.40	1.31	1.42
1	D	330	SER	CB-OG	-8.40	1.31	1.42
1	A	330	SER	CB-OG	-8.40	1.31	1.42
1	B	330	SER	CB-OG	-8.38	1.31	1.42
1	B	410	GLY	N-CA	7.95	1.57	1.46
1	F	410	GLY	N-CA	7.94	1.57	1.46
1	A	410	GLY	N-CA	7.92	1.57	1.46
1	E	410	GLY	N-CA	7.92	1.57	1.46
1	C	410	GLY	N-CA	7.92	1.57	1.46
1	D	410	GLY	N-CA	7.88	1.57	1.46
1	B	208	SER	CB-OG	7.70	1.52	1.42
1	A	208	SER	CB-OG	7.69	1.52	1.42
1	C	208	SER	CB-OG	7.69	1.52	1.42
1	D	208	SER	CB-OG	7.69	1.52	1.42
1	E	208	SER	CB-OG	7.68	1.52	1.42
1	F	208	SER	CB-OG	7.66	1.52	1.42
1	E	273	ASP	N-CA	7.24	1.60	1.46
1	C	273	ASP	N-CA	7.23	1.60	1.46
1	A	273	ASP	N-CA	7.23	1.60	1.46
1	D	273	ASP	N-CA	7.23	1.60	1.46
1	B	273	ASP	N-CA	7.23	1.60	1.46
1	F	273	ASP	N-CA	7.20	1.60	1.46
1	C	372	GLU	CD-OE2	-6.84	1.18	1.25
1	F	372	GLU	CD-OE2	-6.83	1.18	1.25
1	D	372	GLU	CD-OE2	-6.82	1.18	1.25
1	E	372	GLU	CD-OE2	-6.82	1.18	1.25
1	A	372	GLU	CD-OE2	-6.82	1.18	1.25
1	B	372	GLU	CD-OE2	-6.77	1.18	1.25
1	E	169	SER	CA-CB	6.75	1.63	1.52
1	B	169	SER	CA-CB	6.73	1.63	1.52
1	D	169	SER	CA-CB	6.72	1.63	1.52
1	F	169	SER	CA-CB	6.71	1.63	1.52
1	A	169	SER	CA-CB	6.71	1.63	1.52
1	C	169	SER	CA-CB	6.71	1.63	1.52
1	C	624	TYR	CG-CD1	-6.64	1.30	1.39
1	F	624	TYR	CG-CD1	-6.62	1.30	1.39
1	A	624	TYR	CG-CD1	-6.61	1.30	1.39
1	E	624	TYR	CG-CD1	-6.61	1.30	1.39
1	B	624	TYR	CG-CD1	-6.59	1.30	1.39
1	D	624	TYR	CG-CD1	-6.58	1.30	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	535	SER	CB-OG	6.41	1.50	1.42
1	D	535	SER	CB-OG	6.41	1.50	1.42
1	F	535	SER	CB-OG	6.41	1.50	1.42
1	E	535	SER	CB-OG	6.40	1.50	1.42
1	C	535	SER	CB-OG	6.39	1.50	1.42
1	B	535	SER	CB-OG	6.37	1.50	1.42
1	B	329	GLU	CD-OE1	-6.36	1.18	1.25
1	C	329	GLU	CD-OE1	-6.35	1.18	1.25
1	F	329	GLU	CD-OE1	-6.33	1.18	1.25
1	A	329	GLU	CD-OE1	-6.31	1.18	1.25
1	E	329	GLU	CD-OE1	-6.30	1.18	1.25
1	B	186	GLU	CD-OE2	6.29	1.32	1.25
1	D	329	GLU	CD-OE1	-6.28	1.18	1.25
1	C	186	GLU	CD-OE2	6.25	1.32	1.25
1	A	186	GLU	CD-OE2	6.25	1.32	1.25
1	E	186	GLU	CD-OE2	6.24	1.32	1.25
1	D	186	GLU	CD-OE2	6.24	1.32	1.25
1	D	215	ARG	N-CA	6.20	1.58	1.46
1	F	186	GLU	CD-OE2	6.20	1.32	1.25
1	C	499	ARG	CZ-NH2	6.20	1.41	1.33
1	E	215	ARG	N-CA	6.19	1.58	1.46
1	B	215	ARG	N-CA	6.19	1.58	1.46
1	F	215	ARG	N-CA	6.18	1.58	1.46
1	A	215	ARG	N-CA	6.18	1.58	1.46
1	C	215	ARG	N-CA	6.16	1.58	1.46
1	B	499	ARG	CZ-NH2	6.15	1.41	1.33
1	F	499	ARG	CZ-NH2	6.14	1.41	1.33
1	A	499	ARG	CZ-NH2	6.14	1.41	1.33
1	D	499	ARG	CZ-NH2	6.12	1.41	1.33
1	A	371	PHE	CG-CD1	-6.12	1.29	1.38
1	F	371	PHE	CG-CD1	-6.12	1.29	1.38
1	E	499	ARG	CZ-NH2	6.12	1.41	1.33
1	D	371	PHE	CG-CD1	-6.11	1.29	1.38
1	E	371	PHE	CG-CD1	-6.11	1.29	1.38
1	B	371	PHE	CG-CD1	-6.10	1.29	1.38
1	C	371	PHE	CG-CD1	-6.10	1.29	1.38
1	E	183	TYR	CG-CD1	-6.04	1.31	1.39
1	F	183	TYR	CG-CD1	-6.04	1.31	1.39
1	B	496	ASP	CA-CB	-6.03	1.40	1.53
1	A	183	TYR	CG-CD1	-6.03	1.31	1.39
1	E	496	ASP	CA-CB	-6.02	1.40	1.53
1	D	183	TYR	CG-CD1	-6.02	1.31	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	496	ASP	CA-CB	-6.01	1.40	1.53
1	B	183	TYR	CG-CD1	-6.00	1.31	1.39
1	F	496	ASP	CA-CB	-6.00	1.40	1.53
1	D	496	ASP	CA-CB	-5.99	1.40	1.53
1	C	183	TYR	CG-CD1	-5.99	1.31	1.39
1	C	496	ASP	CA-CB	-5.97	1.40	1.53
1	F	248	TRP	CD2-CE2	-5.83	1.34	1.41
1	C	248	TRP	CD2-CE2	-5.82	1.34	1.41
1	D	551	HIS	CA-CB	5.81	1.66	1.53
1	B	59	GLU	CD-OE1	-5.81	1.19	1.25
1	C	551	HIS	CA-CB	5.80	1.66	1.53
1	E	59	GLU	CD-OE1	-5.79	1.19	1.25
1	B	248	TRP	CD2-CE2	-5.78	1.34	1.41
1	A	248	TRP	CD2-CE2	-5.77	1.34	1.41
1	A	551	HIS	CA-CB	5.77	1.66	1.53
1	B	551	HIS	CA-CB	5.77	1.66	1.53
1	F	421	GLU	CD-OE1	5.77	1.31	1.25
1	E	248	TRP	CD2-CE2	-5.76	1.34	1.41
1	F	551	HIS	CA-CB	5.76	1.66	1.53
1	E	551	HIS	CA-CB	5.75	1.66	1.53
1	C	59	GLU	CD-OE1	-5.75	1.19	1.25
1	C	421	GLU	CD-OE1	5.75	1.31	1.25
1	A	59	GLU	CD-OE1	-5.74	1.19	1.25
1	F	59	GLU	CD-OE1	-5.73	1.19	1.25
1	E	421	GLU	CD-OE1	5.72	1.31	1.25
1	D	248	TRP	CD2-CE2	-5.71	1.34	1.41
1	C	367	VAL	C-N	-5.71	1.21	1.34
1	A	421	GLU	CD-OE1	5.71	1.31	1.25
1	D	421	GLU	CD-OE1	5.70	1.31	1.25
1	D	59	GLU	CD-OE1	-5.69	1.19	1.25
1	F	367	VAL	C-N	-5.69	1.21	1.34
1	A	367	VAL	C-N	-5.69	1.21	1.34
1	D	367	VAL	C-N	-5.68	1.21	1.34
1	B	421	GLU	CD-OE1	5.68	1.31	1.25
1	E	367	VAL	C-N	-5.67	1.21	1.34
1	B	215	ARG	NE-CZ	5.67	1.40	1.33
1	B	367	VAL	C-N	-5.67	1.21	1.34
1	F	215	ARG	NE-CZ	5.65	1.40	1.33
1	B	408	PHE	CA-CB	-5.64	1.41	1.53
1	A	215	ARG	NE-CZ	5.63	1.40	1.33
1	D	215	ARG	NE-CZ	5.62	1.40	1.33
1	F	408	PHE	CA-CB	-5.62	1.41	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	215	ARG	NE-CZ	5.61	1.40	1.33
1	A	408	PHE	CA-CB	-5.61	1.41	1.53
1	C	408	PHE	CA-CB	-5.61	1.41	1.53
1	E	408	PHE	CA-CB	-5.60	1.41	1.53
1	D	408	PHE	CA-CB	-5.59	1.41	1.53
1	B	523	SER	CB-OG	5.57	1.49	1.42
1	C	215	ARG	NE-CZ	5.57	1.40	1.33
1	D	310	GLY	N-CA	5.56	1.54	1.46
1	E	310	GLY	N-CA	5.55	1.54	1.46
1	F	523	SER	CB-OG	5.55	1.49	1.42
1	D	391	PHE	CB-CG	-5.54	1.42	1.51
1	F	92	GLN	CA-CB	-5.54	1.41	1.53
1	D	101	SER	CB-OG	5.53	1.49	1.42
1	F	310	GLY	N-CA	5.53	1.54	1.46
1	C	310	GLY	N-CA	5.53	1.54	1.46
1	B	101	SER	CB-OG	5.53	1.49	1.42
1	E	391	PHE	CB-CG	-5.53	1.42	1.51
1	D	523	SER	CB-OG	5.52	1.49	1.42
1	B	310	GLY	N-CA	5.52	1.54	1.46
1	F	391	PHE	CB-CG	-5.52	1.42	1.51
1	C	391	PHE	CB-CG	-5.52	1.42	1.51
1	E	101	SER	CB-OG	5.52	1.49	1.42
1	A	310	GLY	N-CA	5.52	1.54	1.46
1	C	101	SER	CB-OG	5.52	1.49	1.42
1	C	92	GLN	CA-CB	-5.51	1.41	1.53
1	F	101	SER	CB-OG	5.51	1.49	1.42
1	A	92	GLN	CA-CB	-5.51	1.41	1.53
1	A	101	SER	CB-OG	5.51	1.49	1.42
1	E	523	SER	CB-OG	5.51	1.49	1.42
1	B	92	GLN	CA-CB	-5.50	1.41	1.53
1	A	391	PHE	CB-CG	-5.50	1.42	1.51
1	A	523	SER	CB-OG	5.50	1.49	1.42
1	B	113	GLY	N-CA	5.49	1.54	1.46
1	E	92	GLN	CA-CB	-5.49	1.41	1.53
1	D	92	GLN	CA-CB	-5.49	1.41	1.53
1	C	523	SER	CB-OG	5.47	1.49	1.42
1	B	391	PHE	CB-CG	-5.46	1.42	1.51
1	E	113	GLY	N-CA	5.44	1.54	1.46
1	F	113	GLY	N-CA	5.44	1.54	1.46
1	A	113	GLY	N-CA	5.43	1.54	1.46
1	C	113	GLY	N-CA	5.42	1.54	1.46
1	D	113	GLY	N-CA	5.41	1.54	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	561	SER	CB-OG	5.39	1.49	1.42
1	E	561	SER	CB-OG	5.33	1.49	1.42
1	B	561	SER	CB-OG	5.32	1.49	1.42
1	A	561	SER	CB-OG	5.31	1.49	1.42
1	F	561	SER	CB-OG	5.30	1.49	1.42
1	C	561	SER	CB-OG	5.29	1.49	1.42
1	C	245	GLU	CD-OE2	-5.28	1.19	1.25
1	A	245	GLU	CD-OE2	-5.28	1.19	1.25
1	F	245	GLU	CD-OE2	-5.25	1.19	1.25
1	B	245	GLU	CD-OE2	-5.25	1.19	1.25
1	E	245	GLU	CD-OE2	-5.24	1.19	1.25
1	B	216	LYS	C-O	5.23	1.33	1.23
1	D	277	PHE	CG-CD2	-5.23	1.30	1.38
1	D	245	GLU	CD-OE2	-5.21	1.20	1.25
1	A	216	LYS	C-O	5.20	1.33	1.23
1	B	573	SER	CB-OG	-5.20	1.35	1.42
1	E	573	SER	CB-OG	-5.20	1.35	1.42
1	F	216	LYS	C-O	5.20	1.33	1.23
1	B	70	HIS	C-O	5.20	1.33	1.23
1	C	573	SER	CB-OG	-5.20	1.35	1.42
1	C	277	PHE	CG-CD2	-5.20	1.30	1.38
1	D	70	HIS	C-O	5.20	1.33	1.23
1	E	216	LYS	C-O	5.20	1.33	1.23
1	F	277	PHE	CG-CD2	-5.19	1.30	1.38
1	C	216	LYS	C-O	5.19	1.33	1.23
1	A	277	PHE	CG-CD2	-5.18	1.30	1.38
1	D	520	GLU	CD-OE1	5.18	1.31	1.25
1	A	70	HIS	C-O	5.18	1.33	1.23
1	F	70	HIS	C-O	5.17	1.33	1.23
1	E	70	HIS	C-O	5.17	1.33	1.23
1	B	277	PHE	CG-CD2	-5.17	1.31	1.38
1	A	573	SER	CB-OG	-5.16	1.35	1.42
1	C	70	HIS	C-O	5.16	1.33	1.23
1	E	277	PHE	CG-CD2	-5.15	1.31	1.38
1	D	216	LYS	C-O	5.15	1.33	1.23
1	A	520	GLU	CD-OE1	5.15	1.31	1.25
1	F	520	GLU	CD-OE1	5.14	1.31	1.25
1	C	520	GLU	CD-OE1	5.14	1.31	1.25
1	E	520	GLU	CD-OE1	5.13	1.31	1.25
1	B	520	GLU	CD-OE1	5.13	1.31	1.25
1	B	214	ASP	C-O	5.11	1.33	1.23
1	A	214	ASP	C-O	5.10	1.33	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	214	ASP	C-O	5.10	1.33	1.23
1	D	573	SER	CB-OG	-5.10	1.35	1.42
1	F	214	ASP	C-O	5.10	1.33	1.23
1	F	573	SER	CB-OG	-5.09	1.35	1.42
1	C	214	ASP	C-O	5.09	1.33	1.23
1	E	214	ASP	C-O	5.06	1.32	1.23
1	B	101	SER	CA-CB	-5.05	1.45	1.52
1	E	373	THR	CB-OG1	5.04	1.53	1.43
1	D	373	THR	CB-OG1	5.04	1.53	1.43
1	C	101	SER	CA-CB	-5.03	1.45	1.52
1	A	373	THR	CB-OG1	5.02	1.53	1.43
1	B	373	THR	CB-OG1	5.02	1.53	1.43
1	A	101	SER	CA-CB	-5.01	1.45	1.52
1	F	373	THR	CB-OG1	5.01	1.53	1.43
1	E	101	SER	CA-CB	-5.00	1.45	1.52
1	F	95	GLU	CD-OE2	5.00	1.31	1.25
1	B	487	ASP	N-CA	-5.00	1.36	1.46

All (6927) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	628	ARG	NE-CZ-NH2	-45.56	97.52	120.30
1	E	628	ARG	NE-CZ-NH2	-45.53	97.54	120.30
1	C	628	ARG	NE-CZ-NH2	-45.49	97.56	120.30
1	D	628	ARG	NE-CZ-NH2	-45.48	97.56	120.30
1	A	628	ARG	NE-CZ-NH2	-45.47	97.56	120.30
1	B	628	ARG	NE-CZ-NH2	-45.40	97.60	120.30
1	F	80	ARG	NE-CZ-NH2	-29.16	105.72	120.30
1	E	80	ARG	NE-CZ-NH2	-29.11	105.74	120.30
1	A	80	ARG	NE-CZ-NH2	-29.09	105.76	120.30
1	B	80	ARG	NE-CZ-NH2	-29.04	105.78	120.30
1	C	80	ARG	NE-CZ-NH2	-29.04	105.78	120.30
1	D	80	ARG	NE-CZ-NH2	-28.99	105.81	120.30
1	E	299	ALA	CB-CA-C	26.57	149.96	110.10
1	B	299	ALA	CB-CA-C	26.56	149.94	110.10
1	D	299	ALA	CB-CA-C	26.56	149.94	110.10
1	A	299	ALA	CB-CA-C	26.55	149.93	110.10
1	C	299	ALA	CB-CA-C	26.55	149.93	110.10
1	F	299	ALA	CB-CA-C	26.55	149.92	110.10
1	E	78	ARG	NE-CZ-NH2	26.38	133.49	120.30
1	F	78	ARG	NE-CZ-NH2	26.37	133.48	120.30
1	B	78	ARG	NE-CZ-NH2	26.31	133.46	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ARG	NE-CZ-NH2	26.31	133.45	120.30
1	C	78	ARG	NE-CZ-NH2	26.30	133.45	120.30
1	D	78	ARG	NE-CZ-NH2	26.29	133.45	120.30
1	C	109	ARG	NE-CZ-NH2	-24.86	107.87	120.30
1	B	109	ARG	NE-CZ-NH2	-24.82	107.89	120.30
1	F	109	ARG	NE-CZ-NH2	-24.79	107.90	120.30
1	A	109	ARG	NE-CZ-NH2	-24.79	107.91	120.30
1	E	109	ARG	NE-CZ-NH2	-24.78	107.91	120.30
1	D	109	ARG	NE-CZ-NH2	-24.78	107.91	120.30
1	E	628	ARG	NE-CZ-NH1	24.56	132.58	120.30
1	A	628	ARG	NE-CZ-NH1	24.50	132.55	120.30
1	D	628	ARG	NE-CZ-NH1	24.50	132.55	120.30
1	C	628	ARG	NE-CZ-NH1	24.49	132.54	120.30
1	F	628	ARG	NE-CZ-NH1	24.46	132.53	120.30
1	B	628	ARG	NE-CZ-NH1	24.40	132.50	120.30
1	C	632	ASP	CB-CG-OD2	21.75	137.87	118.30
1	F	632	ASP	CB-CG-OD2	21.74	137.87	118.30
1	B	632	ASP	CB-CG-OD2	21.73	137.86	118.30
1	A	632	ASP	CB-CG-OD2	21.73	137.86	118.30
1	B	215	ARG	NE-CZ-NH1	-21.73	109.44	120.30
1	D	632	ASP	CB-CG-OD2	21.73	137.85	118.30
1	F	215	ARG	NE-CZ-NH1	-21.71	109.44	120.30
1	E	215	ARG	NE-CZ-NH1	-21.71	109.45	120.30
1	E	632	ASP	CB-CG-OD2	21.71	137.84	118.30
1	A	215	ARG	NE-CZ-NH1	-21.69	109.46	120.30
1	D	215	ARG	NE-CZ-NH1	-21.63	109.49	120.30
1	C	215	ARG	NE-CZ-NH1	-21.61	109.50	120.30
1	C	69	ARG	NE-CZ-NH2	21.35	130.98	120.30
1	D	69	ARG	NE-CZ-NH2	21.33	130.97	120.30
1	E	69	ARG	NE-CZ-NH2	21.33	130.96	120.30
1	F	69	ARG	NE-CZ-NH2	21.30	130.95	120.30
1	A	69	ARG	NE-CZ-NH2	21.26	130.93	120.30
1	B	69	ARG	NE-CZ-NH2	21.16	130.88	120.30
1	E	427	ASP	CB-CG-OD2	20.86	137.08	118.30
1	A	427	ASP	CB-CG-OD2	20.86	137.08	118.30
1	C	427	ASP	CB-CG-OD2	20.86	137.07	118.30
1	F	427	ASP	CB-CG-OD2	20.84	137.06	118.30
1	D	427	ASP	CB-CG-OD2	20.84	137.06	118.30
1	B	427	ASP	CB-CG-OD2	20.80	137.02	118.30
1	D	235	ARG	NE-CZ-NH1	-18.96	110.82	120.30
1	A	235	ARG	NE-CZ-NH1	-18.89	110.86	120.30
1	B	235	ARG	NE-CZ-NH1	-18.89	110.86	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	235	ARG	NE-CZ-NH1	-18.87	110.86	120.30
1	E	235	ARG	NE-CZ-NH1	-18.80	110.90	120.30
1	C	235	ARG	NE-CZ-NH1	-18.80	110.90	120.30
1	E	316	ARG	NE-CZ-NH1	18.66	129.63	120.30
1	F	316	ARG	NE-CZ-NH1	18.65	129.62	120.30
1	B	316	ARG	NE-CZ-NH1	18.63	129.62	120.30
1	C	316	ARG	NE-CZ-NH1	18.63	129.61	120.30
1	A	316	ARG	NE-CZ-NH1	18.62	129.61	120.30
1	D	316	ARG	NE-CZ-NH1	18.57	129.58	120.30
1	B	100	ARG	NE-CZ-NH1	18.44	129.52	120.30
1	C	100	ARG	NE-CZ-NH1	18.43	129.51	120.30
1	D	100	ARG	NE-CZ-NH1	18.39	129.50	120.30
1	A	100	ARG	NE-CZ-NH1	18.38	129.49	120.30
1	E	100	ARG	NE-CZ-NH1	18.36	129.48	120.30
1	F	100	ARG	NE-CZ-NH1	18.33	129.47	120.30
1	A	180	ARG	NE-CZ-NH2	-18.25	111.17	120.30
1	B	180	ARG	NE-CZ-NH2	-18.24	111.18	120.30
1	E	180	ARG	NE-CZ-NH2	-18.23	111.18	120.30
1	F	180	ARG	NE-CZ-NH2	-18.23	111.19	120.30
1	D	180	ARG	NE-CZ-NH2	-18.19	111.20	120.30
1	C	180	ARG	NE-CZ-NH2	-18.19	111.20	120.30
1	F	632	ASP	CB-CG-OD1	-17.81	102.27	118.30
1	E	632	ASP	CB-CG-OD1	-17.79	102.29	118.30
1	A	632	ASP	CB-CG-OD1	-17.77	102.30	118.30
1	B	632	ASP	CB-CG-OD1	-17.75	102.33	118.30
1	D	632	ASP	CB-CG-OD1	-17.73	102.34	118.30
1	C	632	ASP	CB-CG-OD1	-17.73	102.34	118.30
1	C	64	ARG	NE-CZ-NH2	-17.53	111.54	120.30
1	A	64	ARG	NE-CZ-NH2	-17.47	111.56	120.30
1	E	64	ARG	NE-CZ-NH2	-17.45	111.58	120.30
1	D	64	ARG	NE-CZ-NH2	-17.43	111.59	120.30
1	B	64	ARG	NE-CZ-NH2	-17.41	111.59	120.30
1	F	64	ARG	NE-CZ-NH2	-17.40	111.60	120.30
1	B	235	ARG	NE-CZ-NH2	-17.30	111.65	120.30
1	D	235	ARG	NE-CZ-NH2	-17.30	111.65	120.30
1	C	235	ARG	NE-CZ-NH2	-17.29	111.66	120.30
1	F	264	TYR	CB-CG-CD2	17.26	131.36	121.00
1	A	235	ARG	NE-CZ-NH2	-17.25	111.67	120.30
1	E	235	ARG	NE-CZ-NH2	-17.23	111.68	120.30
1	A	264	TYR	CB-CG-CD2	17.21	131.33	121.00
1	D	264	TYR	CB-CG-CD2	17.21	131.33	121.00
1	F	235	ARG	NE-CZ-NH2	-17.21	111.69	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	264	TYR	CB-CG-CD2	17.19	131.31	121.00
1	B	264	TYR	CB-CG-CD2	17.18	131.31	121.00
1	E	264	TYR	CB-CG-CD2	17.17	131.30	121.00
1	C	177	ARG	NE-CZ-NH2	16.97	128.78	120.30
1	D	316	ARG	CD-NE-CZ	16.93	147.30	123.60
1	A	177	ARG	NE-CZ-NH2	16.91	128.75	120.30
1	F	316	ARG	CD-NE-CZ	16.91	147.27	123.60
1	F	177	ARG	NE-CZ-NH2	16.91	128.75	120.30
1	A	316	ARG	CD-NE-CZ	16.91	147.27	123.60
1	C	316	ARG	CD-NE-CZ	16.91	147.27	123.60
1	E	316	ARG	CD-NE-CZ	16.90	147.25	123.60
1	B	316	ARG	CD-NE-CZ	16.88	147.23	123.60
1	D	177	ARG	NE-CZ-NH2	16.87	128.74	120.30
1	E	177	ARG	NE-CZ-NH2	16.85	128.73	120.30
1	B	177	ARG	NE-CZ-NH2	16.84	128.72	120.30
1	C	390	ILE	O-C-N	16.71	149.43	122.70
1	A	390	ILE	O-C-N	16.69	149.41	122.70
1	F	390	ILE	O-C-N	16.69	149.41	122.70
1	B	390	ILE	O-C-N	16.69	149.40	122.70
1	D	390	ILE	O-C-N	16.67	149.38	122.70
1	E	390	ILE	O-C-N	16.67	149.37	122.70
1	F	314	ASP	CB-CG-OD2	16.59	133.23	118.30
1	C	314	ASP	CB-CG-OD2	16.59	133.23	118.30
1	D	314	ASP	CB-CG-OD2	16.58	133.22	118.30
1	F	218	GLU	OE1-CD-OE2	16.57	143.18	123.30
1	A	314	ASP	CB-CG-OD2	16.56	133.21	118.30
1	B	314	ASP	CB-CG-OD2	16.55	133.20	118.30
1	E	620	ARG	CA-CB-CG	16.54	149.79	113.40
1	B	218	GLU	OE1-CD-OE2	16.54	143.14	123.30
1	A	620	ARG	CA-CB-CG	16.53	149.76	113.40
1	E	314	ASP	CB-CG-OD2	16.53	133.17	118.30
1	F	620	ARG	CA-CB-CG	16.53	149.76	113.40
1	B	620	ARG	CA-CB-CG	16.52	149.74	113.40
1	C	620	ARG	CA-CB-CG	16.52	149.74	113.40
1	D	620	ARG	CA-CB-CG	16.52	149.74	113.40
1	A	218	GLU	OE1-CD-OE2	16.51	143.12	123.30
1	D	218	GLU	OE1-CD-OE2	16.50	143.10	123.30
1	E	218	GLU	OE1-CD-OE2	16.50	143.10	123.30
1	C	218	GLU	OE1-CD-OE2	16.50	143.10	123.30
1	C	499	ARG	NE-CZ-NH2	16.39	128.50	120.30
1	B	499	ARG	NE-CZ-NH2	16.38	128.49	120.30
1	D	499	ARG	NE-CZ-NH2	16.36	128.48	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	499	ARG	NE-CZ-NH2	16.36	128.48	120.30
1	F	499	ARG	NE-CZ-NH2	16.32	128.46	120.30
1	E	499	ARG	NE-CZ-NH2	16.31	128.46	120.30
1	E	253	ARG	NE-CZ-NH1	-16.23	112.19	120.30
1	F	253	ARG	NE-CZ-NH1	-16.22	112.19	120.30
1	A	253	ARG	NE-CZ-NH1	-16.20	112.20	120.30
1	B	253	ARG	NE-CZ-NH1	-16.19	112.20	120.30
1	C	253	ARG	NE-CZ-NH1	-16.17	112.21	120.30
1	D	253	ARG	NE-CZ-NH1	-16.16	112.22	120.30
1	D	235	ARG	NH1-CZ-NH2	16.03	137.03	119.40
1	B	235	ARG	NH1-CZ-NH2	16.00	137.00	119.40
1	A	235	ARG	NH1-CZ-NH2	15.97	136.97	119.40
1	C	235	ARG	NH1-CZ-NH2	15.96	136.95	119.40
1	F	235	ARG	NH1-CZ-NH2	15.95	136.95	119.40
1	E	235	ARG	NH1-CZ-NH2	15.94	136.93	119.40
1	E	288	ASP	CB-CG-OD2	-15.45	104.40	118.30
1	C	288	ASP	CB-CG-OD2	-15.43	104.42	118.30
1	D	78	ARG	NE-CZ-NH1	-15.42	112.59	120.30
1	F	288	ASP	CB-CG-OD2	-15.41	104.43	118.30
1	A	288	ASP	CB-CG-OD2	-15.39	104.45	118.30
1	D	288	ASP	CB-CG-OD2	-15.38	104.46	118.30
1	E	78	ARG	NE-CZ-NH1	-15.38	112.61	120.30
1	C	78	ARG	NE-CZ-NH1	-15.37	112.62	120.30
1	F	78	ARG	NE-CZ-NH1	-15.37	112.62	120.30
1	A	78	ARG	NE-CZ-NH1	-15.34	112.63	120.30
1	B	288	ASP	CB-CG-OD2	-15.33	104.50	118.30
1	B	78	ARG	NE-CZ-NH1	-15.28	112.66	120.30
1	F	244	ASP	CB-CG-OD1	14.99	131.79	118.30
1	C	244	ASP	CB-CG-OD1	14.97	131.78	118.30
1	A	244	ASP	CB-CG-OD1	14.97	131.77	118.30
1	B	244	ASP	CB-CG-OD1	14.94	131.75	118.30
1	D	244	ASP	CB-CG-OD1	14.94	131.75	118.30
1	E	244	ASP	CB-CG-OD1	14.93	131.74	118.30
1	A	624	TYR	CB-CG-CD1	14.91	129.95	121.00
1	E	624	TYR	CB-CG-CD1	14.89	129.94	121.00
1	C	624	TYR	CB-CG-CD1	14.89	129.93	121.00
1	F	624	TYR	CB-CG-CD1	14.88	129.93	121.00
1	B	624	TYR	CB-CG-CD1	14.88	129.93	121.00
1	D	624	TYR	CB-CG-CD1	14.87	129.92	121.00
1	B	80	ARG	CD-NE-CZ	-14.57	103.20	123.60
1	F	80	ARG	CD-NE-CZ	-14.57	103.20	123.60
1	E	80	ARG	CD-NE-CZ	-14.57	103.21	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	ARG	CD-NE-CZ	-14.56	103.22	123.60
1	C	80	ARG	CD-NE-CZ	-14.56	103.22	123.60
1	D	80	ARG	CD-NE-CZ	-14.51	103.29	123.60
1	F	264	TYR	CB-CG-CD1	-14.43	112.34	121.00
1	D	264	TYR	CB-CG-CD1	-14.38	112.37	121.00
1	A	264	TYR	CB-CG-CD1	-14.34	112.40	121.00
1	E	264	TYR	CB-CG-CD1	-14.33	112.40	121.00
1	B	264	TYR	CB-CG-CD1	-14.31	112.41	121.00
1	C	264	TYR	CB-CG-CD1	-14.28	112.43	121.00
1	C	62	ASP	CB-CG-OD2	14.17	131.05	118.30
1	E	62	ASP	CB-CG-OD2	14.14	131.02	118.30
1	F	62	ASP	CB-CG-OD2	14.13	131.02	118.30
1	A	62	ASP	CB-CG-OD2	14.12	131.00	118.30
1	D	62	ASP	CB-CG-OD2	14.09	130.98	118.30
1	B	62	ASP	CB-CG-OD2	14.08	130.97	118.30
1	D	247	HIS	N-CA-CB	13.96	135.72	110.60
1	B	247	HIS	N-CA-CB	13.95	135.71	110.60
1	A	247	HIS	N-CA-CB	13.93	135.67	110.60
1	C	247	HIS	N-CA-CB	13.92	135.66	110.60
1	E	247	HIS	N-CA-CB	13.90	135.61	110.60
1	F	247	HIS	N-CA-CB	13.90	135.62	110.60
1	A	649	ILE	O-C-N	13.81	144.80	122.70
1	F	649	ILE	O-C-N	13.81	144.79	122.70
1	B	649	ILE	O-C-N	13.81	144.79	122.70
1	D	649	ILE	O-C-N	13.80	144.78	122.70
1	C	279	ASP	CB-CG-OD2	-13.79	105.89	118.30
1	C	649	ILE	O-C-N	13.79	144.77	122.70
1	B	279	ASP	CB-CG-OD2	-13.79	105.89	118.30
1	E	649	ILE	O-C-N	13.79	144.76	122.70
1	D	279	ASP	CB-CG-OD2	-13.78	105.90	118.30
1	E	322	GLU	CA-CB-CG	13.78	143.71	113.40
1	A	322	GLU	CA-CB-CG	13.77	143.69	113.40
1	F	411	MET	CA-CB-CG	-13.77	89.89	113.30
1	B	322	GLU	CA-CB-CG	13.77	143.69	113.40
1	C	322	GLU	CA-CB-CG	13.77	143.69	113.40
1	D	322	GLU	CA-CB-CG	13.77	143.69	113.40
1	C	411	MET	CA-CB-CG	-13.76	89.91	113.30
1	F	322	GLU	CA-CB-CG	13.76	143.67	113.40
1	E	279	ASP	CB-CG-OD2	-13.76	105.92	118.30
1	A	279	ASP	CB-CG-OD2	-13.75	105.92	118.30
1	D	411	MET	CA-CB-CG	-13.75	89.92	113.30
1	A	411	MET	CA-CB-CG	-13.74	89.94	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	411	MET	CA-CB-CG	-13.74	89.94	113.30
1	E	411	MET	CA-CB-CG	-13.73	89.97	113.30
1	F	279	ASP	CB-CG-OD2	-13.71	105.96	118.30
1	B	340	TYR	CB-CG-CD2	13.64	129.19	121.00
1	C	340	TYR	CB-CG-CD2	13.63	129.18	121.00
1	E	340	TYR	CB-CG-CD2	13.60	129.16	121.00
1	A	340	TYR	CB-CG-CD2	13.59	129.15	121.00
1	F	340	TYR	CB-CG-CD2	13.59	129.16	121.00
1	D	340	TYR	CB-CG-CD2	13.55	129.13	121.00
1	B	250	ARG	NE-CZ-NH2	-13.48	113.56	120.30
1	D	250	ARG	NE-CZ-NH2	-13.45	113.58	120.30
1	C	250	ARG	NE-CZ-NH2	-13.44	113.58	120.30
1	A	250	ARG	NE-CZ-NH2	-13.44	113.58	120.30
1	F	428	GLU	OE1-CD-OE2	13.44	139.42	123.30
1	E	250	ARG	NE-CZ-NH2	-13.43	113.59	120.30
1	F	250	ARG	NE-CZ-NH2	-13.41	113.59	120.30
1	A	428	GLU	OE1-CD-OE2	13.41	139.39	123.30
1	E	428	GLU	OE1-CD-OE2	13.39	139.37	123.30
1	D	428	GLU	OE1-CD-OE2	13.39	139.37	123.30
1	C	428	GLU	OE1-CD-OE2	13.39	139.37	123.30
1	B	428	GLU	OE1-CD-OE2	13.38	139.36	123.30
1	E	238	ASN	CB-CG-OD1	-13.38	94.84	121.60
1	C	238	ASN	CB-CG-OD1	-13.38	94.84	121.60
1	A	238	ASN	CB-CG-OD1	-13.37	94.86	121.60
1	F	238	ASN	CB-CG-OD1	-13.37	94.86	121.60
1	D	238	ASN	CB-CG-OD1	-13.37	94.87	121.60
1	B	238	ASN	CB-CG-OD1	-13.35	94.90	121.60
1	F	48	ASP	CB-CG-OD2	-13.15	106.47	118.30
1	D	48	ASP	CB-CG-OD2	-13.13	106.48	118.30
1	E	48	ASP	CB-CG-OD2	-13.13	106.49	118.30
1	A	48	ASP	CB-CG-OD2	-13.12	106.49	118.30
1	C	48	ASP	CB-CG-OD2	-13.10	106.51	118.30
1	B	48	ASP	CB-CG-OD2	-13.06	106.54	118.30
1	F	624	TYR	CG-CD2-CE2	12.87	131.60	121.30
1	E	624	TYR	CG-CD2-CE2	12.87	131.59	121.30
1	B	1	ASP	CB-CG-OD1	12.86	129.88	118.30
1	A	1	ASP	CB-CG-OD1	12.85	129.86	118.30
1	C	624	TYR	CG-CD2-CE2	12.84	131.57	121.30
1	D	1	ASP	CB-CG-OD1	12.84	129.85	118.30
1	C	271	ARG	NE-CZ-NH1	12.84	126.72	120.30
1	D	624	TYR	CG-CD2-CE2	12.84	131.57	121.30
1	F	1	ASP	CB-CG-OD1	12.83	129.85	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	624	TYR	CG-CD2-CE2	12.83	131.56	121.30
1	B	624	TYR	CG-CD2-CE2	12.82	131.56	121.30
1	C	1	ASP	CB-CG-OD1	12.82	129.84	118.30
1	E	1	ASP	CB-CG-OD1	12.80	129.82	118.30
1	C	241	ASP	CB-CG-OD2	12.80	129.82	118.30
1	D	271	ARG	NE-CZ-NH1	12.80	126.70	120.30
1	B	271	ARG	NE-CZ-NH1	12.79	126.70	120.30
1	A	241	ASP	CB-CG-OD2	12.77	129.79	118.30
1	B	241	ASP	CB-CG-OD2	12.77	129.79	118.30
1	F	241	ASP	CB-CG-OD2	12.76	129.78	118.30
1	A	271	ARG	NE-CZ-NH1	12.75	126.67	120.30
1	D	241	ASP	CB-CG-OD2	12.75	129.78	118.30
1	E	180	ARG	NE-CZ-NH1	12.75	126.67	120.30
1	E	241	ASP	CB-CG-OD2	12.75	129.77	118.30
1	F	271	ARG	NE-CZ-NH1	12.74	126.67	120.30
1	E	271	ARG	NE-CZ-NH1	12.71	126.65	120.30
1	B	180	ARG	NE-CZ-NH1	12.71	126.65	120.30
1	F	180	ARG	NE-CZ-NH1	12.69	126.65	120.30
1	C	329	GLU	C-N-CA	12.67	153.38	121.70
1	A	329	GLU	C-N-CA	12.67	153.37	121.70
1	B	329	GLU	C-N-CA	12.67	153.37	121.70
1	D	329	GLU	C-N-CA	12.66	153.35	121.70
1	E	329	GLU	C-N-CA	12.66	153.35	121.70
1	A	180	ARG	NE-CZ-NH1	12.65	126.62	120.30
1	F	329	GLU	C-N-CA	12.63	153.29	121.70
1	E	367	VAL	O-C-N	-12.62	102.52	122.70
1	A	367	VAL	O-C-N	-12.60	102.55	122.70
1	F	367	VAL	O-C-N	-12.60	102.55	122.70
1	D	367	VAL	O-C-N	-12.59	102.56	122.70
1	B	367	VAL	O-C-N	-12.58	102.57	122.70
1	C	180	ARG	NE-CZ-NH1	12.57	126.59	120.30
1	C	367	VAL	O-C-N	-12.57	102.58	122.70
1	D	180	ARG	NE-CZ-NH1	12.55	126.58	120.30
1	D	452	VAL	O-C-N	12.51	142.71	122.70
1	D	583	TYR	CB-CG-CD2	-12.50	113.50	121.00
1	B	452	VAL	O-C-N	12.48	142.67	122.70
1	E	452	VAL	O-C-N	12.48	142.67	122.70
1	B	583	TYR	CB-CG-CD2	-12.47	113.52	121.00
1	C	583	TYR	CB-CG-CD2	-12.46	113.53	121.00
1	A	452	VAL	O-C-N	12.46	142.63	122.70
1	A	583	TYR	CB-CG-CD2	-12.46	113.53	121.00
1	E	583	TYR	CB-CG-CD2	-12.45	113.53	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	452	VAL	O-C-N	12.45	142.62	122.70
1	F	452	VAL	O-C-N	12.45	142.62	122.70
1	F	583	TYR	CB-CG-CD2	-12.44	113.54	121.00
1	D	337	VAL	CA-CB-CG2	12.37	129.46	110.90
1	E	337	VAL	CA-CB-CG2	12.37	129.45	110.90
1	F	337	VAL	CA-CB-CG2	12.37	129.45	110.90
1	B	337	VAL	CA-CB-CG2	12.36	129.44	110.90
1	A	337	VAL	CA-CB-CG2	12.35	129.43	110.90
1	C	92	GLN	CA-CB-CG	12.35	140.58	113.40
1	B	92	GLN	CA-CB-CG	12.35	140.57	113.40
1	F	92	GLN	CA-CB-CG	12.35	140.56	113.40
1	C	337	VAL	CA-CB-CG2	12.34	129.41	110.90
1	A	92	GLN	CA-CB-CG	12.34	140.55	113.40
1	E	92	GLN	CA-CB-CG	12.34	140.54	113.40
1	D	92	GLN	CA-CB-CG	12.32	140.51	113.40
1	C	333	TYR	CB-CG-CD1	12.29	128.38	121.00
1	A	333	TYR	CB-CG-CD1	12.28	128.37	121.00
1	E	333	TYR	CB-CG-CD1	12.28	128.37	121.00
1	D	333	TYR	CB-CG-CD1	12.26	128.36	121.00
1	F	333	TYR	CB-CG-CD1	12.26	128.35	121.00
1	C	186	GLU	OE1-CD-OE2	12.26	138.01	123.30
1	D	186	GLU	OE1-CD-OE2	12.25	138.00	123.30
1	B	333	TYR	CB-CG-CD1	12.24	128.34	121.00
1	F	186	GLU	OE1-CD-OE2	12.23	137.98	123.30
1	A	186	GLU	OE1-CD-OE2	12.23	137.98	123.30
1	B	186	GLU	OE1-CD-OE2	12.22	137.96	123.30
1	B	298	GLU	OE1-CD-OE2	12.21	137.95	123.30
1	D	298	GLU	OE1-CD-OE2	12.20	137.94	123.30
1	E	186	GLU	OE1-CD-OE2	12.20	137.93	123.30
1	E	298	GLU	OE1-CD-OE2	12.19	137.93	123.30
1	F	298	GLU	OE1-CD-OE2	12.19	137.93	123.30
1	A	298	GLU	OE1-CD-OE2	12.18	137.92	123.30
1	C	298	GLU	OE1-CD-OE2	12.17	137.91	123.30
1	D	232	ASP	CB-CG-OD1	12.13	129.22	118.30
1	A	232	ASP	CB-CG-OD1	12.13	129.22	118.30
1	B	232	ASP	CB-CG-OD1	12.13	129.22	118.30
1	E	232	ASP	CB-CG-OD1	12.13	129.21	118.30
1	C	232	ASP	CB-CG-OD1	12.12	129.21	118.30
1	F	232	ASP	CB-CG-OD1	12.10	129.19	118.30
1	D	583	TYR	CB-CG-CD1	12.00	128.20	121.00
1	B	25	THR	OG1-CB-CG2	11.95	137.48	110.00
1	F	25	THR	OG1-CB-CG2	11.94	137.47	110.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	THR	OG1-CB-CG2	11.93	137.44	110.00
1	D	25	THR	OG1-CB-CG2	11.93	137.43	110.00
1	C	25	THR	OG1-CB-CG2	11.92	137.42	110.00
1	F	293	GLU	OE1-CD-OE2	-11.92	108.99	123.30
1	F	583	TYR	CB-CG-CD1	11.92	128.15	121.00
1	A	583	TYR	CB-CG-CD1	11.92	128.15	121.00
1	E	25	THR	OG1-CB-CG2	11.92	137.42	110.00
1	C	583	TYR	CB-CG-CD1	11.92	128.15	121.00
1	E	583	TYR	CB-CG-CD1	11.91	128.15	121.00
1	D	293	GLU	OE1-CD-OE2	-11.91	109.01	123.30
1	C	293	GLU	OE1-CD-OE2	-11.89	109.03	123.30
1	A	293	GLU	OE1-CD-OE2	-11.89	109.03	123.30
1	B	583	TYR	CB-CG-CD1	11.89	128.13	121.00
1	B	203	PHE	CB-CG-CD1	11.88	129.11	120.80
1	A	203	PHE	CB-CG-CD1	11.87	129.11	120.80
1	B	387	MET	N-CA-CB	11.86	131.94	110.60
1	E	293	GLU	OE1-CD-OE2	-11.85	109.08	123.30
1	E	203	PHE	CB-CG-CD1	11.85	129.09	120.80
1	F	203	PHE	CB-CG-CD1	11.85	129.09	120.80
1	D	387	MET	N-CA-CB	11.84	131.92	110.60
1	A	387	MET	N-CA-CB	11.84	131.91	110.60
1	B	293	GLU	OE1-CD-OE2	-11.83	109.10	123.30
1	E	109	ARG	NH1-CZ-NH2	11.83	132.42	119.40
1	C	387	MET	N-CA-CB	11.83	131.90	110.60
1	F	387	MET	N-CA-CB	11.83	131.89	110.60
1	C	109	ARG	NH1-CZ-NH2	11.83	132.41	119.40
1	D	203	PHE	CB-CG-CD1	11.82	129.08	120.80
1	E	387	MET	N-CA-CB	11.81	131.86	110.60
1	C	203	PHE	CB-CG-CD1	11.81	129.06	120.80
1	F	302	HIS	O-C-N	11.79	143.25	123.20
1	A	109	ARG	NH1-CZ-NH2	11.79	132.37	119.40
1	D	302	HIS	O-C-N	11.79	143.24	123.20
1	D	566	ASP	CB-CG-OD1	11.79	128.91	118.30
1	F	109	ARG	NH1-CZ-NH2	11.79	132.37	119.40
1	E	460	PHE	O-C-N	11.79	141.56	122.70
1	B	302	HIS	O-C-N	11.79	143.24	123.20
1	B	109	ARG	NH1-CZ-NH2	11.78	132.36	119.40
1	E	302	HIS	O-C-N	11.78	143.23	123.20
1	A	302	HIS	O-C-N	11.78	143.22	123.20
1	C	460	PHE	O-C-N	11.78	141.54	122.70
1	F	460	PHE	O-C-N	11.78	141.54	122.70
1	F	566	ASP	CB-CG-OD1	11.78	128.90	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	PHE	O-C-N	11.76	141.52	122.70
1	D	109	ARG	NH1-CZ-NH2	11.76	132.34	119.40
1	B	460	PHE	O-C-N	11.76	141.51	122.70
1	A	566	ASP	CB-CG-OD1	11.75	128.88	118.30
1	C	302	HIS	O-C-N	11.75	143.17	123.20
1	D	460	PHE	O-C-N	11.75	141.50	122.70
1	E	566	ASP	CB-CG-OD1	11.74	128.86	118.30
1	C	566	ASP	CB-CG-OD1	11.73	128.86	118.30
1	B	219	LEU	CB-CA-C	11.70	132.42	110.20
1	D	219	LEU	CB-CA-C	11.70	132.42	110.20
1	A	219	LEU	CB-CA-C	11.69	132.41	110.20
1	B	566	ASP	CB-CG-OD1	11.69	128.82	118.30
1	F	119	LEU	CB-CG-CD2	-11.69	91.13	111.00
1	F	219	LEU	CB-CA-C	11.69	132.41	110.20
1	C	219	LEU	CB-CA-C	11.68	132.40	110.20
1	E	219	LEU	CB-CA-C	11.68	132.39	110.20
1	A	119	LEU	CB-CG-CD2	-11.67	91.16	111.00
1	B	119	LEU	CB-CG-CD2	-11.67	91.16	111.00
1	D	119	LEU	CB-CG-CD2	-11.67	91.16	111.00
1	C	119	LEU	CB-CG-CD2	-11.66	91.17	111.00
1	E	119	LEU	CB-CG-CD2	-11.66	91.17	111.00
1	E	64	ARG	CD-NE-CZ	11.65	139.90	123.60
1	F	64	ARG	CD-NE-CZ	11.64	139.90	123.60
1	B	64	ARG	CD-NE-CZ	11.64	139.89	123.60
1	D	64	ARG	CD-NE-CZ	11.64	139.90	123.60
1	A	64	ARG	CD-NE-CZ	11.63	139.88	123.60
1	C	64	ARG	CD-NE-CZ	11.63	139.88	123.60
1	A	353	ARG	NE-CZ-NH2	-11.61	114.50	120.30
1	B	103	ALA	N-CA-CB	-11.61	93.85	110.10
1	C	155	TYR	N-CA-CB	11.60	131.49	110.60
1	C	103	ALA	N-CA-CB	-11.60	93.86	110.10
1	D	353	ARG	NE-CZ-NH2	-11.60	114.50	120.30
1	E	155	TYR	N-CA-CB	11.60	131.48	110.60
1	A	155	TYR	N-CA-CB	11.59	131.47	110.60
1	F	353	ARG	NE-CZ-NH2	-11.59	114.50	120.30
1	B	52	ALA	N-CA-CB	11.59	126.33	110.10
1	F	155	TYR	N-CA-CB	11.59	131.46	110.60
1	A	103	ALA	N-CA-CB	-11.59	93.88	110.10
1	D	52	ALA	N-CA-CB	11.58	126.31	110.10
1	B	353	ARG	NE-CZ-NH2	-11.58	114.51	120.30
1	D	155	TYR	N-CA-CB	11.58	131.44	110.60
1	B	155	TYR	N-CA-CB	11.57	131.43	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	52	ALA	N-CA-CB	11.57	126.30	110.10
1	F	103	ALA	N-CA-CB	-11.57	93.90	110.10
1	D	103	ALA	N-CA-CB	-11.57	93.91	110.10
1	E	103	ALA	N-CA-CB	-11.57	93.91	110.10
1	F	52	ALA	N-CA-CB	11.57	126.30	110.10
1	A	52	ALA	N-CA-CB	11.56	126.29	110.10
1	C	52	ALA	N-CA-CB	11.56	126.28	110.10
1	C	353	ARG	NE-CZ-NH2	-11.55	114.52	120.30
1	E	552	ASP	CB-CG-OD2	-11.55	107.90	118.30
1	B	339	TYR	CB-CG-CD2	11.54	127.92	121.00
1	F	339	TYR	CB-CG-CD2	11.54	127.92	121.00
1	A	552	ASP	CB-CG-OD2	-11.53	107.92	118.30
1	C	552	ASP	CB-CG-OD2	-11.53	107.92	118.30
1	B	552	ASP	CB-CG-OD2	-11.51	107.94	118.30
1	E	353	ARG	NE-CZ-NH2	-11.51	114.54	120.30
1	B	17	LEU	CB-CG-CD2	-11.51	91.44	111.00
1	D	552	ASP	CB-CG-OD2	-11.51	107.94	118.30
1	F	17	LEU	CB-CG-CD2	-11.50	91.44	111.00
1	F	552	ASP	CB-CG-OD2	-11.50	107.95	118.30
1	C	17	LEU	CB-CG-CD2	-11.50	91.45	111.00
1	C	568	MET	CG-SD-CE	11.50	118.60	100.20
1	E	17	LEU	CB-CG-CD2	-11.50	91.46	111.00
1	D	568	MET	CG-SD-CE	11.49	118.59	100.20
1	D	17	LEU	CB-CG-CD2	-11.49	91.46	111.00
1	A	17	LEU	CB-CG-CD2	-11.49	91.47	111.00
1	D	339	TYR	CB-CG-CD2	11.49	127.89	121.00
1	A	568	MET	CG-SD-CE	11.49	118.58	100.20
1	B	568	MET	CG-SD-CE	11.49	118.58	100.20
1	A	339	TYR	CB-CG-CD2	11.47	127.89	121.00
1	E	568	MET	CG-SD-CE	11.47	118.56	100.20
1	F	568	MET	CG-SD-CE	11.47	118.55	100.20
1	C	339	TYR	CB-CG-CD2	11.47	127.88	121.00
1	E	339	TYR	CB-CG-CD2	11.46	127.88	121.00
1	A	241	ASP	CB-CG-OD1	-11.45	107.99	118.30
1	D	241	ASP	CB-CG-OD1	-11.45	107.99	118.30
1	B	241	ASP	CB-CG-OD1	-11.45	108.00	118.30
1	C	241	ASP	CB-CG-OD1	-11.45	108.00	118.30
1	F	241	ASP	CB-CG-OD1	-11.44	108.00	118.30
1	E	241	ASP	CB-CG-OD1	-11.43	108.01	118.30
1	D	458	ASN	CA-CB-CG	11.36	138.38	113.40
1	F	458	ASN	CA-CB-CG	11.36	138.39	113.40
1	D	72	TYR	O-C-N	11.35	140.87	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	458	ASN	CA-CB-CG	11.35	138.38	113.40
1	A	72	TYR	O-C-N	11.35	140.86	122.70
1	A	458	ASN	CA-CB-CG	11.35	138.36	113.40
1	F	72	TYR	O-C-N	11.34	140.84	122.70
1	C	458	ASN	CA-CB-CG	11.34	138.34	113.40
1	E	72	TYR	O-C-N	11.33	140.83	122.70
1	B	72	TYR	O-C-N	11.33	140.83	122.70
1	B	458	ASN	CA-CB-CG	11.33	138.32	113.40
1	C	387	MET	CG-SD-CE	11.32	118.32	100.20
1	E	387	MET	CG-SD-CE	11.32	118.31	100.20
1	F	387	MET	CG-SD-CE	11.32	118.31	100.20
1	C	422	LEU	CB-CA-C	11.31	131.70	110.20
1	F	422	LEU	CB-CA-C	11.31	131.70	110.20
1	A	387	MET	CG-SD-CE	11.31	118.30	100.20
1	C	72	TYR	O-C-N	11.31	140.79	122.70
1	D	532	ASP	CB-CG-OD2	11.31	128.48	118.30
1	A	422	LEU	CB-CA-C	11.30	131.67	110.20
1	B	422	LEU	CB-CA-C	11.30	131.67	110.20
1	D	387	MET	CG-SD-CE	11.30	118.28	100.20
1	D	422	LEU	CB-CA-C	11.30	131.67	110.20
1	B	387	MET	CG-SD-CE	11.30	118.28	100.20
1	E	422	LEU	CB-CA-C	11.29	131.66	110.20
1	A	532	ASP	CB-CG-OD2	11.29	128.46	118.30
1	C	532	ASP	CB-CG-OD2	11.29	128.46	118.30
1	E	532	ASP	CB-CG-OD2	11.26	128.43	118.30
1	F	532	ASP	CB-CG-OD2	11.26	128.43	118.30
1	B	532	ASP	CB-CG-OD2	11.25	128.43	118.30
1	D	180	ARG	CD-NE-CZ	11.21	139.30	123.60
1	C	180	ARG	CD-NE-CZ	11.20	139.28	123.60
1	E	112	GLU	OE1-CD-OE2	11.19	136.73	123.30
1	D	112	GLU	OE1-CD-OE2	11.18	136.72	123.30
1	A	112	GLU	OE1-CD-OE2	11.18	136.71	123.30
1	F	180	ARG	CD-NE-CZ	11.18	139.25	123.60
1	A	180	ARG	CD-NE-CZ	11.17	139.24	123.60
1	F	112	GLU	OE1-CD-OE2	11.17	136.70	123.30
1	E	180	ARG	CD-NE-CZ	11.14	139.20	123.60
1	B	112	GLU	OE1-CD-OE2	11.13	136.66	123.30
1	B	180	ARG	CD-NE-CZ	11.13	139.18	123.60
1	C	112	GLU	OE1-CD-OE2	11.12	136.64	123.30
1	C	616	TYR	CB-CG-CD1	-11.10	114.34	121.00
1	E	451	ARG	NE-CZ-NH1	-11.10	114.75	120.30
1	E	509	PHE	CB-CG-CD2	-11.10	113.03	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	509	PHE	CB-CG-CD2	-11.10	113.03	120.80
1	D	616	TYR	CB-CG-CD1	-11.08	114.35	121.00
1	C	451	ARG	NE-CZ-NH1	-11.08	114.76	120.30
1	E	616	TYR	CB-CG-CD1	-11.07	114.36	121.00
1	B	509	PHE	CB-CG-CD2	-11.06	113.06	120.80
1	B	7	ASN	N-CA-CB	11.06	130.51	110.60
1	E	206	GLU	OE1-CD-OE2	11.06	136.57	123.30
1	A	509	PHE	CB-CG-CD2	-11.05	113.06	120.80
1	A	616	TYR	CB-CG-CD1	-11.05	114.37	121.00
1	C	7	ASN	N-CA-CB	11.05	130.50	110.60
1	B	616	TYR	CB-CG-CD2	11.05	127.63	121.00
1	C	206	GLU	OE1-CD-OE2	11.04	136.55	123.30
1	C	509	PHE	CB-CG-CD2	-11.04	113.07	120.80
1	E	7	ASN	N-CA-CB	11.04	130.48	110.60
1	F	7	ASN	N-CA-CB	11.04	130.48	110.60
1	A	7	ASN	N-CA-CB	11.04	130.47	110.60
1	A	206	GLU	OE1-CD-OE2	11.04	136.55	123.30
1	E	616	TYR	CB-CG-CD2	11.04	127.62	121.00
1	D	7	ASN	N-CA-CB	11.03	130.46	110.60
1	F	206	GLU	OE1-CD-OE2	11.03	136.54	123.30
1	A	451	ARG	NE-CZ-NH1	-11.03	114.79	120.30
1	D	509	PHE	CB-CG-CD2	-11.03	113.08	120.80
1	D	149	GLU	CG-CD-OE2	-11.02	96.26	118.30
1	A	616	TYR	CB-CG-CD2	11.02	127.61	121.00
1	B	149	GLU	CG-CD-OE2	-11.02	96.27	118.30
1	C	149	GLU	CG-CD-OE2	-11.02	96.27	118.30
1	D	616	TYR	CB-CG-CD2	11.02	127.61	121.00
1	A	149	GLU	CG-CD-OE2	-11.01	96.27	118.30
1	B	616	TYR	CB-CG-CD1	-11.01	114.39	121.00
1	E	149	GLU	CG-CD-OE2	-11.01	96.28	118.30
1	F	149	GLU	CG-CD-OE2	-11.01	96.28	118.30
1	B	25	THR	CA-CB-OG1	-11.01	85.89	109.00
1	B	206	GLU	OE1-CD-OE2	11.01	136.51	123.30
1	D	206	GLU	OE1-CD-OE2	11.01	136.51	123.30
1	C	616	TYR	CB-CG-CD2	11.00	127.60	121.00
1	C	25	THR	CA-CB-OG1	-11.00	85.91	109.00
1	E	25	THR	CA-CB-OG1	-10.99	85.91	109.00
1	F	616	TYR	CB-CG-CD1	-10.99	114.40	121.00
1	A	25	THR	CA-CB-OG1	-10.99	85.92	109.00
1	F	25	THR	CA-CB-OG1	-10.99	85.93	109.00
1	D	25	THR	CA-CB-OG1	-10.98	85.94	109.00
1	F	83	ALA	N-CA-CB	10.98	125.47	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	ALA	N-CA-CB	10.96	125.45	110.10
1	A	83	ALA	N-CA-CB	10.96	125.44	110.10
1	B	451	ARG	NE-CZ-NH1	-10.95	114.82	120.30
1	E	83	ALA	N-CA-CB	10.95	125.43	110.10
1	D	451	ARG	NE-CZ-NH1	-10.95	114.83	120.30
1	D	83	ALA	N-CA-CB	10.94	125.42	110.10
1	B	552	ASP	CB-CG-OD1	10.94	128.15	118.30
1	C	83	ALA	N-CA-CB	10.94	125.41	110.10
1	C	552	ASP	CB-CG-OD1	10.94	128.14	118.30
1	D	625	PRO	N-CA-CB	-10.94	90.17	103.30
1	F	625	PRO	N-CA-CB	-10.94	90.18	103.30
1	E	625	PRO	N-CA-CB	-10.93	90.18	103.30
1	A	552	ASP	CB-CG-OD1	10.93	128.13	118.30
1	F	552	ASP	CB-CG-OD1	10.92	128.13	118.30
1	A	625	PRO	N-CA-CB	-10.92	90.19	103.30
1	F	616	TYR	CB-CG-CD2	10.92	127.55	121.00
1	D	567	ARG	NE-CZ-NH1	-10.92	114.84	120.30
1	B	625	PRO	N-CA-CB	-10.92	90.20	103.30
1	F	451	ARG	NE-CZ-NH1	-10.92	114.84	120.30
1	C	625	PRO	N-CA-CB	-10.91	90.21	103.30
1	E	552	ASP	CB-CG-OD1	10.91	128.12	118.30
1	C	279	ASP	CA-CB-CG	10.90	137.38	113.40
1	D	552	ASP	CB-CG-OD1	10.90	128.11	118.30
1	F	279	ASP	CA-CB-CG	10.89	137.37	113.40
1	A	279	ASP	CA-CB-CG	10.89	137.36	113.40
1	F	279	ASP	N-CA-CB	-10.89	91.00	110.60
1	E	279	ASP	CA-CB-CG	10.88	137.34	113.40
1	D	279	ASP	N-CA-CB	-10.88	91.01	110.60
1	D	279	ASP	CA-CB-CG	10.88	137.33	113.40
1	F	567	ARG	NE-CZ-NH1	-10.88	114.86	120.30
1	A	279	ASP	N-CA-CB	-10.87	91.03	110.60
1	B	279	ASP	N-CA-CB	-10.87	91.03	110.60
1	B	279	ASP	CA-CB-CG	10.87	137.32	113.40
1	C	279	ASP	N-CA-CB	-10.87	91.04	110.60
1	C	567	ARG	NE-CZ-NH1	-10.86	114.87	120.30
1	E	279	ASP	N-CA-CB	-10.86	91.06	110.60
1	B	567	ARG	NE-CZ-NH1	-10.85	114.88	120.30
1	D	427	ASP	CB-CG-OD1	-10.84	108.55	118.30
1	C	427	ASP	CB-CG-OD1	-10.83	108.55	118.30
1	A	567	ARG	NE-CZ-NH1	-10.83	114.88	120.30
1	E	427	ASP	CB-CG-OD1	-10.83	108.55	118.30
1	F	427	ASP	CB-CG-OD1	-10.83	108.56	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	427	ASP	CB-CG-OD1	-10.82	108.56	118.30
1	B	427	ASP	CB-CG-OD1	-10.80	108.58	118.30
1	C	281	ASP	O-C-N	10.78	141.52	123.20
1	B	281	ASP	O-C-N	10.75	141.48	123.20
1	A	281	ASP	O-C-N	10.75	141.47	123.20
1	C	69	ARG	NE-CZ-NH1	-10.74	114.93	120.30
1	F	281	ASP	O-C-N	10.74	141.45	123.20
1	F	644	HIS	CA-C-O	-10.74	97.56	120.10
1	D	281	ASP	O-C-N	10.72	141.43	123.20
1	E	644	HIS	CA-C-O	-10.72	97.58	120.10
1	F	217	GLY	N-CA-C	-10.72	86.29	113.10
1	A	644	HIS	CA-C-O	-10.72	97.58	120.10
1	B	644	HIS	CA-C-O	-10.72	97.59	120.10
1	C	644	HIS	CA-C-O	-10.72	97.59	120.10
1	E	281	ASP	O-C-N	10.72	141.42	123.20
1	E	567	ARG	NE-CZ-NH1	-10.72	114.94	120.30
1	B	211	TYR	CB-CG-CD2	10.71	127.43	121.00
1	D	217	GLY	N-CA-C	-10.71	86.32	113.10
1	B	217	GLY	N-CA-C	-10.71	86.33	113.10
1	A	217	GLY	N-CA-C	-10.71	86.33	113.10
1	D	644	HIS	CA-C-O	-10.71	97.62	120.10
1	C	217	GLY	N-CA-C	-10.70	86.35	113.10
1	F	211	TYR	CB-CG-CD2	10.70	127.42	121.00
1	E	217	GLY	N-CA-C	-10.69	86.37	113.10
1	E	69	ARG	NE-CZ-NH1	-10.68	114.96	120.30
1	C	211	TYR	CB-CG-CD2	10.67	127.40	121.00
1	F	69	ARG	NE-CZ-NH1	-10.67	114.97	120.30
1	B	322	GLU	OE1-CD-OE2	-10.66	110.50	123.30
1	B	69	ARG	NE-CZ-NH1	-10.66	114.97	120.30
1	D	69	ARG	NE-CZ-NH1	-10.66	114.97	120.30
1	A	69	ARG	NE-CZ-NH1	-10.65	114.98	120.30
1	D	438	ASP	CB-CG-OD1	-10.64	108.72	118.30
1	D	211	TYR	CB-CG-CD2	10.63	127.38	121.00
1	A	211	TYR	CB-CG-CD2	10.63	127.38	121.00
1	C	322	GLU	OE1-CD-OE2	-10.62	110.55	123.30
1	D	322	GLU	OE1-CD-OE2	-10.62	110.56	123.30
1	F	322	GLU	OE1-CD-OE2	-10.62	110.56	123.30
1	A	322	GLU	OE1-CD-OE2	-10.61	110.57	123.30
1	A	438	ASP	CB-CG-OD1	-10.61	108.75	118.30
1	E	322	GLU	OE1-CD-OE2	-10.61	110.57	123.30
1	C	438	ASP	CB-CG-OD1	-10.60	108.76	118.30
1	E	211	TYR	CB-CG-CD2	10.59	127.35	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	500	TRP	CA-CB-CG	10.58	133.81	113.70
1	E	438	ASP	CB-CG-OD1	-10.58	108.78	118.30
1	F	500	TRP	CA-CB-CG	10.57	133.78	113.70
1	D	500	TRP	CA-CB-CG	10.56	133.77	113.70
1	F	100	ARG	NE-CZ-NH2	-10.56	115.02	120.30
1	A	500	TRP	CA-CB-CG	10.56	133.76	113.70
1	C	500	TRP	CA-CB-CG	10.56	133.76	113.70
1	E	500	TRP	CA-CB-CG	10.56	133.76	113.70
1	F	438	ASP	CB-CG-OD1	-10.56	108.80	118.30
1	F	10	LYS	CG-CD-CE	10.55	143.55	111.90
1	E	10	LYS	CG-CD-CE	10.54	143.53	111.90
1	B	438	ASP	CB-CG-OD1	-10.54	108.81	118.30
1	B	10	LYS	CG-CD-CE	10.54	143.52	111.90
1	D	10	LYS	CG-CD-CE	10.54	143.52	111.90
1	A	10	LYS	CG-CD-CE	10.54	143.52	111.90
1	C	10	LYS	CG-CD-CE	10.54	143.50	111.90
1	C	556	SER	N-CA-CB	10.54	126.30	110.50
1	D	100	ARG	NE-CZ-NH2	-10.53	115.04	120.30
1	F	556	SER	N-CA-CB	10.53	126.29	110.50
1	D	556	SER	N-CA-CB	10.52	126.29	110.50
1	E	100	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	E	480	ILE	CA-CB-CG2	10.51	131.93	110.90
1	A	100	ARG	NE-CZ-NH2	-10.51	115.05	120.30
1	A	556	SER	N-CA-CB	10.51	126.26	110.50
1	B	100	ARG	NE-CZ-NH2	-10.51	115.05	120.30
1	A	480	ILE	CA-CB-CG2	10.50	131.91	110.90
1	C	480	ILE	CA-CB-CG2	10.50	131.91	110.90
1	D	576	GLU	OE1-CD-OE2	10.50	135.90	123.30
1	E	576	GLU	OE1-CD-OE2	10.50	135.90	123.30
1	E	169	SER	N-CA-C	10.50	139.35	111.00
1	F	480	ILE	CA-CB-CG2	10.49	131.89	110.90
1	D	480	ILE	CA-CB-CG2	10.49	131.88	110.90
1	B	169	SER	N-CA-C	10.49	139.32	111.00
1	C	390	ILE	CA-C-O	-10.49	98.07	120.10
1	F	169	SER	N-CA-C	10.49	139.32	111.00
1	A	169	SER	N-CA-C	10.49	139.31	111.00
1	C	169	SER	N-CA-C	10.49	139.32	111.00
1	C	576	GLU	OE1-CD-OE2	10.49	135.88	123.30
1	D	169	SER	N-CA-C	10.49	139.31	111.00
1	E	556	SER	N-CA-CB	10.49	126.23	110.50
1	B	576	GLU	OE1-CD-OE2	10.48	135.88	123.30
1	A	390	ILE	CA-C-O	-10.48	98.10	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	390	ILE	CA-C-O	-10.48	98.10	120.10
1	F	390	ILE	CA-C-O	-10.48	98.09	120.10
1	B	480	ILE	CA-CB-CG2	10.48	131.85	110.90
1	A	576	GLU	OE1-CD-OE2	10.47	135.87	123.30
1	B	390	ILE	CA-C-O	-10.47	98.10	120.10
1	B	556	SER	N-CA-CB	10.47	126.21	110.50
1	E	390	ILE	CA-C-O	-10.47	98.11	120.10
1	C	100	ARG	NE-CZ-NH2	-10.46	115.07	120.30
1	F	576	GLU	OE1-CD-OE2	10.45	135.84	123.30
1	B	130	ASP	CB-CG-OD2	-10.44	108.91	118.30
1	A	99	PHE	CA-CB-CG	10.44	138.94	113.90
1	E	99	PHE	CA-CB-CG	10.44	138.95	113.90
1	D	99	PHE	CA-CB-CG	10.43	138.94	113.90
1	C	99	PHE	CA-CB-CG	10.43	138.94	113.90
1	F	99	PHE	CA-CB-CG	10.43	138.93	113.90
1	A	130	ASP	CB-CG-OD2	-10.42	108.92	118.30
1	E	130	ASP	CB-CG-OD2	-10.42	108.92	118.30
1	B	99	PHE	CA-CB-CG	10.41	138.89	113.90
1	E	245	GLU	OE1-CD-OE2	-10.40	110.81	123.30
1	D	245	GLU	OE1-CD-OE2	-10.40	110.82	123.30
1	B	245	GLU	OE1-CD-OE2	-10.40	110.82	123.30
1	C	130	ASP	CB-CG-OD2	-10.40	108.94	118.30
1	D	130	ASP	CB-CG-OD2	-10.40	108.94	118.30
1	F	130	ASP	CB-CG-OD2	-10.39	108.94	118.30
1	F	245	GLU	OE1-CD-OE2	-10.39	110.83	123.30
1	F	191	ASN	CB-CG-OD1	-10.39	100.82	121.60
1	C	245	GLU	OE1-CD-OE2	-10.39	110.83	123.30
1	A	245	GLU	OE1-CD-OE2	-10.39	110.83	123.30
1	E	191	ASN	CB-CG-OD1	-10.39	100.82	121.60
1	A	431	TYR	CB-CG-CD2	-10.38	114.77	121.00
1	D	191	ASN	CB-CG-OD1	-10.38	100.83	121.60
1	E	260	THR	CA-CB-OG1	-10.38	87.19	109.00
1	C	260	THR	CA-CB-OG1	-10.38	87.20	109.00
1	A	191	ASN	CB-CG-OD1	-10.38	100.85	121.60
1	C	191	ASN	CB-CG-OD1	-10.37	100.85	121.60
1	B	191	ASN	CB-CG-OD1	-10.37	100.86	121.60
1	A	260	THR	CA-CB-OG1	-10.36	87.24	109.00
1	B	260	THR	CA-CB-OG1	-10.36	87.24	109.00
1	E	386	TYR	CB-CG-CD2	10.36	127.22	121.00
1	D	431	TYR	CB-CG-CD2	-10.36	114.78	121.00
1	D	260	THR	CA-CB-OG1	-10.36	87.25	109.00
1	F	260	THR	CA-CB-OG1	-10.35	87.26	109.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	431	TYR	CB-CG-CD2	-10.35	114.79	121.00
1	F	431	TYR	CB-CG-CD2	-10.35	114.79	121.00
1	B	386	TYR	CB-CG-CD2	10.34	127.20	121.00
1	B	431	TYR	CB-CG-CD2	-10.34	114.80	121.00
1	C	273	ASP	CB-CG-OD1	-10.32	109.01	118.30
1	C	530	VAL	CA-CB-CG2	-10.32	95.42	110.90
1	D	273	ASP	CB-CG-OD1	-10.32	109.02	118.30
1	C	431	TYR	CB-CG-CD2	-10.31	114.81	121.00
1	E	273	ASP	CB-CG-OD1	-10.30	109.03	118.30
1	F	80	ARG	NH1-CZ-NH2	10.30	130.73	119.40
1	A	530	VAL	CA-CB-CG2	-10.29	95.46	110.90
1	B	150	VAL	CA-CB-CG2	-10.29	95.46	110.90
1	B	273	ASP	CB-CG-OD1	-10.29	109.04	118.30
1	E	530	VAL	CA-CB-CG2	-10.29	95.46	110.90
1	F	530	VAL	CA-CB-CG2	-10.29	95.47	110.90
1	A	273	ASP	CB-CG-OD1	-10.29	109.04	118.30
1	D	530	VAL	CA-CB-CG2	-10.29	95.47	110.90
1	B	530	VAL	CA-CB-CG2	-10.28	95.48	110.90
1	D	150	VAL	CA-CB-CG2	-10.27	95.49	110.90
1	A	386	TYR	CB-CG-CD2	10.26	127.16	121.00
1	F	150	VAL	CA-CB-CG2	-10.26	95.51	110.90
1	E	150	VAL	CA-CB-CG2	-10.26	95.51	110.90
1	F	273	ASP	CB-CG-OD1	-10.26	109.07	118.30
1	A	150	VAL	CA-CB-CG2	-10.25	95.52	110.90
1	C	150	VAL	CA-CB-CG2	-10.25	95.53	110.90
1	D	80	ARG	NH1-CZ-NH2	10.25	130.67	119.40
1	E	393	LYS	N-CA-CB	10.24	129.04	110.60
1	A	393	LYS	N-CA-CB	10.24	129.03	110.60
1	F	386	TYR	CB-CG-CD2	10.24	127.14	121.00
1	A	80	ARG	NH1-CZ-NH2	10.24	130.66	119.40
1	D	393	LYS	N-CA-CB	10.24	129.03	110.60
1	C	386	TYR	CB-CG-CD2	10.23	127.14	121.00
1	F	393	LYS	N-CA-CB	10.23	129.02	110.60
1	B	393	LYS	N-CA-CB	10.23	129.01	110.60
1	C	393	LYS	N-CA-CB	10.21	128.98	110.60
1	E	80	ARG	NH1-CZ-NH2	10.21	130.63	119.40
1	B	80	ARG	NH1-CZ-NH2	10.20	130.62	119.40
1	C	80	ARG	NH1-CZ-NH2	10.20	130.62	119.40
1	D	386	TYR	CB-CG-CD2	10.18	127.11	121.00
1	F	588	ASP	CB-CG-OD2	-10.16	109.15	118.30
1	B	588	ASP	CB-CG-OD2	-10.16	109.16	118.30
1	C	388	ASP	CB-CG-OD1	-10.16	109.16	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	588	ASP	CB-CG-OD2	-10.15	109.16	118.30
1	E	388	ASP	CB-CG-OD1	-10.15	109.17	118.30
1	F	174	LYS	CA-CB-CG	10.15	135.73	113.40
1	B	174	LYS	CA-CB-CG	10.15	135.72	113.40
1	C	588	ASP	CB-CG-OD2	-10.15	109.17	118.30
1	E	588	ASP	CB-CG-OD2	-10.14	109.17	118.30
1	F	388	ASP	CB-CG-OD1	-10.14	109.17	118.30
1	A	388	ASP	CB-CG-OD1	-10.13	109.18	118.30
1	A	174	LYS	CA-CB-CG	10.13	135.68	113.40
1	D	174	LYS	CA-CB-CG	10.13	135.68	113.40
1	D	388	ASP	CB-CG-OD1	-10.12	109.19	118.30
1	E	174	LYS	CA-CB-CG	10.12	135.67	113.40
1	C	174	LYS	CA-CB-CG	10.12	135.66	113.40
1	D	588	ASP	CB-CG-OD2	-10.09	109.22	118.30
1	B	103	ALA	CB-CA-C	10.09	125.23	110.10
1	B	388	ASP	CB-CG-OD1	-10.08	109.23	118.30
1	A	103	ALA	CB-CA-C	10.06	125.20	110.10
1	C	103	ALA	CB-CA-C	10.06	125.19	110.10
1	C	249	ASP	CB-CG-OD2	-10.06	109.25	118.30
1	D	103	ALA	CB-CA-C	10.06	125.19	110.10
1	E	249	ASP	CB-CG-OD2	-10.05	109.25	118.30
1	F	103	ALA	CB-CA-C	10.05	125.18	110.10
1	E	103	ALA	CB-CA-C	10.04	125.17	110.10
1	A	249	ASP	CB-CG-OD2	-10.04	109.26	118.30
1	E	624	TYR	CZ-CE2-CD2	-10.04	110.77	119.80
1	D	249	ASP	CB-CG-OD2	-10.01	109.29	118.30
1	C	624	TYR	CZ-CE2-CD2	-10.01	110.80	119.80
1	F	249	ASP	CB-CG-OD2	-10.00	109.30	118.30
1	A	624	TYR	CZ-CE2-CD2	-9.99	110.81	119.80
1	B	624	TYR	CZ-CE2-CD2	-9.99	110.81	119.80
1	D	408	PHE	CA-CB-CG	9.99	137.88	113.90
1	C	408	PHE	CA-CB-CG	9.99	137.87	113.90
1	B	249	ASP	CB-CG-OD2	-9.98	109.32	118.30
1	B	408	PHE	CA-CB-CG	9.98	137.85	113.90
1	A	408	PHE	CA-CB-CG	9.97	137.84	113.90
1	F	408	PHE	CA-CB-CG	9.97	137.84	113.90
1	F	624	TYR	CZ-CE2-CD2	-9.97	110.82	119.80
1	B	461	THR	CA-C-O	9.96	141.03	120.10
1	D	624	TYR	CZ-CE2-CD2	-9.96	110.83	119.80
1	E	408	PHE	CA-CB-CG	9.96	137.79	113.90
1	A	461	THR	CA-C-O	9.94	140.98	120.10
1	C	461	THR	CA-C-O	9.95	140.98	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	461	THR	CA-C-O	9.95	140.99	120.10
1	E	461	THR	CA-C-O	9.93	140.96	120.10
1	D	461	THR	CA-C-O	9.93	140.94	120.10
1	C	551	HIS	CB-CA-C	-9.92	90.56	110.40
1	D	551	HIS	CB-CA-C	-9.92	90.56	110.40
1	E	551	HIS	CB-CA-C	-9.92	90.56	110.40
1	A	551	HIS	CB-CA-C	-9.92	90.56	110.40
1	F	551	HIS	CB-CA-C	-9.92	90.57	110.40
1	B	551	HIS	CB-CA-C	-9.91	90.58	110.40
1	C	281	ASP	CB-CG-OD2	-9.88	109.41	118.30
1	C	200	ASP	CB-CG-OD2	9.87	127.19	118.30
1	F	330	SER	N-CA-CB	9.87	125.31	110.50
1	C	1	ASP	CA-CB-CG	9.87	135.10	113.40
1	E	1	ASP	CA-CB-CG	9.86	135.09	113.40
1	B	200	ASP	CB-CG-OD2	9.86	127.17	118.30
1	D	1	ASP	CA-CB-CG	9.86	135.09	113.40
1	F	1	ASP	CA-CB-CG	9.86	135.08	113.40
1	D	281	ASP	CB-CG-OD2	-9.85	109.43	118.30
1	C	330	SER	N-CA-CB	9.85	125.28	110.50
1	A	1	ASP	CA-CB-CG	9.85	135.07	113.40
1	B	1	ASP	CA-CB-CG	9.85	135.07	113.40
1	A	200	ASP	CB-CG-OD2	9.84	127.16	118.30
1	B	331	SER	CA-C-O	-9.84	99.44	120.10
1	F	331	SER	CA-C-O	-9.84	99.44	120.10
1	D	200	ASP	CB-CG-OD2	9.83	127.15	118.30
1	E	200	ASP	CB-CG-OD2	9.83	127.15	118.30
1	A	331	SER	CA-C-O	-9.83	99.45	120.10
1	F	281	ASP	CB-CG-OD2	-9.83	109.45	118.30
1	A	281	ASP	CB-CG-OD2	-9.83	109.46	118.30
1	A	330	SER	N-CA-CB	9.83	125.24	110.50
1	E	281	ASP	CB-CG-OD2	-9.83	109.46	118.30
1	E	331	SER	CA-C-O	-9.83	99.46	120.10
1	D	7	ASN	CA-CB-CG	9.82	135.01	113.40
1	C	331	SER	CA-C-O	-9.82	99.48	120.10
1	B	7	ASN	CA-CB-CG	9.82	135.00	113.40
1	D	330	SER	N-CA-CB	9.82	125.23	110.50
1	F	7	ASN	CA-CB-CG	9.82	135.00	113.40
1	A	7	ASN	CA-CB-CG	9.81	134.98	113.40
1	D	331	SER	CA-C-O	-9.81	99.50	120.10
1	B	330	SER	N-CA-CB	9.81	125.21	110.50
1	C	7	ASN	CA-CB-CG	9.80	134.97	113.40
1	D	163	PRO	O-C-N	9.80	139.86	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	273	ASP	CB-CA-C	9.80	130.00	110.40
1	E	330	SER	N-CA-CB	9.80	125.20	110.50
1	B	281	ASP	CB-CG-OD2	-9.79	109.48	118.30
1	E	163	PRO	O-C-N	9.79	139.85	123.20
1	F	200	ASP	CB-CG-OD2	9.79	127.11	118.30
1	F	273	ASP	CB-CA-C	9.79	129.99	110.40
1	C	273	ASP	CB-CA-C	9.79	129.98	110.40
1	E	273	ASP	CB-CA-C	9.79	129.98	110.40
1	A	273	ASP	CB-CA-C	9.79	129.98	110.40
1	B	273	ASP	CB-CA-C	9.79	129.97	110.40
1	C	163	PRO	O-C-N	9.79	139.84	123.20
1	E	7	ASN	CA-CB-CG	9.79	134.93	113.40
1	A	163	PRO	O-C-N	9.78	139.82	123.20
1	B	163	PRO	O-C-N	9.78	139.82	123.20
1	F	163	PRO	O-C-N	9.77	139.81	123.20
1	F	218	GLU	CG-CD-OE2	-9.77	98.76	118.30
1	C	253	ARG	NH1-CZ-NH2	9.77	130.14	119.40
1	A	253	ARG	NH1-CZ-NH2	9.77	130.14	119.40
1	B	218	GLU	CG-CD-OE2	-9.76	98.78	118.30
1	C	218	GLU	CG-CD-OE2	-9.76	98.79	118.30
1	E	218	GLU	CG-CD-OE2	-9.76	98.78	118.30
1	D	331	SER	O-C-N	9.76	138.31	122.70
1	F	253	ARG	NH1-CZ-NH2	9.75	130.13	119.40
1	A	331	SER	O-C-N	9.75	138.30	122.70
1	E	253	ARG	NH1-CZ-NH2	9.75	130.13	119.40
1	D	218	GLU	CG-CD-OE2	-9.75	98.80	118.30
1	A	218	GLU	CG-CD-OE2	-9.75	98.81	118.30
1	F	126	SER	CA-C-O	9.75	140.57	120.10
1	B	126	SER	CA-C-O	9.74	140.56	120.10
1	B	253	ARG	NH1-CZ-NH2	9.74	130.12	119.40
1	C	126	SER	CA-C-O	9.74	140.56	120.10
1	C	331	SER	O-C-N	9.74	138.29	122.70
1	D	253	ARG	NH1-CZ-NH2	9.74	130.12	119.40
1	A	126	SER	CA-C-O	9.74	140.56	120.10
1	D	126	SER	CA-C-O	9.74	140.56	120.10
1	E	126	SER	CA-C-O	9.74	140.56	120.10
1	B	331	SER	O-C-N	9.74	138.28	122.70
1	F	371	PHE	CG-CD2-CE2	9.74	131.51	120.80
1	E	331	SER	O-C-N	9.73	138.27	122.70
1	F	331	SER	O-C-N	9.73	138.27	122.70
1	B	5	THR	C-N-CA	9.73	142.73	122.30
1	B	174	LYS	CB-CA-C	9.73	129.85	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	496	ASP	N-CA-CB	9.72	128.10	110.60
1	C	174	LYS	CB-CA-C	9.72	129.84	110.40
1	D	496	ASP	N-CA-CB	9.72	128.10	110.60
1	E	174	LYS	CB-CA-C	9.72	129.84	110.40
1	F	496	ASP	N-CA-CB	9.72	128.10	110.60
1	E	496	ASP	N-CA-CB	9.72	128.09	110.60
1	A	174	LYS	CB-CA-C	9.72	129.83	110.40
1	E	371	PHE	CG-CD2-CE2	9.71	131.49	120.80
1	F	174	LYS	CB-CA-C	9.71	129.83	110.40
1	A	496	ASP	N-CA-CB	9.71	128.08	110.60
1	B	250	ARG	NH1-CZ-NH2	9.71	130.08	119.40
1	D	296	ILE	CA-C-N	-9.71	95.83	117.20
1	E	5	THR	C-N-CA	9.71	142.70	122.30
1	F	419	ASP	CB-CG-OD1	-9.71	109.56	118.30
1	D	250	ARG	NH1-CZ-NH2	9.71	130.08	119.40
1	B	419	ASP	CB-CG-OD1	-9.71	109.56	118.30
1	D	174	LYS	CB-CA-C	9.71	129.81	110.40
1	C	250	ARG	NH1-CZ-NH2	9.70	130.07	119.40
1	A	5	THR	C-N-CA	9.70	142.67	122.30
1	A	419	ASP	CB-CG-OD1	-9.70	109.57	118.30
1	E	296	ILE	CA-C-N	-9.70	95.86	117.20
1	F	296	ILE	CA-C-N	-9.70	95.86	117.20
1	B	296	ILE	CA-C-N	-9.69	95.87	117.20
1	C	496	ASP	N-CA-CB	9.69	128.05	110.60
1	A	296	ILE	CA-C-N	-9.69	95.88	117.20
1	C	371	PHE	CG-CD2-CE2	9.69	131.46	120.80
1	F	5	THR	C-N-CA	9.69	142.65	122.30
1	D	5	THR	C-N-CA	9.69	142.65	122.30
1	A	250	ARG	NH1-CZ-NH2	9.69	130.05	119.40
1	C	296	ILE	CA-C-N	-9.69	95.89	117.20
1	A	371	PHE	CG-CD2-CE2	9.68	131.45	120.80
1	C	5	THR	C-N-CA	9.68	142.63	122.30
1	C	419	ASP	CB-CG-OD1	-9.68	109.59	118.30
1	C	527	SER	N-CA-CB	9.68	125.02	110.50
1	D	645	VAL	CA-C-N	9.68	138.49	117.20
1	B	527	SER	N-CA-CB	9.67	125.01	110.50
1	E	527	SER	N-CA-CB	9.67	125.00	110.50
1	B	645	VAL	CA-C-N	9.67	138.47	117.20
1	A	527	SER	N-CA-CB	9.66	125.00	110.50
1	E	419	ASP	CB-CG-OD1	-9.66	109.60	118.30
1	A	645	VAL	CA-C-N	9.66	138.45	117.20
1	B	371	PHE	CG-CD2-CE2	9.66	131.43	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	527	SER	N-CA-CB	9.66	124.99	110.50
1	D	419	ASP	CB-CG-OD1	-9.66	109.61	118.30
1	F	645	VAL	CA-C-N	9.66	138.45	117.20
1	E	645	VAL	CA-C-N	9.65	138.43	117.20
1	E	250	ARG	NH1-CZ-NH2	9.65	130.01	119.40
1	D	371	PHE	CG-CD2-CE2	9.65	131.41	120.80
1	D	527	SER	N-CA-CB	9.64	124.97	110.50
1	F	250	ARG	NH1-CZ-NH2	9.64	130.01	119.40
1	C	645	VAL	CA-C-N	9.64	138.40	117.20
1	C	501	PHE	N-CA-CB	-9.62	93.28	110.60
1	F	501	PHE	N-CA-CB	-9.62	93.29	110.60
1	A	501	PHE	N-CA-CB	-9.61	93.30	110.60
1	B	232	ASP	CA-CB-CG	9.61	134.54	113.40
1	F	643	LYS	CA-CB-CG	9.61	134.54	113.40
1	A	643	LYS	CA-CB-CG	9.61	134.53	113.40
1	D	643	LYS	CA-CB-CG	9.61	134.53	113.40
1	F	9	GLN	O-C-N	9.61	138.07	122.70
1	B	501	PHE	N-CA-CB	-9.60	93.31	110.60
1	D	501	PHE	N-CA-CB	-9.60	93.31	110.60
1	E	643	LYS	CA-CB-CG	9.60	134.52	113.40
1	F	232	ASP	CA-CB-CG	9.60	134.53	113.40
1	C	232	ASP	CA-CB-CG	9.60	134.52	113.40
1	E	232	ASP	CA-CB-CG	9.60	134.52	113.40
1	B	643	LYS	CA-CB-CG	9.59	134.51	113.40
1	A	232	ASP	CA-CB-CG	9.59	134.50	113.40
1	C	643	LYS	CA-CB-CG	9.59	134.50	113.40
1	D	9	GLN	O-C-N	9.59	138.04	122.70
1	D	232	ASP	CA-CB-CG	9.59	134.49	113.40
1	E	501	PHE	N-CA-CB	-9.58	93.35	110.60
1	C	77	THR	N-CA-CB	9.57	128.49	110.30
1	E	77	THR	N-CA-CB	9.57	128.49	110.30
1	C	9	GLN	O-C-N	9.57	138.02	122.70
1	A	9	GLN	O-C-N	9.57	138.01	122.70
1	B	77	THR	N-CA-CB	9.57	128.48	110.30
1	F	246	LEU	CA-C-O	-9.57	100.00	120.10
1	B	246	LEU	CA-C-O	-9.56	100.02	120.10
1	B	9	GLN	O-C-N	9.56	138.00	122.70
1	E	9	GLN	O-C-N	9.56	138.00	122.70
1	E	246	LEU	CA-C-O	-9.56	100.02	120.10
1	F	77	THR	N-CA-CB	9.56	128.46	110.30
1	A	77	THR	N-CA-CB	9.56	128.46	110.30
1	A	246	LEU	CA-C-O	-9.56	100.03	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	246	LEU	CA-C-O	-9.56	100.03	120.10
1	F	581	ASN	N-CA-CB	-9.55	93.41	110.60
1	C	246	LEU	CA-C-O	-9.54	100.06	120.10
1	A	581	ASN	N-CA-CB	-9.54	93.43	110.60
1	E	333	TYR	CD1-CE1-CZ	9.54	128.38	119.80
1	C	581	ASN	N-CA-CB	-9.53	93.44	110.60
1	F	242	PRO	N-CA-CB	-9.54	91.86	103.30
1	D	298	GLU	CG-CD-OE2	-9.53	99.24	118.30
1	D	581	ASN	N-CA-CB	-9.53	93.45	110.60
1	B	581	ASN	N-CA-CB	-9.53	93.45	110.60
1	B	298	GLU	CG-CD-OE2	-9.53	99.25	118.30
1	D	77	THR	N-CA-CB	9.52	128.40	110.30
1	E	242	PRO	N-CA-CB	-9.52	91.87	103.30
1	C	242	PRO	N-CA-CB	-9.52	91.88	103.30
1	C	298	GLU	CG-CD-OE2	-9.52	99.26	118.30
1	A	298	GLU	CG-CD-OE2	-9.52	99.27	118.30
1	E	298	GLU	CG-CD-OE2	-9.52	99.26	118.30
1	A	242	PRO	N-CA-CB	-9.52	91.88	103.30
1	D	242	PRO	N-CA-CB	-9.51	91.88	103.30
1	B	242	PRO	N-CA-CB	-9.51	91.89	103.30
1	B	333	TYR	CD1-CE1-CZ	9.51	128.36	119.80
1	D	522	SER	N-CA-C	9.51	136.68	111.00
1	C	333	TYR	CD1-CE1-CZ	9.51	128.36	119.80
1	F	298	GLU	CG-CD-OE2	-9.51	99.29	118.30
1	E	581	ASN	N-CA-CB	-9.51	93.49	110.60
1	E	522	SER	N-CA-C	9.50	136.65	111.00
1	C	522	SER	N-CA-C	9.50	136.65	111.00
1	A	522	SER	N-CA-C	9.49	136.62	111.00
1	A	333	TYR	CD1-CE1-CZ	9.49	128.34	119.80
1	F	333	TYR	CD1-CE1-CZ	9.49	128.34	119.80
1	B	522	SER	N-CA-C	9.48	136.60	111.00
1	F	522	SER	N-CA-C	9.48	136.59	111.00
1	C	413	VAL	CA-CB-CG2	-9.47	96.69	110.90
1	D	333	TYR	CD1-CE1-CZ	9.47	128.32	119.80
1	B	413	VAL	CA-CB-CG2	-9.46	96.71	110.90
1	A	413	VAL	CA-CB-CG2	-9.45	96.72	110.90
1	F	413	VAL	CA-CB-CG2	-9.45	96.72	110.90
1	D	413	VAL	CA-CB-CG2	-9.44	96.74	110.90
1	E	413	VAL	CA-CB-CG2	-9.44	96.74	110.90
1	D	629	ARG	CA-CB-CG	9.37	134.01	113.40
1	B	109	ARG	CD-NE-CZ	-9.36	110.50	123.60
1	F	629	ARG	CA-CB-CG	9.36	133.98	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	109	ARG	CD-NE-CZ	-9.35	110.51	123.60
1	F	373	THR	N-CA-CB	-9.35	92.54	110.30
1	A	109	ARG	CD-NE-CZ	-9.35	110.52	123.60
1	A	629	ARG	CA-CB-CG	9.35	133.96	113.40
1	D	643	LYS	CB-CA-C	-9.35	91.71	110.40
1	E	629	ARG	CA-CB-CG	9.35	133.96	113.40
1	D	343	LEU	CB-CG-CD1	-9.34	95.12	111.00
1	E	643	LYS	CB-CA-C	-9.34	91.72	110.40
1	A	373	THR	N-CA-CB	-9.34	92.56	110.30
1	A	643	LYS	CB-CA-C	-9.34	91.73	110.40
1	F	343	LEU	CB-CG-CD1	-9.34	95.13	111.00
1	F	109	ARG	CD-NE-CZ	-9.33	110.53	123.60
1	B	629	ARG	CA-CB-CG	9.33	133.93	113.40
1	B	643	LYS	CB-CA-C	-9.33	91.73	110.40
1	C	629	ARG	CA-CB-CG	9.33	133.93	113.40
1	C	643	LYS	CB-CA-C	-9.33	91.74	110.40
1	C	343	LEU	CB-CG-CD1	-9.33	95.14	111.00
1	E	279	ASP	CB-CG-OD1	9.33	126.69	118.30
1	E	373	THR	N-CA-CB	-9.33	92.58	110.30
1	F	643	LYS	CB-CA-C	-9.33	91.75	110.40
1	A	343	LEU	CB-CG-CD1	-9.32	95.15	111.00
1	B	343	LEU	CB-CG-CD1	-9.32	95.15	111.00
1	C	109	ARG	CD-NE-CZ	-9.32	110.55	123.60
1	E	109	ARG	CD-NE-CZ	-9.32	110.55	123.60
1	E	79	GLN	CG-CD-NE2	-9.32	94.33	116.70
1	C	79	GLN	CG-CD-NE2	-9.32	94.34	116.70
1	C	373	THR	N-CA-CB	-9.32	92.60	110.30
1	D	373	THR	N-CA-CB	-9.32	92.59	110.30
1	B	373	THR	N-CA-CB	-9.31	92.60	110.30
1	E	343	LEU	CB-CG-CD1	-9.31	95.17	111.00
1	D	220	PHE	CG-CD1-CE1	9.31	131.04	120.80
1	B	79	GLN	CG-CD-NE2	-9.30	94.37	116.70
1	A	79	GLN	CG-CD-NE2	-9.30	94.38	116.70
1	F	79	GLN	CG-CD-NE2	-9.30	94.38	116.70
1	C	220	PHE	CG-CD1-CE1	9.30	131.03	120.80
1	B	279	ASP	CB-CG-OD1	9.29	126.66	118.30
1	D	109	ARG	O-C-N	-9.29	107.84	122.70
1	E	13	ASP	CB-CG-OD1	-9.29	109.94	118.30
1	F	220	PHE	CG-CD1-CE1	9.29	131.02	120.80
1	D	79	GLN	CG-CD-NE2	-9.29	94.41	116.70
1	B	109	ARG	O-C-N	-9.28	107.86	122.70
1	B	539	LEU	CB-CG-CD2	-9.28	95.23	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	279	ASP	CB-CG-OD1	9.27	126.65	118.30
1	A	13	ASP	CB-CG-OD1	-9.27	109.96	118.30
1	A	109	ARG	O-C-N	-9.27	107.87	122.70
1	A	220	PHE	CG-CD1-CE1	9.27	131.00	120.80
1	E	109	ARG	O-C-N	-9.26	107.88	122.70
1	D	539	LEU	CB-CG-CD2	-9.26	95.25	111.00
1	B	13	ASP	CB-CG-OD1	-9.26	109.97	118.30
1	C	109	ARG	O-C-N	-9.26	107.88	122.70
1	B	220	PHE	CG-CD1-CE1	9.26	130.99	120.80
1	A	539	LEU	CB-CG-CD2	-9.26	95.26	111.00
1	E	539	LEU	CB-CG-CD2	-9.26	95.26	111.00
1	A	279	ASP	CB-CG-OD1	9.25	126.63	118.30
1	D	279	ASP	CB-CG-OD1	9.25	126.63	118.30
1	C	13	ASP	CB-CG-OD1	-9.25	109.97	118.30
1	D	13	ASP	CB-CG-OD1	-9.25	109.98	118.30
1	F	109	ARG	O-C-N	-9.25	107.90	122.70
1	F	305	ILE	CA-C-O	-9.25	100.68	120.10
1	A	305	ILE	CA-C-O	-9.24	100.69	120.10
1	B	77	THR	CA-C-O	-9.24	100.69	120.10
1	B	305	ILE	CA-C-O	-9.24	100.69	120.10
1	C	539	LEU	CB-CG-CD2	-9.24	95.29	111.00
1	F	539	LEU	CB-CG-CD2	-9.24	95.29	111.00
1	E	305	ILE	CA-C-O	-9.24	100.70	120.10
1	F	77	THR	CA-C-O	-9.23	100.71	120.10
1	D	77	THR	CA-C-O	-9.23	100.72	120.10
1	F	566	ASP	CB-CG-OD2	-9.23	109.99	118.30
1	A	77	THR	CA-C-O	-9.23	100.72	120.10
1	B	486	GLU	C-N-CA	9.23	144.77	121.70
1	C	279	ASP	CB-CG-OD1	9.23	126.60	118.30
1	C	305	ILE	CA-C-O	-9.23	100.72	120.10
1	D	305	ILE	CA-C-O	-9.22	100.73	120.10
1	E	77	THR	CA-C-O	-9.22	100.73	120.10
1	C	77	THR	CA-C-O	-9.22	100.73	120.10
1	E	193	HIS	CA-CB-CG	9.22	129.28	113.60
1	C	486	GLU	C-N-CA	9.22	144.75	121.70
1	F	13	ASP	CB-CG-OD1	-9.22	110.00	118.30
1	F	486	GLU	C-N-CA	9.22	144.75	121.70
1	D	486	GLU	C-N-CA	9.21	144.73	121.70
1	E	486	GLU	C-N-CA	9.21	144.72	121.70
1	A	486	GLU	C-N-CA	9.21	144.72	121.70
1	D	193	HIS	CA-CB-CG	9.21	129.25	113.60
1	F	40	LEU	N-CA-CB	-9.21	91.99	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	HIS	CA-CB-CG	9.20	129.23	113.60
1	D	40	LEU	N-CA-CB	-9.20	92.01	110.40
1	C	193	HIS	CA-CB-CG	9.19	129.23	113.60
1	E	220	PHE	CG-CD1-CE1	9.20	130.91	120.80
1	E	75	PHE	CA-C-O	-9.19	100.80	120.10
1	A	40	LEU	N-CA-CB	-9.19	92.02	110.40
1	F	193	HIS	CA-CB-CG	9.19	129.22	113.60
1	C	566	ASP	CB-CG-OD2	-9.19	110.03	118.30
1	B	75	PHE	CA-C-O	-9.19	100.81	120.10
1	D	75	PHE	CA-C-O	-9.19	100.81	120.10
1	D	566	ASP	CB-CG-OD2	-9.19	110.03	118.30
1	F	75	PHE	CA-C-O	-9.19	100.81	120.10
1	B	40	LEU	N-CA-CB	-9.18	92.03	110.40
1	C	40	LEU	N-CA-CB	-9.18	92.04	110.40
1	A	75	PHE	CA-C-O	-9.18	100.82	120.10
1	B	193	HIS	CA-CB-CG	9.18	129.21	113.60
1	B	608	GLN	O-C-N	9.18	137.39	122.70
1	C	75	PHE	CA-C-O	-9.18	100.82	120.10
1	E	206	GLU	CG-CD-OE2	-9.18	99.94	118.30
1	F	608	GLN	O-C-N	9.18	137.39	122.70
1	A	206	GLU	CG-CD-OE2	-9.18	99.95	118.30
1	B	632	ASP	O-C-N	9.18	137.38	122.70
1	D	608	GLN	O-C-N	9.18	137.38	122.70
1	F	206	GLU	CG-CD-OE2	-9.18	99.95	118.30
1	C	608	GLN	O-C-N	9.17	137.38	122.70
1	E	40	LEU	N-CA-CB	-9.17	92.05	110.40
1	C	206	GLU	CG-CD-OE2	-9.17	99.96	118.30
1	F	632	ASP	O-C-N	9.17	137.38	122.70
1	A	566	ASP	CB-CG-OD2	-9.17	110.05	118.30
1	A	608	GLN	O-C-N	9.17	137.37	122.70
1	C	632	ASP	O-C-N	9.17	137.37	122.70
1	F	483	CYS	CA-C-O	-9.17	100.85	120.10
1	B	206	GLU	CG-CD-OE2	-9.16	99.97	118.30
1	D	632	ASP	O-C-N	9.16	137.36	122.70
1	E	632	ASP	O-C-N	9.16	137.36	122.70
1	D	206	GLU	CG-CD-OE2	-9.16	99.98	118.30
1	E	608	GLN	O-C-N	9.16	137.36	122.70
1	D	483	CYS	CA-C-O	-9.15	100.88	120.10
1	A	632	ASP	O-C-N	9.15	137.34	122.70
1	B	483	CYS	CA-C-O	-9.15	100.88	120.10
1	E	483	CYS	CA-C-O	-9.15	100.88	120.10
1	A	483	CYS	CA-C-O	-9.15	100.89	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	554	ASP	C-N-CA	9.14	144.56	121.70
1	D	554	ASP	C-N-CA	9.14	144.56	121.70
1	F	554	ASP	C-N-CA	9.14	144.56	121.70
1	F	337	VAL	CA-CB-CG1	-9.14	97.19	110.90
1	A	554	ASP	C-N-CA	9.14	144.54	121.70
1	E	566	ASP	CB-CG-OD2	-9.14	110.08	118.30
1	C	483	CYS	CA-C-O	-9.14	100.91	120.10
1	C	554	ASP	C-N-CA	9.13	144.53	121.70
1	D	337	VAL	CA-CB-CG1	-9.13	97.20	110.90
1	E	554	ASP	C-N-CA	9.13	144.53	121.70
1	C	337	VAL	CA-CB-CG1	-9.13	97.21	110.90
1	E	487	ASP	CB-CG-OD1	9.13	126.51	118.30
1	B	337	VAL	CA-CB-CG1	-9.12	97.21	110.90
1	B	566	ASP	CB-CG-OD2	-9.12	110.09	118.30
1	E	337	VAL	CA-CB-CG1	-9.12	97.22	110.90
1	A	337	VAL	CA-CB-CG1	-9.11	97.23	110.90
1	A	487	ASP	CB-CG-OD1	9.11	126.50	118.30
1	E	506	ASP	CB-CG-OD2	-9.11	110.10	118.30
1	F	287	HIS	N-CA-CB	-9.11	94.20	110.60
1	C	287	HIS	N-CA-CB	-9.11	94.21	110.60
1	A	287	HIS	N-CA-CB	-9.10	94.22	110.60
1	D	287	HIS	N-CA-CB	-9.10	94.23	110.60
1	D	487	ASP	CB-CG-OD1	9.09	126.48	118.30
1	E	287	HIS	N-CA-CB	-9.09	94.24	110.60
1	E	279	ASP	CB-CA-C	9.09	128.58	110.40
1	C	487	ASP	CB-CG-OD1	9.09	126.48	118.30
1	B	287	HIS	N-CA-CB	-9.08	94.25	110.60
1	B	487	ASP	CB-CG-OD1	9.08	126.47	118.30
1	C	506	ASP	CB-CG-OD2	-9.08	110.13	118.30
1	C	279	ASP	CB-CA-C	9.07	128.55	110.40
1	F	506	ASP	CB-CG-OD2	-9.07	110.14	118.30
1	A	506	ASP	CB-CG-OD2	-9.07	110.14	118.30
1	B	279	ASP	CB-CA-C	9.07	128.54	110.40
1	D	63	HIS	N-CA-CB	9.07	126.92	110.60
1	D	279	ASP	CB-CA-C	9.06	128.53	110.40
1	D	506	ASP	CB-CG-OD2	-9.06	110.14	118.30
1	D	650	VAL	CA-CB-CG1	-9.06	97.31	110.90
1	F	63	HIS	N-CA-CB	9.06	126.91	110.60
1	E	63	HIS	N-CA-CB	9.06	126.91	110.60
1	A	63	HIS	N-CA-CB	9.06	126.91	110.60
1	A	279	ASP	CB-CA-C	9.06	128.52	110.40
1	F	279	ASP	CB-CA-C	9.06	128.52	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	650	VAL	CA-CB-CG1	-9.06	97.31	110.90
1	B	572	LYS	C-N-CA	9.05	144.34	121.70
1	F	487	ASP	CB-CG-OD1	9.05	126.45	118.30
1	C	63	HIS	N-CA-CB	9.05	126.89	110.60
1	A	256	PHE	CB-CG-CD2	-9.04	114.47	120.80
1	C	572	LYS	C-N-CA	9.04	144.30	121.70
1	B	256	PHE	CB-CG-CD2	-9.03	114.48	120.80
1	A	650	VAL	CA-CB-CG1	-9.03	97.35	110.90
1	F	256	PHE	CB-CG-CD2	-9.03	114.48	120.80
1	B	63	HIS	N-CA-CB	9.03	126.85	110.60
1	A	572	LYS	C-N-CA	9.03	144.27	121.70
1	D	256	PHE	CB-CG-CD2	-9.03	114.48	120.80
1	E	650	VAL	CA-CB-CG1	-9.03	97.36	110.90
1	D	572	LYS	C-N-CA	9.03	144.26	121.70
1	E	572	LYS	C-N-CA	9.03	144.26	121.70
1	B	650	VAL	CA-CB-CG1	-9.02	97.37	110.90
1	F	572	LYS	C-N-CA	9.02	144.25	121.70
1	F	90	LEU	N-CA-CB	-9.02	92.36	110.40
1	B	506	ASP	CB-CG-OD2	-9.01	110.19	118.30
1	A	90	LEU	N-CA-CB	-9.01	92.39	110.40
1	C	90	LEU	N-CA-CB	-9.01	92.39	110.40
1	D	4	GLY	CA-C-O	9.01	136.81	120.60
1	B	90	LEU	N-CA-CB	-9.00	92.39	110.40
1	C	650	VAL	CA-CB-CG1	-9.00	97.39	110.90
1	D	90	LEU	N-CA-CB	-9.00	92.40	110.40
1	E	44	SER	O-C-N	9.00	137.10	122.70
1	E	90	LEU	N-CA-CB	-9.00	92.40	110.40
1	C	4	GLY	CA-C-O	9.00	136.79	120.60
1	F	4	GLY	CA-C-O	8.99	136.79	120.60
1	F	226	GLN	CA-CB-CG	-8.99	93.62	113.40
1	E	4	GLY	CA-C-O	8.99	136.78	120.60
1	F	606	HIS	CA-CB-CG	-8.99	98.32	113.60
1	A	226	GLN	CA-CB-CG	-8.98	93.64	113.40
1	A	416	VAL	CB-CA-C	8.98	128.47	111.40
1	B	4	GLY	CA-C-O	8.98	136.77	120.60
1	C	416	VAL	CB-CA-C	8.98	128.47	111.40
1	D	294	SER	O-C-N	8.98	137.07	122.70
1	C	256	PHE	CB-CG-CD2	-8.98	114.51	120.80
1	A	4	GLY	CA-C-O	8.98	136.76	120.60
1	A	294	SER	O-C-N	8.98	137.06	122.70
1	B	44	SER	O-C-N	8.98	137.06	122.70
1	C	226	GLN	CA-CB-CG	-8.98	93.65	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	416	VAL	CB-CA-C	8.98	128.46	111.40
1	F	416	VAL	CB-CA-C	8.98	128.46	111.40
1	D	226	GLN	CA-CB-CG	-8.98	93.65	113.40
1	E	256	PHE	CB-CG-CD2	-8.98	114.52	120.80
1	F	294	SER	O-C-N	8.98	137.06	122.70
1	B	294	SER	O-C-N	8.97	137.06	122.70
1	E	294	SER	O-C-N	8.97	137.06	122.70
1	A	44	SER	O-C-N	8.97	137.05	122.70
1	A	606	HIS	CA-CB-CG	-8.97	98.35	113.60
1	B	416	VAL	CB-CA-C	8.97	128.45	111.40
1	D	416	VAL	CB-CA-C	8.97	128.44	111.40
1	D	606	HIS	CA-CB-CG	-8.97	98.35	113.60
1	E	226	GLN	CA-CB-CG	-8.97	93.66	113.40
1	E	606	HIS	CA-CB-CG	-8.97	98.35	113.60
1	B	226	GLN	CA-CB-CG	-8.97	93.67	113.40
1	B	606	HIS	CA-CB-CG	-8.97	98.35	113.60
1	C	294	SER	O-C-N	8.97	137.05	122.70
1	F	44	SER	O-C-N	8.97	137.05	122.70
1	D	44	SER	O-C-N	8.96	137.04	122.70
1	B	92	GLN	CB-CG-CD	-8.96	88.31	111.60
1	A	92	GLN	CB-CG-CD	-8.96	88.31	111.60
1	C	44	SER	O-C-N	8.96	137.03	122.70
1	E	92	GLN	CB-CG-CD	-8.96	88.31	111.60
1	C	92	GLN	CB-CG-CD	-8.96	88.31	111.60
1	D	92	GLN	CB-CG-CD	-8.95	88.32	111.60
1	D	312	THR	CA-CB-CG2	8.95	124.94	112.40
1	C	606	HIS	CA-CB-CG	-8.95	98.38	113.60
1	F	92	GLN	CB-CG-CD	-8.95	88.33	111.60
1	F	85	MET	N-CA-CB	8.95	126.71	110.60
1	B	85	MET	N-CA-CB	8.95	126.70	110.60
1	A	312	THR	CA-CB-CG2	8.94	124.92	112.40
1	D	85	MET	N-CA-CB	8.94	126.70	110.60
1	D	51	ALA	N-CA-CB	-8.94	97.59	110.10
1	C	312	THR	CA-CB-CG2	8.93	124.91	112.40
1	A	85	MET	N-CA-CB	8.93	126.68	110.60
1	F	51	ALA	N-CA-CB	-8.93	97.59	110.10
1	A	51	ALA	N-CA-CB	-8.93	97.60	110.10
1	C	85	MET	N-CA-CB	8.93	126.67	110.60
1	E	312	THR	CA-CB-CG2	8.93	124.90	112.40
1	F	312	THR	CA-CB-CG2	8.93	124.90	112.40
1	E	85	MET	N-CA-CB	8.93	126.67	110.60
1	B	312	THR	CA-CB-CG2	8.92	124.89	112.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	51	ALA	N-CA-CB	-8.90	97.63	110.10
1	E	51	ALA	N-CA-CB	-8.90	97.64	110.10
1	C	413	VAL	O-C-N	8.89	136.92	122.70
1	B	51	ALA	N-CA-CB	-8.88	97.66	110.10
1	C	645	VAL	CA-C-O	-8.88	101.45	120.10
1	E	645	VAL	CA-C-O	-8.88	101.45	120.10
1	D	413	VAL	O-C-N	8.88	136.91	122.70
1	A	645	VAL	CA-C-O	-8.88	101.45	120.10
1	B	413	VAL	O-C-N	8.88	136.91	122.70
1	B	645	VAL	CA-C-O	-8.88	101.46	120.10
1	F	413	VAL	O-C-N	8.88	136.91	122.70
1	F	645	VAL	CA-C-O	-8.88	101.46	120.10
1	A	413	VAL	O-C-N	8.88	136.90	122.70
1	C	290	GLU	CB-CG-CD	8.87	138.16	114.20
1	A	290	GLU	CB-CG-CD	8.87	138.16	114.20
1	E	413	VAL	O-C-N	8.87	136.90	122.70
1	F	290	GLU	CB-CG-CD	8.87	138.16	114.20
1	D	290	GLU	CB-CG-CD	8.87	138.15	114.20
1	D	645	VAL	CA-C-O	-8.87	101.47	120.10
1	B	290	GLU	CB-CG-CD	8.87	138.14	114.20
1	E	290	GLU	CB-CG-CD	8.86	138.12	114.20
1	D	554	ASP	CA-C-O	8.85	138.69	120.10
1	E	554	ASP	CA-C-O	8.85	138.69	120.10
1	C	206	GLU	CA-C-O	-8.85	101.52	120.10
1	B	206	GLU	CA-C-O	-8.84	101.53	120.10
1	C	554	ASP	CA-C-O	8.84	138.67	120.10
1	A	206	GLU	CA-C-O	-8.84	101.54	120.10
1	A	554	ASP	CA-C-O	8.84	138.66	120.10
1	B	247	HIS	O-C-N	8.84	136.84	122.70
1	C	247	HIS	O-C-N	8.84	136.84	122.70
1	F	554	ASP	CA-C-O	8.84	138.65	120.10
1	D	206	GLU	CA-C-O	-8.83	101.55	120.10
1	E	206	GLU	CA-C-O	-8.83	101.55	120.10
1	B	554	ASP	CA-C-O	8.83	138.63	120.10
1	F	206	GLU	CA-C-O	-8.83	101.56	120.10
1	F	247	HIS	O-C-N	8.82	136.82	122.70
1	A	247	HIS	O-C-N	8.82	136.81	122.70
1	D	247	HIS	O-C-N	8.81	136.80	122.70
1	E	247	HIS	O-C-N	8.81	136.79	122.70
1	B	410	GLY	N-CA-C	-8.80	91.09	113.10
1	B	376	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	C	250	ARG	CD-NE-CZ	8.80	135.92	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	410	GLY	N-CA-C	-8.79	91.11	113.10
1	B	496	ASP	N-CA-C	-8.79	87.26	111.00
1	A	410	GLY	N-CA-C	-8.79	91.12	113.10
1	D	410	GLY	N-CA-C	-8.79	91.13	113.10
1	E	496	ASP	N-CA-C	-8.79	87.27	111.00
1	D	376	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	C	410	GLY	N-CA-C	-8.78	91.15	113.10
1	D	250	ARG	CD-NE-CZ	8.78	135.90	123.60
1	B	295	ARG	CD-NE-CZ	-8.78	111.31	123.60
1	D	243	VAL	CB-CA-C	-8.78	94.72	111.40
1	E	376	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	A	496	ASP	N-CA-C	-8.78	87.30	111.00
1	C	361	PHE	N-CA-CB	-8.78	94.80	110.60
1	C	496	ASP	N-CA-C	-8.78	87.31	111.00
1	D	496	ASP	N-CA-C	-8.78	87.31	111.00
1	E	410	GLY	N-CA-C	-8.77	91.17	113.10
1	A	243	VAL	CB-CA-C	-8.77	94.73	111.40
1	A	250	ARG	CD-NE-CZ	8.77	135.88	123.60
1	A	376	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	F	295	ARG	CD-NE-CZ	-8.77	111.32	123.60
1	E	361	PHE	N-CA-CB	-8.77	94.81	110.60
1	F	243	VAL	CB-CA-C	-8.77	94.73	111.40
1	F	496	ASP	N-CA-C	-8.77	87.31	111.00
1	A	361	PHE	N-CA-CB	-8.77	94.81	110.60
1	B	243	VAL	CB-CA-C	-8.77	94.74	111.40
1	B	250	ARG	CD-NE-CZ	8.77	135.88	123.60
1	C	243	VAL	CB-CA-C	-8.77	94.75	111.40
1	E	295	ARG	CD-NE-CZ	-8.77	111.33	123.60
1	D	361	PHE	N-CA-CB	-8.76	94.83	110.60
1	E	243	VAL	CB-CA-C	-8.76	94.75	111.40
1	F	361	PHE	N-CA-CB	-8.76	94.84	110.60
1	B	361	PHE	N-CA-CB	-8.76	94.84	110.60
1	C	295	ARG	CD-NE-CZ	-8.76	111.34	123.60
1	F	250	ARG	CD-NE-CZ	8.75	135.86	123.60
1	B	170	PHE	N-CA-CB	8.75	126.35	110.60
1	D	295	ARG	CD-NE-CZ	-8.75	111.35	123.60
1	A	295	ARG	CD-NE-CZ	-8.75	111.35	123.60
1	C	170	PHE	N-CA-CB	8.74	126.34	110.60
1	E	250	ARG	CD-NE-CZ	8.74	135.84	123.60
1	A	170	PHE	N-CA-CB	8.74	126.33	110.60
1	F	173	THR	N-CA-CB	8.74	126.90	110.30
1	F	376	ARG	NE-CZ-NH1	8.74	124.67	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	173	THR	N-CA-CB	8.73	126.89	110.30
1	E	408	PHE	CB-CG-CD2	-8.73	114.69	120.80
1	F	170	PHE	N-CA-CB	8.73	126.32	110.60
1	D	408	PHE	CB-CG-CD2	-8.73	114.69	120.80
1	E	170	PHE	N-CA-CB	8.73	126.31	110.60
1	E	173	THR	N-CA-CB	8.72	126.87	110.30
1	A	408	PHE	CB-CG-CD2	-8.72	114.70	120.80
1	C	330	SER	O-C-N	8.72	136.65	122.70
1	A	173	THR	N-CA-CB	8.72	126.86	110.30
1	D	170	PHE	N-CA-CB	8.72	126.29	110.60
1	D	330	SER	O-C-N	8.71	136.64	122.70
1	D	574	LYS	CB-CG-CD	8.71	134.26	111.60
1	B	574	LYS	CB-CG-CD	8.71	134.24	111.60
1	C	173	THR	N-CA-CB	8.71	126.84	110.30
1	C	376	ARG	NE-CZ-NH1	8.71	124.65	120.30
1	F	408	PHE	CB-CG-CD2	-8.71	114.71	120.80
1	B	173	THR	N-CA-CB	8.70	126.83	110.30
1	A	330	SER	O-C-N	8.70	136.62	122.70
1	B	330	SER	O-C-N	8.70	136.61	122.70
1	F	574	LYS	CB-CG-CD	8.70	134.21	111.60
1	A	574	LYS	CB-CG-CD	8.69	134.20	111.60
1	C	574	LYS	CB-CG-CD	8.69	134.19	111.60
1	E	574	LYS	CB-CG-CD	8.69	134.19	111.60
1	E	330	SER	O-C-N	8.69	136.60	122.70
1	C	408	PHE	CB-CG-CD2	-8.68	114.73	120.80
1	B	408	PHE	CB-CG-CD2	-8.67	114.73	120.80
1	D	438	ASP	OD1-CG-OD2	8.67	139.77	123.30
1	F	330	SER	O-C-N	8.66	136.55	122.70
1	E	304	TYR	CG-CD2-CE2	8.65	128.22	121.30
1	C	438	ASP	OD1-CG-OD2	8.65	139.73	123.30
1	B	304	TYR	CG-CD2-CE2	8.64	128.21	121.30
1	A	438	ASP	OD1-CG-OD2	8.63	139.70	123.30
1	B	317	GLN	CA-CB-CG	-8.63	94.41	113.40
1	D	304	TYR	CG-CD2-CE2	8.63	128.20	121.30
1	A	304	TYR	CG-CD2-CE2	8.63	128.20	121.30
1	F	304	TYR	CG-CD2-CE2	8.63	128.20	121.30
1	A	317	GLN	CA-CB-CG	-8.62	94.43	113.40
1	E	317	GLN	CA-CB-CG	-8.62	94.44	113.40
1	F	317	GLN	CA-CB-CG	-8.62	94.44	113.40
1	F	438	ASP	OD1-CG-OD2	8.62	139.68	123.30
1	C	317	GLN	CA-CB-CG	-8.62	94.45	113.40
1	D	317	GLN	CA-CB-CG	-8.62	94.44	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	304	TYR	CG-CD2-CE2	8.61	128.19	121.30
1	E	61	ASN	CA-CB-CG	-8.61	94.46	113.40
1	B	438	ASP	OD1-CG-OD2	8.61	139.66	123.30
1	E	438	ASP	OD1-CG-OD2	8.61	139.66	123.30
1	F	61	ASN	CA-CB-CG	-8.61	94.46	113.40
1	C	61	ASN	CA-CB-CG	-8.61	94.47	113.40
1	E	391	PHE	CZ-CE2-CD2	-8.60	109.78	120.10
1	A	61	ASN	CA-CB-CG	-8.60	94.48	113.40
1	B	61	ASN	CA-CB-CG	-8.60	94.48	113.40
1	B	391	PHE	CZ-CE2-CD2	-8.60	109.79	120.10
1	D	61	ASN	CA-CB-CG	-8.59	94.50	113.40
1	C	391	PHE	CZ-CE2-CD2	-8.59	109.79	120.10
1	A	391	PHE	CZ-CE2-CD2	-8.58	109.80	120.10
1	E	316	ARG	NH1-CZ-NH2	-8.58	109.96	119.40
1	D	459	GLU	OE1-CD-OE2	8.58	133.59	123.30
1	B	459	GLU	OE1-CD-OE2	8.57	133.59	123.30
1	F	293	GLU	CG-CD-OE2	8.57	135.44	118.30
1	D	391	PHE	CZ-CE2-CD2	-8.57	109.82	120.10
1	E	89	VAL	CB-CA-C	8.57	127.68	111.40
1	C	25	THR	N-CA-CB	8.56	126.57	110.30
1	B	89	VAL	CB-CA-C	8.56	127.67	111.40
1	C	293	GLU	CG-CD-OE2	8.56	135.42	118.30
1	F	25	THR	N-CA-CB	8.56	126.57	110.30
1	A	89	VAL	CB-CA-C	8.56	127.66	111.40
1	C	89	VAL	CB-CA-C	8.56	127.66	111.40
1	D	25	THR	N-CA-CB	8.56	126.56	110.30
1	D	293	GLU	CG-CD-OE2	8.56	135.41	118.30
1	A	25	THR	N-CA-CB	8.55	126.55	110.30
1	A	293	GLU	CG-CD-OE2	8.55	135.41	118.30
1	A	459	GLU	OE1-CD-OE2	8.55	133.56	123.30
1	F	89	VAL	CB-CA-C	8.55	127.65	111.40
1	E	25	THR	N-CA-CB	8.55	126.55	110.30
1	A	316	ARG	NH1-CZ-NH2	-8.55	110.00	119.40
1	F	459	GLU	OE1-CD-OE2	8.55	133.56	123.30
1	D	316	ARG	NH1-CZ-NH2	-8.55	110.00	119.40
1	E	459	GLU	OE1-CD-OE2	8.55	133.56	123.30
1	F	391	PHE	CZ-CE2-CD2	-8.54	109.85	120.10
1	B	25	THR	N-CA-CB	8.54	126.53	110.30
1	C	316	ARG	NH1-CZ-NH2	-8.54	110.00	119.40
1	D	89	VAL	CB-CA-C	8.54	127.63	111.40
1	B	316	ARG	NH1-CZ-NH2	-8.54	110.01	119.40
1	B	360	LYS	CA-C-O	-8.54	102.17	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	293	GLU	CG-CD-OE2	8.54	135.38	118.30
1	E	311	HIS	CA-CB-CG	-8.53	99.09	113.60
1	A	360	LYS	CA-C-O	-8.53	102.19	120.10
1	C	459	GLU	OE1-CD-OE2	8.53	133.53	123.30
1	F	316	ARG	NH1-CZ-NH2	-8.53	110.02	119.40
1	F	360	LYS	CA-C-O	-8.53	102.19	120.10
1	E	360	LYS	CA-C-O	-8.52	102.21	120.10
1	B	293	GLU	CG-CD-OE2	8.52	135.34	118.30
1	A	311	HIS	CA-CB-CG	-8.51	99.13	113.60
1	D	311	HIS	CA-CB-CG	-8.51	99.13	113.60
1	F	311	HIS	CA-CB-CG	-8.51	99.13	113.60
1	C	311	HIS	CA-CB-CG	-8.51	99.13	113.60
1	C	357	PRO	N-CD-CG	-8.51	90.44	103.20
1	B	340	TYR	CB-CG-CD1	-8.51	115.89	121.00
1	B	311	HIS	CA-CB-CG	-8.51	99.14	113.60
1	C	360	LYS	CA-C-O	-8.51	102.24	120.10
1	D	360	LYS	CA-C-O	-8.50	102.24	120.10
1	B	558	TYR	CB-CG-CD2	-8.50	115.90	121.00
1	D	357	PRO	N-CD-CG	-8.50	90.45	103.20
1	E	357	PRO	N-CD-CG	-8.49	90.46	103.20
1	A	357	PRO	N-CD-CG	-8.49	90.46	103.20
1	E	340	TYR	CB-CG-CD1	-8.49	115.91	121.00
1	B	488	ASN	N-CA-CB	8.49	125.87	110.60
1	E	488	ASN	N-CA-CB	8.49	125.88	110.60
1	F	357	PRO	N-CD-CG	-8.49	90.47	103.20
1	E	558	TYR	CB-CG-CD2	-8.48	115.91	121.00
1	F	340	TYR	CB-CG-CD1	-8.48	115.91	121.00
1	C	488	ASN	N-CA-CB	8.48	125.87	110.60
1	D	488	ASN	N-CA-CB	8.48	125.86	110.60
1	C	558	TYR	CB-CG-CD2	-8.47	115.92	121.00
1	A	488	ASN	N-CA-CB	8.47	125.84	110.60
1	D	558	TYR	CB-CG-CD2	-8.47	115.92	121.00
1	F	488	ASN	N-CA-CB	8.47	125.84	110.60
1	F	356	ASP	CB-CG-OD1	-8.46	110.68	118.30
1	A	356	ASP	CB-CG-OD1	-8.46	110.68	118.30
1	A	340	TYR	CB-CG-CD1	-8.46	115.92	121.00
1	A	558	TYR	CB-CG-CD2	-8.46	115.92	121.00
1	B	356	ASP	CB-CG-OD1	-8.46	110.69	118.30
1	F	558	TYR	CB-CG-CD2	-8.46	115.92	121.00
1	F	29	ASP	CB-CG-OD1	-8.45	110.69	118.30
1	C	29	ASP	CB-CG-OD1	-8.45	110.69	118.30
1	C	340	TYR	CB-CG-CD1	-8.45	115.93	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	PRO	N-CD-CG	-8.45	90.53	103.20
1	C	356	ASP	CB-CG-OD1	-8.44	110.70	118.30
1	D	29	ASP	CB-CG-OD1	-8.44	110.70	118.30
1	A	29	ASP	CB-CG-OD1	-8.44	110.70	118.30
1	B	622	LEU	CB-CG-CD1	8.44	125.35	111.00
1	D	356	ASP	CB-CG-OD1	-8.44	110.70	118.30
1	E	356	ASP	CB-CG-OD1	-8.43	110.71	118.30
1	D	340	TYR	CB-CG-CD1	-8.43	115.94	121.00
1	F	622	LEU	CB-CG-CD1	8.43	125.33	111.00
1	A	622	LEU	CB-CG-CD1	8.43	125.33	111.00
1	D	622	LEU	CB-CG-CD1	8.43	125.33	111.00
1	E	517	GLU	CG-CD-OE2	8.43	135.16	118.30
1	A	517	GLU	CG-CD-OE2	8.42	135.15	118.30
1	B	517	GLU	CG-CD-OE2	8.42	135.14	118.30
1	F	517	GLU	CG-CD-OE2	8.42	135.14	118.30
1	B	29	ASP	CB-CG-OD1	-8.41	110.73	118.30
1	C	517	GLU	CG-CD-OE2	8.41	135.13	118.30
1	F	377	ASP	CB-CG-OD2	8.41	125.87	118.30
1	A	377	ASP	CB-CG-OD2	8.41	125.87	118.30
1	E	29	ASP	CB-CG-OD1	-8.41	110.73	118.30
1	E	622	LEU	CB-CG-CD1	8.41	125.30	111.00
1	C	622	LEU	CB-CG-CD1	8.40	125.29	111.00
1	C	308	SER	O-C-N	8.40	136.14	122.70
1	B	308	SER	O-C-N	8.40	136.13	122.70
1	C	76	ASN	OD1-CG-ND2	8.40	141.21	121.90
1	D	517	GLU	CG-CD-OE2	8.39	135.09	118.30
1	B	530	VAL	CA-CB-CG1	8.39	123.49	110.90
1	D	76	ASN	OD1-CG-ND2	8.39	141.20	121.90
1	F	76	ASN	OD1-CG-ND2	8.39	141.20	121.90
1	A	76	ASN	OD1-CG-ND2	8.38	141.19	121.90
1	E	76	ASN	OD1-CG-ND2	8.38	141.18	121.90
1	E	308	SER	O-C-N	8.38	136.12	122.70
1	C	377	ASP	CB-CG-OD2	8.38	125.84	118.30
1	D	308	SER	O-C-N	8.38	136.11	122.70
1	F	73	SER	N-CA-CB	8.38	123.07	110.50
1	A	308	SER	O-C-N	8.38	136.11	122.70
1	B	350	MET	CG-SD-CE	-8.38	86.80	100.20
1	E	377	ASP	CB-CG-OD2	8.38	125.84	118.30
1	E	532	ASP	OD1-CG-OD2	-8.38	107.38	123.30
1	D	377	ASP	CB-CG-OD2	8.37	125.84	118.30
1	C	532	ASP	OD1-CG-OD2	-8.37	107.39	123.30
1	D	530	VAL	CA-CB-CG1	8.37	123.46	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	SER	N-CA-CB	8.37	123.06	110.50
1	B	76	ASN	OD1-CG-ND2	8.37	141.15	121.90
1	C	350	MET	CG-SD-CE	-8.37	86.81	100.20
1	C	530	VAL	CA-CB-CG1	8.37	123.45	110.90
1	A	350	MET	CG-SD-CE	-8.37	86.81	100.20
1	B	532	ASP	OD1-CG-OD2	-8.37	107.40	123.30
1	E	73	SER	N-CA-CB	8.37	123.05	110.50
1	F	308	SER	O-C-N	8.37	136.09	122.70
1	A	530	VAL	CA-CB-CG1	8.37	123.45	110.90
1	A	532	ASP	OD1-CG-OD2	-8.37	107.41	123.30
1	A	73	SER	N-CA-CB	8.36	123.05	110.50
1	C	245	GLU	CG-CD-OE2	8.36	135.03	118.30
1	F	532	ASP	OD1-CG-OD2	-8.37	107.41	123.30
1	B	307	ASP	CB-CG-OD2	-8.36	110.78	118.30
1	E	350	MET	CG-SD-CE	-8.36	86.82	100.20
1	D	532	ASP	OD1-CG-OD2	-8.36	107.42	123.30
1	F	307	ASP	CB-CG-OD2	-8.36	110.78	118.30
1	D	73	SER	N-CA-CB	8.36	123.03	110.50
1	E	245	GLU	CG-CD-OE2	8.36	135.01	118.30
1	A	245	GLU	CG-CD-OE2	8.36	135.01	118.30
1	F	350	MET	CG-SD-CE	-8.36	86.83	100.20
1	A	307	ASP	CB-CG-OD2	-8.35	110.78	118.30
1	B	377	ASP	CB-CG-OD2	8.35	125.82	118.30
1	F	147	ASN	CB-CG-OD1	-8.35	104.90	121.60
1	D	350	MET	CG-SD-CE	-8.35	86.84	100.20
1	B	241	ASP	N-CA-CB	-8.35	95.58	110.60
1	C	73	SER	N-CA-CB	8.35	123.02	110.50
1	D	245	GLU	CG-CD-OE2	8.35	134.99	118.30
1	E	307	ASP	CB-CG-OD2	-8.35	110.79	118.30
1	F	241	ASP	N-CA-CB	-8.34	95.58	110.60
1	E	530	VAL	CA-CB-CG1	8.34	123.41	110.90
1	B	245	GLU	CG-CD-OE2	8.34	134.97	118.30
1	B	373	THR	CA-CB-CG2	8.34	124.07	112.40
1	B	48	ASP	CA-CB-CG	8.33	131.73	113.40
1	C	48	ASP	CA-CB-CG	8.33	131.73	113.40
1	F	245	GLU	CG-CD-OE2	8.33	134.97	118.30
1	C	307	ASP	CB-CG-OD2	-8.33	110.80	118.30
1	F	48	ASP	CA-CB-CG	8.33	131.72	113.40
1	D	147	ASN	CB-CG-OD1	-8.33	104.95	121.60
1	C	216	LYS	CA-CB-CG	8.32	131.71	113.40
1	C	310	GLY	O-C-N	8.32	136.02	122.70
1	D	307	ASP	CB-CG-OD2	-8.32	110.81	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	147	ASN	CB-CG-OD1	-8.32	104.95	121.60
1	E	216	LYS	CA-CB-CG	8.32	131.71	113.40
1	A	241	ASP	N-CA-CB	-8.32	95.62	110.60
1	E	48	ASP	CA-CB-CG	8.32	131.71	113.40
1	F	221	PHE	CB-CG-CD1	8.32	126.62	120.80
1	B	147	ASN	CB-CG-OD1	-8.32	104.96	121.60
1	F	163	PRO	CB-CA-C	-8.32	91.20	112.00
1	D	8	ALA	O-C-N	-8.32	109.39	122.70
1	D	163	PRO	CB-CA-C	-8.32	91.20	112.00
1	F	216	LYS	CA-CB-CG	8.32	131.70	113.40
1	A	147	ASN	CB-CG-OD1	-8.32	104.97	121.60
1	E	163	PRO	CB-CA-C	-8.32	91.21	112.00
1	E	241	ASP	N-CA-CB	-8.32	95.63	110.60
1	F	530	VAL	CA-CB-CG1	8.32	123.38	110.90
1	A	48	ASP	CA-CB-CG	8.31	131.69	113.40
1	A	216	LYS	CA-CB-CG	8.31	131.69	113.40
1	B	8	ALA	O-C-N	-8.31	109.40	122.70
1	B	163	PRO	CB-CA-C	-8.31	91.22	112.00
1	B	381	PHE	CZ-CE2-CD2	-8.31	110.12	120.10
1	A	163	PRO	CB-CA-C	-8.31	91.22	112.00
1	C	241	ASP	N-CA-CB	-8.31	95.64	110.60
1	D	373	THR	CA-CB-CG2	8.31	124.04	112.40
1	E	221	PHE	CB-CG-CD1	8.31	126.62	120.80
1	B	221	PHE	CB-CG-CD1	8.31	126.61	120.80
1	D	546	ALA	N-CA-CB	8.31	121.73	110.10
1	F	546	ALA	N-CA-CB	8.31	121.73	110.10
1	C	147	ASN	CB-CG-OD1	-8.30	104.99	121.60
1	D	241	ASP	N-CA-CB	-8.31	95.65	110.60
1	E	8	ALA	O-C-N	-8.30	109.41	122.70
1	E	373	THR	CA-CB-CG2	8.30	124.03	112.40
1	F	8	ALA	O-C-N	-8.30	109.41	122.70
1	A	8	ALA	O-C-N	-8.30	109.42	122.70
1	C	163	PRO	CB-CA-C	-8.30	91.25	112.00
1	D	310	GLY	O-C-N	8.30	135.98	122.70
1	A	373	THR	CA-CB-CG2	8.30	124.02	112.40
1	A	546	ALA	N-CA-CB	8.30	121.72	110.10
1	B	546	ALA	N-CA-CB	8.30	121.72	110.10
1	D	216	LYS	CA-CB-CG	8.30	131.66	113.40
1	B	216	LYS	CA-CB-CG	8.30	131.65	113.40
1	C	373	THR	CA-CB-CG2	8.30	124.01	112.40
1	D	48	ASP	CA-CB-CG	8.30	131.65	113.40
1	A	310	GLY	O-C-N	8.29	135.97	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	556	SER	N-CA-C	-8.29	88.62	111.00
1	C	546	ALA	N-CA-CB	8.29	121.70	110.10
1	D	556	SER	N-CA-C	-8.29	88.62	111.00
1	C	556	SER	N-CA-C	-8.29	88.63	111.00
1	A	221	PHE	CB-CG-CD1	8.28	126.60	120.80
1	B	556	SER	N-CA-C	-8.29	88.63	111.00
1	C	326	ASP	CA-CB-CG	8.28	131.63	113.40
1	E	395	THR	CA-CB-OG1	-8.29	91.60	109.00
1	E	546	ALA	N-CA-CB	8.28	121.70	110.10
1	C	8	ALA	O-C-N	-8.28	109.45	122.70
1	E	310	GLY	O-C-N	8.28	135.95	122.70
1	E	556	SER	N-CA-C	-8.28	88.64	111.00
1	F	373	THR	CA-CB-CG2	8.28	123.99	112.40
1	F	556	SER	N-CA-C	-8.28	88.64	111.00
1	B	310	GLY	O-C-N	8.28	135.95	122.70
1	E	326	ASP	CA-CB-CG	8.28	131.61	113.40
1	A	381	PHE	CZ-CE2-CD2	-8.28	110.17	120.10
1	B	326	ASP	CA-CB-CG	8.28	131.61	113.40
1	F	310	GLY	O-C-N	8.27	135.94	122.70
1	A	326	ASP	CA-CB-CG	8.27	131.59	113.40
1	B	395	THR	CA-CB-OG1	-8.27	91.63	109.00
1	D	221	PHE	CB-CG-CD1	8.27	126.59	120.80
1	D	381	PHE	CZ-CE2-CD2	-8.27	110.18	120.10
1	E	381	PHE	CZ-CE2-CD2	-8.27	110.18	120.10
1	C	381	PHE	CZ-CE2-CD2	-8.26	110.18	120.10
1	C	395	THR	CA-CB-OG1	-8.26	91.65	109.00
1	D	326	ASP	CA-CB-CG	8.26	131.58	113.40
1	F	395	THR	CA-CB-OG1	-8.26	91.64	109.00
1	A	395	THR	CA-CB-OG1	-8.26	91.66	109.00
1	C	173	THR	CA-C-N	-8.26	99.03	117.20
1	F	326	ASP	CA-CB-CG	8.26	131.57	113.40
1	B	173	THR	CA-C-N	-8.26	99.04	117.20
1	D	395	THR	CA-CB-OG1	-8.25	91.67	109.00
1	E	155	TYR	O-C-N	8.24	135.89	122.70
1	A	173	THR	CA-C-N	-8.24	99.06	117.20
1	C	155	TYR	O-C-N	8.24	135.89	122.70
1	E	173	THR	CA-C-N	-8.24	99.07	117.20
1	F	173	THR	CA-C-N	-8.24	99.07	117.20
1	D	173	THR	CA-C-N	-8.24	99.08	117.20
1	B	155	TYR	O-C-N	8.23	135.88	122.70
1	C	221	PHE	CB-CG-CD1	8.23	126.56	120.80
1	D	155	TYR	O-C-N	8.23	135.87	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	381	PHE	CZ-CE2-CD2	-8.23	110.22	120.10
1	A	67	GLU	OE1-CD-OE2	8.22	133.17	123.30
1	A	155	TYR	O-C-N	8.22	135.85	122.70
1	B	411	MET	N-CA-C	8.21	133.18	111.00
1	D	67	GLU	OE1-CD-OE2	8.21	133.15	123.30
1	D	220	PHE	CD1-CE1-CZ	-8.21	110.25	120.10
1	B	67	GLU	OE1-CD-OE2	8.21	133.15	123.30
1	C	220	PHE	CD1-CE1-CZ	-8.21	110.25	120.10
1	D	411	MET	N-CA-C	8.21	133.16	111.00
1	D	314	ASP	O-C-N	8.20	135.82	122.70
1	A	411	MET	N-CA-C	8.20	133.14	111.00
1	E	67	GLU	OE1-CD-OE2	8.20	133.14	123.30
1	F	67	GLU	OE1-CD-OE2	8.20	133.14	123.30
1	F	588	ASP	CB-CG-OD1	8.20	125.68	118.30
1	C	411	MET	N-CA-C	8.20	133.13	111.00
1	F	411	MET	N-CA-C	8.20	133.13	111.00
1	C	67	GLU	OE1-CD-OE2	8.19	133.13	123.30
1	F	220	PHE	CD1-CE1-CZ	-8.19	110.27	120.10
1	A	220	PHE	CD1-CE1-CZ	-8.19	110.27	120.10
1	D	333	TYR	CG-CD2-CE2	8.19	127.85	121.30
1	E	411	MET	N-CA-C	8.19	133.10	111.00
1	D	588	ASP	CB-CG-OD1	8.18	125.67	118.30
1	D	606	HIS	CB-CA-C	-8.18	94.04	110.40
1	E	304	TYR	CZ-CE2-CD2	-8.18	112.44	119.80
1	F	606	HIS	CB-CA-C	-8.18	94.03	110.40
1	B	588	ASP	CB-CG-OD1	8.18	125.66	118.30
1	B	220	PHE	CD1-CE1-CZ	-8.18	110.28	120.10
1	C	256	PHE	CZ-CE2-CD2	-8.18	110.28	120.10
1	D	216	LYS	C-N-CA	-8.18	105.13	122.30
1	F	155	TYR	O-C-N	8.18	135.78	122.70
1	F	216	LYS	C-N-CA	-8.18	105.12	122.30
1	F	314	ASP	O-C-N	8.18	135.78	122.70
1	A	588	ASP	CB-CG-OD1	8.18	125.66	118.30
1	B	216	LYS	C-N-CA	-8.18	105.13	122.30
1	A	314	ASP	O-C-N	8.17	135.78	122.70
1	A	606	HIS	CB-CA-C	-8.17	94.05	110.40
1	C	606	HIS	CB-CA-C	-8.17	94.06	110.40
1	B	606	HIS	CB-CA-C	-8.17	94.06	110.40
1	A	215	ARG	CD-NE-CZ	-8.17	112.16	123.60
1	D	256	PHE	CZ-CE2-CD2	-8.17	110.30	120.10
1	E	256	PHE	CZ-CE2-CD2	-8.17	110.30	120.10
1	E	215	ARG	CD-NE-CZ	-8.17	112.17	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	LYS	C-N-CA	-8.16	105.15	122.30
1	C	216	LYS	C-N-CA	-8.16	105.15	122.30
1	D	215	ARG	CD-NE-CZ	-8.16	112.17	123.60
1	A	256	PHE	CZ-CE2-CD2	-8.16	110.31	120.10
1	B	215	ARG	CD-NE-CZ	-8.16	112.17	123.60
1	E	588	ASP	CB-CG-OD1	8.16	125.65	118.30
1	E	606	HIS	CB-CA-C	-8.16	94.07	110.40
1	F	592	ASP	CB-CG-OD2	-8.16	110.95	118.30
1	F	215	ARG	CD-NE-CZ	-8.16	112.17	123.60
1	C	314	ASP	O-C-N	8.16	135.75	122.70
1	C	304	TYR	CZ-CE2-CD2	-8.16	112.46	119.80
1	A	304	TYR	CZ-CE2-CD2	-8.15	112.46	119.80
1	B	314	ASP	O-C-N	8.15	135.75	122.70
1	C	474	ARG	CB-CG-CD	8.15	132.80	111.60
1	D	304	TYR	CZ-CE2-CD2	-8.15	112.46	119.80
1	E	216	LYS	C-N-CA	-8.15	105.17	122.30
1	A	624	TYR	CB-CG-CD2	-8.15	116.11	121.00
1	C	215	ARG	CD-NE-CZ	-8.15	112.19	123.60
1	A	474	ARG	CB-CG-CD	8.15	132.79	111.60
1	B	256	PHE	CZ-CE2-CD2	-8.15	110.32	120.10
1	E	314	ASP	O-C-N	8.15	135.73	122.70
1	C	624	TYR	CB-CG-CD2	-8.14	116.11	121.00
1	F	333	TYR	CG-CD2-CE2	8.14	127.81	121.30
1	B	304	TYR	CZ-CE2-CD2	-8.14	112.47	119.80
1	E	624	TYR	CB-CG-CD2	-8.14	116.11	121.00
1	F	474	ARG	CB-CG-CD	8.14	132.77	111.60
1	B	474	ARG	CB-CG-CD	8.14	132.76	111.60
1	D	474	ARG	CB-CG-CD	8.14	132.76	111.60
1	E	226	GLN	CB-CA-C	8.14	126.68	110.40
1	F	304	TYR	CZ-CE2-CD2	-8.14	112.48	119.80
1	C	492	THR	CA-CB-CG2	8.13	123.79	112.40
1	C	588	ASP	CB-CG-OD1	8.13	125.62	118.30
1	E	220	PHE	CD1-CE1-CZ	-8.14	110.34	120.10
1	E	302	HIS	N-CA-CB	8.13	125.24	110.60
1	D	67	GLU	CB-CA-C	-8.13	94.14	110.40
1	E	474	ARG	CB-CG-CD	8.13	132.74	111.60
1	F	226	GLN	CB-CA-C	8.13	126.66	110.40
1	A	299	ALA	N-CA-CB	-8.13	98.72	110.10
1	B	299	ALA	N-CA-CB	-8.13	98.72	110.10
1	B	624	TYR	CB-CG-CD2	-8.13	116.12	121.00
1	D	226	GLN	CB-CA-C	8.13	126.66	110.40
1	D	302	HIS	N-CA-CB	8.13	125.23	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	492	THR	CA-CB-CG2	8.12	123.78	112.40
1	A	226	GLN	CB-CA-C	8.12	126.64	110.40
1	B	226	GLN	CB-CA-C	8.12	126.64	110.40
1	C	302	HIS	N-CA-CB	8.12	125.22	110.60
1	E	67	GLU	CB-CA-C	-8.12	94.16	110.40
1	E	409	SER	N-CA-CB	-8.12	98.32	110.50
1	F	256	PHE	CZ-CE2-CD2	-8.12	110.36	120.10
1	E	299	ALA	N-CA-CB	-8.12	98.73	110.10
1	B	333	TYR	CG-CD2-CE2	8.12	127.80	121.30
1	C	226	GLN	CB-CA-C	8.12	126.63	110.40
1	C	299	ALA	N-CA-CB	-8.12	98.73	110.10
1	D	592	ASP	CB-CG-OD2	-8.12	110.99	118.30
1	B	592	ASP	CB-CG-OD2	-8.12	111.00	118.30
1	F	299	ALA	N-CA-CB	-8.12	98.74	110.10
1	A	333	TYR	CG-CD2-CE2	8.11	127.79	121.30
1	F	67	GLU	CB-CA-C	-8.11	94.17	110.40
1	A	302	HIS	N-CA-CB	8.11	125.20	110.60
1	A	592	ASP	CB-CG-OD2	-8.11	111.00	118.30
1	D	299	ALA	N-CA-CB	-8.11	98.75	110.10
1	E	273	ASP	CA-CB-CG	8.11	131.24	113.40
1	E	333	TYR	CG-CD2-CE2	8.11	127.79	121.30
1	C	333	TYR	CG-CD2-CE2	8.11	127.78	121.30
1	A	492	THR	CA-CB-CG2	8.10	123.75	112.40
1	C	67	GLU	CB-CA-C	-8.10	94.19	110.40
1	D	409	SER	N-CA-CB	-8.10	98.34	110.50
1	A	67	GLU	CB-CA-C	-8.10	94.20	110.40
1	B	409	SER	N-CA-CB	-8.10	98.35	110.50
1	C	273	ASP	CA-CB-CG	8.10	131.22	113.40
1	B	302	HIS	N-CA-CB	8.10	125.17	110.60
1	E	492	THR	CA-CB-CG2	8.10	123.73	112.40
1	F	273	ASP	CA-CB-CG	8.10	131.21	113.40
1	A	409	SER	N-CA-CB	-8.09	98.36	110.50
1	B	67	GLU	CB-CA-C	-8.09	94.22	110.40
1	B	290	GLU	OE1-CD-OE2	-8.09	113.59	123.30
1	C	592	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	A	273	ASP	CA-CB-CG	8.09	131.20	113.40
1	B	492	THR	CA-CB-CG2	8.09	123.72	112.40
1	D	492	THR	CA-CB-CG2	8.09	123.73	112.40
1	D	521	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	F	302	HIS	N-CA-CB	8.09	125.16	110.60
1	B	273	ASP	CA-CB-CG	8.09	131.19	113.40
1	F	409	SER	N-CA-CB	-8.09	98.37	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	273	ASP	CA-CB-CG	8.09	131.19	113.40
1	D	290	GLU	OE1-CD-OE2	-8.09	113.60	123.30
1	D	624	TYR	CB-CG-CD2	-8.09	116.15	121.00
1	C	644	HIS	CA-CB-CG	8.08	127.34	113.60
1	C	409	SER	N-CA-CB	-8.08	98.38	110.50
1	B	644	HIS	CA-CB-CG	8.08	127.33	113.60
1	C	290	GLU	OE1-CD-OE2	-8.08	113.61	123.30
1	D	250	ARG	NE-CZ-NH1	-8.08	116.26	120.30
1	F	290	GLU	OE1-CD-OE2	-8.08	113.61	123.30
1	F	624	TYR	CB-CG-CD2	-8.08	116.16	121.00
1	F	644	HIS	CA-CB-CG	8.07	127.33	113.60
1	C	250	ARG	NE-CZ-NH1	-8.07	116.26	120.30
1	A	290	GLU	OE1-CD-OE2	-8.07	113.62	123.30
1	A	644	HIS	CA-CB-CG	8.06	127.31	113.60
1	D	644	HIS	CA-CB-CG	8.06	127.31	113.60
1	B	205	TRP	CA-C-O	-8.06	103.17	120.10
1	C	205	TRP	CA-C-O	-8.06	103.17	120.10
1	D	491	ILE	CA-C-N	8.06	134.93	117.20
1	A	205	TRP	CA-C-O	-8.06	103.18	120.10
1	A	491	ILE	CA-C-N	8.05	134.92	117.20
1	C	491	ILE	CA-C-N	8.05	134.92	117.20
1	E	592	ASP	CB-CG-OD2	-8.05	111.05	118.30
1	F	491	ILE	CA-C-N	8.05	134.92	117.20
1	F	521	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	B	250	ARG	NE-CZ-NH1	-8.05	116.28	120.30
1	C	608	GLN	CB-CG-CD	8.05	132.53	111.60
1	E	205	TRP	CA-C-O	-8.05	103.20	120.10
1	D	205	TRP	CA-C-O	-8.04	103.20	120.10
1	E	491	ILE	CA-C-N	8.04	134.90	117.20
1	E	644	HIS	CA-CB-CG	8.04	127.28	113.60
1	F	205	TRP	CA-C-O	-8.04	103.21	120.10
1	A	608	GLN	CB-CG-CD	8.04	132.50	111.60
1	E	290	GLU	OE1-CD-OE2	-8.04	113.65	123.30
1	A	250	ARG	NE-CZ-NH1	-8.04	116.28	120.30
1	F	608	GLN	CB-CG-CD	8.04	132.50	111.60
1	B	521	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	B	608	GLN	CB-CG-CD	8.04	132.49	111.60
1	F	489	ASN	N-CA-C	-8.04	89.31	111.00
1	B	491	ILE	CA-C-N	8.03	134.87	117.20
1	E	608	GLN	CB-CG-CD	8.03	132.47	111.60
1	D	489	ASN	N-CA-C	-8.03	89.33	111.00
1	E	101	SER	CB-CA-C	8.02	125.34	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	489	ASN	N-CA-C	-8.02	89.34	111.00
1	E	489	ASN	N-CA-C	-8.02	89.34	111.00
1	A	489	ASN	N-CA-C	-8.02	89.35	111.00
1	D	395	THR	O-C-N	8.02	135.53	122.70
1	C	427	ASP	N-CA-CB	-8.02	96.17	110.60
1	A	395	THR	O-C-N	8.01	135.52	122.70
1	C	489	ASN	N-CA-C	-8.01	89.37	111.00
1	F	49	HIS	N-CA-CB	8.01	125.03	110.60
1	D	608	GLN	CB-CG-CD	8.01	132.43	111.60
1	F	101	SER	CB-CA-C	8.01	125.32	110.10
1	A	101	SER	CB-CA-C	8.01	125.32	110.10
1	A	427	ASP	N-CA-CB	-8.01	96.18	110.60
1	B	101	SER	CB-CA-C	8.01	125.32	110.10
1	C	101	SER	CB-CA-C	8.01	125.32	110.10
1	D	49	HIS	N-CA-CB	8.01	125.02	110.60
1	F	332	LYS	CA-CB-CG	-8.01	95.78	113.40
1	C	395	THR	O-C-N	8.01	135.51	122.70
1	D	101	SER	CB-CA-C	8.01	125.31	110.10
1	E	427	ASP	N-CA-CB	-8.01	96.19	110.60
1	F	395	THR	O-C-N	8.01	135.51	122.70
1	E	49	HIS	N-CA-CB	8.01	125.01	110.60
1	E	395	THR	O-C-N	8.01	135.51	122.70
1	F	285	HIS	CA-C-O	-8.00	103.30	120.10
1	C	285	HIS	CA-C-O	-8.00	103.30	120.10
1	B	427	ASP	N-CA-CB	-8.00	96.20	110.60
1	D	285	HIS	CA-C-O	-8.00	103.30	120.10
1	F	427	ASP	N-CA-CB	-8.00	96.20	110.60
1	A	285	HIS	CA-C-O	-8.00	103.31	120.10
1	A	49	HIS	N-CA-CB	7.99	124.99	110.60
1	A	521	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	D	332	LYS	CA-CB-CG	-7.99	95.81	113.40
1	A	332	LYS	CA-CB-CG	-7.99	95.82	113.40
1	C	521	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	D	427	ASP	N-CA-CB	-7.99	96.22	110.60
1	B	49	HIS	N-CA-CB	7.99	124.98	110.60
1	B	285	HIS	CA-C-O	-7.99	103.33	120.10
1	C	332	LYS	CA-CB-CG	-7.99	95.83	113.40
1	E	84	LEU	CB-CA-C	7.98	125.37	110.20
1	C	49	HIS	N-CA-CB	7.98	124.97	110.60
1	C	345	ASN	OD1-CG-ND2	7.98	140.25	121.90
1	E	169	SER	N-CA-CB	-7.98	98.53	110.50
1	E	285	HIS	CA-C-O	-7.98	103.34	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	332	LYS	CA-CB-CG	-7.98	95.85	113.40
1	B	332	LYS	CA-CB-CG	-7.98	95.85	113.40
1	B	390	ILE	N-CA-C	-7.98	89.46	111.00
1	B	395	THR	O-C-N	7.98	135.47	122.70
1	C	40	LEU	CB-CG-CD2	-7.98	97.44	111.00
1	D	390	ILE	N-CA-C	-7.98	89.46	111.00
1	E	390	ILE	N-CA-C	-7.98	89.46	111.00
1	D	82	GLU	CG-CD-OE2	7.98	134.25	118.30
1	E	40	LEU	CB-CG-CD2	-7.98	97.44	111.00
1	F	390	ILE	N-CA-C	-7.97	89.47	111.00
1	A	390	ILE	N-CA-C	-7.97	89.47	111.00
1	C	82	GLU	CG-CD-OE2	7.97	134.25	118.30
1	F	84	LEU	CB-CA-C	7.97	125.34	110.20
1	C	390	ILE	N-CA-C	-7.97	89.49	111.00
1	A	82	GLU	CG-CD-OE2	7.97	134.23	118.30
1	A	84	LEU	CB-CA-C	7.97	125.34	110.20
1	F	40	LEU	CB-CG-CD2	-7.97	97.46	111.00
1	B	345	ASN	OD1-CG-ND2	7.96	140.22	121.90
1	D	84	LEU	CB-CA-C	7.96	125.33	110.20
1	E	250	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	F	82	GLU	CG-CD-OE2	7.96	134.23	118.30
1	F	169	SER	N-CA-CB	-7.96	98.55	110.50
1	F	305	ILE	O-C-N	7.96	135.44	122.70
1	B	84	LEU	CB-CA-C	7.96	125.33	110.20
1	D	72	TYR	CA-C-O	-7.96	103.38	120.10
1	E	175	LYS	CA-CB-CG	7.96	130.92	113.40
1	F	250	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	B	175	LYS	CA-CB-CG	7.96	130.91	113.40
1	A	169	SER	N-CA-CB	-7.96	98.56	110.50
1	B	82	GLU	CG-CD-OE2	7.96	134.22	118.30
1	F	340	TYR	CZ-CE2-CD2	-7.96	112.64	119.80
1	A	40	LEU	CB-CG-CD2	-7.96	97.47	111.00
1	E	82	GLU	CG-CD-OE2	7.96	134.22	118.30
1	A	345	ASN	OD1-CG-ND2	7.96	140.20	121.90
1	F	345	ASN	OD1-CG-ND2	7.95	140.19	121.90
1	B	40	LEU	CB-CG-CD2	-7.95	97.48	111.00
1	D	345	ASN	OD1-CG-ND2	7.95	140.18	121.90
1	A	72	TYR	CA-C-O	-7.95	103.41	120.10
1	B	169	SER	N-CA-CB	-7.95	98.58	110.50
1	D	40	LEU	CB-CG-CD2	-7.95	97.49	111.00
1	B	221	PHE	CG-CD2-CE2	7.94	129.54	120.80
1	C	84	LEU	CB-CA-C	7.94	125.29	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	72	TYR	CA-C-O	-7.94	103.43	120.10
1	A	175	LYS	CA-CB-CG	7.94	130.87	113.40
1	C	169	SER	N-CA-CB	-7.94	98.59	110.50
1	B	340	TYR	CZ-CE2-CD2	-7.94	112.66	119.80
1	C	72	TYR	CA-C-O	-7.94	103.43	120.10
1	E	334	SER	CB-CA-C	-7.94	95.02	110.10
1	C	340	TYR	CZ-CE2-CD2	-7.93	112.66	119.80
1	D	494	THR	N-CA-C	7.93	132.43	111.00
1	C	175	LYS	CA-CB-CG	7.93	130.85	113.40
1	D	169	SER	N-CA-CB	-7.93	98.60	110.50
1	E	72	TYR	CA-C-O	-7.93	103.44	120.10
1	E	494	THR	N-CA-C	7.93	132.42	111.00
1	B	494	THR	N-CA-C	7.93	132.41	111.00
1	E	345	ASN	OD1-CG-ND2	7.93	140.14	121.90
1	D	175	LYS	CA-CB-CG	7.93	130.85	113.40
1	E	305	ILE	O-C-N	7.93	135.39	122.70
1	F	175	LYS	CA-CB-CG	7.93	130.84	113.40
1	B	305	ILE	O-C-N	7.93	135.38	122.70
1	C	494	THR	N-CA-C	7.93	132.40	111.00
1	E	521	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	F	494	THR	N-CA-C	7.93	132.40	111.00
1	A	494	THR	N-CA-C	7.92	132.39	111.00
1	C	305	ILE	O-C-N	7.92	135.38	122.70
1	C	334	SER	CB-CA-C	-7.92	95.05	110.10
1	E	152	ASP	CB-CG-OD1	7.92	125.43	118.30
1	A	334	SER	CB-CA-C	-7.92	95.05	110.10
1	A	305	ILE	O-C-N	7.92	135.37	122.70
1	B	72	TYR	CA-C-O	-7.92	103.47	120.10
1	D	152	ASP	CB-CG-OD1	7.92	125.43	118.30
1	D	334	SER	CB-CA-C	-7.92	95.05	110.10
1	F	334	SER	CB-CA-C	-7.92	95.06	110.10
1	C	247	HIS	CA-C-O	-7.91	103.49	120.10
1	C	653	LEU	CB-CA-C	7.91	125.23	110.20
1	D	247	HIS	CA-C-O	-7.91	103.49	120.10
1	B	334	SER	CB-CA-C	-7.91	95.08	110.10
1	D	305	ILE	O-C-N	7.91	135.35	122.70
1	C	152	ASP	CB-CG-OD1	7.90	125.41	118.30
1	C	221	PHE	CG-CD2-CE2	7.90	129.49	120.80
1	A	221	PHE	CG-CD2-CE2	7.90	129.49	120.80
1	A	340	TYR	CZ-CE2-CD2	-7.90	112.69	119.80
1	B	653	LEU	CB-CA-C	7.90	125.21	110.20
1	A	653	LEU	CB-CA-C	7.90	125.21	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	221	PHE	CG-CD2-CE2	7.90	129.49	120.80
1	F	653	LEU	CB-CA-C	7.90	125.21	110.20
1	B	247	HIS	CA-C-O	-7.90	103.51	120.10
1	E	247	HIS	CA-C-O	-7.90	103.51	120.10
1	A	247	HIS	CA-C-O	-7.90	103.52	120.10
1	A	265	GLY	CA-C-N	7.90	131.99	116.20
1	D	653	LEU	CB-CA-C	7.90	125.20	110.20
1	D	265	GLY	CA-C-N	7.89	131.99	116.20
1	E	653	LEU	CB-CA-C	7.89	125.20	110.20
1	A	152	ASP	CB-CG-OD1	7.89	125.40	118.30
1	C	502	CYS	N-CA-CB	7.89	124.80	110.60
1	B	152	ASP	CB-CG-OD1	7.89	125.40	118.30
1	E	265	GLY	CA-C-N	7.89	131.98	116.20
1	E	340	TYR	CZ-CE2-CD2	-7.89	112.70	119.80
1	D	502	CYS	N-CA-CB	7.89	124.80	110.60
1	F	141	THR	CA-CB-CG2	-7.89	101.36	112.40
1	C	17	LEU	CA-C-O	-7.89	103.54	120.10
1	C	265	GLY	CA-C-N	7.89	131.97	116.20
1	E	221	PHE	CG-CD2-CE2	7.89	129.48	120.80
1	B	265	GLY	CA-C-N	7.88	131.97	116.20
1	E	160	THR	CA-CB-CG2	-7.88	101.36	112.40
1	F	221	PHE	CG-CD2-CE2	7.88	129.47	120.80
1	B	17	LEU	CA-C-O	-7.88	103.55	120.10
1	D	160	THR	CA-CB-CG2	-7.88	101.36	112.40
1	F	416	VAL	CA-CB-CG1	7.88	122.72	110.90
1	D	141	THR	CA-CB-CG2	-7.88	101.37	112.40
1	A	17	LEU	CA-C-O	-7.88	103.56	120.10
1	A	502	CYS	N-CA-CB	7.88	124.78	110.60
1	E	141	THR	CA-CB-CG2	-7.88	101.37	112.40
1	C	228	THR	OG1-CB-CG2	7.88	128.12	110.00
1	D	340	TYR	CZ-CE2-CD2	-7.88	112.71	119.80
1	F	152	ASP	CB-CG-OD1	7.88	125.39	118.30
1	F	502	CYS	N-CA-CB	7.88	124.78	110.60
1	F	247	HIS	CA-C-O	-7.88	103.56	120.10
1	C	416	VAL	CA-CB-CG1	7.87	122.71	110.90
1	F	265	GLY	CA-C-N	7.87	131.95	116.20
1	A	141	THR	CA-CB-CG2	-7.87	101.38	112.40
1	B	390	ILE	N-CA-CB	7.87	128.90	110.80
1	F	183	TYR	CZ-CE2-CD2	-7.87	112.72	119.80
1	D	17	LEU	CA-C-O	-7.87	103.57	120.10
1	C	183	TYR	CZ-CE2-CD2	-7.87	112.72	119.80
1	E	17	LEU	CA-C-O	-7.87	103.58	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	244	ASP	OD1-CG-OD2	-7.87	108.36	123.30
1	E	390	ILE	N-CA-CB	7.87	128.89	110.80
1	F	17	LEU	CA-C-O	-7.87	103.58	120.10
1	A	183	TYR	CZ-CE2-CD2	-7.86	112.72	119.80
1	A	244	ASP	OD1-CG-OD2	-7.86	108.36	123.30
1	B	183	TYR	CZ-CE2-CD2	-7.86	112.72	119.80
1	B	502	CYS	N-CA-CB	7.86	124.75	110.60
1	B	199	MET	CA-CB-CG	7.86	126.66	113.30
1	C	160	THR	CA-CB-CG2	-7.86	101.40	112.40
1	D	244	ASP	OD1-CG-OD2	-7.86	108.37	123.30
1	E	502	CYS	N-CA-CB	7.86	124.75	110.60
1	F	244	ASP	OD1-CG-OD2	-7.86	108.36	123.30
1	B	244	ASP	OD1-CG-OD2	-7.86	108.37	123.30
1	A	160	THR	CA-CB-CG2	-7.86	101.40	112.40
1	E	228	THR	OG1-CB-CG2	7.86	128.07	110.00
1	E	429	PHE	CB-CG-CD1	-7.86	115.30	120.80
1	F	228	THR	OG1-CB-CG2	7.86	128.07	110.00
1	F	309	ASP	C-N-CA	-7.86	105.80	122.30
1	A	390	ILE	N-CA-CB	7.86	128.87	110.80
1	B	416	VAL	CA-CB-CG1	7.86	122.68	110.90
1	D	228	THR	OG1-CB-CG2	7.86	128.07	110.00
1	F	160	THR	CA-CB-CG2	-7.86	101.40	112.40
1	A	228	THR	OG1-CB-CG2	7.85	128.06	110.00
1	C	390	ILE	N-CA-CB	7.85	128.86	110.80
1	D	183	TYR	CZ-CE2-CD2	-7.85	112.73	119.80
1	D	199	MET	CA-CB-CG	7.85	126.65	113.30
1	A	309	ASP	C-N-CA	-7.85	105.82	122.30
1	C	141	THR	CA-CB-CG2	-7.85	101.41	112.40
1	A	416	VAL	CA-CB-CG1	7.85	122.67	110.90
1	B	141	THR	CA-CB-CG2	-7.85	101.41	112.40
1	E	309	ASP	C-N-CA	-7.85	105.82	122.30
1	F	390	ILE	N-CA-CB	7.85	128.85	110.80
1	B	228	THR	OG1-CB-CG2	7.85	128.05	110.00
1	D	510	GLN	CB-CA-C	-7.85	94.71	110.40
1	E	244	ASP	OD1-CG-OD2	-7.85	108.39	123.30
1	D	390	ILE	N-CA-CB	7.84	128.84	110.80
1	C	309	ASP	C-N-CA	-7.84	105.83	122.30
1	D	309	ASP	C-N-CA	-7.84	105.83	122.30
1	B	160	THR	CA-CB-CG2	-7.84	101.42	112.40
1	B	510	GLN	CB-CA-C	-7.84	94.72	110.40
1	C	510	GLN	CB-CA-C	-7.84	94.72	110.40
1	E	171	THR	N-CA-C	7.84	132.17	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	183	TYR	CZ-CE2-CD2	-7.84	112.74	119.80
1	E	228	THR	CA-CB-OG1	-7.84	92.53	109.00
1	A	429	PHE	CB-CG-CD1	-7.84	115.31	120.80
1	E	416	VAL	CA-CB-CG1	7.84	122.66	110.90
1	A	510	GLN	CB-CA-C	-7.84	94.72	110.40
1	A	199	MET	CA-CB-CG	7.84	126.62	113.30
1	E	510	GLN	CB-CA-C	-7.84	94.73	110.40
1	B	228	THR	CA-CB-OG1	-7.83	92.55	109.00
1	B	309	ASP	C-N-CA	-7.83	105.85	122.30
1	B	429	PHE	CB-CG-CD1	-7.83	115.32	120.80
1	C	429	PHE	CB-CG-CD1	-7.83	115.32	120.80
1	D	416	VAL	CA-CB-CG1	7.83	122.65	110.90
1	F	171	THR	N-CA-C	7.83	132.15	111.00
1	D	205	TRP	CA-C-N	7.83	134.43	117.20
1	F	228	THR	CA-CB-OG1	-7.83	92.56	109.00
1	A	228	THR	CA-CB-OG1	-7.83	92.56	109.00
1	B	171	THR	N-CA-C	7.83	132.13	111.00
1	C	228	THR	CA-CB-OG1	-7.83	92.56	109.00
1	F	199	MET	CA-CB-CG	7.83	126.61	113.30
1	C	65	LEU	CA-C-N	7.83	134.42	117.20
1	B	486	GLU	O-C-N	-7.82	110.18	122.70
1	D	65	LEU	CA-C-N	7.82	134.41	117.20
1	D	228	THR	CA-CB-OG1	-7.82	92.57	109.00
1	E	199	MET	CA-CB-CG	7.82	126.60	113.30
1	F	510	GLN	CB-CA-C	-7.82	94.75	110.40
1	B	631	PRO	CA-C-O	-7.82	101.43	120.20
1	C	171	THR	N-CA-C	7.82	132.12	111.00
1	F	75	PHE	O-C-N	7.82	135.21	122.70
1	F	429	PHE	CB-CG-CD1	-7.82	115.33	120.80
1	B	550	GLY	CA-C-O	-7.82	106.53	120.60
1	D	631	PRO	CA-C-O	-7.82	101.44	120.20
1	A	171	THR	N-CA-C	7.82	132.10	111.00
1	E	177	ARG	CD-NE-CZ	-7.82	112.66	123.60
1	C	199	MET	CA-CB-CG	7.81	126.58	113.30
1	C	631	PRO	CA-C-O	-7.81	101.45	120.20
1	E	205	TRP	CA-C-N	7.81	134.39	117.20
1	F	486	GLU	O-C-N	-7.81	110.20	122.70
1	F	631	PRO	CA-C-O	-7.81	101.45	120.20
1	E	65	LEU	CA-C-N	7.81	134.38	117.20
1	A	65	LEU	CA-C-N	7.81	134.38	117.20
1	A	205	TRP	CA-C-N	7.81	134.38	117.20
1	B	65	LEU	CA-C-N	7.81	134.38	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	550	GLY	CA-C-O	-7.80	106.55	120.60
1	D	171	THR	N-CA-C	7.80	132.07	111.00
1	A	631	PRO	CA-C-O	-7.80	101.47	120.20
1	B	205	TRP	CA-C-N	7.80	134.37	117.20
1	F	177	ARG	CD-NE-CZ	-7.80	112.68	123.60
1	D	177	ARG	CD-NE-CZ	-7.80	112.68	123.60
1	B	177	ARG	CD-NE-CZ	-7.80	112.68	123.60
1	B	483	CYS	CA-CB-SG	-7.80	99.96	114.00
1	E	75	PHE	O-C-N	7.80	135.18	122.70
1	F	550	GLY	CA-C-O	-7.80	106.56	120.60
1	E	483	CYS	CA-CB-SG	-7.80	99.96	114.00
1	C	205	TRP	CA-C-N	7.80	134.35	117.20
1	C	486	GLU	O-C-N	-7.80	110.23	122.70
1	D	550	GLY	CA-C-O	-7.80	106.56	120.60
1	E	486	GLU	O-C-N	-7.80	110.23	122.70
1	F	65	LEU	CA-C-N	7.80	134.35	117.20
1	F	205	TRP	CA-C-N	7.80	134.35	117.20
1	F	483	CYS	CA-CB-SG	-7.80	99.97	114.00
1	A	483	CYS	CA-CB-SG	-7.79	99.97	114.00
1	E	631	PRO	CA-C-O	-7.79	101.49	120.20
1	D	429	PHE	CB-CG-CD1	-7.79	115.34	120.80
1	D	483	CYS	CA-CB-SG	-7.79	99.97	114.00
1	A	177	ARG	CD-NE-CZ	-7.79	112.69	123.60
1	C	550	GLY	CA-C-O	-7.79	106.58	120.60
1	D	75	PHE	O-C-N	7.79	135.17	122.70
1	C	75	PHE	O-C-N	7.79	135.16	122.70
1	D	92	GLN	CG-CD-OE1	-7.79	106.02	121.60
1	A	486	GLU	O-C-N	-7.79	110.24	122.70
1	E	550	GLY	CA-C-O	-7.79	106.58	120.60
1	B	75	PHE	O-C-N	7.78	135.15	122.70
1	B	92	GLN	CG-CD-OE1	-7.78	106.03	121.60
1	C	92	GLN	CG-CD-OE1	-7.78	106.03	121.60
1	C	483	CYS	CA-CB-SG	-7.78	99.99	114.00
1	D	396	ASP	N-CA-CB	-7.78	96.59	110.60
1	A	75	PHE	O-C-N	7.78	135.15	122.70
1	C	177	ARG	CD-NE-CZ	-7.78	112.71	123.60
1	F	92	GLN	CG-CD-OE1	-7.78	106.04	121.60
1	D	486	GLU	O-C-N	-7.77	110.26	122.70
1	D	504	GLU	OE1-CD-OE2	7.77	132.63	123.30
1	E	396	ASP	N-CA-CB	-7.77	96.61	110.60
1	D	25	THR	CB-CA-C	-7.77	90.63	111.60
1	D	482	LEU	CA-C-O	-7.77	103.79	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	GLN	CG-CD-OE1	-7.76	106.07	121.60
1	C	396	ASP	N-CA-CB	-7.76	96.62	110.60
1	E	92	GLN	CG-CD-OE1	-7.76	106.07	121.60
1	A	396	ASP	N-CA-CB	-7.76	96.63	110.60
1	A	25	THR	CB-CA-C	-7.76	90.64	111.60
1	B	504	GLU	OE1-CD-OE2	7.76	132.62	123.30
1	F	25	THR	CB-CA-C	-7.76	90.65	111.60
1	F	396	ASP	N-CA-CB	-7.76	96.64	110.60
1	F	482	LEU	CA-C-O	-7.76	103.81	120.10
1	B	25	THR	CB-CA-C	-7.76	90.66	111.60
1	E	25	THR	CB-CA-C	-7.75	90.67	111.60
1	C	25	THR	CB-CA-C	-7.75	90.67	111.60
1	D	487	ASP	N-CA-C	7.75	131.93	111.00
1	E	487	ASP	N-CA-C	7.75	131.93	111.00
1	A	482	LEU	CA-C-O	-7.75	103.83	120.10
1	C	482	LEU	CA-C-O	-7.75	103.83	120.10
1	A	487	ASP	N-CA-C	7.75	131.92	111.00
1	E	504	GLU	OE1-CD-OE2	7.75	132.59	123.30
1	E	482	LEU	CA-C-O	-7.74	103.84	120.10
1	B	487	ASP	N-CA-C	7.74	131.91	111.00
1	C	487	ASP	N-CA-C	7.74	131.90	111.00
1	F	360	LYS	O-C-N	7.74	135.08	122.70
1	B	396	ASP	N-CA-CB	-7.74	96.67	110.60
1	B	482	LEU	CA-C-O	-7.74	103.86	120.10
1	F	504	GLU	OE1-CD-OE2	7.74	132.58	123.30
1	B	360	LYS	O-C-N	7.73	135.07	122.70
1	E	360	LYS	O-C-N	7.73	135.07	122.70
1	A	360	LYS	O-C-N	7.73	135.07	122.70
1	F	487	ASP	N-CA-C	7.73	131.87	111.00
1	B	32	ASP	CB-CG-OD1	7.73	125.25	118.30
1	E	199	MET	CG-SD-CE	7.72	112.56	100.20
1	A	504	GLU	OE1-CD-OE2	7.72	132.57	123.30
1	B	199	MET	CG-SD-CE	7.72	112.56	100.20
1	D	360	LYS	O-C-N	7.72	135.05	122.70
1	F	199	MET	CG-SD-CE	7.72	112.55	100.20
1	F	644	HIS	O-C-N	7.72	135.05	122.70
1	B	368	MET	N-CA-CB	-7.72	96.70	110.60
1	C	199	MET	CG-SD-CE	7.72	112.55	100.20
1	C	360	LYS	O-C-N	7.72	135.05	122.70
1	D	199	MET	CG-SD-CE	7.72	112.55	100.20
1	F	489	ASN	N-CA-CB	7.72	124.50	110.60
1	B	644	HIS	O-C-N	7.72	135.05	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	644	HIS	O-C-N	7.71	135.04	122.70
1	A	199	MET	CG-SD-CE	7.71	112.54	100.20
1	C	32	ASP	CB-CG-OD1	7.71	125.24	118.30
1	C	504	GLU	OE1-CD-OE2	7.71	132.55	123.30
1	D	489	ASN	N-CA-CB	7.71	124.47	110.60
1	B	439	SER	CA-C-O	-7.70	103.92	120.10
1	D	368	MET	N-CA-CB	-7.70	96.73	110.60
1	A	644	HIS	O-C-N	7.70	135.02	122.70
1	C	368	MET	N-CA-CB	-7.70	96.74	110.60
1	D	499	ARG	NH1-CZ-NH2	-7.70	110.93	119.40
1	E	607	ALA	CB-CA-C	7.70	121.65	110.10
1	F	439	SER	CA-C-O	-7.70	103.93	120.10
1	C	489	ASN	N-CA-CB	7.70	124.46	110.60
1	C	607	ALA	CB-CA-C	7.70	121.65	110.10
1	D	438	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	D	439	SER	CA-C-O	-7.70	103.94	120.10
1	E	368	MET	N-CA-CB	-7.70	96.75	110.60
1	E	644	HIS	O-C-N	7.70	135.01	122.70
1	F	453	HIS	N-CA-CB	-7.70	96.75	110.60
1	C	438	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	C	439	SER	CA-C-O	-7.69	103.95	120.10
1	A	368	MET	N-CA-CB	-7.69	96.76	110.60
1	A	439	SER	CA-C-O	-7.69	103.95	120.10
1	F	32	ASP	CB-CG-OD1	7.69	125.22	118.30
1	F	368	MET	N-CA-CB	-7.69	96.76	110.60
1	D	32	ASP	CB-CG-OD1	7.69	125.22	118.30
1	A	32	ASP	CB-CG-OD1	7.69	125.22	118.30
1	A	489	ASN	N-CA-CB	7.68	124.43	110.60
1	A	607	ALA	CB-CA-C	7.68	121.63	110.10
1	D	607	ALA	CB-CA-C	7.68	121.63	110.10
1	F	438	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	E	489	ASN	N-CA-CB	7.68	124.43	110.60
1	F	607	ALA	CB-CA-C	7.68	121.62	110.10
1	B	438	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	B	453	HIS	N-CA-CB	-7.68	96.78	110.60
1	C	453	HIS	N-CA-CB	-7.68	96.78	110.60
1	C	499	ARG	NH1-CZ-NH2	-7.68	110.95	119.40
1	A	453	HIS	N-CA-CB	-7.67	96.79	110.60
1	D	453	HIS	N-CA-CB	-7.67	96.78	110.60
1	C	22	TYR	O-C-N	7.67	134.97	122.70
1	F	22	TYR	O-C-N	7.67	134.97	122.70
1	B	489	ASN	N-CA-CB	7.67	124.41	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	607	ALA	CB-CA-C	7.67	121.60	110.10
1	D	644	HIS	O-C-N	7.67	134.97	122.70
1	E	439	SER	CA-C-O	-7.67	104.00	120.10
1	B	499	ARG	NH1-CZ-NH2	-7.67	110.97	119.40
1	E	453	HIS	N-CA-CB	-7.67	96.80	110.60
1	A	499	ARG	NH1-CZ-NH2	-7.66	110.97	119.40
1	F	179	GLN	CB-CA-C	7.66	125.73	110.40
1	E	22	TYR	O-C-N	7.66	134.96	122.70
1	A	438	ASP	CB-CG-OD2	-7.66	111.41	118.30
1	D	290	GLU	CG-CD-OE2	7.66	133.62	118.30
1	B	22	TYR	O-C-N	7.66	134.95	122.70
1	C	290	GLU	CG-CD-OE2	7.66	133.62	118.30
1	D	31	LYS	N-CA-CB	7.66	124.38	110.60
1	A	22	TYR	O-C-N	7.66	134.95	122.70
1	D	179	GLN	CB-CA-C	7.66	125.71	110.40
1	E	179	GLN	CB-CA-C	7.66	125.71	110.40
1	F	31	LYS	N-CA-CB	7.66	124.38	110.60
1	B	179	GLN	CB-CA-C	7.65	125.70	110.40
1	C	179	GLN	CB-CA-C	7.65	125.70	110.40
1	D	510	GLN	O-C-N	7.65	134.94	122.70
1	E	49	HIS	CA-CB-CG	-7.65	100.59	113.60
1	B	290	GLU	CG-CD-OE2	7.65	133.60	118.30
1	A	179	GLN	CB-CA-C	7.65	125.69	110.40
1	F	290	GLU	CG-CD-OE2	7.65	133.59	118.30
1	A	290	GLU	CG-CD-OE2	7.64	133.59	118.30
1	D	22	TYR	O-C-N	7.64	134.93	122.70
1	E	31	LYS	N-CA-CB	7.64	124.36	110.60
1	A	31	LYS	N-CA-CB	7.64	124.35	110.60
1	C	31	LYS	N-CA-CB	7.64	124.35	110.60
1	C	49	HIS	CA-CB-CG	-7.64	100.61	113.60
1	B	31	LYS	N-CA-CB	7.64	124.34	110.60
1	E	499	ARG	NH1-CZ-NH2	-7.64	111.00	119.40
1	E	438	ASP	CB-CG-OD2	-7.63	111.43	118.30
1	E	510	GLN	O-C-N	7.63	134.91	122.70
1	A	49	HIS	CA-CB-CG	-7.63	100.62	113.60
1	B	49	HIS	CA-CB-CG	-7.63	100.62	113.60
1	F	49	HIS	CA-CB-CG	-7.63	100.62	113.60
1	E	32	ASP	CB-CG-OD1	7.63	125.17	118.30
1	D	76	ASN	CB-CG-OD1	-7.63	106.34	121.60
1	F	499	ARG	NH1-CZ-NH2	-7.63	111.01	119.40
1	A	510	GLN	O-C-N	7.62	134.89	122.70
1	B	511	LYS	N-CA-CB	7.62	124.31	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	277	PHE	CB-CA-C	-7.61	95.17	110.40
1	E	290	GLU	CG-CD-OE2	7.61	133.53	118.30
1	F	510	GLN	O-C-N	7.61	134.88	122.70
1	D	49	HIS	CA-CB-CG	-7.61	100.66	113.60
1	A	76	ASN	CB-CG-OD1	-7.61	106.38	121.60
1	B	510	GLN	O-C-N	7.61	134.87	122.70
1	D	511	LYS	N-CA-CB	7.61	124.29	110.60
1	F	76	ASN	CB-CG-OD1	-7.61	106.39	121.60
1	C	510	GLN	O-C-N	7.60	134.87	122.70
1	E	76	ASN	CB-CG-OD1	-7.60	106.40	121.60
1	C	76	ASN	CB-CG-OD1	-7.60	106.40	121.60
1	F	277	PHE	CB-CA-C	-7.60	95.21	110.40
1	D	277	PHE	CB-CA-C	-7.60	95.21	110.40
1	B	277	PHE	CB-CA-C	-7.59	95.21	110.40
1	D	25	THR	O-C-N	7.59	134.85	122.70
1	A	277	PHE	CB-CA-C	-7.59	95.22	110.40
1	B	25	THR	O-C-N	7.59	134.84	122.70
1	B	76	ASN	CB-CG-OD1	-7.59	106.42	121.60
1	C	511	LYS	N-CA-CB	7.59	124.27	110.60
1	A	511	LYS	N-CA-CB	7.59	124.26	110.60
1	F	511	LYS	N-CA-CB	7.59	124.26	110.60
1	F	391	PHE	CB-CG-CD2	7.59	126.11	120.80
1	D	391	PHE	CB-CG-CD2	7.58	126.11	120.80
1	E	277	PHE	CB-CA-C	-7.58	95.25	110.40
1	E	511	LYS	N-CA-CB	7.57	124.23	110.60
1	C	177	ARG	NE-CZ-NH1	-7.56	116.52	120.30
1	A	25	THR	O-C-N	7.56	134.79	122.70
1	B	457	HIS	O-C-N	7.56	134.79	122.70
1	D	122	SER	O-C-N	7.56	134.79	122.70
1	C	25	THR	O-C-N	7.55	134.79	122.70
1	C	306	THR	CA-CB-OG1	-7.55	93.14	109.00
1	C	309	ASP	CA-CB-CG	-7.55	96.78	113.40
1	F	25	THR	O-C-N	7.55	134.79	122.70
1	D	457	HIS	O-C-N	7.55	134.78	122.70
1	C	126	SER	N-CA-CB	7.55	121.83	110.50
1	F	306	THR	CA-CB-OG1	-7.55	93.14	109.00
1	F	183	TYR	O-C-N	7.55	134.78	122.70
1	D	306	THR	CA-CB-OG1	-7.55	93.15	109.00
1	A	183	TYR	O-C-N	7.54	134.77	122.70
1	E	183	TYR	O-C-N	7.54	134.77	122.70
1	B	306	THR	CA-CB-OG1	-7.54	93.16	109.00
1	A	306	THR	CA-CB-OG1	-7.54	93.17	109.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	391	PHE	CB-CG-CD2	7.54	126.08	120.80
1	A	309	ASP	CA-CB-CG	-7.54	96.82	113.40
1	B	122	SER	O-C-N	7.54	134.76	122.70
1	E	126	SER	N-CA-CB	7.54	121.81	110.50
1	E	306	THR	CA-CB-OG1	-7.54	93.17	109.00
1	C	122	SER	O-C-N	7.54	134.76	122.70
1	E	309	ASP	CA-CB-CG	-7.54	96.82	113.40
1	F	126	SER	N-CA-CB	7.54	121.81	110.50
1	B	126	SER	N-CA-CB	7.54	121.80	110.50
1	E	122	SER	O-C-N	7.53	134.75	122.70
1	F	309	ASP	CA-CB-CG	-7.53	96.83	113.40
1	A	126	SER	N-CA-CB	7.53	121.80	110.50
1	D	309	ASP	CA-CB-CG	-7.53	96.84	113.40
1	A	457	HIS	O-C-N	7.53	134.74	122.70
1	B	309	ASP	CA-CB-CG	-7.53	96.84	113.40
1	C	183	TYR	O-C-N	7.53	134.74	122.70
1	B	391	PHE	CB-CG-CD2	7.52	126.07	120.80
1	A	122	SER	O-C-N	7.52	134.74	122.70
1	B	183	TYR	O-C-N	7.52	134.73	122.70
1	E	278	GLU	OE1-CD-OE2	7.52	132.32	123.30
1	D	183	TYR	O-C-N	7.52	134.73	122.70
1	C	313	ILE	CA-CB-CG2	7.51	125.93	110.90
1	E	25	THR	O-C-N	7.51	134.72	122.70
1	B	313	ILE	CA-CB-CG2	7.51	125.93	110.90
1	A	313	ILE	CA-CB-CG2	7.51	125.92	110.90
1	C	391	PHE	CB-CG-CD2	7.51	126.06	120.80
1	D	126	SER	N-CA-CB	7.51	121.76	110.50
1	E	391	PHE	CB-CG-CD2	7.51	126.06	120.80
1	F	382	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	C	466	MET	N-CA-CB	-7.50	97.09	110.60
1	F	122	SER	O-C-N	7.50	134.71	122.70
1	D	313	ILE	CA-CB-CG2	7.50	125.91	110.90
1	F	313	ILE	CA-CB-CG2	7.50	125.90	110.90
1	C	278	GLU	OE1-CD-OE2	7.50	132.30	123.30
1	F	466	MET	N-CA-CB	-7.50	97.10	110.60
1	F	495	LEU	CB-CG-CD1	7.50	123.75	111.00
1	C	457	HIS	O-C-N	7.50	134.69	122.70
1	E	457	HIS	O-C-N	7.50	134.69	122.70
1	F	457	HIS	O-C-N	7.50	134.69	122.70
1	E	612	HIS	CA-CB-CG	7.50	126.34	113.60
1	E	313	ILE	CA-CB-CG2	7.49	125.89	110.90
1	E	466	MET	N-CA-CB	-7.49	97.11	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	GLU	OE1-CD-OE2	7.49	132.29	123.30
1	A	466	MET	N-CA-CB	-7.49	97.12	110.60
1	D	612	HIS	CA-CB-CG	7.49	126.33	113.60
1	F	177	ARG	NE-CZ-NH1	-7.49	116.56	120.30
1	B	495	LEU	CB-CG-CD1	7.49	123.73	111.00
1	E	495	LEU	CB-CG-CD1	7.49	123.73	111.00
1	B	466	MET	N-CA-CB	-7.49	97.12	110.60
1	C	612	HIS	CA-CB-CG	7.49	126.32	113.60
1	D	278	GLU	OE1-CD-OE2	7.49	132.28	123.30
1	B	69	ARG	CB-CG-CD	7.48	131.04	111.60
1	F	632	ASP	N-CA-CB	7.48	124.06	110.60
1	C	382	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	D	424	THR	CA-CB-CG2	-7.48	101.93	112.40
1	A	495	LEU	CB-CG-CD1	7.48	123.71	111.00
1	F	424	THR	CA-CB-CG2	-7.48	101.93	112.40
1	A	177	ARG	NE-CZ-NH1	-7.47	116.56	120.30
1	B	177	ARG	NE-CZ-NH1	-7.47	116.56	120.30
1	C	495	LEU	CB-CG-CD1	7.47	123.71	111.00
1	D	466	MET	N-CA-CB	-7.47	97.15	110.60
1	F	612	HIS	CA-CB-CG	7.47	126.31	113.60
1	B	554	ASP	N-CA-CB	7.47	124.05	110.60
1	B	612	HIS	CA-CB-CG	7.47	126.30	113.60
1	E	554	ASP	N-CA-CB	7.47	124.05	110.60
1	A	612	HIS	CA-CB-CG	7.47	126.30	113.60
1	D	382	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	D	252	ILE	N-CA-C	-7.47	90.84	111.00
1	D	495	LEU	CB-CG-CD1	7.47	123.69	111.00
1	C	554	ASP	N-CA-CB	7.47	124.04	110.60
1	C	632	ASP	N-CA-CB	7.46	124.03	110.60
1	F	252	ILE	N-CA-C	-7.46	90.85	111.00
1	A	554	ASP	N-CA-CB	7.46	124.03	110.60
1	A	69	ARG	CB-CG-CD	7.46	131.00	111.60
1	A	309	ASP	CB-CG-OD1	-7.46	111.58	118.30
1	B	309	ASP	CB-CG-OD1	-7.46	111.58	118.30
1	C	384	HIS	O-C-N	7.46	134.64	122.70
1	A	632	ASP	N-CA-CB	7.46	124.03	110.60
1	E	309	ASP	CB-CG-OD1	-7.46	111.59	118.30
1	C	69	ARG	CB-CG-CD	7.46	130.99	111.60
1	E	252	ILE	N-CA-C	-7.46	90.86	111.00
1	D	384	HIS	O-C-N	7.46	134.63	122.70
1	E	69	ARG	CB-CG-CD	7.46	130.99	111.60
1	E	424	THR	CA-CB-CG2	-7.46	101.96	112.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	252	ILE	N-CA-C	-7.46	90.87	111.00
1	B	632	ASP	N-CA-CB	7.45	124.02	110.60
1	C	213	LEU	CA-C-O	-7.45	104.45	120.10
1	D	43	THR	N-CA-CB	-7.45	96.14	110.30
1	D	454	ARG	CB-CA-C	7.45	125.31	110.40
1	E	450	ALA	CB-CA-C	7.45	121.28	110.10
1	E	632	ASP	N-CA-CB	7.45	124.02	110.60
1	F	384	HIS	O-C-N	7.45	134.63	122.70
1	F	554	ASP	N-CA-CB	7.45	124.02	110.60
1	A	252	ILE	N-CA-C	-7.45	90.88	111.00
1	A	382	ARG	NE-CZ-NH2	-7.45	116.57	120.30
1	B	50	GLY	N-CA-C	7.45	131.73	113.10
1	B	424	THR	CA-CB-CG2	-7.45	101.97	112.40
1	C	424	THR	CA-CB-CG2	-7.45	101.97	112.40
1	E	469	ASN	CB-CG-OD1	7.45	136.50	121.60
1	A	424	THR	CA-CB-CG2	-7.45	101.97	112.40
1	D	632	ASP	N-CA-CB	7.45	124.01	110.60
1	E	384	HIS	O-C-N	7.45	134.62	122.70
1	B	252	ILE	N-CA-C	-7.45	90.89	111.00
1	B	278	GLU	OE1-CD-OE2	7.45	132.24	123.30
1	D	69	ARG	CB-CG-CD	7.45	130.96	111.60
1	C	606	HIS	N-CA-C	7.45	131.10	111.00
1	F	50	GLY	N-CA-C	7.45	131.71	113.10
1	F	450	ALA	CB-CA-C	7.45	121.27	110.10
1	A	469	ASN	CB-CG-OD1	7.44	136.49	121.60
1	F	43	THR	N-CA-CB	-7.44	96.16	110.30
1	F	69	ARG	CB-CG-CD	7.44	130.95	111.60
1	F	278	GLU	OE1-CD-OE2	7.44	132.23	123.30
1	B	454	ARG	CB-CA-C	7.44	125.28	110.40
1	C	128	LEU	CA-C-O	-7.44	104.48	120.10
1	C	454	ARG	CB-CA-C	7.44	125.28	110.40
1	C	469	ASN	CB-CG-OD1	7.44	136.48	121.60
1	E	43	THR	N-CA-CB	-7.44	96.17	110.30
1	A	43	THR	N-CA-CB	-7.44	96.17	110.30
1	A	384	HIS	O-C-N	7.44	134.60	122.70
1	A	454	ARG	CB-CA-C	7.44	125.28	110.40
1	B	213	LEU	CA-C-O	-7.44	104.48	120.10
1	B	606	HIS	N-CA-C	7.44	131.08	111.00
1	E	128	LEU	CA-C-O	-7.44	104.48	120.10
1	E	213	LEU	CA-C-O	-7.44	104.48	120.10
1	D	50	GLY	N-CA-C	7.44	131.69	113.10
1	E	454	ARG	CB-CA-C	7.44	125.27	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	606	HIS	N-CA-C	7.44	131.08	111.00
1	C	43	THR	N-CA-CB	-7.43	96.17	110.30
1	C	180	ARG	CG-CD-NE	7.43	127.41	111.80
1	A	606	HIS	N-CA-C	7.43	131.06	111.00
1	B	469	ASN	CB-CG-OD1	7.43	136.46	121.60
1	A	50	GLY	N-CA-C	7.43	131.67	113.10
1	A	213	LEU	CA-C-O	-7.43	104.50	120.10
1	B	382	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	C	50	GLY	N-CA-C	7.43	131.67	113.10
1	D	128	LEU	CA-C-O	-7.43	104.50	120.10
1	D	309	ASP	CB-CG-OD1	-7.43	111.61	118.30
1	F	469	ASN	CB-CG-OD1	7.43	136.46	121.60
1	D	529	THR	CA-CB-OG1	-7.43	93.40	109.00
1	C	400	PRO	O-C-N	7.43	134.58	122.70
1	D	554	ASP	N-CA-CB	7.43	123.97	110.60
1	F	560	ARG	NE-CZ-NH1	-7.43	116.59	120.30
1	A	128	LEU	CA-C-O	-7.42	104.51	120.10
1	B	43	THR	N-CA-CB	-7.42	96.20	110.30
1	D	213	LEU	CA-C-O	-7.42	104.51	120.10
1	E	560	ARG	NE-CZ-NH1	-7.42	116.59	120.30
1	F	606	HIS	N-CA-C	7.42	131.04	111.00
1	A	450	ALA	CB-CA-C	7.42	121.23	110.10
1	B	128	LEU	CA-C-O	-7.42	104.51	120.10
1	B	624	TYR	CD1-CE1-CZ	7.42	126.48	119.80
1	D	180	ARG	CG-CD-NE	7.42	127.39	111.80
1	F	309	ASP	CB-CG-OD1	-7.42	111.62	118.30
1	D	469	ASN	CB-CG-OD1	7.42	136.44	121.60
1	A	340	TYR	CD1-CE1-CZ	-7.42	113.12	119.80
1	C	450	ALA	CB-CA-C	7.42	121.23	110.10
1	D	60	LEU	CB-CG-CD2	-7.42	98.39	111.00
1	E	50	GLY	N-CA-C	7.42	131.65	113.10
1	F	213	LEU	CA-C-O	-7.42	104.52	120.10
1	B	450	ALA	CB-CA-C	7.42	121.22	110.10
1	C	388	ASP	CA-C-O	-7.42	104.53	120.10
1	D	606	HIS	N-CA-C	7.42	131.03	111.00
1	F	454	ARG	CB-CA-C	7.42	125.23	110.40
1	F	529	THR	CA-CB-OG1	-7.42	93.42	109.00
1	A	180	ARG	CG-CD-NE	7.42	127.37	111.80
1	B	384	HIS	O-C-N	7.41	134.56	122.70
1	C	309	ASP	CB-CG-OD1	-7.41	111.63	118.30
1	A	60	LEU	CB-CG-CD2	-7.41	98.40	111.00
1	F	180	ARG	CG-CD-NE	7.41	127.36	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	529	THR	CA-CB-OG1	-7.41	93.44	109.00
1	B	340	TYR	CD1-CE1-CZ	-7.41	113.13	119.80
1	C	340	TYR	CD1-CE1-CZ	-7.41	113.13	119.80
1	C	529	THR	CA-CB-OG1	-7.41	93.44	109.00
1	E	60	LEU	CB-CG-CD2	-7.41	98.41	111.00
1	F	128	LEU	CA-C-O	-7.41	104.54	120.10
1	D	340	TYR	CD1-CE1-CZ	-7.41	113.14	119.80
1	E	400	PRO	O-C-N	7.41	134.55	122.70
1	F	400	PRO	O-C-N	7.41	134.55	122.70
1	E	624	TYR	CD1-CE1-CZ	7.40	126.46	119.80
1	D	270	VAL	CB-CA-C	7.40	125.47	111.40
1	E	177	ARG	NE-CZ-NH1	-7.40	116.60	120.30
1	F	499	ARG	CD-NE-CZ	7.40	133.96	123.60
1	A	388	ASP	CA-C-O	-7.40	104.57	120.10
1	B	60	LEU	CB-CG-CD2	-7.40	98.42	111.00
1	E	529	THR	CA-CB-OG1	-7.40	93.46	109.00
1	B	180	ARG	CG-CD-NE	7.40	127.33	111.80
1	B	270	VAL	CB-CA-C	7.40	125.45	111.40
1	D	614	GLU	N-CA-CB	-7.40	97.29	110.60
1	F	614	GLU	N-CA-CB	-7.40	97.29	110.60
1	A	400	PRO	O-C-N	7.39	134.53	122.70
1	C	60	LEU	CB-CG-CD2	-7.39	98.43	111.00
1	D	450	ALA	CB-CA-C	7.39	121.19	110.10
1	D	624	TYR	CD1-CE1-CZ	7.39	126.45	119.80
1	E	180	ARG	CG-CD-NE	7.39	127.33	111.80
1	B	400	PRO	O-C-N	7.39	134.53	122.70
1	E	388	ASP	CA-C-O	-7.39	104.58	120.10
1	F	60	LEU	CB-CG-CD2	-7.39	98.43	111.00
1	E	382	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	F	290	GLU	CA-C-O	-7.39	104.58	120.10
1	F	340	TYR	CD1-CE1-CZ	-7.39	113.15	119.80
1	B	529	THR	CA-CB-OG1	-7.39	93.48	109.00
1	C	108	GLU	OE1-CD-OE2	7.39	132.17	123.30
1	C	270	VAL	CB-CA-C	7.39	125.44	111.40
1	E	290	GLU	CA-C-O	-7.39	104.58	120.10
1	E	340	TYR	CD1-CE1-CZ	-7.39	113.15	119.80
1	D	400	PRO	O-C-N	7.39	134.52	122.70
1	F	246	LEU	CA-C-N	7.39	133.45	117.20
1	C	117	TYR	N-CA-CB	7.39	123.90	110.60
1	A	270	VAL	CB-CA-C	7.38	125.43	111.40
1	B	554	ASP	CB-CA-C	7.38	125.17	110.40
1	C	290	GLU	CA-C-O	-7.38	104.59	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	290	GLU	CA-C-O	-7.38	104.59	120.10
1	D	388	ASP	CA-C-O	-7.38	104.59	120.10
1	F	108	GLU	OE1-CD-OE2	7.38	132.16	123.30
1	A	108	GLU	OE1-CD-OE2	7.38	132.16	123.30
1	B	290	GLU	CA-C-O	-7.38	104.59	120.10
1	B	388	ASP	CA-C-O	-7.38	104.60	120.10
1	C	499	ARG	CD-NE-CZ	7.38	133.93	123.60
1	D	108	GLU	OE1-CD-OE2	7.38	132.16	123.30
1	D	397	SER	N-CA-CB	-7.38	99.43	110.50
1	D	585	ALA	CB-CA-C	7.38	121.17	110.10
1	E	270	VAL	CB-CA-C	7.38	125.42	111.40
1	E	614	GLU	N-CA-CB	-7.38	97.31	110.60
1	F	388	ASP	CA-C-O	-7.38	104.60	120.10
1	B	148	SER	O-C-N	7.38	134.51	122.70
1	D	177	ARG	NE-CZ-NH1	-7.38	116.61	120.30
1	C	554	ASP	CB-CA-C	7.38	125.15	110.40
1	D	246	LEU	CA-C-N	7.38	133.43	117.20
1	D	554	ASP	CB-CA-C	7.38	125.15	110.40
1	E	148	SER	O-C-N	7.38	134.50	122.70
1	C	614	GLU	N-CA-CB	-7.38	97.33	110.60
1	F	554	ASP	CB-CA-C	7.38	125.15	110.40
1	A	290	GLU	CA-C-O	-7.37	104.61	120.10
1	A	554	ASP	CB-CA-C	7.37	125.15	110.40
1	E	117	TYR	N-CA-CB	7.37	123.87	110.60
1	F	270	VAL	CB-CA-C	7.37	125.41	111.40
1	A	614	GLU	N-CA-CB	-7.37	97.33	110.60
1	B	499	ARG	CD-NE-CZ	7.37	133.92	123.60
1	E	108	GLU	OE1-CD-OE2	7.37	132.15	123.30
1	E	499	ARG	CD-NE-CZ	7.37	133.92	123.60
1	F	585	ALA	CB-CA-C	7.37	121.16	110.10
1	F	624	TYR	CD1-CE1-CZ	7.37	126.43	119.80
1	D	117	TYR	N-CA-CB	7.37	123.87	110.60
1	B	614	GLU	N-CA-CB	-7.37	97.33	110.60
1	D	371	PHE	CB-CG-CD1	7.37	125.96	120.80
1	A	499	ARG	CD-NE-CZ	7.37	133.91	123.60
1	A	117	TYR	N-CA-CB	7.37	123.86	110.60
1	A	585	ALA	CB-CA-C	7.37	121.15	110.10
1	B	246	LEU	CA-C-N	7.37	133.40	117.20
1	E	371	PHE	CB-CG-CD1	7.37	125.95	120.80
1	F	148	SER	O-C-N	7.37	134.49	122.70
1	A	246	LEU	CA-C-N	7.36	133.40	117.20
1	B	560	ARG	NE-CZ-NH1	-7.36	116.62	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	246	LEU	CA-C-N	7.36	133.40	117.20
1	A	624	TYR	CD1-CE1-CZ	7.36	126.43	119.80
1	C	397	SER	N-CA-CB	-7.36	99.46	110.50
1	C	534	PRO	CB-CA-C	-7.36	93.60	112.00
1	E	534	PRO	CB-CA-C	-7.36	93.59	112.00
1	A	397	SER	N-CA-CB	-7.36	99.46	110.50
1	A	560	ARG	NE-CZ-NH1	-7.36	116.62	120.30
1	F	117	TYR	N-CA-CB	7.36	123.85	110.60
1	F	534	PRO	CB-CA-C	-7.36	93.60	112.00
1	A	534	PRO	CB-CA-C	-7.36	93.61	112.00
1	B	117	TYR	N-CA-CB	7.36	123.84	110.60
1	B	534	PRO	CB-CA-C	-7.36	93.61	112.00
1	D	148	SER	O-C-N	7.36	134.47	122.70
1	E	585	ALA	CB-CA-C	7.36	121.14	110.10
1	A	148	SER	O-C-N	7.36	134.47	122.70
1	C	474	ARG	CB-CA-C	7.36	125.11	110.40
1	D	499	ARG	CD-NE-CZ	7.35	133.89	123.60
1	C	624	TYR	CD1-CE1-CZ	7.35	126.42	119.80
1	D	91	ASN	CB-CG-OD1	7.35	136.30	121.60
1	D	560	ARG	NE-CZ-NH1	-7.35	116.62	120.30
1	F	91	ASN	CB-CG-OD1	7.35	136.30	121.60
1	B	371	PHE	CB-CG-CD1	7.35	125.94	120.80
1	C	560	ARG	NE-CZ-NH1	-7.35	116.63	120.30
1	D	534	PRO	CB-CA-C	-7.35	93.63	112.00
1	B	397	SER	N-CA-CB	-7.34	99.48	110.50
1	B	474	ARG	CB-CA-C	7.34	125.09	110.40
1	E	554	ASP	CB-CA-C	7.34	125.09	110.40
1	B	585	ALA	CB-CA-C	7.34	121.11	110.10
1	E	474	ARG	CB-CA-C	7.34	125.08	110.40
1	F	474	ARG	CB-CA-C	7.34	125.08	110.40
1	A	474	ARG	CB-CA-C	7.34	125.08	110.40
1	C	246	LEU	CA-C-N	7.34	133.35	117.20
1	F	371	PHE	CB-CG-CD1	7.34	125.94	120.80
1	F	395	THR	CA-C-O	-7.34	104.69	120.10
1	C	148	SER	O-C-N	7.34	134.44	122.70
1	E	91	ASN	CB-CG-OD1	7.34	136.27	121.60
1	A	91	ASN	CB-CG-OD1	7.33	136.27	121.60
1	A	371	PHE	CB-CG-CD1	7.33	125.93	120.80
1	E	397	SER	N-CA-CB	-7.33	99.50	110.50
1	F	397	SER	N-CA-CB	-7.33	99.50	110.50
1	D	474	ARG	CB-CA-C	7.33	125.06	110.40
1	B	91	ASN	CB-CG-OD1	7.32	136.25	121.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	395	THR	CA-C-O	-7.32	104.72	120.10
1	C	91	ASN	CB-CG-OD1	7.32	136.24	121.60
1	C	585	ALA	CB-CA-C	7.32	121.08	110.10
1	D	547	VAL	O-C-N	7.31	134.40	122.70
1	E	250	ARG	CG-CD-NE	-7.31	96.44	111.80
1	B	108	GLU	OE1-CD-OE2	7.31	132.07	123.30
1	D	395	THR	CA-C-O	-7.31	104.75	120.10
1	A	395	THR	CA-C-O	-7.31	104.75	120.10
1	D	45	ILE	O-C-N	7.31	134.39	122.70
1	B	547	VAL	O-C-N	7.30	134.39	122.70
1	B	395	THR	CA-C-O	-7.30	104.77	120.10
1	D	352	GLY	CA-C-O	-7.30	107.45	120.60
1	F	250	ARG	CG-CD-NE	-7.30	96.46	111.80
1	A	45	ILE	O-C-N	7.30	134.38	122.70
1	D	4	GLY	CA-C-N	-7.30	101.14	117.20
1	E	45	ILE	O-C-N	7.30	134.38	122.70
1	C	395	THR	CA-C-O	-7.30	104.77	120.10
1	F	45	ILE	O-C-N	7.30	134.38	122.70
1	B	560	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	C	248	TRP	O-C-N	7.30	134.37	122.70
1	A	250	ARG	CG-CD-NE	-7.29	96.48	111.80
1	C	371	PHE	CB-CG-CD1	7.29	125.91	120.80
1	D	250	ARG	CG-CD-NE	-7.29	96.48	111.80
1	F	4	GLY	CA-C-N	-7.29	101.16	117.20
1	A	248	TRP	O-C-N	7.29	134.37	122.70
1	A	547	VAL	O-C-N	7.29	134.37	122.70
1	F	352	GLY	CA-C-O	-7.29	107.48	120.60
1	A	4	GLY	CA-C-N	-7.29	101.16	117.20
1	B	250	ARG	CG-CD-NE	-7.29	96.49	111.80
1	C	45	ILE	O-C-N	7.29	134.36	122.70
1	C	352	GLY	CA-C-O	-7.29	107.48	120.60
1	C	4	GLY	CA-C-N	-7.29	101.17	117.20
1	F	65	LEU	N-CA-CB	-7.29	95.83	110.40
1	B	45	ILE	O-C-N	7.29	134.36	122.70
1	F	248	TRP	O-C-N	7.29	134.36	122.70
1	C	468	ASN	CB-CG-OD1	-7.28	107.03	121.60
1	D	310	GLY	N-CA-C	-7.28	94.89	113.10
1	E	4	GLY	CA-C-N	-7.28	101.18	117.20
1	F	468	ASN	CB-CG-OD1	-7.28	107.03	121.60
1	C	65	LEU	N-CA-CB	-7.28	95.83	110.40
1	D	637	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	E	248	TRP	O-C-N	7.28	134.35	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	352	GLY	CA-C-O	-7.28	107.50	120.60
1	F	556	SER	O-C-N	7.28	134.35	122.70
1	E	65	LEU	N-CA-CB	-7.28	95.84	110.40
1	A	468	ASN	CB-CG-OD1	-7.28	107.04	121.60
1	E	547	VAL	O-C-N	7.28	134.34	122.70
1	B	4	GLY	CA-C-N	-7.28	101.20	117.20
1	C	35	GLU	N-CA-CB	-7.28	97.50	110.60
1	C	250	ARG	CG-CD-NE	-7.28	96.52	111.80
1	D	257	ALA	O-C-N	7.28	134.92	121.10
1	D	296	ILE	O-C-N	7.28	134.34	122.70
1	C	310	GLY	N-CA-C	-7.27	94.91	113.10
1	D	248	TRP	O-C-N	7.27	134.34	122.70
1	A	352	GLY	CA-C-O	-7.27	107.51	120.60
1	B	65	LEU	N-CA-CB	-7.27	95.86	110.40
1	B	257	ALA	O-C-N	7.27	134.92	121.10
1	D	468	ASN	CB-CG-OD1	-7.27	107.06	121.60
1	E	468	ASN	CB-CG-OD1	-7.27	107.05	121.60
1	A	65	LEU	N-CA-CB	-7.27	95.86	110.40
1	B	352	GLY	CA-C-O	-7.27	107.51	120.60
1	B	423	ILE	CB-CA-C	7.27	126.14	111.60
1	F	423	ILE	CB-CA-C	7.27	126.14	111.60
1	F	637	ASP	CB-CG-OD2	-7.27	111.76	118.30
1	C	423	ILE	CB-CA-C	7.27	126.14	111.60
1	D	65	LEU	N-CA-CB	-7.27	95.86	110.40
1	A	257	ALA	O-C-N	7.27	134.91	121.10
1	A	310	GLY	N-CA-C	-7.27	94.93	113.10
1	B	310	GLY	N-CA-C	-7.27	94.93	113.10
1	C	547	VAL	O-C-N	7.27	134.33	122.70
1	C	556	SER	O-C-N	7.27	134.33	122.70
1	D	104	ALA	N-CA-C	-7.27	91.38	111.00
1	E	257	ALA	O-C-N	7.27	134.91	121.10
1	E	310	GLY	N-CA-C	-7.27	94.93	113.10
1	B	248	TRP	O-C-N	7.27	134.33	122.70
1	B	556	SER	O-C-N	7.27	134.33	122.70
1	E	423	ILE	CB-CA-C	7.27	126.13	111.60
1	D	35	GLU	N-CA-CB	-7.26	97.52	110.60
1	F	310	GLY	N-CA-C	-7.26	94.94	113.10
1	F	547	VAL	O-C-N	7.26	134.32	122.70
1	A	423	ILE	CB-CA-C	7.26	126.12	111.60
1	A	104	ALA	N-CA-C	-7.26	91.40	111.00
1	B	104	ALA	N-CA-C	-7.26	91.40	111.00
1	D	556	SER	O-C-N	7.26	134.31	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	560	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	B	468	ASN	CB-CG-OD1	-7.26	107.08	121.60
1	D	423	ILE	CB-CA-C	7.26	126.11	111.60
1	E	104	ALA	N-CA-C	-7.26	91.41	111.00
1	B	631	PRO	O-C-N	7.25	134.31	122.70
1	F	560	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	A	35	GLU	N-CA-CB	-7.25	97.55	110.60
1	F	257	ALA	O-C-N	7.25	134.88	121.10
1	B	544	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	A	296	ILE	O-C-N	7.25	134.29	122.70
1	C	104	ALA	N-CA-C	-7.25	91.43	111.00
1	C	637	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	E	453	HIS	CA-CB-CG	-7.25	101.28	113.60
1	B	296	ILE	O-C-N	7.25	134.29	122.70
1	C	620	ARG	CG-CD-NE	-7.25	96.58	111.80
1	A	556	SER	O-C-N	7.24	134.29	122.70
1	B	35	GLU	N-CA-CB	-7.24	97.56	110.60
1	F	104	ALA	N-CA-C	-7.24	91.44	111.00
1	F	296	ILE	O-C-N	7.24	134.29	122.70
1	F	453	HIS	CA-CB-CG	-7.24	101.29	113.60
1	B	453	HIS	CA-CB-CG	-7.24	101.29	113.60
1	C	257	ALA	O-C-N	7.24	134.85	121.10
1	A	453	HIS	CA-CB-CG	-7.24	101.30	113.60
1	F	35	GLU	N-CA-CB	-7.24	97.58	110.60
1	C	296	ILE	O-C-N	7.23	134.28	122.70
1	C	453	HIS	CA-CB-CG	-7.23	101.30	113.60
1	D	620	ARG	CG-CD-NE	-7.23	96.61	111.80
1	E	556	SER	O-C-N	7.23	134.28	122.70
1	E	620	ARG	CG-CD-NE	-7.23	96.61	111.80
1	B	620	ARG	CG-CD-NE	-7.23	96.61	111.80
1	F	357	PRO	CA-C-O	-7.23	102.84	120.20
1	B	357	PRO	CA-C-O	-7.23	102.85	120.20
1	D	453	HIS	CA-CB-CG	-7.23	101.31	113.60
1	D	631	PRO	O-C-N	7.23	134.27	122.70
1	E	35	GLU	N-CA-CB	-7.23	97.59	110.60
1	F	620	ARG	CG-CD-NE	-7.23	96.62	111.80
1	A	620	ARG	CG-CD-NE	-7.23	96.62	111.80
1	A	637	ASP	CB-CG-OD2	-7.23	111.80	118.30
1	E	637	ASP	CB-CG-OD2	-7.23	111.80	118.30
1	A	357	PRO	CA-C-O	-7.22	102.87	120.20
1	D	357	PRO	CA-C-O	-7.22	102.86	120.20
1	C	357	PRO	CA-C-O	-7.22	102.87	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	631	PRO	O-C-N	7.22	134.25	122.70
1	D	8	ALA	CB-CA-C	7.22	120.93	110.10
1	B	637	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	C	544	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	E	357	PRO	CA-C-O	-7.21	102.89	120.20
1	A	544	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	E	631	PRO	O-C-N	7.21	134.24	122.70
1	A	631	PRO	O-C-N	7.21	134.23	122.70
1	E	296	ILE	O-C-N	7.21	134.24	122.70
1	F	544	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	A	8	ALA	CB-CA-C	7.20	120.90	110.10
1	D	316	ARG	CB-CG-CD	7.20	130.32	111.60
1	D	560	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	E	431	TYR	CD1-CE1-CZ	-7.20	113.32	119.80
1	F	8	ALA	CB-CA-C	7.20	120.90	110.10
1	C	8	ALA	CB-CA-C	7.19	120.89	110.10
1	B	8	ALA	CB-CA-C	7.19	120.88	110.10
1	B	431	TYR	CD1-CE1-CZ	-7.19	113.33	119.80
1	F	631	PRO	O-C-N	7.19	134.21	122.70
1	C	173	THR	O-C-N	7.19	134.20	122.70
1	C	316	ARG	CB-CG-CD	7.19	130.29	111.60
1	C	431	TYR	CD1-CE1-CZ	-7.19	113.33	119.80
1	F	431	TYR	CD1-CE1-CZ	-7.19	113.33	119.80
1	B	314	ASP	OD1-CG-OD2	-7.19	109.64	123.30
1	A	316	ARG	CB-CG-CD	7.19	130.28	111.60
1	C	560	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	D	544	ASP	CB-CG-OD2	-7.18	111.83	118.30
1	F	316	ARG	CB-CG-CD	7.18	130.28	111.60
1	B	316	ARG	CB-CG-CD	7.18	130.27	111.60
1	B	481	PHE	CA-C-N	7.18	133.00	117.20
1	D	481	PHE	CA-C-N	7.18	133.00	117.20
1	E	8	ALA	CB-CA-C	7.18	120.88	110.10
1	E	316	ARG	CB-CG-CD	7.18	130.28	111.60
1	E	560	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	C	314	ASP	OD1-CG-OD2	-7.18	109.66	123.30
1	A	314	ASP	OD1-CG-OD2	-7.18	109.66	123.30
1	B	92	GLN	OE1-CD-NE2	7.18	138.41	121.90
1	B	576	GLU	CA-CB-CG	-7.18	97.60	113.40
1	D	431	TYR	CD1-CE1-CZ	-7.18	113.34	119.80
1	E	237	SER	CA-C-N	7.18	132.99	117.20
1	E	314	ASP	OD1-CG-OD2	-7.17	109.67	123.30
1	F	314	ASP	OD1-CG-OD2	-7.17	109.67	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	576	GLU	CA-CB-CG	-7.17	97.62	113.40
1	A	362	ASN	CB-CA-C	7.17	124.74	110.40
1	D	92	GLN	OE1-CD-NE2	7.17	138.39	121.90
1	E	206	GLU	CA-C-N	7.17	132.98	117.20
1	B	173	THR	O-C-N	7.17	134.17	122.70
1	B	139	GLN	CA-CB-CG	7.17	129.17	113.40
1	C	237	SER	CA-C-N	7.17	132.97	117.20
1	C	245	GLU	O-C-N	-7.17	111.23	122.70
1	E	544	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	F	173	THR	O-C-N	7.17	134.17	122.70
1	A	206	GLU	CA-C-N	7.17	132.97	117.20
1	A	431	TYR	CD1-CE1-CZ	-7.17	113.35	119.80
1	A	481	PHE	CA-C-N	7.17	132.97	117.20
1	C	92	GLN	OE1-CD-NE2	7.17	138.38	121.90
1	F	362	ASN	CB-CA-C	7.17	124.73	110.40
1	A	173	THR	O-C-N	7.17	134.16	122.70
1	C	328	ILE	CA-C-N	7.17	132.96	117.20
1	C	576	GLU	CA-CB-CG	-7.17	97.64	113.40
1	F	481	PHE	CA-C-N	7.17	132.96	117.20
1	A	576	GLU	CA-CB-CG	-7.16	97.64	113.40
1	B	206	GLU	CA-C-N	7.16	132.96	117.20
1	C	206	GLU	CA-C-N	7.16	132.96	117.20
1	C	481	PHE	CA-C-N	7.16	132.96	117.20
1	D	314	ASP	OD1-CG-OD2	-7.16	109.69	123.30
1	D	362	ASN	CB-CA-C	7.16	124.73	110.40
1	E	362	ASN	CB-CA-C	7.16	124.73	110.40
1	D	237	SER	CA-C-N	7.16	132.96	117.20
1	D	328	ILE	CA-C-N	7.16	132.96	117.20
1	C	362	ASN	CB-CA-C	7.16	124.72	110.40
1	D	576	GLU	CA-CB-CG	-7.16	97.64	113.40
1	E	245	GLU	O-C-N	-7.16	111.25	122.70
1	F	576	GLU	CA-CB-CG	-7.16	97.65	113.40
1	D	174	LYS	N-CA-C	-7.16	91.68	111.00
1	E	328	ILE	CA-C-N	7.16	132.94	117.20
1	F	92	GLN	OE1-CD-NE2	7.16	138.36	121.90
1	A	328	ILE	CA-C-N	7.16	132.94	117.20
1	C	75	PHE	N-CA-CB	7.16	123.48	110.60
1	E	139	GLN	CA-CB-CG	7.16	129.14	113.40
1	F	206	GLU	CA-C-N	7.16	132.94	117.20
1	A	92	GLN	OE1-CD-NE2	7.15	138.35	121.90
1	E	174	LYS	N-CA-C	-7.15	91.69	111.00
1	D	206	GLU	CA-C-N	7.15	132.94	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	174	LYS	N-CA-C	-7.15	91.69	111.00
1	A	237	SER	CA-C-N	7.15	132.93	117.20
1	B	174	LYS	N-CA-C	-7.15	91.69	111.00
1	B	328	ILE	CA-C-N	7.15	132.93	117.20
1	E	481	PHE	CA-C-N	7.15	132.93	117.20
1	F	237	SER	CA-C-N	7.15	132.93	117.20
1	F	75	PHE	N-CA-CB	7.15	123.47	110.60
1	A	139	GLN	CA-CB-CG	7.15	129.12	113.40
1	B	362	ASN	CB-CA-C	7.15	124.69	110.40
1	D	173	THR	O-C-N	7.15	134.13	122.70
1	F	328	ILE	CA-C-N	7.15	132.92	117.20
1	A	174	LYS	N-CA-C	-7.15	91.70	111.00
1	B	237	SER	CA-C-N	7.15	132.92	117.20
1	D	75	PHE	N-CA-CB	7.15	123.46	110.60
1	D	139	GLN	CA-CB-CG	7.15	129.12	113.40
1	F	139	GLN	CA-CB-CG	7.14	129.12	113.40
1	C	139	GLN	CA-CB-CG	7.14	129.11	113.40
1	F	245	GLU	O-C-N	-7.14	111.28	122.70
1	E	92	GLN	OE1-CD-NE2	7.14	138.32	121.90
1	A	245	GLU	O-C-N	-7.14	111.28	122.70
1	A	75	PHE	N-CA-CB	7.13	123.44	110.60
1	C	174	LYS	N-CA-C	-7.13	91.73	111.00
1	B	245	GLU	O-C-N	-7.13	111.29	122.70
1	F	79	GLN	CG-CD-OE1	7.13	135.86	121.60
1	E	302	HIS	CB-CA-C	-7.13	96.14	110.40
1	F	302	HIS	CB-CA-C	-7.13	96.14	110.40
1	D	245	GLU	O-C-N	-7.13	111.30	122.70
1	B	302	HIS	CB-CA-C	-7.13	96.15	110.40
1	C	79	GLN	CG-CD-OE1	7.13	135.85	121.60
1	B	75	PHE	N-CA-CB	7.12	123.42	110.60
1	E	75	PHE	N-CA-CB	7.12	123.42	110.60
1	E	79	GLN	CG-CD-OE1	7.12	135.85	121.60
1	A	79	GLN	CG-CD-OE1	7.12	135.84	121.60
1	E	173	THR	O-C-N	7.12	134.09	122.70
1	D	302	HIS	CB-CA-C	-7.12	96.17	110.40
1	A	302	HIS	CB-CA-C	-7.11	96.17	110.40
1	B	339	TYR	CG-CD2-CE2	7.11	126.99	121.30
1	B	79	GLN	CG-CD-OE1	7.11	135.82	121.60
1	D	79	GLN	CG-CD-OE1	7.11	135.82	121.60
1	E	649	ILE	CA-C-N	-7.11	101.56	117.20
1	B	391	PHE	CG-CD2-CE2	7.11	128.62	120.80
1	A	649	ILE	CA-C-N	-7.11	101.57	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	649	ILE	CA-C-N	-7.11	101.57	117.20
1	F	649	ILE	CA-C-N	-7.10	101.58	117.20
1	D	391	PHE	CG-CD2-CE2	7.10	128.61	120.80
1	B	649	ILE	CA-C-N	-7.09	101.59	117.20
1	C	302	HIS	CB-CA-C	-7.09	96.21	110.40
1	C	649	ILE	CA-C-N	-7.09	101.60	117.20
1	F	151	ILE	CB-CG1-CD1	7.09	133.75	113.90
1	C	122	SER	CA-CB-OG	-7.09	92.07	111.20
1	D	107	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	E	497	GLU	N-CA-CB	7.09	123.36	110.60
1	F	491	ILE	CA-C-O	-7.08	105.22	120.10
1	A	151	ILE	CB-CG1-CD1	7.08	133.74	113.90
1	B	151	ILE	CB-CG1-CD1	7.08	133.74	113.90
1	C	151	ILE	CB-CG1-CD1	7.08	133.74	113.90
1	A	391	PHE	CG-CD2-CE2	7.08	128.59	120.80
1	C	339	TYR	CG-CD2-CE2	7.08	126.96	121.30
1	C	391	PHE	CG-CD2-CE2	7.08	128.59	120.80
1	D	242	PRO	CA-CB-CG	-7.08	90.55	104.00
1	D	562	CYS	CB-CA-C	-7.08	96.24	110.40
1	E	151	ILE	CB-CG1-CD1	7.08	133.73	113.90
1	F	227	LEU	CB-CG-CD1	-7.08	98.96	111.00
1	E	339	TYR	CG-CD2-CE2	7.08	126.96	121.30
1	B	122	SER	CA-CB-OG	-7.08	92.09	111.20
1	E	391	PHE	CG-CD2-CE2	7.08	128.59	120.80
1	A	491	ILE	CA-C-O	-7.08	105.24	120.10
1	A	562	CYS	CB-CA-C	-7.08	96.25	110.40
1	B	562	CYS	CB-CA-C	-7.08	96.25	110.40
1	E	227	LEU	CB-CG-CD1	-7.08	98.97	111.00
1	D	151	ILE	CB-CG1-CD1	7.07	133.71	113.90
1	D	491	ILE	CA-C-O	-7.07	105.24	120.10
1	B	242	PRO	CA-CB-CG	-7.07	90.56	104.00
1	A	122	SER	CA-CB-OG	-7.07	92.11	111.20
1	B	491	ILE	CA-C-O	-7.07	105.25	120.10
1	D	122	SER	CA-CB-OG	-7.07	92.11	111.20
1	E	562	CYS	CB-CA-C	-7.07	96.26	110.40
1	F	497	GLU	N-CA-CB	7.07	123.33	110.60
1	A	227	LEU	CB-CG-CD1	-7.07	98.98	111.00
1	B	227	LEU	CB-CG-CD1	-7.07	98.98	111.00
1	F	122	SER	CA-CB-OG	-7.07	92.11	111.20
1	F	562	CYS	CB-CA-C	-7.07	96.26	110.40
1	A	242	PRO	CA-CB-CG	-7.07	90.57	104.00
1	C	491	ILE	CA-C-O	-7.07	105.26	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	227	LEU	CB-CG-CD1	-7.07	98.98	111.00
1	E	491	ILE	CA-C-O	-7.07	105.26	120.10
1	C	227	LEU	CB-CG-CD1	-7.07	98.99	111.00
1	C	562	CYS	CB-CA-C	-7.06	96.27	110.40
1	D	190	MET	CG-SD-CE	-7.06	88.90	100.20
1	E	122	SER	CA-CB-OG	-7.06	92.13	111.20
1	F	190	MET	CG-SD-CE	-7.06	88.90	100.20
1	A	107	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	F	391	PHE	CG-CD2-CE2	7.06	128.57	120.80
1	B	190	MET	CG-SD-CE	-7.06	88.91	100.20
1	C	107	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	D	497	GLU	N-CA-CB	7.06	123.31	110.60
1	C	190	MET	CG-SD-CE	-7.06	88.91	100.20
1	E	242	PRO	CA-CB-CG	-7.06	90.59	104.00
1	F	339	TYR	CG-CD2-CE2	7.06	126.95	121.30
1	A	497	GLU	N-CA-CB	7.06	123.30	110.60
1	E	190	MET	CG-SD-CE	-7.06	88.91	100.20
1	A	190	MET	CG-SD-CE	-7.05	88.91	100.20
1	D	339	TYR	CG-CD2-CE2	7.05	126.94	121.30
1	B	84	LEU	N-CA-CB	-7.05	96.30	110.40
1	D	24	PRO	N-CD-CG	-7.05	92.62	103.20
1	C	242	PRO	CA-CB-CG	-7.05	90.61	104.00
1	A	339	TYR	CG-CD2-CE2	7.05	126.94	121.30
1	E	24	PRO	N-CD-CG	-7.05	92.63	103.20
1	C	24	PRO	N-CD-CG	-7.04	92.63	103.20
1	A	84	LEU	N-CA-CB	-7.04	96.31	110.40
1	F	107	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	24	PRO	N-CD-CG	-7.04	92.64	103.20
1	B	497	GLU	N-CA-CB	7.04	123.28	110.60
1	D	149	GLU	CG-CD-OE1	7.04	132.38	118.30
1	E	248	TRP	CA-C-O	-7.04	105.32	120.10
1	B	149	GLU	CG-CD-OE1	7.04	132.38	118.30
1	C	497	GLU	N-CA-CB	7.04	123.27	110.60
1	F	242	PRO	CA-CB-CG	-7.04	90.62	104.00
1	B	107	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	D	547	VAL	CA-CB-CG2	7.04	121.45	110.90
1	E	547	VAL	CA-CB-CG2	7.04	121.45	110.90
1	F	84	LEU	N-CA-CB	-7.03	96.33	110.40
1	F	248	TRP	CA-C-O	-7.03	105.33	120.10
1	B	24	PRO	N-CD-CG	-7.03	92.66	103.20
1	B	231	PHE	CD1-CE1-CZ	7.03	128.54	120.10
1	C	248	TRP	CA-C-O	-7.03	105.34	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	84	LEU	N-CA-CB	-7.03	96.34	110.40
1	E	107	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	A	231	PHE	CD1-CE1-CZ	7.03	128.53	120.10
1	C	84	LEU	N-CA-CB	-7.03	96.34	110.40
1	A	149	GLU	CG-CD-OE1	7.03	132.36	118.30
1	B	547	VAL	CA-CB-CG2	7.03	121.44	110.90
1	E	231	PHE	CD1-CE1-CZ	7.03	128.53	120.10
1	C	547	VAL	CA-CB-CG2	7.03	121.44	110.90
1	D	6	GLY	N-CA-C	-7.03	95.54	113.10
1	D	84	LEU	N-CA-CB	-7.03	96.35	110.40
1	E	149	GLU	CG-CD-OE1	7.03	132.35	118.30
1	F	231	PHE	CD1-CE1-CZ	7.03	128.53	120.10
1	A	248	TRP	CA-C-O	-7.02	105.35	120.10
1	C	231	PHE	CD1-CE1-CZ	7.02	128.53	120.10
1	C	353	ARG	CD-NE-CZ	7.02	133.43	123.60
1	B	248	TRP	CA-C-O	-7.02	105.35	120.10
1	E	211	TYR	CB-CA-C	7.02	124.44	110.40
1	B	130	ASP	OD1-CG-OD2	7.02	136.64	123.30
1	C	6	GLY	N-CA-C	-7.02	95.55	113.10
1	A	547	VAL	CA-CB-CG2	7.02	121.42	110.90
1	C	149	GLU	CG-CD-OE1	7.02	132.34	118.30
1	A	6	GLY	N-CA-C	-7.02	95.56	113.10
1	E	130	ASP	OD1-CG-OD2	7.02	136.63	123.30
1	F	211	TYR	CB-CA-C	7.02	124.43	110.40
1	C	484	PRO	O-C-N	7.01	133.92	122.70
1	D	248	TRP	CA-C-O	-7.01	105.37	120.10
1	F	24	PRO	N-CD-CG	-7.01	92.68	103.20
1	F	6	GLY	N-CA-C	-7.01	95.57	113.10
1	F	149	GLU	CG-CD-OE1	7.01	132.32	118.30
1	D	231	PHE	CD1-CE1-CZ	7.01	128.51	120.10
1	B	340	TYR	CG-CD2-CE2	7.01	126.91	121.30
1	B	484	PRO	O-C-N	7.01	133.91	122.70
1	D	211	TYR	CB-CA-C	7.01	124.42	110.40
1	D	394	HIS	CA-C-N	-7.01	101.78	117.20
1	D	484	PRO	O-C-N	7.01	133.91	122.70
1	F	484	PRO	O-C-N	7.01	133.91	122.70
1	A	211	TYR	CB-CA-C	7.00	124.41	110.40
1	A	130	ASP	OD1-CG-OD2	7.00	136.61	123.30
1	C	211	TYR	CB-CA-C	7.00	124.41	110.40
1	F	130	ASP	OD1-CG-OD2	7.00	136.60	123.30
1	B	6	GLY	N-CA-C	-7.00	95.59	113.10
1	E	394	HIS	CA-C-N	-7.00	101.80	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	6	GLY	N-CA-C	-7.00	95.60	113.10
1	F	394	HIS	CA-C-N	-7.00	101.81	117.20
1	B	211	TYR	CB-CA-C	7.00	124.39	110.40
1	C	394	HIS	CA-C-N	-7.00	101.81	117.20
1	D	353	ARG	CD-NE-CZ	7.00	133.39	123.60
1	E	22	TYR	CA-C-O	-6.99	105.42	120.10
1	C	340	TYR	CG-CD2-CE2	6.99	126.89	121.30
1	A	394	HIS	CA-C-N	-6.99	101.82	117.20
1	A	484	PRO	O-C-N	6.99	133.88	122.70
1	B	383	LEU	N-CA-CB	6.99	124.38	110.40
1	C	383	LEU	N-CA-CB	6.99	124.38	110.40
1	D	130	ASP	OD1-CG-OD2	6.99	136.57	123.30
1	E	353	ARG	CD-NE-CZ	6.99	133.38	123.60
1	F	547	VAL	CA-CB-CG2	6.99	121.38	110.90
1	A	353	ARG	CD-NE-CZ	6.99	133.38	123.60
1	F	353	ARG	CD-NE-CZ	6.98	133.38	123.60
1	A	383	LEU	N-CA-CB	6.98	124.36	110.40
1	B	120	TYR	CB-CG-CD2	6.98	125.19	121.00
1	F	383	LEU	N-CA-CB	6.98	124.36	110.40
1	B	353	ARG	CD-NE-CZ	6.98	133.37	123.60
1	C	130	ASP	OD1-CG-OD2	6.97	136.55	123.30
1	F	272	PRO	CA-CB-CG	-6.97	90.75	104.00
1	B	394	HIS	CA-C-N	-6.97	101.86	117.20
1	D	383	LEU	N-CA-CB	6.97	124.34	110.40
1	C	22	TYR	CA-C-O	-6.97	105.46	120.10
1	D	22	TYR	CA-C-O	-6.97	105.47	120.10
1	E	340	TYR	CG-CD2-CE2	6.97	126.88	121.30
1	F	239	TRP	CD1-CG-CD2	-6.97	100.72	106.30
1	A	22	TYR	CA-C-O	-6.97	105.47	120.10
1	E	383	LEU	N-CA-CB	6.97	124.33	110.40
1	B	22	TYR	CA-C-O	-6.96	105.48	120.10
1	D	272	PRO	CA-CB-CG	-6.96	90.77	104.00
1	F	22	TYR	CA-C-O	-6.96	105.47	120.10
1	F	340	TYR	CG-CD2-CE2	6.96	126.87	121.30
1	E	239	TRP	CD1-CG-CD2	-6.96	100.73	106.30
1	B	272	PRO	CA-CB-CG	-6.96	90.77	104.00
1	E	484	PRO	O-C-N	6.96	133.84	122.70
1	E	251	ILE	O-C-N	6.96	133.84	122.70
1	A	239	TRP	CD1-CG-CD2	-6.96	100.73	106.30
1	D	369	GLU	O-C-N	6.96	133.83	122.70
1	D	570	LEU	CB-CG-CD2	-6.96	99.17	111.00
1	A	251	ILE	O-C-N	6.95	133.82	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	251	ILE	O-C-N	6.95	133.83	122.70
1	A	272	PRO	CA-CB-CG	-6.95	90.80	104.00
1	F	570	LEU	CB-CG-CD2	-6.95	99.19	111.00
1	C	67	GLU	CB-CG-CD	-6.94	95.46	114.20
1	C	272	PRO	CA-CB-CG	-6.94	90.81	104.00
1	C	369	GLU	O-C-N	6.94	133.81	122.70
1	A	340	TYR	CG-CD2-CE2	6.94	126.85	121.30
1	E	67	GLU	CB-CG-CD	-6.94	95.46	114.20
1	A	67	GLU	CB-CG-CD	-6.94	95.46	114.20
1	C	251	ILE	O-C-N	6.94	133.80	122.70
1	F	67	GLU	CB-CG-CD	-6.94	95.47	114.20
1	F	251	ILE	O-C-N	6.94	133.80	122.70
1	D	67	GLU	CB-CG-CD	-6.93	95.48	114.20
1	E	272	PRO	CA-CB-CG	-6.93	90.83	104.00
1	F	120	TYR	CB-CG-CD2	6.93	125.16	121.00
1	A	570	LEU	CB-CG-CD2	-6.93	99.22	111.00
1	B	67	GLU	CB-CG-CD	-6.93	95.49	114.20
1	C	570	LEU	CB-CG-CD2	-6.93	99.22	111.00
1	B	239	TRP	CD1-CG-CD2	-6.93	100.76	106.30
1	C	239	TRP	CD1-CG-CD2	-6.93	100.76	106.30
1	B	369	GLU	O-C-N	6.92	133.78	122.70
1	B	570	LEU	CB-CG-CD2	-6.92	99.23	111.00
1	E	156	SER	N-CA-CB	6.92	120.89	110.50
1	B	251	ILE	O-C-N	6.92	133.77	122.70
1	B	276	HIS	CA-CB-CG	-6.92	101.84	113.60
1	B	386	TYR	CB-CG-CD1	-6.92	116.85	121.00
1	E	570	LEU	CB-CG-CD2	-6.92	99.24	111.00
1	F	156	SER	N-CA-CB	6.92	120.87	110.50
1	B	156	SER	N-CA-CB	6.91	120.87	110.50
1	E	372	GLU	CA-CB-CG	-6.91	98.19	113.40
1	E	369	GLU	O-C-N	6.91	133.76	122.70
1	F	276	HIS	CA-CB-CG	-6.91	101.85	113.60
1	A	156	SER	N-CA-CB	6.91	120.86	110.50
1	D	156	SER	N-CA-CB	6.91	120.87	110.50
1	D	239	TRP	CD1-CG-CD2	-6.91	100.78	106.30
1	B	128	LEU	O-C-N	6.90	134.93	123.20
1	D	276	HIS	CA-CB-CG	-6.90	101.87	113.60
1	D	340	TYR	CG-CD2-CE2	6.90	126.82	121.30
1	A	369	GLU	O-C-N	6.90	133.74	122.70
1	A	276	HIS	CA-CB-CG	-6.90	101.88	113.60
1	D	120	TYR	CB-CG-CD2	6.90	125.14	121.00
1	E	650	VAL	CG1-CB-CG2	6.90	121.94	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	TYR	CB-CG-CD2	6.89	125.14	121.00
1	A	372	GLU	CA-CB-CG	-6.89	98.24	113.40
1	E	276	HIS	CA-CB-CG	-6.89	101.88	113.60
1	C	128	LEU	O-C-N	6.89	134.91	123.20
1	F	372	GLU	CA-CB-CG	-6.89	98.24	113.40
1	D	372	GLU	CA-CB-CG	-6.89	98.24	113.40
1	E	128	LEU	O-C-N	6.89	134.91	123.20
1	B	372	GLU	CA-CB-CG	-6.88	98.26	113.40
1	C	372	GLU	CA-CB-CG	-6.88	98.26	113.40
1	B	650	VAL	CG1-CB-CG2	6.88	121.91	110.90
1	C	276	HIS	CA-CB-CG	-6.88	101.91	113.60
1	E	120	TYR	CB-CG-CD2	6.88	125.13	121.00
1	A	650	VAL	CG1-CB-CG2	6.88	121.90	110.90
1	C	650	VAL	CG1-CB-CG2	6.87	121.89	110.90
1	A	128	LEU	O-C-N	6.87	134.88	123.20
1	C	156	SER	N-CA-CB	6.87	120.80	110.50
1	E	386	TYR	CB-CG-CD1	-6.87	116.88	121.00
1	C	120	TYR	CB-CG-CD2	6.86	125.12	121.00
1	D	128	LEU	O-C-N	6.86	134.87	123.20
1	D	650	VAL	CG1-CB-CG2	6.86	121.88	110.90
1	E	335	SER	O-C-N	6.86	133.68	122.70
1	F	650	VAL	CG1-CB-CG2	6.86	121.88	110.90
1	C	385	LYS	N-CA-CB	6.86	122.94	110.60
1	D	68	GLN	CG-CD-OE1	6.85	135.31	121.60
1	C	216	LYS	O-C-N	6.85	134.85	123.20
1	E	68	GLN	CG-CD-OE1	6.85	135.30	121.60
1	F	369	GLU	O-C-N	6.85	133.66	122.70
1	B	313	ILE	CG1-CB-CG2	-6.85	96.33	111.40
1	C	313	ILE	CG1-CB-CG2	-6.85	96.33	111.40
1	C	582	LEU	CB-CA-C	6.85	123.21	110.20
1	F	335	SER	O-C-N	6.85	133.66	122.70
1	C	68	GLN	CG-CD-OE1	6.85	135.29	121.60
1	A	582	LEU	CB-CA-C	6.85	123.21	110.20
1	D	216	LYS	O-C-N	6.85	134.84	123.20
1	E	582	LEU	CB-CA-C	6.85	123.21	110.20
1	F	128	LEU	O-C-N	6.85	134.84	123.20
1	E	313	ILE	CG1-CB-CG2	-6.84	96.34	111.40
1	D	582	LEU	CB-CA-C	6.84	123.20	110.20
1	A	335	SER	O-C-N	6.84	133.64	122.70
1	A	385	LYS	N-CA-CB	6.84	122.91	110.60
1	B	68	GLN	CG-CD-OE1	6.84	135.28	121.60
1	E	3	LEU	N-CA-CB	6.84	124.08	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	567	ARG	CD-NE-CZ	-6.84	114.03	123.60
1	A	68	GLN	CG-CD-OE1	6.84	135.28	121.60
1	A	313	ILE	CG1-CB-CG2	-6.84	96.36	111.40
1	B	216	LYS	O-C-N	6.84	134.82	123.20
1	D	82	GLU	OE1-CD-OE2	-6.84	115.09	123.30
1	F	313	ILE	CG1-CB-CG2	-6.84	96.36	111.40
1	B	335	SER	O-C-N	6.84	133.64	122.70
1	D	385	LYS	N-CA-CB	6.84	122.91	110.60
1	F	3	LEU	N-CA-CB	6.84	124.07	110.40
1	F	216	LYS	O-C-N	6.84	134.82	123.20
1	F	68	GLN	CG-CD-OE1	6.83	135.27	121.60
1	B	582	LEU	CB-CA-C	6.83	123.18	110.20
1	E	216	LYS	O-C-N	6.83	134.81	123.20
1	D	313	ILE	CG1-CB-CG2	-6.83	96.37	111.40
1	A	3	LEU	N-CA-CB	6.83	124.06	110.40
1	C	335	SER	O-C-N	6.83	133.63	122.70
1	B	385	LYS	N-CA-CB	6.83	122.89	110.60
1	D	335	SER	O-C-N	6.83	133.62	122.70
1	E	385	LYS	N-CA-CB	6.83	122.89	110.60
1	A	216	LYS	O-C-N	6.82	134.80	123.20
1	E	609	CYS	CA-CB-SG	-6.82	101.72	114.00
1	F	385	LYS	N-CA-CB	6.82	122.88	110.60
1	B	3	LEU	N-CA-CB	6.82	124.04	110.40
1	C	363	LEU	CB-CG-CD1	-6.82	99.40	111.00
1	F	582	LEU	CB-CA-C	6.82	123.16	110.20
1	B	567	ARG	CD-NE-CZ	-6.82	114.06	123.60
1	C	3	LEU	N-CA-CB	6.82	124.03	110.40
1	D	3	LEU	N-CA-CB	6.82	124.03	110.40
1	E	483	CYS	CB-CA-C	-6.82	96.77	110.40
1	F	609	CYS	CA-CB-SG	-6.82	101.73	114.00
1	E	82	GLU	OE1-CD-OE2	-6.81	115.13	123.30
1	C	567	ARG	CD-NE-CZ	-6.81	114.06	123.60
1	D	609	CYS	CA-CB-SG	-6.81	101.74	114.00
1	F	567	ARG	CD-NE-CZ	-6.81	114.07	123.60
1	A	567	ARG	CD-NE-CZ	-6.81	114.07	123.60
1	F	363	LEU	CB-CG-CD1	-6.81	99.43	111.00
1	F	483	CYS	CB-CA-C	-6.81	96.78	110.40
1	A	363	LEU	CB-CG-CD1	-6.81	99.43	111.00
1	E	147	ASN	CB-CA-C	-6.81	96.79	110.40
1	B	483	CYS	CB-CA-C	-6.80	96.79	110.40
1	C	537	GLN	CA-CB-CG	-6.80	98.43	113.40
1	C	609	CYS	CA-CB-SG	-6.80	101.75	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	537	GLN	CA-CB-CG	-6.80	98.43	113.40
1	A	609	CYS	CA-CB-SG	-6.80	101.75	114.00
1	B	147	ASN	CB-CA-C	-6.80	96.80	110.40
1	F	386	TYR	CB-CG-CD1	-6.80	116.92	121.00
1	A	386	TYR	CB-CG-CD1	-6.80	116.92	121.00
1	F	179	GLN	N-CA-C	-6.80	92.64	111.00
1	A	483	CYS	CB-CA-C	-6.80	96.81	110.40
1	C	386	TYR	CB-CG-CD1	-6.80	116.92	121.00
1	E	177	ARG	CB-CG-CD	-6.80	93.92	111.60
1	D	147	ASN	CB-CA-C	-6.79	96.81	110.40
1	C	177	ARG	CB-CG-CD	-6.79	93.94	111.60
1	E	179	GLN	N-CA-C	-6.79	92.66	111.00
1	A	177	ARG	CB-CG-CD	-6.79	93.94	111.60
1	B	609	CYS	CA-CB-SG	-6.79	101.77	114.00
1	D	177	ARG	CB-CG-CD	-6.79	93.94	111.60
1	D	483	CYS	CB-CA-C	-6.79	96.82	110.40
1	E	363	LEU	CB-CG-CD1	-6.79	99.45	111.00
1	E	537	GLN	CA-CB-CG	-6.79	98.46	113.40
1	B	363	LEU	CB-CG-CD1	-6.79	99.46	111.00
1	A	82	GLU	OE1-CD-OE2	-6.79	115.15	123.30
1	A	537	GLN	CA-CB-CG	-6.79	98.47	113.40
1	A	147	ASN	CB-CA-C	-6.79	96.83	110.40
1	A	179	GLN	N-CA-C	-6.79	92.67	111.00
1	D	179	GLN	N-CA-C	-6.79	92.67	111.00
1	F	358	HIS	CA-CB-CG	-6.79	102.06	113.60
1	B	179	GLN	N-CA-C	-6.79	92.68	111.00
1	B	221	PHE	CZ-CE2-CD2	-6.79	111.96	120.10
1	D	567	ARG	CD-NE-CZ	-6.79	114.10	123.60
1	F	147	ASN	CB-CA-C	-6.79	96.83	110.40
1	C	483	CYS	CB-CA-C	-6.78	96.83	110.40
1	F	177	ARG	CB-CG-CD	-6.78	93.96	111.60
1	C	179	GLN	N-CA-C	-6.78	92.69	111.00
1	F	82	GLU	OE1-CD-OE2	-6.78	115.16	123.30
1	B	358	HIS	CA-CB-CG	-6.78	102.07	113.60
1	C	147	ASN	CB-CA-C	-6.78	96.84	110.40
1	C	358	HIS	CA-CB-CG	-6.78	102.08	113.60
1	E	358	HIS	CA-CB-CG	-6.78	102.07	113.60
1	B	177	ARG	CB-CG-CD	-6.78	93.98	111.60
1	B	537	GLN	CA-CB-CG	-6.78	98.49	113.40
1	A	358	HIS	CA-CB-CG	-6.78	102.08	113.60
1	D	363	LEU	CB-CG-CD1	-6.78	99.48	111.00
1	D	537	GLN	CA-CB-CG	-6.78	98.50	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	221	PHE	CZ-CE2-CD2	-6.77	111.97	120.10
1	B	126	SER	CA-C-N	-6.77	102.30	117.20
1	E	492	THR	C-N-CA	6.77	138.63	121.70
1	B	82	GLU	OE1-CD-OE2	-6.77	115.18	123.30
1	B	461	THR	O-C-N	-6.77	111.87	122.70
1	D	181	VAL	CA-CB-CG2	6.77	121.05	110.90
1	A	221	PHE	CZ-CE2-CD2	-6.77	111.98	120.10
1	D	358	HIS	CA-CB-CG	-6.77	102.10	113.60
1	D	492	THR	C-N-CA	6.77	138.62	121.70
1	A	388	ASP	N-CA-CB	6.77	122.78	110.60
1	D	364	PRO	CA-C-O	-6.77	103.96	120.20
1	F	23	GLU	CB-CA-C	-6.77	96.87	110.40
1	C	126	SER	CA-C-N	-6.76	102.32	117.20
1	C	364	PRO	CA-C-O	-6.76	103.97	120.20
1	C	82	GLU	OE1-CD-OE2	-6.76	115.19	123.30
1	D	388	ASP	N-CA-CB	6.76	122.77	110.60
1	F	388	ASP	N-CA-CB	6.76	122.77	110.60
1	E	126	SER	CA-C-N	-6.76	102.32	117.20
1	F	126	SER	CA-C-N	-6.76	102.33	117.20
1	A	126	SER	CA-C-N	-6.76	102.33	117.20
1	F	364	PRO	CA-C-O	-6.76	103.98	120.20
1	B	23	GLU	CB-CA-C	-6.76	96.89	110.40
1	B	364	PRO	CA-C-O	-6.76	103.98	120.20
1	E	388	ASP	N-CA-CB	6.76	122.76	110.60
1	A	364	PRO	CA-C-O	-6.75	103.99	120.20
1	F	492	THR	C-N-CA	6.75	138.59	121.70
1	B	388	ASP	N-CA-CB	6.75	122.75	110.60
1	B	492	THR	C-N-CA	6.75	138.58	121.70
1	C	388	ASP	N-CA-CB	6.75	122.76	110.60
1	C	492	THR	C-N-CA	6.75	138.58	121.70
1	E	364	PRO	CA-C-O	-6.75	103.99	120.20
1	F	461	THR	O-C-N	-6.75	111.90	122.70
1	B	132	ILE	N-CA-C	6.75	129.22	111.00
1	D	23	GLU	CB-CA-C	-6.75	96.90	110.40
1	D	221	PHE	CZ-CE2-CD2	-6.75	112.00	120.10
1	D	386	TYR	CB-CG-CD1	-6.75	116.95	121.00
1	A	461	THR	O-C-N	-6.75	111.91	122.70
1	E	576	GLU	CG-CD-OE1	-6.75	104.81	118.30
1	A	492	THR	C-N-CA	6.75	138.56	121.70
1	A	23	GLU	CB-CA-C	-6.74	96.91	110.40
1	C	576	GLU	CG-CD-OE1	-6.74	104.81	118.30
1	D	126	SER	CA-C-N	-6.74	102.36	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	461	THR	O-C-N	-6.74	111.91	122.70
1	C	221	PHE	CZ-CE2-CD2	-6.74	112.01	120.10
1	D	278	GLU	CA-C-N	-6.74	102.37	117.20
1	C	17	LEU	O-C-N	6.74	133.49	122.70
1	C	23	GLU	CB-CA-C	-6.74	96.92	110.40
1	D	17	LEU	O-C-N	6.74	133.48	122.70
1	D	576	GLU	CG-CD-OE1	-6.74	104.82	118.30
1	E	17	LEU	O-C-N	6.74	133.49	122.70
1	F	221	PHE	CZ-CE2-CD2	-6.74	112.01	120.10
1	B	80	ARG	O-C-N	6.74	133.48	122.70
1	C	132	ILE	N-CA-C	6.74	129.19	111.00
1	A	132	ILE	N-CA-C	6.74	129.19	111.00
1	C	212	HIS	CA-C-O	-6.74	105.95	120.10
1	A	278	GLU	CA-C-N	-6.74	102.38	117.20
1	B	278	GLU	CA-C-N	-6.74	102.38	117.20
1	E	189	GLY	O-C-N	6.74	133.48	122.70
1	F	278	GLU	CA-C-N	-6.74	102.38	117.20
1	C	278	GLU	CA-C-N	-6.73	102.39	117.20
1	D	212	HIS	CA-C-O	-6.73	105.96	120.10
1	F	511	LYS	CA-C-N	-6.73	102.39	117.20
1	A	17	LEU	O-C-N	6.73	133.47	122.70
1	B	17	LEU	O-C-N	6.73	133.47	122.70
1	B	189	GLY	O-C-N	6.73	133.47	122.70
1	C	364	PRO	O-C-N	6.73	133.89	121.10
1	E	132	ILE	N-CA-C	6.73	129.18	111.00
1	F	132	ILE	N-CA-C	6.73	129.18	111.00
1	F	212	HIS	CA-C-O	-6.73	105.96	120.10
1	A	511	LYS	CA-C-N	-6.73	102.39	117.20
1	A	576	GLU	CG-CD-OE1	-6.73	104.84	118.30
1	C	460	PHE	CA-C-O	-6.73	105.97	120.10
1	D	132	ILE	N-CA-C	6.73	129.18	111.00
1	D	461	THR	O-C-N	-6.73	111.93	122.70
1	F	94	LYS	CB-CA-C	6.73	123.86	110.40
1	F	576	GLU	CG-CD-OE1	-6.73	104.84	118.30
1	A	212	HIS	CA-C-O	-6.73	105.97	120.10
1	B	460	PHE	CA-C-O	-6.73	105.97	120.10
1	A	181	VAL	CA-CB-CG2	6.73	120.99	110.90
1	E	511	LYS	CA-C-N	-6.73	102.40	117.20
1	F	149	GLU	OE1-CD-OE2	6.73	131.37	123.30
1	A	460	PHE	CA-C-O	-6.73	105.97	120.10
1	B	207	ASP	CA-CB-CG	6.73	128.20	113.40
1	D	80	ARG	O-C-N	6.73	133.46	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	ARG	O-C-N	6.72	133.46	122.70
1	B	94	LYS	CB-CA-C	6.72	123.85	110.40
1	D	472	GLY	O-C-N	6.72	133.46	122.70
1	F	80	ARG	O-C-N	6.72	133.46	122.70
1	C	461	THR	O-C-N	-6.72	111.94	122.70
1	D	364	PRO	O-C-N	6.72	133.87	121.10
1	E	23	GLU	CB-CA-C	-6.72	96.95	110.40
1	E	80	ARG	O-C-N	6.72	133.46	122.70
1	E	212	HIS	CA-C-O	-6.72	105.98	120.10
1	E	460	PHE	CA-C-O	-6.72	105.98	120.10
1	D	460	PHE	CA-C-O	-6.72	105.99	120.10
1	F	460	PHE	CA-C-O	-6.72	105.99	120.10
1	B	212	HIS	CA-C-O	-6.72	105.99	120.10
1	C	149	GLU	OE1-CD-OE2	6.72	131.36	123.30
1	D	94	LYS	CB-CA-C	6.72	123.84	110.40
1	F	17	LEU	O-C-N	6.72	133.45	122.70
1	F	181	VAL	CA-CB-CG2	6.72	120.98	110.90
1	F	189	GLY	O-C-N	6.72	133.45	122.70
1	C	181	VAL	CA-CB-CG2	6.72	120.97	110.90
1	C	465	THR	O-C-N	6.72	133.45	122.70
1	A	189	GLY	O-C-N	6.71	133.44	122.70
1	B	576	GLU	CG-CD-OE1	-6.71	104.87	118.30
1	C	305	ILE	CA-CB-CG1	-6.71	98.24	111.00
1	F	364	PRO	O-C-N	6.71	133.86	121.10
1	A	94	LYS	CB-CA-C	6.71	123.83	110.40
1	A	364	PRO	O-C-N	6.71	133.85	121.10
1	C	94	LYS	CB-CA-C	6.71	123.83	110.40
1	D	465	THR	O-C-N	6.71	133.44	122.70
1	E	278	GLU	CA-C-N	-6.71	102.43	117.20
1	A	207	ASP	CA-CB-CG	6.71	128.17	113.40
1	B	511	LYS	CA-C-N	-6.71	102.43	117.20
1	D	189	GLY	O-C-N	6.71	133.44	122.70
1	D	511	LYS	CA-C-N	-6.71	102.44	117.20
1	E	94	LYS	CB-CA-C	6.71	123.82	110.40
1	E	144	MET	CG-SD-CE	6.71	110.94	100.20
1	E	181	VAL	CA-CB-CG2	6.71	120.97	110.90
1	B	144	MET	CG-SD-CE	6.71	110.94	100.20
1	B	364	PRO	O-C-N	6.71	133.85	121.10
1	C	207	ASP	CA-CB-CG	6.71	128.16	113.40
1	D	207	ASP	CA-CB-CG	6.71	128.16	113.40
1	D	152	ASP	OD1-CG-OD2	-6.71	110.56	123.30
1	D	409	SER	C-N-CA	-6.71	108.22	122.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	149	GLU	OE1-CD-OE2	6.71	131.35	123.30
1	C	511	LYS	CA-C-N	-6.71	102.45	117.20
1	E	207	ASP	CA-CB-CG	6.71	128.15	113.40
1	A	149	GLU	OE1-CD-OE2	6.70	131.34	123.30
1	B	305	ILE	CA-CB-CG1	-6.70	98.26	111.00
1	D	305	ILE	CA-CB-CG1	-6.70	98.26	111.00
1	F	207	ASP	CA-CB-CG	6.70	128.15	113.40
1	B	409	SER	C-N-CA	-6.70	108.23	122.30
1	E	152	ASP	OD1-CG-OD2	-6.70	110.57	123.30
1	E	305	ILE	CA-CB-CG1	-6.70	98.27	111.00
1	F	553	LEU	N-CA-CB	-6.70	97.00	110.40
1	A	409	SER	C-N-CA	-6.70	108.23	122.30
1	C	80	ARG	O-C-N	6.70	133.42	122.70
1	C	152	ASP	OD1-CG-OD2	-6.70	110.57	123.30
1	C	469	ASN	CB-CA-C	6.70	123.80	110.40
1	C	472	GLY	O-C-N	6.70	133.42	122.70
1	E	409	SER	C-N-CA	-6.70	108.23	122.30
1	A	305	ILE	CA-CB-CG1	-6.70	98.28	111.00
1	B	181	VAL	CA-CB-CG2	6.70	120.94	110.90
1	C	189	GLY	O-C-N	6.70	133.41	122.70
1	D	558	TYR	CB-CG-CD1	6.70	125.02	121.00
1	A	144	MET	CG-SD-CE	6.70	110.91	100.20
1	D	149	GLU	OE1-CD-OE2	6.70	131.34	123.30
1	E	364	PRO	O-C-N	6.70	133.82	121.10
1	E	465	THR	O-C-N	6.70	133.41	122.70
1	F	144	MET	CG-SD-CE	6.70	110.91	100.20
1	F	409	SER	C-N-CA	-6.69	108.24	122.30
1	B	149	GLU	OE1-CD-OE2	6.69	131.33	123.30
1	F	305	ILE	CA-CB-CG1	-6.69	98.28	111.00
1	F	465	THR	O-C-N	6.69	133.41	122.70
1	A	152	ASP	OD1-CG-OD2	-6.69	110.59	123.30
1	A	465	THR	O-C-N	6.69	133.40	122.70
1	B	152	ASP	OD1-CG-OD2	-6.69	110.59	123.30
1	B	465	THR	O-C-N	6.69	133.40	122.70
1	C	553	LEU	N-CA-CB	-6.69	97.02	110.40
1	A	472	GLY	O-C-N	6.69	133.40	122.70
1	F	472	GLY	O-C-N	6.69	133.40	122.70
1	C	144	MET	CG-SD-CE	6.68	110.89	100.20
1	D	144	MET	CG-SD-CE	6.68	110.90	100.20
1	E	558	TYR	CB-CG-CD1	6.68	125.01	121.00
1	B	230	ARG	N-CA-CB	6.68	122.63	110.60
1	E	10	LYS	CD-CE-NZ	6.68	127.07	111.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	553	LEU	N-CA-CB	-6.68	97.04	110.40
1	D	553	LEU	N-CA-CB	-6.68	97.04	110.40
1	E	374	ALA	O-C-N	6.68	133.39	122.70
1	B	10	LYS	CD-CE-NZ	6.68	127.06	111.70
1	B	558	TYR	CB-CG-CD1	6.68	125.01	121.00
1	D	374	ALA	O-C-N	6.68	133.39	122.70
1	F	10	LYS	CD-CE-NZ	6.68	127.06	111.70
1	F	152	ASP	OD1-CG-OD2	-6.68	110.61	123.30
1	A	10	LYS	CD-CE-NZ	6.68	127.06	111.70
1	C	409	SER	C-N-CA	-6.68	108.28	122.30
1	D	10	LYS	CD-CE-NZ	6.68	127.05	111.70
1	A	230	ARG	N-CA-CB	6.67	122.61	110.60
1	A	469	ASN	CB-CA-C	6.67	123.75	110.40
1	E	23	GLU	OE1-CD-OE2	6.67	131.31	123.30
1	E	469	ASN	CB-CA-C	6.67	123.75	110.40
1	E	553	LEU	N-CA-CB	-6.67	97.05	110.40
1	B	553	LEU	N-CA-CB	-6.67	97.05	110.40
1	C	374	ALA	O-C-N	6.67	133.38	122.70
1	C	10	LYS	CD-CE-NZ	6.67	127.05	111.70
1	C	23	GLU	OE1-CD-OE2	6.67	131.31	123.30
1	C	230	ARG	N-CA-CB	6.67	122.61	110.60
1	E	234	GLU	OE1-CD-OE2	6.67	131.31	123.30
1	B	472	GLY	O-C-N	6.67	133.37	122.70
1	C	234	GLU	OE1-CD-OE2	6.67	131.30	123.30
1	C	297	HIS	CB-CA-C	-6.67	97.07	110.40
1	D	297	HIS	CB-CA-C	-6.67	97.07	110.40
1	E	491	ILE	CA-CB-CG2	-6.67	97.57	110.90
1	D	13	ASP	CB-CG-OD2	6.67	124.30	118.30
1	B	491	ILE	CA-CB-CG2	-6.66	97.57	110.90
1	E	297	HIS	CB-CA-C	-6.66	97.07	110.40
1	C	543	ALA	O-C-N	6.66	133.36	122.70
1	E	230	ARG	N-CA-CB	6.66	122.59	110.60
1	A	297	HIS	CB-CA-C	-6.66	97.08	110.40
1	F	560	ARG	NH1-CZ-NH2	6.66	126.73	119.40
1	A	23	GLU	OE1-CD-OE2	6.66	131.29	123.30
1	E	472	GLY	O-C-N	6.66	133.35	122.70
1	F	234	GLU	OE1-CD-OE2	6.66	131.29	123.30
1	F	469	ASN	CB-CA-C	6.66	123.72	110.40
1	C	16	HIS	CA-CB-CG	-6.66	102.28	113.60
1	C	558	TYR	CB-CG-CD1	6.66	124.99	121.00
1	D	123	VAL	CB-CA-C	6.66	124.05	111.40
1	E	16	HIS	CA-CB-CG	-6.66	102.28	113.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	297	HIS	CB-CA-C	-6.66	97.09	110.40
1	B	469	ASN	CB-CA-C	6.66	123.71	110.40
1	D	491	ILE	CA-CB-CG2	-6.66	97.59	110.90
1	A	374	ALA	O-C-N	6.65	133.35	122.70
1	A	491	ILE	CA-CB-CG2	-6.65	97.59	110.90
1	B	234	GLU	OE1-CD-OE2	6.65	131.28	123.30
1	C	123	VAL	CB-CA-C	6.65	124.04	111.40
1	D	23	GLU	OE1-CD-OE2	6.65	131.28	123.30
1	D	543	ALA	O-C-N	6.65	133.34	122.70
1	F	23	GLU	OE1-CD-OE2	6.65	131.28	123.30
1	C	491	ILE	CA-CB-CG2	-6.65	97.60	110.90
1	D	230	ARG	N-CA-CB	6.65	122.57	110.60
1	D	469	ASN	CB-CA-C	6.65	123.70	110.40
1	F	230	ARG	N-CA-CB	6.65	122.57	110.60
1	C	13	ASP	CB-CG-OD2	6.65	124.28	118.30
1	D	16	HIS	CA-CB-CG	-6.65	102.30	113.60
1	B	543	ALA	O-C-N	6.65	133.34	122.70
1	B	560	ARG	NH1-CZ-NH2	6.65	126.71	119.40
1	E	123	VAL	CB-CA-C	6.65	124.03	111.40
1	E	190	MET	O-C-N	6.65	133.34	122.70
1	F	297	HIS	CB-CA-C	-6.65	97.10	110.40
1	A	13	ASP	CB-CG-OD2	6.64	124.28	118.30
1	A	16	HIS	CA-CB-CG	-6.64	102.30	113.60
1	B	23	GLU	OE1-CD-OE2	6.64	131.27	123.30
1	E	218	GLU	CB-CA-C	-6.64	97.11	110.40
1	F	374	ALA	O-C-N	6.64	133.33	122.70
1	D	234	GLU	OE1-CD-OE2	6.64	131.27	123.30
1	F	218	GLU	CB-CA-C	-6.64	97.12	110.40
1	A	543	ALA	O-C-N	6.64	133.32	122.70
1	A	558	TYR	CB-CG-CD1	6.64	124.98	121.00
1	B	374	ALA	O-C-N	6.64	133.32	122.70
1	D	190	MET	O-C-N	6.64	133.32	122.70
1	F	16	HIS	CA-CB-CG	-6.64	102.31	113.60
1	F	190	MET	O-C-N	6.64	133.32	122.70
1	A	234	GLU	OE1-CD-OE2	6.64	131.27	123.30
1	C	402	THR	CA-CB-CG2	6.64	121.69	112.40
1	F	13	ASP	CB-CG-OD2	6.64	124.28	118.30
1	A	190	MET	O-C-N	6.63	133.31	122.70
1	F	123	VAL	CB-CA-C	6.63	124.01	111.40
1	D	25	THR	CA-C-N	-6.63	102.61	117.20
1	A	123	VAL	CB-CA-C	6.63	124.00	111.40
1	B	123	VAL	CB-CA-C	6.63	124.00	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	ASP	OD1-CG-OD2	-6.63	110.70	123.30
1	B	190	MET	O-C-N	6.63	133.31	122.70
1	E	194	HIS	N-CA-CB	6.63	122.53	110.60
1	A	560	ARG	NH1-CZ-NH2	6.63	126.69	119.40
1	E	560	ARG	NH1-CZ-NH2	6.63	126.69	119.40
1	E	629	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	F	491	ILE	CA-CB-CG2	-6.63	97.65	110.90
1	B	13	ASP	CB-CG-OD2	6.62	124.26	118.30
1	C	194	HIS	N-CA-CB	6.62	122.52	110.60
1	E	543	ALA	O-C-N	6.62	133.30	122.70
1	C	190	MET	O-C-N	6.62	133.29	122.70
1	D	194	HIS	N-CA-CB	6.62	122.52	110.60
1	E	13	ASP	CB-CG-OD2	6.62	124.26	118.30
1	F	194	HIS	N-CA-CB	6.62	122.52	110.60
1	B	25	THR	CA-C-N	-6.62	102.64	117.20
1	B	194	HIS	N-CA-CB	6.62	122.51	110.60
1	C	263	LYS	CD-CE-NZ	6.62	126.92	111.70
1	E	616	TYR	N-CA-CB	-6.62	98.69	110.60
1	F	543	ALA	O-C-N	6.62	133.29	122.70
1	C	218	GLU	CB-CA-C	-6.62	97.17	110.40
1	A	25	THR	CA-C-N	-6.62	102.64	117.20
1	A	218	GLU	CB-CA-C	-6.62	97.17	110.40
1	B	354	GLN	OE1-CD-NE2	-6.62	106.69	121.90
1	D	354	GLN	OE1-CD-NE2	-6.62	106.69	121.90
1	F	72	TYR	CB-CG-CD1	-6.62	117.03	121.00
1	B	16	HIS	CA-CB-CG	-6.61	102.36	113.60
1	C	549	GLY	C-N-CA	-6.61	108.41	122.30
1	E	200	ASP	OD1-CG-OD2	-6.61	110.73	123.30
1	D	200	ASP	OD1-CG-OD2	-6.61	110.74	123.30
1	F	25	THR	CA-C-N	-6.61	102.65	117.20
1	A	200	ASP	OD1-CG-OD2	-6.61	110.74	123.30
1	C	25	THR	CA-C-N	-6.61	102.66	117.20
1	E	549	GLY	C-N-CA	-6.61	108.42	122.30
1	A	194	HIS	N-CA-CB	6.61	122.49	110.60
1	B	218	GLU	CB-CA-C	-6.61	97.19	110.40
1	D	462	TYR	O-C-N	6.61	133.27	122.70
1	B	200	ASP	OD1-CG-OD2	-6.60	110.75	123.30
1	D	48	ASP	CB-CG-OD1	6.60	124.24	118.30
1	D	218	GLU	CB-CA-C	-6.60	97.19	110.40
1	F	354	GLN	OE1-CD-NE2	-6.60	106.72	121.90
1	F	549	GLY	C-N-CA	-6.60	108.43	122.30
1	B	616	TYR	N-CA-CB	-6.60	98.72	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	THR	CA-CB-CG2	6.60	121.64	112.40
1	E	402	THR	CA-CB-CG2	6.60	121.64	112.40
1	A	354	GLN	OE1-CD-NE2	-6.60	106.72	121.90
1	D	144	MET	CA-CB-CG	6.60	124.52	113.30
1	D	263	LYS	CD-CE-NZ	6.60	126.88	111.70
1	D	560	ARG	NH1-CZ-NH2	6.60	126.66	119.40
1	F	263	LYS	CD-CE-NZ	6.60	126.87	111.70
1	F	402	THR	CA-CB-CG2	6.60	121.64	112.40
1	A	263	LYS	CD-CE-NZ	6.59	126.87	111.70
1	A	549	GLY	C-N-CA	-6.59	108.45	122.30
1	D	402	THR	CA-CB-CG2	6.59	121.63	112.40
1	E	25	THR	CA-C-N	-6.59	102.69	117.20
1	F	200	ASP	OD1-CG-OD2	-6.59	110.77	123.30
1	A	616	TYR	N-CA-CB	-6.59	98.73	110.60
1	C	354	GLN	OE1-CD-NE2	-6.59	106.73	121.90
1	B	263	LYS	CD-CE-NZ	6.59	126.86	111.70
1	C	560	ARG	NH1-CZ-NH2	6.59	126.65	119.40
1	F	616	TYR	N-CA-CB	-6.59	98.74	110.60
1	C	357	PRO	C-N-CA	-6.59	105.23	121.70
1	E	263	LYS	CD-CE-NZ	6.59	126.86	111.70
1	F	144	MET	CA-CB-CG	6.59	124.50	113.30
1	D	549	GLY	C-N-CA	-6.59	108.47	122.30
1	F	518	THR	N-CA-CB	6.59	122.82	110.30
1	B	402	THR	CA-CB-CG2	6.59	121.62	112.40
1	B	549	GLY	C-N-CA	-6.59	108.47	122.30
1	C	199	MET	N-CA-C	-6.59	93.22	111.00
1	F	462	TYR	O-C-N	6.59	133.24	122.70
1	F	558	TYR	CB-CG-CD1	6.59	124.95	121.00
1	B	72	TYR	CB-CG-CD1	-6.58	117.05	121.00
1	B	244	ASP	CA-CB-CG	6.58	127.89	113.40
1	E	177	ARG	N-CA-C	6.58	128.78	111.00
1	F	177	ARG	N-CA-C	6.58	128.78	111.00
1	C	177	ARG	N-CA-C	6.58	128.77	111.00
1	D	177	ARG	N-CA-C	6.58	128.78	111.00
1	D	518	THR	N-CA-CB	6.58	122.81	110.30
1	E	144	MET	CA-CB-CG	6.58	124.49	113.30
1	A	462	TYR	O-C-N	6.58	133.23	122.70
1	C	91	ASN	CB-CG-ND2	-6.58	100.91	116.70
1	D	207	ASP	CB-CG-OD2	6.58	124.22	118.30
1	D	616	TYR	N-CA-CB	-6.58	98.76	110.60
1	F	199	MET	N-CA-C	-6.58	93.23	111.00
1	F	651	HIS	O-C-N	6.58	133.23	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ARG	N-CA-C	6.58	128.76	111.00
1	B	91	ASN	CB-CG-ND2	-6.58	100.91	116.70
1	E	91	ASN	CB-CG-ND2	-6.58	100.91	116.70
1	D	91	ASN	CB-CG-ND2	-6.58	100.92	116.70
1	E	354	GLN	OE1-CD-NE2	-6.58	106.77	121.90
1	A	91	ASN	CB-CG-ND2	-6.58	100.92	116.70
1	A	144	MET	CA-CB-CG	6.58	124.48	113.30
1	A	244	ASP	CA-CB-CG	6.58	127.87	113.40
1	A	357	PRO	C-N-CA	-6.58	105.26	121.70
1	C	616	TYR	N-CA-CB	-6.58	98.76	110.60
1	D	244	ASP	CA-CB-CG	6.58	127.86	113.40
1	E	98	CYS	CB-CA-C	6.58	123.55	110.40
1	B	177	ARG	N-CA-C	6.57	128.75	111.00
1	C	462	TYR	O-C-N	6.57	133.22	122.70
1	F	357	PRO	C-N-CA	-6.57	105.27	121.70
1	F	629	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	B	199	MET	N-CA-C	-6.57	93.26	111.00
1	D	357	PRO	C-N-CA	-6.57	105.27	121.70
1	A	199	MET	N-CA-C	-6.57	93.26	111.00
1	C	244	ASP	CA-CB-CG	6.57	127.85	113.40
1	E	48	ASP	CB-CG-OD1	6.57	124.21	118.30
1	E	518	THR	N-CA-CB	6.57	122.78	110.30
1	F	91	ASN	CB-CG-ND2	-6.57	100.93	116.70
1	F	642	ILE	CA-C-O	-6.57	106.30	120.10
1	E	199	MET	N-CA-C	-6.57	93.26	111.00
1	A	48	ASP	CB-CG-OD1	6.57	124.21	118.30
1	B	48	ASP	CB-CG-OD1	6.57	124.21	118.30
1	C	561	SER	CB-CA-C	6.57	122.58	110.10
1	E	275	ILE	CB-CA-C	-6.57	98.46	111.60
1	B	642	ILE	CA-C-O	-6.57	106.31	120.10
1	C	275	ILE	CB-CA-C	-6.57	98.47	111.60
1	C	629	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	E	244	ASP	CA-CB-CG	6.57	127.84	113.40
1	B	462	TYR	O-C-N	6.56	133.20	122.70
1	D	199	MET	N-CA-C	-6.56	93.28	111.00
1	B	357	PRO	C-N-CA	-6.56	105.30	121.70
1	C	518	THR	N-CA-CB	6.56	122.77	110.30
1	A	518	THR	N-CA-CB	6.56	122.77	110.30
1	F	48	ASP	CB-CG-OD1	6.56	124.20	118.30
1	A	642	ILE	CA-C-O	-6.56	106.33	120.10
1	B	144	MET	CA-CB-CG	6.56	124.45	113.30
1	D	278	GLU	CA-CB-CG	-6.56	98.97	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	642	ILE	CA-C-O	-6.56	106.33	120.10
1	E	357	PRO	C-N-CA	-6.56	105.30	121.70
1	E	642	ILE	CA-C-O	-6.56	106.33	120.10
1	B	561	SER	CB-CA-C	6.56	122.56	110.10
1	F	278	GLU	CA-CB-CG	-6.56	98.97	113.40
1	C	278	GLU	CA-CB-CG	-6.56	98.98	113.40
1	D	275	ILE	CB-CA-C	-6.56	98.49	111.60
1	A	275	ILE	CB-CA-C	-6.55	98.49	111.60
1	C	98	CYS	CB-CA-C	6.55	123.51	110.40
1	E	462	TYR	O-C-N	6.55	133.19	122.70
1	F	275	ILE	CB-CA-C	-6.55	98.49	111.60
1	C	72	TYR	CB-CG-CD1	-6.55	117.07	121.00
1	E	561	SER	CB-CA-C	6.55	122.55	110.10
1	C	48	ASP	CB-CG-OD1	6.55	124.20	118.30
1	C	144	MET	CA-CB-CG	6.55	124.44	113.30
1	E	278	GLU	CA-CB-CG	-6.55	98.99	113.40
1	F	244	ASP	CA-CB-CG	6.55	127.81	113.40
1	B	278	GLU	CA-CB-CG	-6.55	98.99	113.40
1	A	98	CYS	CB-CA-C	6.55	123.50	110.40
1	A	278	GLU	CA-CB-CG	-6.55	99.00	113.40
1	A	629	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	B	275	ILE	CB-CA-C	-6.55	98.51	111.60
1	B	651	HIS	O-C-N	6.55	133.18	122.70
1	C	207	ASP	CB-CG-OD2	6.55	124.19	118.30
1	C	642	ILE	CA-C-O	-6.55	106.35	120.10
1	A	207	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	561	SER	CB-CA-C	6.54	122.53	110.10
1	A	651	HIS	O-C-N	6.54	133.17	122.70
1	E	532	ASP	CB-CG-OD1	6.54	124.19	118.30
1	F	72	TYR	CB-CG-CD2	6.54	124.92	121.00
1	F	561	SER	CB-CA-C	6.54	122.53	110.10
1	D	561	SER	CB-CA-C	6.54	122.53	110.10
1	F	211	TYR	CB-CG-CD1	-6.54	117.08	121.00
1	B	518	THR	N-CA-CB	6.54	122.72	110.30
1	D	336	ASN	CB-CA-C	6.54	123.48	110.40
1	C	651	HIS	O-C-N	6.54	133.16	122.70
1	D	198	HIS	N-CA-CB	-6.54	98.83	110.60
1	E	651	HIS	O-C-N	6.54	133.16	122.70
1	B	98	CYS	CB-CA-C	6.54	123.47	110.40
1	D	98	CYS	CB-CA-C	6.54	123.47	110.40
1	D	651	HIS	O-C-N	6.54	133.16	122.70
1	F	98	CYS	CB-CA-C	6.54	123.47	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	TYR	CB-CG-CD1	-6.53	117.08	121.00
1	A	211	TYR	CB-CG-CD1	-6.53	117.08	121.00
1	B	207	ASP	CB-CG-OD2	6.53	124.18	118.30
1	F	207	ASP	CB-CG-OD2	6.53	124.18	118.30
1	A	72	TYR	CB-CG-CD1	-6.53	117.08	121.00
1	D	245	GLU	CA-C-N	6.53	131.56	117.20
1	F	245	GLU	CA-C-N	6.53	131.55	117.20
1	E	245	GLU	CA-C-N	6.52	131.55	117.20
1	B	198	HIS	N-CA-CB	-6.52	98.86	110.60
1	E	207	ASP	CB-CG-OD2	6.52	124.17	118.30
1	A	127	LYS	CG-CD-CE	6.52	131.46	111.90
1	B	532	ASP	CB-CG-OD1	6.52	124.17	118.30
1	D	127	LYS	CG-CD-CE	6.52	131.46	111.90
1	E	72	TYR	CB-CG-CD2	6.52	124.91	121.00
1	F	127	LYS	CG-CD-CE	6.52	131.46	111.90
1	B	127	LYS	CG-CD-CE	6.52	131.45	111.90
1	C	183	TYR	CG-CD2-CE2	6.52	126.52	121.30
1	C	198	HIS	N-CA-CB	-6.52	98.87	110.60
1	C	336	ASN	CB-CA-C	6.52	123.43	110.40
1	C	245	GLU	CA-C-N	6.51	131.53	117.20
1	D	181	VAL	CB-CA-C	6.51	123.78	111.40
1	E	72	TYR	CB-CG-CD1	-6.51	117.09	121.00
1	E	127	LYS	CG-CD-CE	6.51	131.44	111.90
1	F	532	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	245	GLU	CA-C-N	6.51	131.53	117.20
1	D	3	LEU	CA-C-O	6.51	133.78	120.10
1	D	72	TYR	CB-CG-CD1	-6.51	117.09	121.00
1	D	629	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	336	ASN	CB-CA-C	6.51	123.42	110.40
1	B	245	GLU	CA-C-N	6.51	131.52	117.20
1	B	336	ASN	CB-CA-C	6.51	123.42	110.40
1	D	412	VAL	O-C-N	6.51	133.11	122.70
1	A	198	HIS	N-CA-CB	-6.51	98.89	110.60
1	F	198	HIS	N-CA-CB	-6.50	98.89	110.60
1	F	333	TYR	O-C-N	-6.50	112.30	122.70
1	A	181	VAL	CB-CA-C	6.50	123.75	111.40
1	F	336	ASN	CB-CA-C	6.50	123.41	110.40
1	B	3	LEU	CA-C-O	6.50	133.75	120.10
1	C	127	LYS	CG-CD-CE	6.50	131.40	111.90
1	E	181	VAL	CB-CA-C	6.50	123.75	111.40
1	E	412	VAL	O-C-N	6.50	133.10	122.70
1	E	333	TYR	O-C-N	-6.50	112.31	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	LEU	CA-C-O	6.49	133.74	120.10
1	A	412	VAL	O-C-N	6.49	133.09	122.70
1	C	333	TYR	O-C-N	-6.49	112.31	122.70
1	C	532	ASP	CB-CG-OD1	6.49	124.14	118.30
1	D	441	GLU	OE1-CD-OE2	6.49	131.09	123.30
1	C	3	LEU	CA-C-O	6.49	133.73	120.10
1	E	198	HIS	N-CA-CB	-6.49	98.92	110.60
1	F	412	VAL	O-C-N	6.49	133.09	122.70
1	A	333	TYR	O-C-N	-6.49	112.32	122.70
1	B	629	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	E	3	LEU	CA-C-O	6.49	133.73	120.10
1	E	211	TYR	CB-CG-CD1	-6.49	117.11	121.00
1	E	441	GLU	OE1-CD-OE2	6.49	131.08	123.30
1	C	181	VAL	CB-CA-C	6.48	123.72	111.40
1	D	211	TYR	CB-CG-CD1	-6.48	117.11	121.00
1	E	336	ASN	CB-CA-C	6.48	123.37	110.40
1	F	3	LEU	CA-C-O	6.48	133.72	120.10
1	D	72	TYR	CB-CG-CD2	6.48	124.89	121.00
1	A	532	ASP	CB-CG-OD1	6.48	124.13	118.30
1	F	361	PHE	CA-C-N	-6.48	102.94	117.20
1	F	494	THR	CA-C-N	6.48	131.46	117.20
1	A	494	THR	CA-C-N	6.48	131.45	117.20
1	B	213	LEU	O-C-N	6.48	133.06	122.70
1	B	546	ALA	O-C-N	6.48	133.06	122.70
1	D	494	THR	CA-C-N	6.48	131.45	117.20
1	B	333	TYR	O-C-N	-6.48	112.34	122.70
1	F	145	PHE	CA-C-O	-6.48	106.50	120.10
1	F	181	VAL	CB-CA-C	6.48	123.70	111.40
1	B	181	VAL	CB-CA-C	6.47	123.70	111.40
1	B	452	VAL	CB-CA-C	-6.47	99.10	111.40
1	C	441	GLU	OE1-CD-OE2	6.47	131.07	123.30
1	C	494	THR	CA-C-N	6.47	131.44	117.20
1	D	333	TYR	O-C-N	-6.47	112.34	122.70
1	D	361	PHE	CA-C-N	-6.47	102.96	117.20
1	E	494	THR	CA-C-N	6.47	131.44	117.20
1	F	452	VAL	CB-CA-C	-6.47	99.10	111.40
1	C	452	VAL	CB-CA-C	-6.47	99.11	111.40
1	C	546	ALA	O-C-N	6.47	133.05	122.70
1	D	214	ASP	CB-CA-C	-6.47	97.46	110.40
1	E	217	GLY	CA-C-O	-6.47	108.96	120.60
1	F	183	TYR	CG-CD2-CE2	6.47	126.47	121.30
1	A	72	TYR	CB-CG-CD2	6.47	124.88	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	441	GLU	OE1-CD-OE2	6.47	131.06	123.30
1	B	494	THR	CA-C-N	6.47	131.43	117.20
1	D	452	VAL	CB-CA-C	-6.47	99.11	111.40
1	E	452	VAL	CB-CA-C	-6.47	99.11	111.40
1	B	214	ASP	CB-CA-C	-6.46	97.47	110.40
1	D	546	ALA	O-C-N	6.46	133.04	122.70
1	A	452	VAL	CB-CA-C	-6.46	99.12	111.40
1	C	412	VAL	O-C-N	6.46	133.04	122.70
1	A	361	PHE	CA-C-N	-6.46	102.99	117.20
1	B	361	PHE	CA-C-N	-6.46	102.98	117.20
1	C	213	LEU	O-C-N	6.46	133.04	122.70
1	E	593	THR	CA-CB-OG1	-6.46	95.43	109.00
1	F	217	GLY	CA-C-O	-6.46	108.97	120.60
1	A	145	PHE	CA-C-O	-6.46	106.53	120.10
1	B	93	CYS	CA-CB-SG	-6.46	102.37	114.00
1	C	211	TYR	CB-CG-CD1	-6.46	117.12	121.00
1	D	593	THR	CA-CB-OG1	-6.46	95.43	109.00
1	B	145	PHE	CA-C-O	-6.46	106.53	120.10
1	A	373	THR	CA-CB-OG1	-6.46	95.44	109.00
1	D	451	ARG	CB-CG-CD	6.46	128.39	111.60
1	E	373	THR	CA-CB-OG1	-6.46	95.44	109.00
1	E	451	ARG	CB-CG-CD	6.46	128.39	111.60
1	F	546	ALA	O-C-N	6.46	133.03	122.70
1	C	86	LEU	CB-CA-C	6.46	122.46	110.20
1	D	217	GLY	CA-C-O	-6.46	108.98	120.60
1	A	214	ASP	CB-CA-C	-6.45	97.49	110.40
1	A	217	GLY	CA-C-O	-6.45	108.98	120.60
1	B	373	THR	CA-CB-OG1	-6.45	95.45	109.00
1	C	93	CYS	CA-CB-SG	-6.45	102.38	114.00
1	D	93	CYS	CA-CB-SG	-6.45	102.38	114.00
1	D	465	THR	CA-CB-CG2	-6.45	103.36	112.40
1	E	145	PHE	CA-C-O	-6.45	106.55	120.10
1	E	383	LEU	CA-C-N	6.45	131.40	117.20
1	A	93	CYS	CA-CB-SG	-6.45	102.39	114.00
1	E	361	PHE	CA-C-N	-6.45	103.00	117.20
1	B	412	VAL	O-C-N	6.45	133.02	122.70
1	C	145	PHE	CA-C-O	-6.45	106.55	120.10
1	C	361	PHE	CA-C-N	-6.45	103.01	117.20
1	C	593	THR	CA-CB-OG1	-6.45	95.45	109.00
1	D	542	GLN	N-CA-CB	-6.45	98.99	110.60
1	E	546	ALA	O-C-N	6.45	133.02	122.70
1	A	451	ARG	CB-CG-CD	6.45	128.36	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	72	TYR	CB-CG-CD2	6.45	124.87	121.00
1	C	217	GLY	CA-C-O	-6.45	108.99	120.60
1	C	373	THR	CA-CB-OG1	-6.45	95.46	109.00
1	D	48	ASP	N-CA-CB	6.45	122.21	110.60
1	E	239	TRP	CD1-NE1-CE2	-6.45	103.20	109.00
1	F	214	ASP	CB-CA-C	-6.45	97.50	110.40
1	F	373	THR	CA-CB-OG1	-6.45	95.46	109.00
1	D	373	THR	CA-CB-OG1	-6.45	95.46	109.00
1	F	451	ARG	CB-CG-CD	6.45	128.36	111.60
1	A	546	ALA	O-C-N	6.45	133.01	122.70
1	A	593	THR	CA-CB-OG1	-6.45	95.46	109.00
1	D	213	LEU	O-C-N	6.45	133.01	122.70
1	D	532	ASP	CB-CG-OD1	6.45	124.10	118.30
1	A	183	TYR	CG-CD2-CE2	6.44	126.45	121.30
1	B	451	ARG	CB-CG-CD	6.44	128.35	111.60
1	B	542	GLN	N-CA-CB	-6.44	99.00	110.60
1	E	93	CYS	CA-CB-SG	-6.44	102.40	114.00
1	A	542	GLN	N-CA-CB	-6.44	99.00	110.60
1	F	383	LEU	CA-C-N	6.44	131.37	117.20
1	F	465	THR	CA-CB-CG2	-6.44	103.38	112.40
1	A	213	LEU	O-C-N	6.44	133.00	122.70
1	B	441	GLU	OE1-CD-OE2	6.44	131.03	123.30
1	B	465	THR	CA-CB-CG2	-6.44	103.38	112.40
1	C	451	ARG	CB-CG-CD	6.44	128.35	111.60
1	D	86	LEU	CB-CA-C	6.44	122.44	110.20
1	D	145	PHE	CA-C-O	-6.44	106.58	120.10
1	E	86	LEU	CB-CA-C	6.44	122.44	110.20
1	F	542	GLN	N-CA-CB	-6.44	99.01	110.60
1	D	183	TYR	CG-CD2-CE2	6.44	126.45	121.30
1	F	93	CYS	CA-CB-SG	-6.44	102.41	114.00
1	C	214	ASP	CB-CA-C	-6.44	97.53	110.40
1	E	42	ASP	CB-CG-OD1	-6.44	112.51	118.30
1	F	593	THR	CA-CB-OG1	-6.44	95.48	109.00
1	B	383	LEU	CA-C-N	6.44	131.36	117.20
1	D	383	LEU	CA-C-N	6.44	131.36	117.20
1	A	383	LEU	CA-C-N	6.43	131.36	117.20
1	B	217	GLY	CA-C-O	-6.43	109.02	120.60
1	F	213	LEU	O-C-N	6.43	133.00	122.70
1	A	48	ASP	N-CA-CB	6.43	122.18	110.60
1	A	86	LEU	CB-CA-C	6.43	122.42	110.20
1	B	183	TYR	CG-CD2-CE2	6.43	126.45	121.30
1	B	593	THR	CA-CB-OG1	-6.43	95.49	109.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	383	LEU	CA-C-N	6.43	131.35	117.20
1	E	214	ASP	CB-CA-C	-6.43	97.54	110.40
1	B	86	LEU	CB-CA-C	6.43	122.42	110.20
1	B	72	TYR	CB-CG-CD2	6.43	124.86	121.00
1	E	465	THR	CA-CB-CG2	-6.43	103.40	112.40
1	C	43	THR	N-CA-C	-6.43	93.65	111.00
1	E	213	LEU	O-C-N	6.43	132.98	122.70
1	F	42	ASP	CB-CG-OD1	-6.42	112.52	118.30
1	F	86	LEU	CB-CA-C	6.42	122.41	110.20
1	F	441	GLU	OE1-CD-OE2	6.42	131.01	123.30
1	A	465	THR	CA-CB-CG2	-6.42	103.41	112.40
1	C	48	ASP	N-CA-CB	6.42	122.15	110.60
1	C	542	GLN	N-CA-CB	-6.42	99.05	110.60
1	D	42	ASP	CB-CG-OD1	-6.42	112.52	118.30
1	E	542	GLN	N-CA-CB	-6.42	99.05	110.60
1	F	422	LEU	CB-CG-CD1	-6.42	100.09	111.00
1	D	43	THR	N-CA-C	-6.42	93.68	111.00
1	E	183	TYR	CG-CD2-CE2	6.42	126.43	121.30
1	B	48	ASP	N-CA-CB	6.41	122.14	110.60
1	E	48	ASP	N-CA-CB	6.41	122.14	110.60
1	A	43	THR	N-CA-C	-6.41	93.69	111.00
1	B	422	LEU	CB-CG-CD1	-6.41	100.10	111.00
1	C	422	LEU	CB-CG-CD1	-6.41	100.10	111.00
1	D	111	ASN	N-CA-CB	-6.41	99.06	110.60
1	E	422	LEU	CB-CG-CD1	-6.41	100.10	111.00
1	A	422	LEU	CB-CG-CD1	-6.41	100.10	111.00
1	B	43	THR	N-CA-C	-6.41	93.69	111.00
1	D	501	PHE	CG-CD2-CE2	6.41	127.85	120.80
1	E	33	ILE	CA-C-N	-6.41	103.10	117.20
1	E	43	THR	N-CA-C	-6.41	93.70	111.00
1	C	33	ILE	CA-C-N	-6.41	103.10	117.20
1	F	48	ASP	N-CA-CB	6.41	122.13	110.60
1	A	42	ASP	CB-CG-OD1	-6.41	112.54	118.30
1	B	346	THR	CA-CB-CG2	-6.40	103.44	112.40
1	C	42	ASP	CB-CG-OD1	-6.40	112.54	118.30
1	D	422	LEU	CB-CG-CD1	-6.40	100.12	111.00
1	B	33	ILE	CA-C-N	-6.40	103.12	117.20
1	B	42	ASP	CB-CG-OD1	-6.40	112.54	118.30
1	C	465	THR	CA-CB-CG2	-6.40	103.44	112.40
1	C	487	ASP	OD1-CG-OD2	-6.39	111.15	123.30
1	F	43	THR	N-CA-C	-6.39	93.73	111.00
1	A	33	ILE	CA-C-N	-6.39	103.14	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	487	ASP	OD1-CG-OD2	-6.39	111.16	123.30
1	F	111	ASN	N-CA-CB	-6.39	99.10	110.60
1	A	111	ASN	N-CA-CB	-6.39	99.10	110.60
1	A	239	TRP	CD1-NE1-CE2	-6.39	103.25	109.00
1	D	487	ASP	OD1-CG-OD2	-6.39	111.17	123.30
1	A	487	ASP	OD1-CG-OD2	-6.38	111.17	123.30
1	B	111	ASN	N-CA-CB	-6.38	99.11	110.60
1	C	346	THR	CA-CB-CG2	-6.38	103.47	112.40
1	E	111	ASN	N-CA-CB	-6.38	99.11	110.60
1	F	33	ILE	CA-C-N	-6.38	103.16	117.20
1	C	100	ARG	CD-NE-CZ	-6.38	114.67	123.60
1	C	111	ASN	N-CA-CB	-6.38	99.12	110.60
1	D	346	THR	CA-CB-CG2	-6.38	103.47	112.40
1	A	346	THR	CA-CB-CG2	-6.38	103.47	112.40
1	F	346	THR	CA-CB-CG2	-6.38	103.47	112.40
1	E	487	ASP	OD1-CG-OD2	-6.37	111.19	123.30
1	F	190	MET	CB-CG-SD	-6.37	93.28	112.40
1	D	33	ILE	CA-C-N	-6.37	103.18	117.20
1	B	423	ILE	CB-CG1-CD1	-6.37	96.06	113.90
1	E	39	PRO	O-C-N	6.37	132.89	122.70
1	F	39	PRO	O-C-N	6.37	132.89	122.70
1	F	487	ASP	OD1-CG-OD2	-6.37	111.20	123.30
1	E	346	THR	CA-CB-CG2	-6.37	103.49	112.40
1	B	501	PHE	CG-CD2-CE2	6.37	127.80	120.80
1	D	239	TRP	CD1-NE1-CE2	-6.37	103.27	109.00
1	F	239	TRP	CD1-NE1-CE2	-6.37	103.27	109.00
1	A	423	ILE	CB-CG1-CD1	-6.36	96.08	113.90
1	E	423	ILE	CB-CG1-CD1	-6.36	96.08	113.90
1	F	423	ILE	CB-CG1-CD1	-6.36	96.08	113.90
1	E	190	MET	CB-CG-SD	-6.36	93.31	112.40
1	B	100	ARG	CD-NE-CZ	-6.36	114.70	123.60
1	B	190	MET	CB-CG-SD	-6.36	93.32	112.40
1	B	239	TRP	CD1-NE1-CE2	-6.36	103.28	109.00
1	A	39	PRO	O-C-N	6.36	132.87	122.70
1	A	190	MET	CB-CG-SD	-6.36	93.33	112.40
1	B	39	PRO	O-C-N	6.36	132.87	122.70
1	C	239	TRP	CD1-NE1-CE2	-6.36	103.28	109.00
1	D	39	PRO	O-C-N	6.36	132.87	122.70
1	D	190	MET	CB-CG-SD	-6.36	93.33	112.40
1	F	100	ARG	CD-NE-CZ	-6.36	114.70	123.60
1	B	186	GLU	N-CA-CB	-6.36	99.16	110.60
1	D	423	ILE	CB-CG1-CD1	-6.36	96.10	113.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	186	GLU	N-CA-CB	-6.35	99.16	110.60
1	C	621	PRO	CA-C-N	6.35	131.18	117.20
1	A	100	ARG	CD-NE-CZ	-6.35	114.71	123.60
1	A	621	PRO	CA-C-N	6.35	131.18	117.20
1	B	180	ARG	O-C-N	6.35	132.86	122.70
1	C	190	MET	CB-CG-SD	-6.35	93.34	112.40
1	C	423	ILE	CB-CG1-CD1	-6.35	96.11	113.90
1	D	89	VAL	CA-CB-CG1	6.35	120.43	110.90
1	E	100	ARG	CD-NE-CZ	-6.35	114.71	123.60
1	C	11	GLN	O-C-N	6.35	132.86	122.70
1	F	621	PRO	CA-C-N	6.35	131.17	117.20
1	C	152	ASP	CB-CG-OD2	6.35	124.01	118.30
1	D	152	ASP	CB-CG-OD2	6.35	124.02	118.30
1	D	621	PRO	CA-C-N	6.35	131.17	117.20
1	B	152	ASP	CB-CG-OD2	6.35	124.01	118.30
1	D	100	ARG	CD-NE-CZ	-6.35	114.71	123.60
1	A	152	ASP	CB-CG-OD2	6.35	124.01	118.30
1	B	621	PRO	CA-C-N	6.34	131.16	117.20
1	C	180	ARG	O-C-N	6.34	132.85	122.70
1	F	322	GLU	N-CA-CB	6.34	122.02	110.60
1	E	621	PRO	CA-C-N	6.34	131.15	117.20
1	F	186	GLU	N-CA-CB	-6.34	99.19	110.60
1	A	419	ASP	CB-CG-OD2	6.34	124.01	118.30
1	B	419	ASP	CB-CG-OD2	6.34	124.01	118.30
1	D	296	ILE	CB-CG1-CD1	-6.34	96.15	113.90
1	D	203	PHE	CG-CD2-CE2	6.34	127.77	120.80
1	C	89	VAL	CA-CB-CG1	6.34	120.40	110.90
1	D	186	GLU	N-CA-CB	-6.34	99.19	110.60
1	E	89	VAL	CA-CB-CG1	6.34	120.41	110.90
1	E	152	ASP	CB-CG-OD2	6.34	124.00	118.30
1	F	152	ASP	CB-CG-OD2	6.34	124.00	118.30
1	A	186	GLU	N-CA-CB	-6.33	99.20	110.60
1	B	296	ILE	CB-CG1-CD1	-6.33	96.16	113.90
1	E	322	GLU	N-CA-CB	6.33	122.00	110.60
1	A	501	PHE	CG-CD2-CE2	6.33	127.77	120.80
1	E	186	GLU	N-CA-CB	-6.33	99.20	110.60
1	A	89	VAL	CA-CB-CG1	6.33	120.40	110.90
1	B	312	THR	CA-CB-OG1	-6.33	95.70	109.00
1	C	39	PRO	O-C-N	6.33	132.83	122.70
1	C	322	GLU	N-CA-CB	6.33	122.00	110.60
1	F	296	ILE	CB-CG1-CD1	-6.33	96.17	113.90
1	A	322	GLU	N-CA-CB	6.33	121.99	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	322	GLU	N-CA-CB	6.33	121.99	110.60
1	E	296	ILE	CB-CG1-CD1	-6.33	96.18	113.90
1	A	296	ILE	CB-CG1-CD1	-6.33	96.19	113.90
1	E	501	PHE	CG-CD2-CE2	6.33	127.76	120.80
1	F	89	VAL	CA-CB-CG1	6.33	120.39	110.90
1	C	296	ILE	CB-CG1-CD1	-6.32	96.20	113.90
1	C	419	ASP	CB-CG-OD2	6.32	123.99	118.30
1	F	312	THR	CA-CB-OG1	-6.32	95.72	109.00
1	F	368	MET	CG-SD-CE	-6.32	90.08	100.20
1	B	322	GLU	N-CA-CB	6.32	121.98	110.60
1	F	501	PHE	CG-CD2-CE2	6.32	127.75	120.80
1	B	89	VAL	CA-CB-CG1	6.32	120.38	110.90
1	E	312	THR	CA-CB-OG1	-6.32	95.72	109.00
1	C	336	ASN	CA-C-N	6.32	131.10	117.20
1	A	180	ARG	O-C-N	6.32	132.81	122.70
1	A	312	THR	CA-CB-OG1	-6.32	95.74	109.00
1	A	11	GLN	O-C-N	6.31	132.80	122.70
1	D	254	GLU	CG-CD-OE1	-6.31	105.67	118.30
1	D	270	VAL	CA-C-O	-6.31	106.84	120.10
1	E	180	ARG	O-C-N	6.31	132.80	122.70
1	B	203	PHE	CG-CD2-CE2	6.31	127.74	120.80
1	C	254	GLU	CG-CD-OE1	-6.31	105.68	118.30
1	D	180	ARG	O-C-N	6.31	132.80	122.70
1	A	270	VAL	CA-C-O	-6.31	106.85	120.10
1	C	501	PHE	CG-CD2-CE2	6.31	127.74	120.80
1	B	270	VAL	CA-C-O	-6.31	106.85	120.10
1	F	180	ARG	O-C-N	6.31	132.79	122.70
1	F	270	VAL	CA-C-O	-6.31	106.86	120.10
1	F	419	ASP	CB-CG-OD2	6.31	123.97	118.30
1	A	336	ASN	CA-C-N	6.30	131.07	117.20
1	B	11	GLN	O-C-N	6.30	132.79	122.70
1	D	336	ASN	CA-C-N	6.30	131.07	117.20
1	E	419	ASP	CB-CG-OD2	6.30	123.97	118.30
1	B	254	GLU	CG-CD-OE1	-6.30	105.69	118.30
1	D	312	THR	CA-CB-OG1	-6.30	95.76	109.00
1	A	254	GLU	CG-CD-OE1	-6.30	105.70	118.30
1	A	368	MET	CG-SD-CE	-6.30	90.12	100.20
1	E	270	VAL	CA-C-O	-6.30	106.87	120.10
1	F	15	ASN	CB-CG-OD1	-6.30	109.00	121.60
1	F	254	GLU	CG-CD-OE1	-6.30	105.69	118.30
1	B	123	VAL	CA-CB-CG2	-6.30	101.45	110.90
1	C	270	VAL	CA-C-O	-6.30	106.87	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	312	THR	CA-CB-OG1	-6.30	95.77	109.00
1	E	203	PHE	CG-CD2-CE2	6.30	127.73	120.80
1	B	336	ASN	CA-C-N	6.30	131.06	117.20
1	C	236	LEU	CB-CA-C	-6.30	98.24	110.20
1	D	368	MET	CG-SD-CE	-6.30	90.13	100.20
1	E	11	GLN	O-C-N	6.30	132.77	122.70
1	F	123	VAL	CA-CB-CG2	-6.29	101.46	110.90
1	C	368	MET	CG-SD-CE	-6.29	90.13	100.20
1	D	236	LEU	CB-CA-C	-6.29	98.24	110.20
1	F	203	PHE	CG-CD2-CE2	6.29	127.72	120.80
1	F	336	ASN	CA-C-N	6.29	131.05	117.20
1	E	368	MET	CG-SD-CE	-6.29	90.13	100.20
1	A	123	VAL	CA-CB-CG2	-6.29	101.47	110.90
1	A	236	LEU	CB-CA-C	-6.29	98.25	110.20
1	E	15	ASN	CB-CG-OD1	-6.29	109.02	121.60
1	B	15	ASN	CB-CG-OD1	-6.29	109.02	121.60
1	B	443	ILE	CA-C-O	-6.29	106.90	120.10
1	C	123	VAL	CA-CB-CG2	-6.29	101.47	110.90
1	C	443	ILE	CA-C-O	-6.29	106.90	120.10
1	E	254	GLU	CG-CD-OE1	-6.29	105.73	118.30
1	E	336	ASN	CA-C-N	6.28	131.02	117.20
1	A	203	PHE	CG-CD2-CE2	6.28	127.71	120.80
1	D	15	ASN	CB-CG-OD1	-6.28	109.04	121.60
1	E	123	VAL	CA-CB-CG2	-6.28	101.48	110.90
1	F	11	GLN	O-C-N	6.28	132.75	122.70
1	A	15	ASN	CB-CG-OD1	-6.28	109.04	121.60
1	A	443	ILE	CA-C-O	-6.28	106.92	120.10
1	B	236	LEU	CB-CA-C	-6.28	98.27	110.20
1	C	203	PHE	CG-CD2-CE2	6.28	127.70	120.80
1	D	11	GLN	O-C-N	6.28	132.74	122.70
1	F	236	LEU	CB-CA-C	-6.28	98.27	110.20
1	B	368	MET	CG-SD-CE	-6.28	90.16	100.20
1	C	15	ASN	CB-CG-OD1	-6.28	109.05	121.60
1	C	557	ALA	O-C-N	6.28	132.74	122.70
1	D	419	ASP	CB-CG-OD2	6.28	123.95	118.30
1	C	214	ASP	CB-CG-OD2	6.27	123.95	118.30
1	F	443	ILE	CA-C-O	-6.27	106.92	120.10
1	E	236	LEU	CB-CA-C	-6.27	98.28	110.20
1	C	66	LEU	CA-CB-CG	6.27	129.72	115.30
1	E	443	ILE	CA-C-O	-6.27	106.94	120.10
1	F	210	GLY	N-CA-C	6.27	128.77	113.10
1	D	443	ILE	CA-C-O	-6.27	106.94	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	452	VAL	CA-C-O	-6.27	106.94	120.10
1	E	210	GLY	N-CA-C	6.27	128.77	113.10
1	D	557	ALA	O-C-N	6.26	132.72	122.70
1	E	557	ALA	O-C-N	6.26	132.72	122.70
1	D	123	VAL	CA-CB-CG2	-6.26	101.50	110.90
1	D	210	GLY	N-CA-C	6.26	128.76	113.10
1	D	66	LEU	CA-CB-CG	6.26	129.70	115.30
1	F	66	LEU	CA-CB-CG	6.26	129.70	115.30
1	F	557	ALA	O-C-N	6.26	132.72	122.70
1	B	452	VAL	CA-C-O	-6.26	106.95	120.10
1	A	210	GLY	N-CA-C	6.26	128.75	113.10
1	A	557	ALA	O-C-N	6.25	132.71	122.70
1	E	441	GLU	O-C-N	6.25	132.71	122.70
1	A	66	LEU	CA-CB-CG	6.25	129.68	115.30
1	C	426	PHE	C-N-CA	6.25	137.33	121.70
1	A	452	VAL	CA-C-O	-6.25	106.98	120.10
1	C	452	VAL	CA-C-O	-6.25	106.98	120.10
1	E	187	ASP	CB-CG-OD1	-6.25	112.68	118.30
1	F	510	GLN	CA-C-O	-6.25	106.98	120.10
1	A	426	PHE	C-N-CA	6.25	137.31	121.70
1	D	426	PHE	C-N-CA	6.25	137.31	121.70
1	E	66	LEU	CA-CB-CG	6.25	129.67	115.30
1	B	426	PHE	C-N-CA	6.25	137.31	121.70
1	C	187	ASP	CB-CG-OD1	-6.25	112.68	118.30
1	C	510	GLN	CA-C-O	-6.25	106.98	120.10
1	A	441	GLU	O-C-N	6.24	132.69	122.70
1	D	324	LEU	CB-CG-CD1	6.24	121.61	111.00
1	B	66	LEU	CA-CB-CG	6.24	129.65	115.30
1	B	557	ALA	O-C-N	6.24	132.68	122.70
1	D	441	GLU	O-C-N	6.24	132.69	122.70
1	E	324	LEU	CB-CG-CD1	6.24	121.61	111.00
1	F	426	PHE	C-N-CA	6.24	137.30	121.70
1	A	560	ARG	CA-C-N	-6.24	103.47	117.20
1	B	210	GLY	N-CA-C	6.24	128.70	113.10
1	C	210	GLY	N-CA-C	6.24	128.69	113.10
1	E	426	PHE	C-N-CA	6.24	137.29	121.70
1	F	324	LEU	CB-CG-CD1	6.24	121.61	111.00
1	B	214	ASP	CB-CG-OD2	6.24	123.91	118.30
1	B	324	LEU	CB-CG-CD1	6.24	121.60	111.00
1	D	560	ARG	CA-C-N	-6.24	103.48	117.20
1	E	452	VAL	CA-C-O	-6.24	107.00	120.10
1	F	452	VAL	CA-C-O	-6.24	107.01	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	560	ARG	CA-C-N	-6.24	103.48	117.20
1	C	560	ARG	CA-C-N	-6.23	103.49	117.20
1	F	187	ASP	CB-CG-OD1	-6.23	112.69	118.30
1	B	441	GLU	O-C-N	6.23	132.67	122.70
1	D	510	GLN	CA-C-O	-6.23	107.02	120.10
1	A	324	LEU	CB-CG-CD1	6.23	121.59	111.00
1	A	510	GLN	CA-C-O	-6.23	107.02	120.10
1	B	510	GLN	CA-C-O	-6.23	107.02	120.10
1	A	187	ASP	CB-CG-OD1	-6.23	112.70	118.30
1	C	324	LEU	CB-CG-CD1	6.22	121.58	111.00
1	A	214	ASP	CB-CG-OD2	6.22	123.90	118.30
1	B	560	ARG	CA-C-N	-6.22	103.51	117.20
1	E	557	ALA	CA-C-N	-6.22	103.51	117.20
1	F	224	HIS	N-CA-CB	-6.22	99.40	110.60
1	C	557	ALA	CA-C-N	-6.22	103.52	117.20
1	E	560	ARG	CA-C-N	-6.22	103.52	117.20
1	F	214	ASP	CB-CG-OD2	6.22	123.90	118.30
1	E	510	GLN	CA-C-O	-6.22	107.04	120.10
1	C	441	GLU	O-C-N	6.22	132.65	122.70
1	D	392	LYS	CD-CE-NZ	6.22	126.00	111.70
1	F	382	ARG	N-CA-CB	-6.22	99.41	110.60
1	C	392	LYS	CD-CE-NZ	6.21	125.99	111.70
1	D	557	ALA	CA-C-N	-6.21	103.53	117.20
1	B	557	ALA	CA-C-N	-6.21	103.53	117.20
1	E	392	LYS	CD-CE-NZ	6.21	125.98	111.70
1	E	450	ALA	N-CA-CB	-6.21	101.41	110.10
1	D	645	VAL	N-CA-CB	-6.21	97.84	111.50
1	E	382	ARG	N-CA-CB	-6.21	99.42	110.60
1	A	392	LYS	CD-CE-NZ	6.21	125.97	111.70
1	A	557	ALA	CA-C-N	-6.21	103.55	117.20
1	B	392	LYS	CD-CE-NZ	6.21	125.97	111.70
1	D	187	ASP	CB-CG-OD1	-6.21	112.72	118.30
1	D	306	THR	OG1-CB-CG2	6.21	124.28	110.00
1	E	645	VAL	N-CA-CB	-6.21	97.85	111.50
1	F	645	VAL	N-CA-CB	-6.20	97.85	111.50
1	E	239	TRP	CG-CD1-NE1	6.20	116.30	110.10
1	B	645	VAL	N-CA-CB	-6.20	97.86	111.50
1	C	635	VAL	O-C-N	6.20	132.62	122.70
1	D	224	HIS	N-CA-CB	-6.20	99.44	110.60
1	F	306	THR	OG1-CB-CG2	6.20	124.26	110.00
1	F	392	LYS	CD-CE-NZ	6.20	125.96	111.70
1	F	441	GLU	O-C-N	6.20	132.62	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	442	ASN	CB-CA-C	6.20	122.80	110.40
1	D	561	SER	N-CA-CB	-6.20	101.20	110.50
1	A	224	HIS	N-CA-CB	-6.20	99.44	110.60
1	C	645	VAL	N-CA-CB	-6.20	97.87	111.50
1	A	306	THR	OG1-CB-CG2	6.20	124.25	110.00
1	E	635	VAL	O-C-N	6.20	132.61	122.70
1	F	557	ALA	CA-C-N	-6.20	103.57	117.20
1	A	382	ARG	N-CA-CB	-6.19	99.45	110.60
1	A	450	ALA	N-CA-CB	-6.19	101.43	110.10
1	A	645	VAL	N-CA-CB	-6.19	97.88	111.50
1	B	32	ASP	CB-CA-C	6.19	122.78	110.40
1	C	382	ARG	N-CA-CB	-6.19	99.46	110.60
1	D	295	ARG	CB-CA-C	6.19	122.78	110.40
1	E	307	ASP	CB-CG-OD1	6.19	123.87	118.30
1	C	224	HIS	N-CA-CB	-6.19	99.46	110.60
1	E	607	ALA	N-CA-CB	6.19	118.77	110.10
1	C	387	MET	CA-CB-CG	6.19	123.82	113.30
1	B	224	HIS	N-CA-CB	-6.19	99.47	110.60
1	C	306	THR	OG1-CB-CG2	6.19	124.23	110.00
1	C	561	SER	N-CA-CB	-6.19	101.22	110.50
1	E	224	HIS	N-CA-CB	-6.19	99.46	110.60
1	D	406	LEU	O-C-N	-6.18	112.81	122.70
1	E	561	SER	N-CA-CB	-6.18	101.22	110.50
1	F	307	ASP	CB-CG-OD1	6.18	123.87	118.30
1	A	561	SER	N-CA-CB	-6.18	101.23	110.50
1	D	450	ALA	N-CA-CB	-6.18	101.44	110.10
1	E	306	THR	OG1-CB-CG2	6.18	124.22	110.00
1	E	349	VAL	CB-CA-C	-6.18	99.65	111.40
1	F	442	ASN	CB-CA-C	6.18	122.76	110.40
1	F	615	ALA	N-CA-CB	-6.18	101.44	110.10
1	F	561	SER	N-CA-CB	-6.18	101.23	110.50
1	B	295	ARG	CB-CA-C	6.18	122.76	110.40
1	C	349	VAL	CB-CA-C	-6.18	99.66	111.40
1	E	442	ASN	CB-CA-C	6.18	122.76	110.40
1	F	32	ASP	CB-CA-C	6.18	122.76	110.40
1	F	239	TRP	CG-CD1-NE1	6.18	116.28	110.10
1	B	442	ASN	CB-CA-C	6.18	122.76	110.40
1	B	187	ASP	CB-CG-OD1	-6.18	112.74	118.30
1	B	306	THR	OG1-CB-CG2	6.18	124.20	110.00
1	B	349	VAL	CB-CA-C	-6.18	99.66	111.40
1	D	382	ARG	N-CA-CB	-6.18	99.48	110.60
1	E	214	ASP	CB-CG-OD2	6.18	123.86	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	442	ASN	CB-CA-C	6.17	122.75	110.40
1	C	450	ALA	N-CA-CB	-6.17	101.46	110.10
1	F	387	MET	CA-CB-CG	6.17	123.80	113.30
1	B	450	ALA	N-CA-CB	-6.17	101.46	110.10
1	A	406	LEU	O-C-N	-6.17	112.83	122.70
1	A	635	VAL	O-C-N	6.17	132.57	122.70
1	C	615	ALA	N-CA-CB	-6.17	101.46	110.10
1	D	442	ASN	CB-CA-C	6.17	122.74	110.40
1	F	406	LEU	O-C-N	-6.17	112.83	122.70
1	B	382	ARG	N-CA-CB	-6.17	99.50	110.60
1	C	607	ALA	N-CA-CB	6.17	118.74	110.10
1	E	32	ASP	CB-CA-C	6.17	122.74	110.40
1	F	450	ALA	N-CA-CB	-6.17	101.46	110.10
1	B	247	HIS	C-N-CA	-6.17	106.28	121.70
1	C	245	GLU	N-CA-CB	-6.17	99.50	110.60
1	D	214	ASP	CB-CG-OD2	6.17	123.85	118.30
1	F	349	VAL	CB-CA-C	-6.17	99.68	111.40
1	E	355	GLY	O-C-N	6.17	132.56	122.70
1	A	239	TRP	CG-CD1-NE1	6.16	116.26	110.10
1	C	32	ASP	CB-CA-C	6.16	122.73	110.40
1	D	607	ALA	N-CA-CB	6.16	118.73	110.10
1	E	439	SER	N-CA-CB	-6.16	101.25	110.50
1	A	32	ASP	CB-CA-C	6.16	122.72	110.40
1	A	295	ARG	CB-CA-C	6.16	122.72	110.40
1	A	607	ALA	N-CA-CB	6.16	118.73	110.10
1	C	295	ARG	CB-CA-C	6.16	122.72	110.40
1	C	328	ILE	O-C-N	-6.16	112.84	122.70
1	A	298	GLU	C-N-CA	-6.16	106.30	121.70
1	A	387	MET	CA-CB-CG	6.16	123.77	113.30
1	B	411	MET	CB-CA-C	-6.16	98.08	110.40
1	C	406	LEU	O-C-N	-6.16	112.84	122.70
1	C	411	MET	CB-CA-C	-6.16	98.08	110.40
1	D	245	GLU	N-CA-CB	-6.16	99.51	110.60
1	D	349	VAL	CB-CA-C	-6.16	99.69	111.40
1	E	406	LEU	O-C-N	-6.16	112.84	122.70
1	F	247	HIS	C-N-CA	-6.16	106.30	121.70
1	F	298	GLU	C-N-CA	-6.16	106.30	121.70
1	F	411	MET	CB-CA-C	-6.16	98.08	110.40
1	A	307	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	349	VAL	CB-CA-C	-6.16	99.70	111.40
1	A	411	MET	CB-CA-C	-6.16	98.08	110.40
1	B	239	TRP	CG-CD1-NE1	6.16	116.26	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	298	GLU	C-N-CA	-6.16	106.31	121.70
1	B	578	MET	O-C-N	6.16	132.55	122.70
1	C	247	HIS	C-N-CA	-6.16	106.31	121.70
1	D	411	MET	CB-CA-C	-6.16	98.09	110.40
1	D	454	ARG	CA-CB-CG	6.16	126.94	113.40
1	E	298	GLU	C-N-CA	-6.16	106.31	121.70
1	E	411	MET	CB-CA-C	-6.16	98.09	110.40
1	F	635	VAL	O-C-N	6.16	132.55	122.70
1	A	245	GLU	N-CA-CB	-6.16	99.52	110.60
1	B	307	ASP	CB-CG-OD1	6.16	123.84	118.30
1	D	387	MET	CA-CB-CG	6.16	123.77	113.30
1	E	104	ALA	O-C-N	6.16	132.55	122.70
1	B	298	GLU	C-N-CA	-6.15	106.31	121.70
1	B	607	ALA	N-CA-CB	6.15	118.72	110.10
1	C	239	TRP	CG-CD1-NE1	6.15	116.25	110.10
1	B	406	LEU	O-C-N	-6.15	112.86	122.70
1	B	615	ALA	N-CA-CB	-6.15	101.49	110.10
1	C	239	TRP	CB-CA-C	6.15	122.71	110.40
1	D	298	GLU	C-N-CA	-6.15	106.32	121.70
1	E	245	GLU	N-CA-CB	-6.15	99.52	110.60
1	E	247	HIS	C-N-CA	-6.15	106.32	121.70
1	A	615	ALA	N-CA-CB	-6.15	101.49	110.10
1	B	561	SER	N-CA-CB	-6.15	101.27	110.50
1	C	450	ALA	CA-C-O	6.15	133.02	120.10
1	F	153	LYS	O-C-N	6.15	132.54	122.70
1	F	272	PRO	N-CD-CG	-6.15	93.98	103.20
1	A	247	HIS	C-N-CA	-6.15	106.33	121.70
1	B	268	PHE	CZ-CE2-CD2	-6.15	112.72	120.10
1	E	295	ARG	CB-CA-C	6.15	122.69	110.40
1	E	387	MET	CA-CB-CG	6.15	123.75	113.30
1	F	245	GLU	N-CA-CB	-6.15	99.53	110.60
1	D	32	ASP	CB-CA-C	6.15	122.69	110.40
1	A	450	ALA	CA-C-O	6.14	133.00	120.10
1	B	104	ALA	O-C-N	6.14	132.53	122.70
1	B	245	GLU	N-CA-CB	-6.14	99.54	110.60
1	D	635	VAL	O-C-N	6.14	132.53	122.70
1	E	615	ALA	N-CA-CB	-6.14	101.50	110.10
1	F	295	ARG	CB-CA-C	6.14	122.69	110.40
1	A	104	ALA	O-C-N	6.14	132.53	122.70
1	B	387	MET	CA-CB-CG	6.14	123.74	113.30
1	D	355	GLY	O-C-N	6.14	132.53	122.70
1	F	55	THR	CA-C-N	-6.14	103.69	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	355	GLY	O-C-N	6.14	132.53	122.70
1	A	454	ARG	CA-CB-CG	6.14	126.91	113.40
1	B	182	ALA	CA-C-O	6.14	133.00	120.10
1	D	615	ALA	N-CA-CB	-6.14	101.50	110.10
1	B	454	ARG	CA-CB-CG	6.14	126.91	113.40
1	C	55	THR	CA-C-N	-6.14	103.69	117.20
1	C	104	ALA	O-C-N	6.14	132.52	122.70
1	D	104	ALA	O-C-N	6.14	132.52	122.70
1	E	239	TRP	CB-CA-C	6.14	122.68	110.40
1	F	607	ALA	N-CA-CB	6.14	118.69	110.10
1	B	450	ALA	CA-C-O	6.14	132.99	120.10
1	C	454	ARG	CA-CB-CG	6.14	126.90	113.40
1	E	454	ARG	CA-CB-CG	6.14	126.90	113.40
1	A	328	ILE	O-C-N	-6.14	112.88	122.70
1	B	355	GLY	O-C-N	6.14	132.52	122.70
1	B	635	VAL	O-C-N	6.14	132.52	122.70
1	D	247	HIS	C-N-CA	-6.14	106.36	121.70
1	D	439	SER	N-CA-CB	-6.14	101.30	110.50
1	D	333	TYR	CD1-CG-CD2	-6.13	111.15	117.90
1	D	328	ILE	O-C-N	-6.13	112.89	122.70
1	A	239	TRP	CB-CA-C	6.13	122.67	110.40
1	B	328	ILE	O-C-N	-6.13	112.89	122.70
1	D	272	PRO	N-CD-CG	-6.13	94.00	103.20
1	E	182	ALA	CA-C-O	6.13	132.98	120.10
1	E	380	PHE	CB-CG-CD2	-6.13	116.51	120.80
1	F	328	ILE	O-C-N	-6.13	112.89	122.70
1	F	395	THR	N-CA-CB	6.13	121.95	110.30
1	A	55	THR	CA-C-N	-6.13	103.72	117.20
1	C	268	PHE	CZ-CE2-CD2	-6.13	112.75	120.10
1	D	450	ALA	CA-C-O	6.13	132.97	120.10
1	E	55	THR	CA-C-N	-6.13	103.71	117.20
1	F	578	MET	O-C-N	6.13	132.51	122.70
1	A	395	THR	N-CA-CB	6.13	121.94	110.30
1	B	164	GLY	N-CA-C	6.13	128.42	113.10
1	B	239	TRP	CB-CA-C	6.13	122.66	110.40
1	E	395	THR	N-CA-CB	6.13	121.95	110.30
1	A	153	LYS	O-C-N	6.13	132.50	122.70
1	A	355	GLY	O-C-N	6.13	132.50	122.70
1	A	439	SER	N-CA-CB	-6.13	101.31	110.50
1	C	153	LYS	O-C-N	6.13	132.50	122.70
1	E	333	TYR	CD1-CG-CD2	-6.13	111.16	117.90
1	E	450	ALA	CA-C-O	6.13	132.97	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	578	MET	O-C-N	6.13	132.50	122.70
1	A	578	MET	O-C-N	6.12	132.50	122.70
1	B	380	PHE	CB-CG-CD2	-6.12	116.51	120.80
1	D	55	THR	CA-C-N	-6.12	103.72	117.20
1	E	164	GLY	N-CA-C	6.12	128.41	113.10
1	A	272	PRO	N-CD-CG	-6.12	94.02	103.20
1	C	182	ALA	CA-C-O	6.12	132.96	120.10
1	C	393	LYS	CB-CA-C	-6.12	98.15	110.40
1	D	393	LYS	CB-CA-C	-6.12	98.15	110.40
1	E	328	ILE	O-C-N	-6.12	112.90	122.70
1	F	454	ARG	CA-CB-CG	6.12	126.87	113.40
1	A	333	TYR	CD1-CG-CD2	-6.12	111.17	117.90
1	D	164	GLY	N-CA-C	6.12	128.41	113.10
1	D	239	TRP	CG-CD1-NE1	6.12	116.22	110.10
1	D	307	ASP	CB-CG-OD1	6.12	123.81	118.30
1	D	395	THR	N-CA-CB	6.12	121.93	110.30
1	E	481	PHE	N-CA-CB	-6.12	99.58	110.60
1	F	182	ALA	CA-C-O	6.12	132.95	120.10
1	F	104	ALA	O-C-N	6.12	132.49	122.70
1	F	239	TRP	CB-CA-C	6.12	122.64	110.40
1	B	55	THR	CA-C-N	-6.12	103.74	117.20
1	B	439	SER	N-CA-CB	-6.12	101.32	110.50
1	B	481	PHE	N-CA-CB	-6.12	99.59	110.60
1	D	481	PHE	N-CA-CB	-6.12	99.58	110.60
1	B	153	LYS	O-C-N	6.12	132.49	122.70
1	A	182	ALA	CA-C-O	6.12	132.94	120.10
1	A	481	PHE	N-CA-CB	-6.12	99.59	110.60
1	D	182	ALA	CA-C-O	6.12	132.94	120.10
1	F	268	PHE	CZ-CE2-CD2	-6.12	112.76	120.10
1	F	393	LYS	CB-CA-C	-6.12	98.17	110.40
1	F	450	ALA	CA-C-O	6.12	132.94	120.10
1	A	268	PHE	CZ-CE2-CD2	-6.11	112.76	120.10
1	A	393	LYS	CB-CA-C	-6.11	98.17	110.40
1	B	393	LYS	CB-CA-C	-6.11	98.17	110.40
1	C	307	ASP	CB-CG-OD1	6.11	123.80	118.30
1	C	355	GLY	O-C-N	6.11	132.48	122.70
1	C	481	PHE	N-CA-CB	-6.11	99.60	110.60
1	D	380	PHE	CB-CG-CD2	-6.11	116.52	120.80
1	E	272	PRO	N-CD-CG	-6.11	94.03	103.20
1	F	609	CYS	CB-CA-C	-6.11	98.18	110.40
1	C	96	TRP	CB-CA-C	6.11	122.62	110.40
1	C	272	PRO	N-CD-CG	-6.11	94.03	103.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	395	THR	N-CA-CB	6.11	121.91	110.30
1	C	439	SER	N-CA-CB	-6.11	101.33	110.50
1	F	439	SER	N-CA-CB	-6.11	101.33	110.50
1	F	481	PHE	N-CA-CB	-6.11	99.60	110.60
1	E	268	PHE	CZ-CE2-CD2	-6.11	112.77	120.10
1	F	164	GLY	N-CA-C	6.11	128.37	113.10
1	B	333	TYR	CD1-CG-CD2	-6.11	111.18	117.90
1	B	395	THR	N-CA-CB	6.11	121.90	110.30
1	D	239	TRP	CB-CA-C	6.11	122.61	110.40
1	D	609	CYS	CB-CA-C	-6.11	98.19	110.40
1	A	164	GLY	N-CA-C	6.11	128.36	113.10
1	B	272	PRO	N-CD-CG	-6.11	94.04	103.20
1	C	578	MET	O-C-N	6.11	132.47	122.70
1	D	59	GLU	OE1-CD-OE2	6.11	130.63	123.30
1	E	609	CYS	CB-CA-C	-6.11	98.19	110.40
1	F	96	TRP	CB-CA-C	6.11	122.61	110.40
1	D	96	TRP	CB-CA-C	6.10	122.61	110.40
1	E	153	LYS	O-C-N	6.10	132.47	122.70
1	A	96	TRP	CB-CA-C	6.10	122.61	110.40
1	B	609	CYS	CB-CA-C	-6.10	98.19	110.40
1	B	622	LEU	CB-CA-C	6.10	121.79	110.20
1	C	333	TYR	CD1-CG-CD2	-6.10	111.19	117.90
1	D	146	THR	CA-CB-OG1	-6.10	96.19	109.00
1	C	164	GLY	N-CA-C	6.10	128.35	113.10
1	D	153	LYS	O-C-N	6.10	132.46	122.70
1	E	96	TRP	CB-CA-C	6.10	122.60	110.40
1	E	393	LYS	CB-CA-C	-6.10	98.20	110.40
1	C	609	CYS	CB-CA-C	-6.10	98.20	110.40
1	E	107	ARG	CG-CD-NE	-6.10	99.00	111.80
1	A	609	CYS	CB-CA-C	-6.09	98.21	110.40
1	A	622	LEU	CB-CA-C	6.09	121.78	110.20
1	F	8	ALA	N-CA-CB	-6.09	101.57	110.10
1	F	59	GLU	OE1-CD-OE2	6.09	130.61	123.30
1	B	96	TRP	CB-CA-C	6.09	122.58	110.40
1	B	107	ARG	CG-CD-NE	-6.09	99.01	111.80
1	B	528	VAL	CA-CB-CG1	-6.09	101.77	110.90
1	E	124	ILE	CA-C-O	-6.09	107.31	120.10
1	F	622	LEU	CB-CA-C	6.09	121.77	110.20
1	B	111	ASN	OD1-CG-ND2	6.09	135.90	121.90
1	C	622	LEU	CB-CA-C	6.09	121.77	110.20
1	C	107	ARG	CG-CD-NE	-6.09	99.02	111.80
1	D	578	MET	O-C-N	6.09	132.44	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	333	TYR	CD1-CG-CD2	-6.09	111.20	117.90
1	C	522	SER	N-CA-CB	-6.08	101.37	110.50
1	D	268	PHE	CZ-CE2-CD2	-6.08	112.80	120.10
1	D	522	SER	N-CA-CB	-6.08	101.37	110.50
1	E	622	LEU	CB-CA-C	6.08	121.76	110.20
1	A	107	ARG	CG-CD-NE	-6.08	99.02	111.80
1	D	622	LEU	CB-CA-C	6.08	121.76	110.20
1	F	111	ASN	OD1-CG-ND2	6.08	135.89	121.90
1	E	8	ALA	N-CA-CB	-6.08	101.59	110.10
1	D	111	ASN	OD1-CG-ND2	6.08	135.88	121.90
1	F	107	ARG	CG-CD-NE	-6.08	99.03	111.80
1	F	237	SER	CA-C-O	-6.08	107.33	120.10
1	B	59	GLU	OE1-CD-OE2	6.08	130.59	123.30
1	B	124	ILE	CA-C-O	-6.08	107.34	120.10
1	B	146	THR	CA-CB-OG1	-6.08	96.24	109.00
1	D	124	ILE	CA-C-O	-6.08	107.34	120.10
1	A	8	ALA	N-CA-CB	-6.07	101.60	110.10
1	B	237	SER	CA-C-O	-6.07	107.35	120.10
1	B	433	LEU	N-CA-CB	-6.07	98.25	110.40
1	C	146	THR	CA-CB-OG1	-6.07	96.24	109.00
1	F	124	ILE	CA-C-O	-6.07	107.34	120.10
1	A	124	ILE	CA-C-O	-6.07	107.35	120.10
1	C	237	SER	CA-C-O	-6.07	107.35	120.10
1	C	423	ILE	N-CA-CB	-6.07	96.83	110.80
1	C	8	ALA	N-CA-CB	-6.07	101.60	110.10
1	C	528	VAL	CA-CB-CG1	-6.07	101.80	110.90
1	D	433	LEU	N-CA-CB	-6.07	98.26	110.40
1	E	423	ILE	N-CA-CB	-6.07	96.84	110.80
1	A	528	VAL	CA-CB-CG1	-6.07	101.80	110.90
1	A	146	THR	CA-CB-OG1	-6.07	96.26	109.00
1	B	41	GLY	CA-C-O	-6.07	109.68	120.60
1	C	41	GLY	CA-C-O	-6.07	109.68	120.60
1	C	111	ASN	OD1-CG-ND2	6.07	135.85	121.90
1	C	433	LEU	N-CA-CB	-6.07	98.27	110.40
1	D	41	GLY	CA-C-O	-6.07	109.68	120.60
1	F	433	LEU	N-CA-CB	-6.07	98.26	110.40
1	A	380	PHE	CB-CG-CD2	-6.07	116.55	120.80
1	E	111	ASN	OD1-CG-ND2	6.07	135.85	121.90
1	E	146	THR	CA-CB-OG1	-6.07	96.26	109.00
1	A	59	GLU	OE1-CD-OE2	6.06	130.58	123.30
1	D	107	ARG	CG-CD-NE	-6.06	99.07	111.80
1	D	481	PHE	O-C-N	-6.06	113.00	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	GLY	CA-C-O	-6.06	109.69	120.60
1	A	111	ASN	OD1-CG-ND2	6.06	135.84	121.90
1	C	124	ILE	CA-C-O	-6.06	107.37	120.10
1	F	299	ALA	N-CA-C	-6.06	94.63	111.00
1	F	423	ILE	N-CA-CB	-6.06	96.86	110.80
1	A	433	LEU	N-CA-CB	-6.06	98.28	110.40
1	D	423	ILE	N-CA-CB	-6.06	96.86	110.80
1	E	41	GLY	CA-C-O	-6.06	109.69	120.60
1	F	556	SER	CB-CA-C	6.06	121.61	110.10
1	F	585	ALA	N-CA-C	-6.06	94.64	111.00
1	A	237	SER	CA-C-O	-6.06	107.37	120.10
1	A	423	ILE	N-CA-CB	-6.06	96.86	110.80
1	B	8	ALA	N-CA-CB	-6.06	101.62	110.10
1	B	299	ALA	N-CA-C	-6.06	94.64	111.00
1	E	237	SER	CA-C-O	-6.06	107.38	120.10
1	E	433	LEU	N-CA-CB	-6.06	98.28	110.40
1	F	41	GLY	CA-C-O	-6.06	109.69	120.60
1	F	345	ASN	CA-C-O	-6.06	107.37	120.10
1	D	299	ALA	N-CA-C	-6.06	94.65	111.00
1	D	237	SER	CA-C-O	-6.06	107.38	120.10
1	D	528	VAL	CA-CB-CG1	-6.06	101.82	110.90
1	A	556	SER	CB-CA-C	6.05	121.61	110.10
1	B	423	ILE	N-CA-CB	-6.05	96.88	110.80
1	B	522	SER	N-CA-CB	-6.05	101.42	110.50
1	E	299	ALA	N-CA-C	-6.05	94.66	111.00
1	E	528	VAL	CA-CB-CG1	-6.05	101.82	110.90
1	F	528	VAL	CA-CB-CG1	-6.05	101.82	110.90
1	A	585	ALA	N-CA-C	-6.05	94.66	111.00
1	C	59	GLU	OE1-CD-OE2	6.05	130.56	123.30
1	D	556	SER	CB-CA-C	6.05	121.60	110.10
1	A	522	SER	N-CA-CB	-6.05	101.42	110.50
1	B	585	ALA	N-CA-C	-6.05	94.67	111.00
1	C	585	ALA	N-CA-C	-6.05	94.67	111.00
1	E	333	TYR	CB-CA-C	6.05	122.50	110.40
1	E	585	ALA	N-CA-C	-6.05	94.67	111.00
1	B	481	PHE	O-C-N	-6.05	113.02	122.70
1	F	68	GLN	O-C-N	6.05	132.38	122.70
1	F	522	SER	N-CA-CB	-6.05	101.43	110.50
1	A	299	ALA	N-CA-C	-6.05	94.67	111.00
1	D	585	ALA	N-CA-C	-6.05	94.67	111.00
1	E	59	GLU	OE1-CD-OE2	6.05	130.56	123.30
1	C	299	ALA	N-CA-C	-6.04	94.68	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	556	SER	CB-CA-C	6.04	121.59	110.10
1	B	339	TYR	CD1-CG-CD2	-6.04	111.25	117.90
1	B	345	ASN	CA-C-O	-6.04	107.41	120.10
1	C	380	PHE	CB-CG-CD2	-6.04	116.57	120.80
1	B	68	GLN	O-C-N	6.04	132.37	122.70
1	B	486	GLU	CA-C-N	6.04	130.49	117.20
1	E	107	ARG	CD-NE-CZ	-6.04	115.14	123.60
1	F	146	THR	CA-CB-OG1	-6.04	96.31	109.00
1	B	556	SER	CB-CA-C	6.04	121.58	110.10
1	D	8	ALA	N-CA-CB	-6.04	101.64	110.10
1	B	362	ASN	N-CA-CB	-6.04	99.73	110.60
1	E	68	GLN	O-C-N	6.04	132.36	122.70
1	E	522	SER	N-CA-CB	-6.04	101.44	110.50
1	F	214	ASP	C-N-CA	-6.04	106.60	121.70
1	A	345	ASN	CA-C-O	-6.04	107.42	120.10
1	C	345	ASN	CA-C-O	-6.04	107.42	120.10
1	E	556	SER	CB-CA-C	6.04	121.57	110.10
1	C	333	TYR	CB-CA-C	6.04	122.47	110.40
1	E	339	TYR	CD1-CG-CD2	-6.03	111.26	117.90
1	E	345	ASN	CA-C-O	-6.03	107.43	120.10
1	F	362	ASN	N-CA-CB	-6.03	99.74	110.60
1	F	380	PHE	CB-CG-CD2	-6.03	116.58	120.80
1	F	486	GLU	CA-C-N	6.03	130.46	117.20
1	A	68	GLN	O-C-N	6.03	132.34	122.70
1	D	68	GLN	O-C-N	6.03	132.34	122.70
1	D	236	LEU	CB-CG-CD2	-6.03	100.75	111.00
1	F	398	PHE	CB-CG-CD1	-6.03	116.58	120.80
1	A	481	PHE	O-C-N	-6.03	113.06	122.70
1	C	214	ASP	C-N-CA	-6.03	106.63	121.70
1	D	214	ASP	C-N-CA	-6.03	106.64	121.70
1	D	333	TYR	CB-CA-C	6.03	122.45	110.40
1	A	362	ASN	N-CA-CB	-6.02	99.76	110.60
1	D	345	ASN	CA-C-O	-6.02	107.45	120.10
1	E	214	ASP	C-N-CA	-6.02	106.64	121.70
1	A	214	ASP	C-N-CA	-6.02	106.64	121.70
1	F	148	SER	CA-C-N	-6.02	103.95	117.20
1	A	333	TYR	CB-CA-C	6.02	122.44	110.40
1	B	236	LEU	CB-CG-CD2	-6.02	100.76	111.00
1	E	398	PHE	CB-CG-CD1	-6.02	116.58	120.80
1	B	333	TYR	CB-CA-C	6.02	122.44	110.40
1	C	339	TYR	CD1-CG-CD2	-6.02	111.28	117.90
1	D	107	ARG	CD-NE-CZ	-6.02	115.17	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	107	ARG	CD-NE-CZ	-6.02	115.17	123.60
1	A	486	GLU	CA-C-N	6.02	130.44	117.20
1	B	148	SER	CA-C-N	-6.02	103.96	117.20
1	C	68	GLN	O-C-N	6.02	132.33	122.70
1	C	486	GLU	CA-C-N	6.02	130.44	117.20
1	D	494	THR	CA-C-O	-6.02	107.47	120.10
1	A	107	ARG	CD-NE-CZ	-6.02	115.18	123.60
1	C	216	LYS	N-CA-C	-6.02	94.76	111.00
1	D	148	SER	CA-C-N	-6.02	103.96	117.20
1	E	56	LEU	CA-C-O	-6.02	107.47	120.10
1	E	486	GLU	CA-C-N	6.02	130.44	117.20
1	A	216	LYS	N-CA-C	-6.01	94.76	111.00
1	B	214	ASP	C-N-CA	-6.01	106.67	121.70
1	C	107	ARG	CD-NE-CZ	-6.01	115.18	123.60
1	D	216	LYS	N-CA-C	-6.01	94.76	111.00
1	E	481	PHE	O-C-N	-6.01	113.08	122.70
1	E	494	THR	CA-C-O	-6.01	107.47	120.10
1	F	339	TYR	CD1-CG-CD2	-6.01	111.28	117.90
1	B	216	LYS	N-CA-C	-6.01	94.77	111.00
1	D	486	GLU	CA-C-N	6.01	130.43	117.20
1	F	494	THR	CA-C-O	-6.01	107.47	120.10
1	A	494	THR	CA-C-O	-6.01	107.47	120.10
1	D	362	ASN	N-CA-CB	-6.01	99.78	110.60
1	E	236	LEU	CB-CG-CD2	-6.01	100.78	111.00
1	F	236	LEU	CB-CG-CD2	-6.01	100.78	111.00
1	F	392	LYS	CA-CB-CG	6.01	126.62	113.40
1	A	148	SER	CA-C-N	-6.01	103.98	117.20
1	C	148	SER	CA-C-N	-6.01	103.98	117.20
1	C	362	ASN	N-CA-CB	-6.01	99.79	110.60
1	F	216	LYS	N-CA-C	-6.01	94.78	111.00
1	B	107	ARG	CD-NE-CZ	-6.01	115.19	123.60
1	B	398	PHE	CB-CG-CD1	-6.01	116.59	120.80
1	E	216	LYS	N-CA-C	-6.01	94.78	111.00
1	A	236	LEU	CB-CG-CD2	-6.00	100.79	111.00
1	A	339	TYR	CD1-CG-CD2	-6.00	111.30	117.90
1	A	398	PHE	CB-CG-CD1	-6.00	116.60	120.80
1	B	56	LEU	CA-C-O	-6.00	107.49	120.10
1	C	56	LEU	CA-C-O	-6.00	107.49	120.10
1	E	80	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	E	148	SER	CA-C-N	-6.00	103.99	117.20
1	A	56	LEU	CA-C-O	-6.00	107.50	120.10
1	B	298	GLU	CB-CG-CD	-6.00	98.01	114.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	339	TYR	CD1-CG-CD2	-6.00	111.30	117.90
1	E	362	ASN	N-CA-CB	-6.00	99.80	110.60
1	F	333	TYR	CB-CA-C	6.00	122.40	110.40
1	F	481	PHE	O-C-N	-6.00	113.10	122.70
1	B	392	LYS	CA-CB-CG	6.00	126.59	113.40
1	C	481	PHE	O-C-N	-6.00	113.11	122.70
1	E	392	LYS	CA-CB-CG	5.99	126.58	113.40
1	F	56	LEU	CA-C-O	-5.99	107.51	120.10
1	C	236	LEU	CB-CG-CD2	-5.99	100.81	111.00
1	D	238	ASN	OD1-CG-ND2	5.99	135.68	121.90
1	D	314	ASP	CA-C-O	-5.99	107.52	120.10
1	A	78	ARG	CB-CG-CD	5.99	127.17	111.60
1	B	494	THR	CA-C-O	-5.99	107.52	120.10
1	D	56	LEU	CA-C-O	-5.99	107.52	120.10
1	C	78	ARG	CB-CG-CD	5.99	127.17	111.60
1	F	292	THR	CA-CB-OG1	-5.99	96.43	109.00
1	C	230	ARG	CD-NE-CZ	-5.99	115.22	123.60
1	C	494	THR	CA-C-O	-5.99	107.53	120.10
1	E	630	ILE	CA-C-O	5.99	132.67	120.10
1	A	292	THR	CA-CB-OG1	-5.98	96.44	109.00
1	A	392	LYS	CA-CB-CG	5.98	126.56	113.40
1	B	292	THR	CA-CB-OG1	-5.98	96.44	109.00
1	C	238	ASN	OD1-CG-ND2	5.98	135.66	121.90
1	D	298	GLU	CB-CG-CD	-5.98	98.05	114.20
1	D	492	THR	CA-C-O	5.98	132.66	120.10
1	F	298	GLU	CB-CG-CD	-5.98	98.05	114.20
1	B	78	ARG	CB-CG-CD	5.98	127.15	111.60
1	B	630	ILE	CA-C-O	5.98	132.66	120.10
1	C	30	LEU	CB-CA-C	5.98	121.56	110.20
1	C	298	GLU	CB-CG-CD	-5.98	98.05	114.20
1	E	298	GLU	CB-CG-CD	-5.98	98.06	114.20
1	E	492	THR	CA-C-O	5.98	132.66	120.10
1	F	30	LEU	CB-CA-C	5.98	121.56	110.20
1	A	238	ASN	OD1-CG-ND2	5.98	135.65	121.90
1	C	630	ILE	CA-C-O	5.98	132.65	120.10
1	D	78	ARG	CB-CG-CD	5.98	127.14	111.60
1	D	398	PHE	CB-CG-CD1	-5.98	116.62	120.80
1	F	238	ASN	OD1-CG-ND2	5.98	135.65	121.90
1	F	630	ILE	CA-C-O	5.98	132.65	120.10
1	C	492	THR	CA-C-O	5.98	132.65	120.10
1	F	78	ARG	CB-CG-CD	5.98	127.14	111.60
1	A	298	GLU	CB-CG-CD	-5.97	98.07	114.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	630	ILE	CA-C-O	5.97	132.65	120.10
1	F	314	ASP	CA-C-O	-5.97	107.55	120.10
1	B	492	THR	CA-C-O	5.97	132.64	120.10
1	D	10	LYS	CB-CA-C	5.97	122.35	110.40
1	D	292	THR	CA-CB-OG1	-5.97	96.46	109.00
1	E	292	THR	CA-CB-OG1	-5.97	96.46	109.00
1	F	492	THR	CA-C-O	5.97	132.64	120.10
1	B	238	ASN	OD1-CG-ND2	5.97	135.63	121.90
1	C	392	LYS	CA-CB-CG	5.97	126.53	113.40
1	E	78	ARG	CB-CG-CD	5.97	127.12	111.60
1	E	517	GLU	OE1-CD-OE2	-5.97	116.14	123.30
1	F	10	LYS	CB-CA-C	5.97	122.34	110.40
1	F	628	ARG	NH1-CZ-NH2	5.97	125.97	119.40
1	A	314	ASP	CA-C-O	-5.97	107.57	120.10
1	B	295	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	E	30	LEU	CB-CA-C	5.97	121.54	110.20
1	C	292	THR	CA-CB-OG1	-5.97	96.47	109.00
1	C	314	ASP	CA-C-O	-5.97	107.57	120.10
1	E	10	LYS	CB-CA-C	5.97	122.33	110.40
1	A	10	LYS	CB-CA-C	5.96	122.33	110.40
1	A	492	THR	CA-C-O	5.96	132.62	120.10
1	C	622	LEU	CB-CG-CD2	-5.96	100.86	111.00
1	E	238	ASN	OD1-CG-ND2	5.96	135.62	121.90
1	F	7	ASN	C-N-CA	-5.96	106.79	121.70
1	F	430	GLN	N-CA-CB	-5.96	99.87	110.60
1	B	314	ASP	CA-C-O	-5.96	107.58	120.10
1	C	398	PHE	CB-CG-CD1	-5.96	116.63	120.80
1	C	581	ASN	CA-C-N	5.96	130.31	117.20
1	D	27	TYR	CB-CG-CD1	5.96	124.58	121.00
1	D	254	GLU	CG-CD-OE2	5.96	130.22	118.30
1	E	314	ASP	CA-C-O	-5.96	107.58	120.10
1	F	254	GLU	CG-CD-OE2	5.96	130.22	118.30
1	A	30	LEU	CB-CA-C	5.96	121.52	110.20
1	D	165	THR	CA-CB-OG1	-5.96	96.49	109.00
1	D	295	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	A	7	ASN	C-N-CA	-5.96	106.81	121.70
1	B	273	ASP	CA-C-O	5.96	132.61	120.10
1	C	7	ASN	C-N-CA	-5.96	106.81	121.70
1	C	165	THR	CA-CB-OG1	-5.96	96.49	109.00
1	D	30	LEU	CB-CA-C	5.96	121.52	110.20
1	D	581	ASN	CA-C-N	5.96	130.30	117.20
1	D	622	LEU	CB-CG-CD2	-5.96	100.87	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	7	ASN	C-N-CA	-5.96	106.81	121.70
1	D	392	LYS	CA-CB-CG	5.96	126.50	113.40
1	D	630	ILE	CA-C-O	5.96	132.60	120.10
1	A	622	LEU	CB-CG-CD2	-5.95	100.88	111.00
1	B	10	LYS	CB-CA-C	5.95	122.31	110.40
1	C	10	LYS	CB-CA-C	5.95	122.31	110.40
1	C	517	GLU	OE1-CD-OE2	-5.95	116.16	123.30
1	F	622	LEU	CB-CG-CD2	-5.95	100.88	111.00
1	B	581	ASN	CA-C-N	5.95	130.29	117.20
1	B	30	LEU	CB-CA-C	5.95	121.51	110.20
1	E	165	THR	CA-CB-OG1	-5.95	96.50	109.00
1	F	165	THR	CA-CB-OG1	-5.95	96.50	109.00
1	F	517	GLU	OE1-CD-OE2	-5.95	116.16	123.30
1	B	80	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	B	430	GLN	N-CA-CB	-5.95	99.89	110.60
1	C	215	ARG	N-CA-CB	-5.95	99.89	110.60
1	C	430	GLN	N-CA-CB	-5.95	99.89	110.60
1	E	230	ARG	CD-NE-CZ	-5.95	115.27	123.60
1	F	451	ARG	CD-NE-CZ	-5.95	115.27	123.60
1	A	430	GLN	N-CA-CB	-5.95	99.89	110.60
1	C	27	TYR	CB-CG-CD1	5.95	124.57	121.00
1	A	165	THR	CA-CB-OG1	-5.95	96.51	109.00
1	B	59	GLU	O-C-N	5.95	132.21	122.70
1	C	594	GLU	CA-CB-CG	5.95	126.48	113.40
1	D	7	ASN	C-N-CA	-5.95	106.84	121.70
1	D	215	ARG	N-CA-CB	-5.95	99.90	110.60
1	D	267	GLU	CG-CD-OE2	5.95	130.19	118.30
1	B	517	GLU	OE1-CD-OE2	-5.94	116.17	123.30
1	B	622	LEU	CB-CG-CD2	-5.94	100.90	111.00
1	C	80	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	C	628	ARG	NH1-CZ-NH2	5.94	125.94	119.40
1	E	215	ARG	N-CA-CB	-5.94	99.91	110.60
1	E	273	ASP	CA-C-O	5.94	132.58	120.10
1	E	430	GLN	N-CA-CB	-5.94	99.91	110.60
1	F	512	VAL	CA-CB-CG2	-5.94	101.99	110.90
1	F	594	GLU	CA-CB-CG	5.94	126.47	113.40
1	A	215	ARG	N-CA-CB	-5.94	99.91	110.60
1	A	230	ARG	CD-NE-CZ	-5.94	115.28	123.60
1	C	254	GLU	CG-CD-OE2	5.94	130.18	118.30
1	D	594	GLU	CA-CB-CG	5.94	126.47	113.40
1	C	446	VAL	O-C-N	5.94	132.20	122.70
1	E	267	GLU	CG-CD-OE2	5.94	130.18	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	31	LYS	CB-CG-CD	-5.94	96.16	111.60
1	B	7	ASN	C-N-CA	-5.94	106.86	121.70
1	C	59	GLU	O-C-N	5.94	132.20	122.70
1	E	446	VAL	O-C-N	5.94	132.20	122.70
1	E	455	LEU	O-C-N	5.94	132.20	122.70
1	E	483	CYS	N-CA-CB	-5.94	99.91	110.60
1	A	581	ASN	CA-C-N	5.94	130.26	117.20
1	B	165	THR	CA-CB-OG1	-5.94	96.53	109.00
1	D	31	LYS	CB-CG-CD	-5.94	96.17	111.60
1	A	254	GLU	CG-CD-OE2	5.93	130.17	118.30
1	A	446	VAL	O-C-N	5.93	132.20	122.70
1	A	517	GLU	OE1-CD-OE2	-5.93	116.18	123.30
1	B	215	ARG	N-CA-CB	-5.93	99.92	110.60
1	B	509	PHE	CB-CG-CD1	5.93	124.95	120.80
1	D	230	ARG	CD-NE-CZ	-5.93	115.29	123.60
1	E	594	GLU	CA-CB-CG	5.93	126.46	113.40
1	E	622	LEU	CB-CG-CD2	-5.93	100.91	111.00
1	D	273	ASP	CA-C-O	5.93	132.56	120.10
1	D	446	VAL	O-C-N	5.93	132.19	122.70
1	D	628	ARG	NH1-CZ-NH2	5.93	125.93	119.40
1	F	581	ASN	CA-C-N	5.93	130.25	117.20
1	B	254	GLU	CG-CD-OE2	5.93	130.16	118.30
1	C	512	VAL	CA-CB-CG2	-5.93	102.00	110.90
1	E	628	ARG	NH1-CZ-NH2	5.93	125.92	119.40
1	A	594	GLU	CA-CB-CG	5.93	126.44	113.40
1	B	31	LYS	CB-CG-CD	-5.93	96.18	111.60
1	B	446	VAL	O-C-N	5.93	132.19	122.70
1	D	59	GLU	O-C-N	5.93	132.19	122.70
1	D	430	GLN	N-CA-CB	-5.93	99.92	110.60
1	E	27	TYR	CB-CG-CD1	5.93	124.56	121.00
1	F	59	GLU	O-C-N	5.93	132.19	122.70
1	A	273	ASP	CA-C-O	5.93	132.55	120.10
1	B	628	ARG	NH1-CZ-NH2	5.93	125.92	119.40
1	F	446	VAL	O-C-N	5.93	132.19	122.70
1	A	295	ARG	NE-CZ-NH2	5.93	123.26	120.30
1	C	267	GLU	CG-CD-OE2	5.93	130.15	118.30
1	E	31	LYS	CB-CG-CD	-5.93	96.19	111.60
1	E	581	ASN	CA-C-N	5.93	130.24	117.20
1	F	230	ARG	CD-NE-CZ	-5.93	115.30	123.60
1	F	483	CYS	N-CA-CB	-5.93	99.93	110.60
1	A	80	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	230	ARG	CD-NE-CZ	-5.92	115.31	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	594	GLU	CA-CB-CG	5.92	126.43	113.40
1	C	273	ASP	CA-C-O	5.92	132.54	120.10
1	A	31	LYS	CB-CG-CD	-5.92	96.20	111.60
1	A	512	VAL	CA-CB-CG2	-5.92	102.02	110.90
1	C	451	ARG	CD-NE-CZ	-5.92	115.31	123.60
1	E	59	GLU	O-C-N	5.92	132.18	122.70
1	A	27	TYR	CB-CG-CD1	5.92	124.55	121.00
1	A	59	GLU	O-C-N	5.92	132.17	122.70
1	A	628	ARG	NH1-CZ-NH2	5.92	125.91	119.40
1	F	215	ARG	NH1-CZ-NH2	5.92	125.91	119.40
1	F	215	ARG	N-CA-CB	-5.92	99.94	110.60
1	A	267	GLU	CG-CD-OE2	5.92	130.13	118.30
1	A	451	ARG	CD-NE-CZ	-5.92	115.31	123.60
1	B	215	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	E	254	GLU	CG-CD-OE2	5.92	130.14	118.30
1	F	267	GLU	CG-CD-OE2	5.92	130.14	118.30
1	A	215	ARG	NH1-CZ-NH2	5.92	125.91	119.40
1	A	483	CYS	N-CA-CB	-5.92	99.95	110.60
1	C	31	LYS	CB-CG-CD	-5.92	96.22	111.60
1	F	509	PHE	CB-CG-CD1	5.92	124.94	120.80
1	C	455	LEU	O-C-N	5.92	132.16	122.70
1	B	27	TYR	CB-CG-CD1	5.91	124.55	121.00
1	B	451	ARG	CD-NE-CZ	-5.91	115.32	123.60
1	D	512	VAL	CA-CB-CG2	-5.91	102.03	110.90
1	B	215	ARG	NH1-CZ-NH2	5.91	125.90	119.40
1	E	512	VAL	CA-CB-CG2	-5.91	102.03	110.90
1	B	267	GLU	CG-CD-OE2	5.91	130.12	118.30
1	B	512	VAL	CA-CB-CG2	-5.91	102.03	110.90
1	D	483	CYS	N-CA-CB	-5.91	99.96	110.60
1	E	509	PHE	CB-CG-CD1	5.91	124.94	120.80
1	B	483	CYS	N-CA-CB	-5.91	99.97	110.60
1	E	215	ARG	NH1-CZ-NH2	5.91	125.90	119.40
1	F	295	ARG	NE-CZ-NH2	5.91	123.25	120.30
1	F	455	LEU	O-C-N	5.91	132.15	122.70
1	B	455	LEU	O-C-N	5.91	132.15	122.70
1	E	18	LEU	CA-C-N	5.91	130.19	117.20
1	C	215	ARG	NE-CZ-NH2	5.91	123.25	120.30
1	C	483	CYS	N-CA-CB	-5.91	99.97	110.60
1	D	492	THR	O-C-N	-5.91	113.25	122.70
1	F	20	LYS	CA-CB-CG	-5.91	100.41	113.40
1	B	261	SER	O-C-N	5.90	132.15	122.70
1	D	451	ARG	CD-NE-CZ	-5.90	115.33	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	517	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	E	284	ALA	C-N-CA	5.90	136.46	121.70
1	F	530	VAL	N-CA-CB	-5.90	98.51	111.50
1	A	455	LEU	O-C-N	5.90	132.15	122.70
1	C	284	ALA	C-N-CA	5.90	136.46	121.70
1	B	284	ALA	C-N-CA	5.90	136.45	121.70
1	D	455	LEU	O-C-N	5.90	132.14	122.70
1	F	273	ASP	CA-C-O	5.90	132.49	120.10
1	E	20	LYS	CA-CB-CG	-5.90	100.42	113.40
1	B	18	LEU	CA-C-N	5.90	130.18	117.20
1	D	482	LEU	CB-CG-CD2	5.90	121.03	111.00
1	A	284	ALA	C-N-CA	5.89	136.44	121.70
1	E	61	ASN	CB-CG-OD1	-5.89	109.81	121.60
1	E	215	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	E	422	LEU	CB-CG-CD2	5.89	121.02	111.00
1	F	492	THR	O-C-N	-5.89	113.27	122.70
1	A	61	ASN	CB-CG-OD1	-5.89	109.82	121.60
1	F	61	ASN	CB-CG-OD1	-5.89	109.82	121.60
1	A	18	LEU	CA-C-N	5.89	130.16	117.20
1	D	215	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	D	530	VAL	N-CA-CB	-5.89	98.54	111.50
1	F	284	ALA	C-N-CA	5.89	136.42	121.70
1	A	20	LYS	CA-CB-CG	-5.89	100.45	113.40
1	E	492	THR	O-C-N	-5.89	113.28	122.70
1	B	170	PHE	O-C-N	5.89	132.12	122.70
1	B	422	LEU	CB-CG-CD2	5.89	121.01	111.00
1	C	422	LEU	CB-CG-CD2	5.89	121.01	111.00
1	C	482	LEU	CB-CG-CD2	5.89	121.01	111.00
1	D	284	ALA	C-N-CA	5.89	136.42	121.70
1	D	432	SER	N-CA-CB	-5.89	101.67	110.50
1	E	398	PHE	CG-CD1-CE1	-5.89	114.32	120.80
1	C	509	PHE	CB-CG-CD1	5.88	124.92	120.80
1	D	20	LYS	CA-CB-CG	-5.88	100.45	113.40
1	E	451	ARG	CD-NE-CZ	-5.88	115.36	123.60
1	E	530	VAL	N-CA-CB	-5.88	98.56	111.50
1	C	261	SER	O-C-N	5.88	132.11	122.70
1	E	414	ASN	C-N-CA	-5.88	109.94	122.30
1	A	261	SER	O-C-N	5.88	132.11	122.70
1	C	20	LYS	CA-CB-CG	-5.88	100.46	113.40
1	C	530	VAL	N-CA-CB	-5.88	98.56	111.50
1	D	18	LEU	CA-C-N	5.88	130.14	117.20
1	E	295	ARG	NE-CZ-NH2	5.88	123.24	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	170	PHE	O-C-N	5.88	132.11	122.70
1	B	482	LEU	CB-CG-CD2	5.88	121.00	111.00
1	E	432	SER	N-CA-CB	-5.88	101.68	110.50
1	F	18	LEU	CA-C-N	5.88	130.14	117.20
1	A	422	LEU	CB-CG-CD2	5.88	120.99	111.00
1	A	482	LEU	CB-CG-CD2	5.88	120.99	111.00
1	A	530	VAL	N-CA-CB	-5.88	98.57	111.50
1	C	295	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	C	642	ILE	CG1-CB-CG2	-5.88	98.47	111.40
1	D	3	LEU	CA-C-N	-5.88	104.44	116.20
1	E	414	ASN	O-C-N	5.88	133.19	123.20
1	F	80	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	20	LYS	CA-CB-CG	-5.88	100.47	113.40
1	C	18	LEU	CA-C-N	5.88	130.13	117.20
1	C	61	ASN	CB-CG-OD1	-5.88	109.85	121.60
1	C	492	THR	O-C-N	-5.88	113.30	122.70
1	D	61	ASN	CB-CG-OD1	-5.88	109.84	121.60
1	D	295	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	F	432	SER	N-CA-CB	-5.88	101.69	110.50
1	D	170	PHE	O-C-N	5.88	132.10	122.70
1	A	509	PHE	CB-CG-CD1	5.87	124.91	120.80
1	A	642	ILE	CG1-CB-CG2	-5.87	98.48	111.40
1	B	77	THR	O-C-N	5.87	132.10	122.70
1	B	178	GLU	CB-CA-C	-5.87	98.65	110.40
1	B	414	ASN	C-N-CA	-5.87	109.97	122.30
1	D	78	ARG	CD-NE-CZ	-5.87	115.38	123.60
1	D	178	GLU	CB-CA-C	-5.87	98.65	110.40
1	F	27	TYR	CB-CG-CD1	5.87	124.53	121.00
1	F	178	GLU	CB-CA-C	-5.87	98.65	110.40
1	F	224	HIS	CB-CA-C	5.87	122.15	110.40
1	F	642	ILE	CG1-CB-CG2	-5.87	98.48	111.40
1	A	78	ARG	CD-NE-CZ	-5.87	115.38	123.60
1	A	178	GLU	CB-CA-C	-5.87	98.66	110.40
1	B	78	ARG	CD-NE-CZ	-5.87	115.38	123.60
1	D	422	LEU	CB-CG-CD2	5.87	120.98	111.00
1	A	170	PHE	O-C-N	5.87	132.09	122.70
1	E	261	SER	O-C-N	5.87	132.09	122.70
1	A	77	THR	O-C-N	5.87	132.09	122.70
1	B	530	VAL	N-CA-CB	-5.87	98.59	111.50
1	C	520	GLU	O-C-N	5.87	132.09	122.70
1	D	215	ARG	NH1-CZ-NH2	5.87	125.86	119.40
1	F	414	ASN	C-N-CA	-5.87	109.98	122.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	492	THR	O-C-N	-5.87	113.31	122.70
1	E	178	GLU	CB-CA-C	-5.87	98.67	110.40
1	A	414	ASN	C-N-CA	-5.87	109.98	122.30
1	B	520	GLU	O-C-N	5.87	132.08	122.70
1	E	77	THR	O-C-N	5.87	132.09	122.70
1	F	482	LEU	CB-CG-CD2	5.87	120.97	111.00
1	B	492	THR	O-C-N	-5.86	113.32	122.70
1	B	642	ILE	CG1-CB-CG2	-5.86	98.50	111.40
1	D	414	ASN	C-N-CA	-5.86	109.98	122.30
1	D	520	GLU	O-C-N	5.86	132.08	122.70
1	E	78	ARG	CD-NE-CZ	-5.86	115.39	123.60
1	E	642	ILE	N-CA-C	-5.86	95.17	111.00
1	E	642	ILE	CG1-CB-CG2	-5.86	98.50	111.40
1	B	61	ASN	CB-CG-OD1	-5.86	109.88	121.60
1	E	482	LEU	CB-CG-CD2	5.86	120.97	111.00
1	A	432	SER	N-CA-CB	-5.86	101.71	110.50
1	B	311	HIS	CA-C-O	-5.86	107.79	120.10
1	D	115	PHE	CB-CG-CD1	5.86	124.90	120.80
1	E	170	PHE	O-C-N	5.86	132.08	122.70
1	F	78	ARG	CD-NE-CZ	-5.86	115.39	123.60
1	A	215	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	C	215	ARG	NH1-CZ-NH2	5.86	125.84	119.40
1	D	224	HIS	CB-CA-C	5.86	122.12	110.40
1	D	642	ILE	CG1-CB-CG2	-5.86	98.51	111.40
1	F	422	LEU	CB-CG-CD2	5.86	120.96	111.00
1	C	170	PHE	O-C-N	5.86	132.07	122.70
1	E	75	PHE	CG-CD1-CE1	-5.86	114.36	120.80
1	F	77	THR	O-C-N	5.86	132.07	122.70
1	F	261	SER	O-C-N	5.86	132.07	122.70
1	F	311	HIS	CA-C-O	-5.86	107.80	120.10
1	F	642	ILE	N-CA-C	-5.86	95.19	111.00
1	B	75	PHE	CG-CD1-CE1	-5.86	114.36	120.80
1	B	349	VAL	CG1-CB-CG2	5.86	120.27	110.90
1	C	77	THR	O-C-N	5.86	132.07	122.70
1	C	414	ASN	C-N-CA	-5.86	110.00	122.30
1	C	642	ILE	N-CA-C	-5.86	95.19	111.00
1	D	77	THR	O-C-N	5.86	132.07	122.70
1	D	261	SER	O-C-N	5.86	132.07	122.70
1	E	224	HIS	CB-CA-C	5.86	122.11	110.40
1	F	520	GLU	O-C-N	5.86	132.07	122.70
1	A	414	ASN	O-C-N	5.85	133.15	123.20
1	A	642	ILE	N-CA-C	-5.85	95.19	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	LEU	CA-C-N	-5.85	104.50	116.20
1	B	642	ILE	N-CA-C	-5.85	95.20	111.00
1	C	224	HIS	CB-CA-C	5.85	122.10	110.40
1	C	311	HIS	CA-C-O	-5.85	107.81	120.10
1	E	520	GLU	O-C-N	5.85	132.06	122.70
1	F	206	GLU	CB-CG-CD	-5.85	98.40	114.20
1	B	432	SER	N-CA-CB	-5.85	101.72	110.50
1	C	3	LEU	CA-C-N	-5.85	104.50	116.20
1	C	78	ARG	CD-NE-CZ	-5.85	115.41	123.60
1	F	215	ARG	NE-CZ-NH2	5.85	123.22	120.30
1	A	224	HIS	CB-CA-C	5.85	122.10	110.40
1	B	3	LEU	CA-C-N	-5.85	104.50	116.20
1	C	178	GLU	CB-CA-C	-5.85	98.70	110.40
1	C	432	SER	N-CA-CB	-5.85	101.73	110.50
1	D	206	GLU	CB-CG-CD	-5.85	98.41	114.20
1	D	414	ASN	O-C-N	5.85	133.14	123.20
1	A	295	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	C	75	PHE	CG-CD1-CE1	-5.84	114.37	120.80
1	D	311	HIS	CA-C-O	-5.84	107.83	120.10
1	E	242	PRO	CA-C-N	5.84	130.06	117.20
1	C	414	ASN	O-C-N	5.84	133.13	123.20
1	F	414	ASN	O-C-N	5.84	133.13	123.20
1	A	206	GLU	CB-CG-CD	-5.84	98.43	114.20
1	A	520	GLU	O-C-N	5.84	132.05	122.70
1	F	3	LEU	CA-C-N	-5.84	104.52	116.20
1	A	75	PHE	CG-CD1-CE1	-5.84	114.38	120.80
1	D	242	PRO	CA-C-N	5.84	130.05	117.20
1	D	387	MET	CB-CA-C	-5.84	98.72	110.40
1	D	642	ILE	N-CA-C	-5.84	95.23	111.00
1	E	206	GLU	CB-CG-CD	-5.84	98.44	114.20
1	A	311	HIS	CA-C-O	-5.84	107.84	120.10
1	B	206	GLU	CB-CG-CD	-5.84	98.44	114.20
1	B	387	MET	CB-CA-C	-5.84	98.73	110.40
1	C	206	GLU	CB-CG-CD	-5.84	98.44	114.20
1	D	75	PHE	CG-CD1-CE1	-5.84	114.38	120.80
1	E	3	LEU	CA-C-N	-5.84	104.53	116.20
1	E	311	HIS	CA-C-O	-5.84	107.84	120.10
1	B	224	HIS	CB-CA-C	5.83	122.07	110.40
1	B	414	ASN	O-C-N	5.83	133.12	123.20
1	C	115	PHE	CB-CG-CD1	5.83	124.89	120.80
1	A	376	ARG	CB-CA-C	-5.83	98.73	110.40
1	E	387	MET	CB-CA-C	-5.83	98.73	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	611	VAL	CA-CB-CG1	5.83	119.65	110.90
1	F	376	ARG	CB-CA-C	-5.83	98.73	110.40
1	F	387	MET	CB-CA-C	-5.83	98.73	110.40
1	A	349	VAL	CG1-CB-CG2	5.83	120.23	110.90
1	F	367	VAL	CB-CA-C	5.83	122.48	111.40
1	A	387	MET	CB-CA-C	-5.83	98.74	110.40
1	A	242	PRO	CA-C-N	5.83	130.02	117.20
1	C	349	VAL	CG1-CB-CG2	5.83	120.23	110.90
1	C	376	ARG	CB-CA-C	-5.83	98.74	110.40
1	B	376	ARG	CB-CA-C	-5.83	98.75	110.40
1	D	349	VAL	CG1-CB-CG2	5.83	120.22	110.90
1	F	115	PHE	CB-CG-CD1	5.83	124.88	120.80
1	C	108	GLU	CB-CA-C	5.83	122.05	110.40
1	C	162	LYS	CB-CA-C	5.83	122.05	110.40
1	C	295	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	D	509	PHE	CB-CG-CD1	5.83	124.88	120.80
1	E	376	ARG	CB-CA-C	-5.83	98.75	110.40
1	B	207	ASP	CB-CA-C	5.82	122.05	110.40
1	D	162	LYS	CB-CA-C	5.82	122.05	110.40
1	B	398	PHE	CG-CD1-CE1	-5.82	114.40	120.80
1	F	398	PHE	CG-CD1-CE1	-5.82	114.40	120.80
1	B	242	PRO	CA-C-N	5.82	130.00	117.20
1	B	295	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	D	376	ARG	CB-CA-C	-5.82	98.76	110.40
1	E	349	VAL	CG1-CB-CG2	5.82	120.21	110.90
1	A	398	PHE	CG-CD1-CE1	-5.82	114.40	120.80
1	C	267	GLU	CG-CD-OE1	-5.82	106.66	118.30
1	F	75	PHE	CG-CD1-CE1	-5.82	114.40	120.80
1	F	242	PRO	CA-C-N	5.82	130.00	117.20
1	A	207	ASP	CB-CA-C	5.82	122.03	110.40
1	C	207	ASP	CB-CA-C	5.82	122.03	110.40
1	C	398	PHE	CG-CD1-CE1	-5.82	114.40	120.80
1	D	267	GLU	CG-CD-OE1	-5.82	106.67	118.30
1	E	108	GLU	CB-CA-C	5.82	122.03	110.40
1	B	162	LYS	CB-CA-C	5.81	122.03	110.40
1	D	108	GLU	CB-CA-C	5.81	122.03	110.40
1	A	115	PHE	CB-CG-CD1	5.81	124.87	120.80
1	C	387	MET	CB-CA-C	-5.81	98.78	110.40
1	E	267	GLU	CG-CD-OE1	-5.81	106.67	118.30
1	F	162	LYS	CB-CA-C	5.81	122.03	110.40
1	B	115	PHE	CB-CG-CD1	5.81	124.87	120.80
1	B	367	VAL	CB-CA-C	5.81	122.44	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	242	PRO	CA-C-N	5.81	129.98	117.20
1	E	295	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	A	162	LYS	CB-CA-C	5.81	122.02	110.40
1	D	207	ASP	CB-CA-C	5.81	122.02	110.40
1	D	350	MET	CA-C-O	-5.81	107.90	120.10
1	D	500	TRP	O-C-N	5.81	132.00	122.70
1	A	350	MET	CA-C-O	-5.81	107.91	120.10
1	E	162	LYS	CB-CA-C	5.81	122.01	110.40
1	F	611	VAL	CA-CB-CG1	5.81	119.61	110.90
1	A	267	GLU	CG-CD-OE1	-5.81	106.69	118.30
1	A	367	VAL	CB-CA-C	5.80	122.43	111.40
1	A	611	VAL	CA-CB-CG1	5.80	119.61	110.90
1	C	350	MET	CA-C-O	-5.80	107.91	120.10
1	C	367	VAL	CB-CA-C	5.80	122.43	111.40
1	E	350	MET	CA-C-O	-5.80	107.91	120.10
1	E	367	VAL	CB-CA-C	5.80	122.43	111.40
1	A	108	GLU	CB-CA-C	5.80	122.01	110.40
1	C	524	LYS	CB-CA-C	5.80	122.00	110.40
1	E	207	ASP	CB-CA-C	5.80	122.00	110.40
1	F	207	ASP	CB-CA-C	5.80	122.00	110.40
1	B	267	GLU	CG-CD-OE1	-5.80	106.70	118.30
1	F	350	MET	CA-C-O	-5.80	107.92	120.10
1	F	295	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	D	398	PHE	CG-CD1-CE1	-5.80	114.42	120.80
1	B	424	THR	O-C-N	5.79	131.97	122.70
1	D	367	VAL	CB-CA-C	5.79	122.41	111.40
1	D	424	THR	O-C-N	5.79	131.97	122.70
1	D	611	VAL	CA-CB-CG1	5.79	119.59	110.90
1	F	349	VAL	CG1-CB-CG2	5.79	120.17	110.90
1	B	611	VAL	CA-CB-CG1	5.79	119.59	110.90
1	C	611	VAL	CA-CB-CG1	5.79	119.59	110.90
1	A	457	HIS	CB-CA-C	-5.79	98.82	110.40
1	E	424	THR	O-C-N	5.79	131.97	122.70
1	F	500	TRP	O-C-N	5.79	131.96	122.70
1	F	524	LYS	CB-CA-C	5.79	121.98	110.40
1	C	457	HIS	CB-CA-C	-5.79	98.82	110.40
1	D	80	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	B	350	MET	CA-C-O	-5.79	107.95	120.10
1	B	457	HIS	CB-CA-C	-5.79	98.83	110.40
1	E	457	HIS	CB-CA-C	-5.79	98.83	110.40
1	F	108	GLU	CB-CA-C	5.79	121.97	110.40
1	F	457	HIS	CB-CA-C	-5.78	98.83	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	294	SER	CA-CB-OG	-5.78	95.59	111.20
1	E	524	LYS	CB-CA-C	5.78	121.96	110.40
1	B	294	SER	CA-CB-OG	-5.78	95.59	111.20
1	F	267	GLU	CG-CD-OE1	-5.78	106.74	118.30
1	C	424	THR	O-C-N	5.78	131.95	122.70
1	E	115	PHE	CB-CG-CD1	5.78	124.85	120.80
1	A	294	SER	CA-CB-OG	-5.78	95.60	111.20
1	A	424	THR	O-C-N	5.78	131.94	122.70
1	C	335	SER	CA-C-O	-5.78	107.97	120.10
1	C	500	TRP	O-C-N	5.78	131.94	122.70
1	E	294	SER	CA-CB-OG	-5.78	95.60	111.20
1	A	524	LYS	CB-CA-C	5.78	121.95	110.40
1	E	335	SER	CA-C-O	-5.78	107.97	120.10
1	F	335	SER	CA-C-O	-5.78	107.97	120.10
1	B	108	GLU	CB-CA-C	5.77	121.95	110.40
1	D	457	HIS	CB-CA-C	-5.77	98.86	110.40
1	F	294	SER	CA-CB-OG	-5.77	95.61	111.20
1	B	184	PHE	CB-CG-CD1	5.77	124.84	120.80
1	D	8	ALA	C-N-CA	5.77	136.12	121.70
1	D	294	SER	CA-CB-OG	-5.77	95.63	111.20
1	D	489	ASN	CB-CA-C	5.77	121.93	110.40
1	D	439	SER	CB-CA-C	-5.77	99.14	110.10
1	D	569	LEU	CA-C-O	-5.77	107.99	120.10
1	F	569	LEU	CA-C-O	-5.77	107.99	120.10
1	A	335	SER	CA-C-O	-5.76	108.00	120.10
1	D	532	ASP	CA-CB-CG	5.76	126.08	113.40
1	B	8	ALA	C-N-CA	5.76	136.11	121.70
1	A	500	TRP	O-C-N	5.76	131.92	122.70
1	E	110	MET	CB-CG-SD	-5.76	95.11	112.40
1	F	489	ASN	CB-CA-C	5.76	121.92	110.40
1	A	8	ALA	C-N-CA	5.76	136.10	121.70
1	B	335	SER	CA-C-O	-5.76	108.01	120.10
1	B	489	ASN	CB-CA-C	5.76	121.92	110.40
1	B	500	TRP	O-C-N	5.76	131.92	122.70
1	B	569	LEU	CA-C-O	-5.76	108.01	120.10
1	C	8	ALA	C-N-CA	5.76	136.10	121.70
1	E	8	ALA	C-N-CA	5.76	136.10	121.70
1	E	532	ASP	CA-CB-CG	5.76	126.07	113.40
1	E	569	LEU	CA-C-O	-5.76	108.00	120.10
1	A	439	SER	CB-CA-C	-5.76	99.16	110.10
1	D	110	MET	CB-CG-SD	-5.76	95.13	112.40
1	F	110	MET	CB-CG-SD	-5.76	95.12	112.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	489	ASN	CB-CA-C	5.76	121.91	110.40
1	A	569	LEU	CA-C-O	-5.76	108.01	120.10
1	B	524	LYS	CB-CA-C	5.76	121.91	110.40
1	C	569	LEU	CA-C-O	-5.76	108.01	120.10
1	D	153	LYS	CA-CB-CG	-5.76	100.73	113.40
1	A	532	ASP	CA-CB-CG	5.75	126.06	113.40
1	E	362	ASN	CB-CG-OD1	-5.75	110.09	121.60
1	A	110	MET	CB-CG-SD	-5.75	95.14	112.40
1	B	439	SER	CB-CA-C	-5.75	99.17	110.10
1	B	467	SER	CB-CA-C	-5.75	99.17	110.10
1	C	532	ASP	CA-CB-CG	5.75	126.06	113.40
1	D	335	SER	CA-C-O	-5.75	108.02	120.10
1	D	524	LYS	CB-CA-C	5.75	121.91	110.40
1	E	448	ILE	CA-C-O	-5.75	108.02	120.10
1	E	500	TRP	O-C-N	5.75	131.91	122.70
1	F	448	ILE	CA-C-O	-5.75	108.02	120.10
1	F	474	ARG	N-CA-CB	-5.75	100.25	110.60
1	D	448	ILE	CA-C-O	-5.75	108.02	120.10
1	D	467	SER	CB-CA-C	-5.75	99.17	110.10
1	E	153	LYS	CA-CB-CG	-5.75	100.75	113.40
1	A	153	LYS	CA-CB-CG	-5.75	100.75	113.40
1	B	110	MET	CB-CG-SD	-5.75	95.16	112.40
1	F	153	LYS	CA-CB-CG	-5.75	100.75	113.40
1	F	434	ILE	C-N-CA	-5.75	107.33	121.70
1	B	532	ASP	CA-CB-CG	5.75	126.04	113.40
1	C	153	LYS	CA-CB-CG	-5.75	100.76	113.40
1	C	489	ASN	CB-CA-C	5.75	121.89	110.40
1	E	357	PRO	CA-CB-CG	-5.75	93.08	104.00
1	E	489	ASN	CB-CA-C	5.75	121.89	110.40
1	F	8	ALA	C-N-CA	5.75	136.06	121.70
1	A	448	ILE	CA-C-O	-5.75	108.03	120.10
1	C	451	ARG	NH1-CZ-NH2	5.75	125.72	119.40
1	E	451	ARG	NH1-CZ-NH2	5.75	125.72	119.40
1	A	451	ARG	NH1-CZ-NH2	5.74	125.72	119.40
1	C	110	MET	CB-CG-SD	-5.74	95.17	112.40
1	C	467	SER	CB-CA-C	-5.74	99.19	110.10
1	D	362	ASN	CB-CG-OD1	-5.74	110.11	121.60
1	E	439	SER	CB-CA-C	-5.74	99.19	110.10
1	C	439	SER	CB-CA-C	-5.74	99.19	110.10
1	F	439	SER	CB-CA-C	-5.74	99.19	110.10
1	A	434	ILE	C-N-CA	-5.74	107.35	121.70
1	A	467	SER	CB-CA-C	-5.74	99.19	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	448	ILE	CA-C-O	-5.74	108.05	120.10
1	F	184	PHE	CB-CG-CD1	5.74	124.82	120.80
1	F	424	THR	O-C-N	5.74	131.88	122.70
1	C	357	PRO	CA-CB-CG	-5.74	93.10	104.00
1	C	448	ILE	CA-C-O	-5.74	108.05	120.10
1	D	434	ILE	C-N-CA	-5.74	107.35	121.70
1	A	474	ARG	N-CA-CB	-5.74	100.27	110.60
1	B	272	PRO	CB-CG-CD	-5.74	84.12	106.50
1	E	434	ILE	C-N-CA	-5.74	107.36	121.70
1	B	153	LYS	CA-CB-CG	-5.74	100.78	113.40
1	E	467	SER	CB-CA-C	-5.74	99.20	110.10
1	F	362	ASN	CB-CG-OD1	-5.74	110.13	121.60
1	F	532	ASP	CA-CB-CG	5.74	126.02	113.40
1	C	474	ARG	N-CA-CB	-5.73	100.28	110.60
1	F	272	PRO	CB-CG-CD	-5.73	84.15	106.50
1	A	272	PRO	CB-CG-CD	-5.73	84.16	106.50
1	A	362	ASN	CB-CG-OD1	-5.73	110.14	121.60
1	B	408	PHE	CA-C-N	-5.73	104.59	117.20
1	C	434	ILE	C-N-CA	-5.73	107.37	121.70
1	D	323	LEU	CB-CG-CD2	-5.73	101.26	111.00
1	E	272	PRO	CB-CG-CD	-5.73	84.15	106.50
1	E	474	ARG	N-CA-CB	-5.73	100.29	110.60
1	F	467	SER	CB-CA-C	-5.73	99.21	110.10
1	B	362	ASN	CB-CG-OD1	-5.73	110.14	121.60
1	C	272	PRO	CB-CG-CD	-5.73	84.16	106.50
1	D	240	LEU	O-C-N	-5.73	113.53	122.70
1	D	272	PRO	CB-CG-CD	-5.73	84.16	106.50
1	C	567	ARG	NH1-CZ-NH2	5.73	125.70	119.40
1	C	362	ASN	CB-CG-OD1	-5.72	110.15	121.60
1	E	323	LEU	CB-CG-CD2	-5.72	101.27	111.00
1	F	451	ARG	NH1-CZ-NH2	5.72	125.70	119.40
1	A	184	PHE	CB-CG-CD1	5.72	124.81	120.80
1	A	357	PRO	CA-CB-CG	-5.72	93.13	104.00
1	B	474	ARG	N-CA-CB	-5.72	100.30	110.60
1	F	357	PRO	CA-CB-CG	-5.72	93.13	104.00
1	A	408	PHE	CA-C-N	-5.72	104.61	117.20
1	B	304	TYR	CB-CG-CD2	5.72	124.43	121.00
1	B	357	PRO	CA-CB-CG	-5.72	93.13	104.00
1	B	434	ILE	C-N-CA	-5.72	107.40	121.70
1	B	451	ARG	NH1-CZ-NH2	5.72	125.69	119.40
1	D	357	PRO	CA-CB-CG	-5.72	93.13	104.00
1	B	567	ARG	NH1-CZ-NH2	5.72	125.69	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	474	ARG	N-CA-CB	-5.72	100.31	110.60
1	E	408	PHE	CA-C-N	-5.72	104.62	117.20
1	D	408	PHE	CA-C-N	-5.72	104.62	117.20
1	A	323	LEU	CB-CG-CD2	-5.71	101.28	111.00
1	B	323	LEU	CB-CG-CD2	-5.71	101.29	111.00
1	C	270	VAL	N-CA-CB	-5.71	98.93	111.50
1	C	408	PHE	CA-C-N	-5.71	104.63	117.20
1	D	567	ARG	NH1-CZ-NH2	5.71	125.68	119.40
1	F	567	ARG	NH1-CZ-NH2	5.71	125.68	119.40
1	D	517	GLU	CA-CB-CG	5.71	125.97	113.40
1	B	31	LYS	CA-C-O	-5.71	108.11	120.10
1	F	90	LEU	CB-CA-C	5.71	121.05	110.20
1	A	567	ARG	NH1-CZ-NH2	5.71	125.68	119.40
1	C	465	THR	C-N-CA	-5.71	107.44	121.70
1	D	31	LYS	CA-C-O	-5.71	108.12	120.10
1	E	465	THR	C-N-CA	-5.71	107.43	121.70
1	F	408	PHE	CA-C-N	-5.71	104.65	117.20
1	A	31	LYS	CA-C-O	-5.71	108.12	120.10
1	B	90	LEU	CB-CA-C	5.70	121.03	110.20
1	C	31	LYS	CA-C-O	-5.70	108.12	120.10
1	D	465	THR	C-N-CA	-5.70	107.44	121.70
1	F	323	LEU	CB-CG-CD2	-5.70	101.31	111.00
1	F	564	ILE	CA-C-O	5.70	132.07	120.10
1	A	90	LEU	CB-CA-C	5.70	121.03	110.20
1	A	465	THR	C-N-CA	-5.70	107.45	121.70
1	C	89	VAL	CG1-CB-CG2	-5.70	101.78	110.90
1	C	323	LEU	CB-CG-CD2	-5.70	101.31	111.00
1	E	90	LEU	CB-CA-C	5.70	121.03	110.20
1	E	270	VAL	N-CA-CB	-5.70	98.97	111.50
1	A	240	LEU	O-C-N	-5.70	113.59	122.70
1	B	564	ILE	CA-C-O	5.70	132.06	120.10
1	C	47	ASN	CB-CA-C	-5.70	99.01	110.40
1	D	184	PHE	CB-CG-CD1	5.70	124.79	120.80
1	F	31	LYS	CA-C-O	-5.70	108.14	120.10
1	A	270	VAL	N-CA-CB	-5.69	98.97	111.50
1	B	465	THR	C-N-CA	-5.69	107.47	121.70
1	E	240	LEU	O-C-N	-5.69	113.59	122.70
1	E	564	ILE	CA-C-O	5.69	132.06	120.10
1	C	240	LEU	O-C-N	-5.69	113.59	122.70
1	C	285	HIS	CA-CB-CG	-5.69	103.92	113.60
1	C	564	ILE	CA-C-O	5.69	132.06	120.10
1	D	90	LEU	CB-CA-C	5.69	121.02	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	451	ARG	NH1-CZ-NH2	5.69	125.66	119.40
1	C	517	GLU	CA-CB-CG	5.69	125.92	113.40
1	E	184	PHE	CB-CG-CD1	5.69	124.78	120.80
1	F	304	TYR	CB-CG-CD2	5.69	124.41	121.00
1	F	465	THR	C-N-CA	-5.69	107.47	121.70
1	A	285	HIS	CA-CB-CG	-5.69	103.93	113.60
1	A	564	ILE	CA-C-O	5.69	132.05	120.10
1	F	240	LEU	O-C-N	-5.69	113.60	122.70
1	F	517	GLU	CA-CB-CG	5.69	125.92	113.40
1	B	216	LYS	N-CA-CB	5.69	120.84	110.60
1	E	31	LYS	CA-C-O	-5.69	108.16	120.10
1	F	47	ASN	CB-CA-C	-5.69	99.02	110.40
1	F	112	GLU	CA-CB-CG	-5.69	100.89	113.40
1	B	240	LEU	O-C-N	-5.69	113.60	122.70
1	D	270	VAL	N-CA-CB	-5.69	98.99	111.50
1	E	517	GLU	CA-CB-CG	5.69	125.91	113.40
1	E	567	ARG	NH1-CZ-NH2	5.69	125.65	119.40
1	F	89	VAL	CG1-CB-CG2	-5.69	101.80	110.90
1	A	517	GLU	CA-CB-CG	5.68	125.91	113.40
1	B	27	TYR	N-CA-CB	-5.68	100.37	110.60
1	B	47	ASN	CB-CA-C	-5.68	99.03	110.40
1	B	285	HIS	CA-CB-CG	-5.68	103.94	113.60
1	C	112	GLU	CA-CB-CG	-5.68	100.89	113.40
1	E	304	TYR	CB-CG-CD2	5.68	124.41	121.00
1	F	270	VAL	N-CA-CB	-5.68	99.00	111.50
1	C	652	HIS	CA-CB-CG	-5.68	103.94	113.60
1	D	112	GLU	CA-CB-CG	-5.68	100.90	113.40
1	B	270	VAL	N-CA-CB	-5.68	99.00	111.50
1	D	47	ASN	CB-CA-C	-5.68	99.04	110.40
1	D	564	ILE	CA-C-O	5.68	132.03	120.10
1	F	551	HIS	N-CA-C	5.68	126.34	111.00
1	A	551	HIS	N-CA-C	5.68	126.34	111.00
1	B	517	GLU	CA-CB-CG	5.68	125.89	113.40
1	C	551	HIS	N-CA-C	5.68	126.33	111.00
1	D	89	VAL	CG1-CB-CG2	-5.68	101.81	110.90
1	D	216	LYS	N-CA-CB	5.68	120.82	110.60
1	D	551	HIS	N-CA-C	5.68	126.34	111.00
1	E	216	LYS	N-CA-CB	5.68	120.82	110.60
1	A	112	GLU	CA-CB-CG	-5.68	100.91	113.40
1	B	112	GLU	CA-CB-CG	-5.68	100.91	113.40
1	B	551	HIS	N-CA-C	5.68	126.33	111.00
1	E	112	GLU	CA-CB-CG	-5.68	100.91	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ASN	CB-CA-C	-5.67	99.05	110.40
1	C	559	GLU	OE1-CD-OE2	5.67	130.11	123.30
1	D	285	HIS	CA-CB-CG	-5.67	103.95	113.60
1	F	27	TYR	N-CA-CB	-5.67	100.38	110.60
1	F	285	HIS	CA-CB-CG	-5.67	103.95	113.60
1	A	89	VAL	CG1-CB-CG2	-5.67	101.82	110.90
1	C	90	LEU	CB-CA-C	5.67	120.98	110.20
1	E	47	ASN	CB-CA-C	-5.67	99.06	110.40
1	A	216	LYS	N-CA-CB	5.67	120.81	110.60
1	B	652	HIS	CA-CB-CG	-5.67	103.96	113.60
1	D	652	HIS	CA-CB-CG	-5.67	103.96	113.60
1	E	285	HIS	CA-CB-CG	-5.67	103.96	113.60
1	A	652	HIS	CA-CB-CG	-5.67	103.97	113.60
1	E	551	HIS	N-CA-C	5.67	126.30	111.00
1	A	304	TYR	CB-CG-CD2	5.66	124.40	121.00
1	B	89	VAL	CG1-CB-CG2	-5.66	101.84	110.90
1	F	216	LYS	N-CA-CB	5.66	120.80	110.60
1	E	27	TYR	N-CA-CB	-5.66	100.41	110.60
1	F	652	HIS	CA-CB-CG	-5.66	103.97	113.60
1	C	27	TYR	N-CA-CB	-5.66	100.41	110.60
1	E	89	VAL	CG1-CB-CG2	-5.66	101.84	110.90
1	C	184	PHE	CB-CG-CD1	5.66	124.76	120.80
1	D	304	TYR	CB-CG-CD2	5.66	124.39	121.00
1	E	559	GLU	OE1-CD-OE2	5.66	130.09	123.30
1	A	27	TYR	N-CA-CB	-5.66	100.42	110.60
1	B	1	ASP	CA-C-O	5.66	131.98	120.10
1	D	27	TYR	N-CA-CB	-5.66	100.42	110.60
1	A	559	GLU	OE1-CD-OE2	5.65	130.08	123.30
1	C	216	LYS	N-CA-CB	5.65	120.78	110.60
1	E	652	HIS	CA-CB-CG	-5.65	103.99	113.60
1	F	648	LYS	N-CA-CB	5.65	120.78	110.60
1	A	560	ARG	CA-C-O	5.65	131.97	120.10
1	C	376	ARG	CB-CG-CD	5.65	126.29	111.60
1	C	463	LYS	CB-CA-C	5.65	121.70	110.40
1	E	648	LYS	N-CA-CB	5.65	120.77	110.60
1	A	463	LYS	CB-CA-C	5.65	121.70	110.40
1	B	648	LYS	N-CA-CB	5.65	120.77	110.60
1	E	1	ASP	CA-C-O	5.65	131.96	120.10
1	E	560	ARG	CA-C-O	5.65	131.96	120.10
1	B	397	SER	C-N-CA	-5.65	107.58	121.70
1	E	181	VAL	C-N-CA	5.65	135.81	121.70
1	C	560	ARG	CA-C-O	5.64	131.95	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	559	GLU	OE1-CD-OE2	5.64	130.07	123.30
1	E	463	LYS	CB-CA-C	5.64	121.69	110.40
1	F	1	ASP	CA-C-O	5.64	131.95	120.10
1	A	376	ARG	CB-CG-CD	5.64	126.27	111.60
1	B	376	ARG	CB-CG-CD	5.64	126.27	111.60
1	B	463	LYS	CB-CA-C	5.64	121.69	110.40
1	B	653	LEU	CA-CB-CG	-5.64	102.33	115.30
1	F	397	SER	C-N-CA	-5.64	107.60	121.70
1	F	463	LYS	CB-CA-C	5.64	121.68	110.40
1	B	560	ARG	CA-C-O	5.64	131.94	120.10
1	A	648	LYS	N-CA-CB	5.64	120.75	110.60
1	C	397	SER	C-N-CA	-5.64	107.61	121.70
1	E	397	SER	C-N-CA	-5.64	107.61	121.70
1	C	304	TYR	CB-CG-CD2	5.64	124.38	121.00
1	B	637	ASP	CA-CB-CG	5.63	125.79	113.40
1	D	463	LYS	CB-CA-C	5.63	121.67	110.40
1	D	632	ASP	CB-CA-C	5.63	121.67	110.40
1	E	376	ARG	CB-CG-CD	5.63	126.25	111.60
1	E	435	ASN	CB-CA-C	5.63	121.67	110.40
1	C	181	VAL	C-N-CA	5.63	135.78	121.70
1	D	376	ARG	CB-CG-CD	5.63	126.25	111.60
1	B	559	GLU	OE1-CD-OE2	5.63	130.06	123.30
1	C	648	LYS	N-CA-CB	5.63	120.74	110.60
1	F	59	GLU	CA-C-O	-5.63	108.28	120.10
1	F	376	ARG	CB-CG-CD	5.63	126.24	111.60
1	F	560	ARG	CA-C-O	5.63	131.93	120.10
1	A	1	ASP	CA-C-O	5.63	131.92	120.10
1	B	59	GLU	CA-C-O	-5.63	108.28	120.10
1	D	560	ARG	CA-C-O	5.63	131.92	120.10
1	A	181	VAL	C-N-CA	5.63	135.77	121.70
1	A	397	SER	C-N-CA	-5.63	107.63	121.70
1	D	181	VAL	C-N-CA	5.63	135.77	121.70
1	D	242	PRO	N-CD-CG	-5.63	94.76	103.20
1	D	653	LEU	CA-CB-CG	-5.63	102.35	115.30
1	C	435	ASN	CB-CA-C	5.63	121.65	110.40
1	D	397	SER	C-N-CA	-5.63	107.63	121.70
1	F	181	VAL	C-N-CA	5.63	135.76	121.70
1	F	653	LEU	CA-CB-CG	-5.63	102.36	115.30
1	B	632	ASP	CB-CA-C	5.62	121.65	110.40
1	F	385	LYS	CA-CB-CG	-5.62	101.03	113.40
1	A	632	ASP	CB-CA-C	5.62	121.64	110.40
1	A	653	LEU	CA-CB-CG	-5.62	102.36	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	ASP	CA-C-O	5.62	131.91	120.10
1	B	435	ASN	CB-CA-C	5.62	121.64	110.40
1	B	524	LYS	CA-CB-CG	-5.62	101.03	113.40
1	E	632	ASP	CB-CA-C	5.62	121.64	110.40
1	D	460	PHE	CZ-CE2-CD2	-5.62	113.36	120.10
1	A	435	ASN	CB-CA-C	5.62	121.64	110.40
1	B	61	ASN	CB-CA-C	5.62	121.64	110.40
1	B	181	VAL	C-N-CA	5.62	135.75	121.70
1	B	385	LYS	CA-CB-CG	-5.62	101.04	113.40
1	C	653	LEU	CA-CB-CG	-5.62	102.38	115.30
1	D	385	LYS	CA-CB-CG	-5.62	101.04	113.40
1	A	637	ASP	CA-CB-CG	5.62	125.76	113.40
1	E	59	GLU	CA-C-O	-5.62	108.31	120.10
1	E	166	PHE	CD1-CE1-CZ	-5.62	113.36	120.10
1	A	59	GLU	CA-C-O	-5.62	108.31	120.10
1	A	166	PHE	CD1-CE1-CZ	-5.62	113.36	120.10
1	D	435	ASN	CB-CA-C	5.62	121.63	110.40
1	D	637	ASP	CA-CB-CG	5.62	125.75	113.40
1	D	648	LYS	N-CA-CB	5.62	120.71	110.60
1	E	653	LEU	CA-CB-CG	-5.62	102.39	115.30
1	F	166	PHE	CD1-CE1-CZ	-5.62	113.36	120.10
1	A	385	LYS	CA-CB-CG	-5.61	101.05	113.40
1	C	242	PRO	N-CD-CG	-5.61	94.78	103.20
1	C	632	ASP	CB-CA-C	5.61	121.63	110.40
1	E	536	PHE	O-C-N	5.61	131.68	122.70
1	F	559	GLU	OE1-CD-OE2	5.61	130.04	123.30
1	C	637	ASP	CA-CB-CG	5.61	125.75	113.40
1	E	385	LYS	CA-CB-CG	-5.61	101.05	113.40
1	F	632	ASP	CB-CA-C	5.61	121.62	110.40
1	A	242	PRO	N-CD-CG	-5.61	94.78	103.20
1	C	59	GLU	CA-C-O	-5.61	108.32	120.10
1	D	1	ASP	CA-C-O	5.61	131.88	120.10
1	D	59	GLU	CA-C-O	-5.61	108.32	120.10
1	E	30	LEU	CA-CB-CG	-5.61	102.40	115.30
1	E	637	ASP	CA-CB-CG	5.61	125.74	113.40
1	F	536	PHE	O-C-N	5.61	131.68	122.70
1	E	524	LYS	CA-CB-CG	-5.61	101.06	113.40
1	A	524	LYS	CA-CB-CG	-5.61	101.06	113.40
1	B	502	CYS	CB-CA-C	-5.61	99.19	110.40
1	D	524	LYS	CA-CB-CG	-5.61	101.07	113.40
1	F	637	ASP	CA-CB-CG	5.61	125.73	113.40
1	A	30	LEU	CA-CB-CG	-5.60	102.41	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	385	LYS	CA-CB-CG	-5.60	101.07	113.40
1	D	408	PHE	N-CA-CB	5.60	120.69	110.60
1	C	536	PHE	O-C-N	5.60	131.66	122.70
1	A	460	PHE	CZ-CE2-CD2	-5.60	113.38	120.10
1	B	166	PHE	CD1-CE1-CZ	-5.60	113.38	120.10
1	B	242	PRO	N-CD-CG	-5.60	94.80	103.20
1	C	61	ASN	CB-CA-C	5.60	121.60	110.40
1	D	30	LEU	CA-CB-CG	-5.60	102.42	115.30
1	D	166	PHE	CD1-CE1-CZ	-5.60	113.38	120.10
1	F	30	LEU	CA-CB-CG	-5.60	102.42	115.30
1	F	302	HIS	CA-C-O	-5.60	108.34	120.10
1	A	61	ASN	CB-CA-C	5.60	121.59	110.40
1	A	502	CYS	CB-CA-C	-5.60	99.21	110.40
1	B	408	PHE	N-CA-CB	5.60	120.67	110.60
1	B	460	PHE	CZ-CE2-CD2	-5.60	113.38	120.10
1	C	30	LEU	CA-CB-CG	-5.60	102.43	115.30
1	C	166	PHE	CD1-CE1-CZ	-5.60	113.38	120.10
1	F	435	ASN	CB-CA-C	5.60	121.59	110.40
1	C	524	LYS	CA-CB-CG	-5.60	101.09	113.40
1	A	536	PHE	O-C-N	5.59	131.65	122.70
1	B	302	HIS	CA-C-O	-5.59	108.35	120.10
1	C	394	HIS	O-C-N	5.59	131.65	122.70
1	E	318	PRO	N-CD-CG	-5.59	94.81	103.20
1	F	61	ASN	CB-CA-C	5.59	121.59	110.40
1	F	242	PRO	N-CD-CG	-5.59	94.81	103.20
1	F	524	LYS	CA-CB-CG	-5.59	101.09	113.40
1	C	408	PHE	N-CA-CB	5.59	120.67	110.60
1	D	536	PHE	O-C-N	5.59	131.65	122.70
1	F	568	MET	CA-CB-CG	5.59	122.81	113.30
1	B	30	LEU	CA-CB-CG	-5.59	102.44	115.30
1	B	536	PHE	O-C-N	5.59	131.64	122.70
1	E	65	LEU	CA-C-O	-5.59	108.36	120.10
1	E	242	PRO	N-CD-CG	-5.59	94.82	103.20
1	E	394	HIS	O-C-N	5.59	131.64	122.70
1	A	408	PHE	N-CA-CB	5.59	120.66	110.60
1	B	590	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	E	61	ASN	CB-CA-C	5.59	121.57	110.40
1	F	408	PHE	N-CA-CB	5.59	120.66	110.60
1	D	61	ASN	CB-CA-C	5.58	121.57	110.40
1	A	302	HIS	CA-C-O	-5.58	108.37	120.10
1	E	302	HIS	CA-C-O	-5.58	108.37	120.10
1	E	374	ALA	N-CA-CB	5.58	117.92	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	568	MET	CA-CB-CG	5.58	122.79	113.30
1	B	275	ILE	CG1-CB-CG2	-5.58	99.12	111.40
1	C	502	CYS	CB-CA-C	-5.58	99.24	110.40
1	D	302	HIS	CA-C-O	-5.58	108.38	120.10
1	D	502	CYS	CB-CA-C	-5.58	99.24	110.40
1	D	643	LYS	C-N-CA	-5.58	107.75	121.70
1	E	502	CYS	CB-CA-C	-5.58	99.24	110.40
1	E	460	PHE	CZ-CE2-CD2	-5.58	113.40	120.10
1	C	460	PHE	CZ-CE2-CD2	-5.58	113.41	120.10
1	D	590	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	A	275	ILE	CG1-CB-CG2	-5.58	99.13	111.40
1	F	502	CYS	CB-CA-C	-5.58	99.25	110.40
1	A	643	LYS	C-N-CA	-5.58	107.76	121.70
1	C	42	ASP	N-CA-C	-5.58	95.95	111.00
1	C	89	VAL	N-CA-C	-5.58	95.95	111.00
1	C	643	LYS	C-N-CA	-5.58	107.76	121.70
1	D	319	LYS	CB-CA-C	-5.58	99.25	110.40
1	F	89	VAL	N-CA-C	-5.58	95.95	111.00
1	C	302	HIS	CA-C-O	-5.57	108.39	120.10
1	D	275	ILE	CG1-CB-CG2	-5.57	99.14	111.40
1	D	460	PHE	CG-CD2-CE2	5.57	126.93	120.80
1	E	264	TYR	CD1-CE1-CZ	-5.57	114.78	119.80
1	E	324	LEU	CB-CG-CD2	-5.57	101.53	111.00
1	C	65	LEU	CA-C-O	-5.57	108.40	120.10
1	C	568	MET	CA-CB-CG	5.57	122.77	113.30
1	D	264	TYR	CD1-CE1-CZ	-5.57	114.78	119.80
1	F	374	ALA	N-CA-CB	5.57	117.90	110.10
1	A	324	LEU	CB-CG-CD2	-5.57	101.53	111.00
1	A	568	MET	CA-CB-CG	5.57	122.77	113.30
1	B	319	LYS	CB-CA-C	-5.57	99.26	110.40
1	B	527	SER	O-C-N	5.57	131.61	122.70
1	D	65	LEU	CA-C-O	-5.57	108.40	120.10
1	E	89	VAL	N-CA-C	-5.57	95.96	111.00
1	A	89	VAL	N-CA-C	-5.57	95.96	111.00
1	D	324	LEU	CB-CG-CD2	-5.57	101.53	111.00
1	D	568	MET	CA-CB-CG	5.57	122.77	113.30
1	E	495	LEU	N-CA-CB	5.57	121.54	110.40
1	A	42	ASP	N-CA-C	-5.57	95.97	111.00
1	A	65	LEU	CA-C-O	-5.57	108.41	120.10
1	B	42	ASP	N-CA-C	-5.57	95.97	111.00
1	B	89	VAL	N-CA-C	-5.57	95.97	111.00
1	B	324	LEU	CB-CG-CD2	-5.57	101.54	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	394	HIS	O-C-N	5.57	131.61	122.70
1	E	297	HIS	CA-CB-CG	-5.57	104.14	113.60
1	E	408	PHE	N-CA-CB	5.57	120.62	110.60
1	E	643	LYS	C-N-CA	-5.57	107.78	121.70
1	F	42	ASP	N-CA-C	-5.57	95.97	111.00
1	F	324	LEU	CB-CG-CD2	-5.57	101.53	111.00
1	F	439	SER	C-N-CA	-5.57	110.61	122.30
1	F	460	PHE	CZ-CE2-CD2	-5.57	113.42	120.10
1	F	643	LYS	C-N-CA	-5.57	107.78	121.70
1	A	318	PRO	N-CD-CG	-5.57	94.85	103.20
1	B	264	TYR	CD1-CE1-CZ	-5.57	114.79	119.80
1	C	297	HIS	CA-CB-CG	-5.57	104.14	113.60
1	C	374	ALA	N-CA-CB	5.57	117.89	110.10
1	D	374	ALA	N-CA-CB	5.57	117.89	110.10
1	D	439	SER	C-N-CA	-5.57	110.61	122.30
1	F	319	LYS	CB-CA-C	-5.57	99.27	110.40
1	F	495	LEU	N-CA-CB	5.57	121.53	110.40
1	B	318	PRO	N-CD-CG	-5.56	94.85	103.20
1	B	394	HIS	O-C-N	5.56	131.60	122.70
1	E	275	ILE	CG1-CB-CG2	-5.56	99.16	111.40
1	F	65	LEU	CA-C-O	-5.56	108.42	120.10
1	A	374	ALA	N-CA-CB	5.56	117.89	110.10
1	A	394	HIS	O-C-N	5.56	131.60	122.70
1	B	374	ALA	N-CA-CB	5.56	117.89	110.10
1	B	439	SER	C-N-CA	-5.56	110.62	122.30
1	C	318	PRO	N-CD-CG	-5.56	94.86	103.20
1	C	324	LEU	CB-CG-CD2	-5.56	101.54	111.00
1	C	460	PHE	CG-CD2-CE2	5.56	126.92	120.80
1	D	297	HIS	CA-CB-CG	-5.56	104.14	113.60
1	D	439	SER	O-C-N	5.56	132.66	123.20
1	F	318	PRO	N-CD-CG	-5.56	94.86	103.20
1	A	319	LYS	CB-CA-C	-5.56	99.28	110.40
1	C	429	PHE	N-CA-CB	-5.56	100.59	110.60
1	A	264	TYR	CD1-CE1-CZ	-5.56	114.80	119.80
1	A	439	SER	C-N-CA	-5.56	110.62	122.30
1	A	495	LEU	N-CA-CB	5.56	121.52	110.40
1	B	65	LEU	CA-C-O	-5.56	108.43	120.10
1	B	431	TYR	CB-CA-C	5.56	121.52	110.40
1	B	643	LYS	C-N-CA	-5.56	107.80	121.70
1	D	42	ASP	N-CA-C	-5.56	95.99	111.00
1	D	495	LEU	N-CA-CB	5.56	121.52	110.40
1	B	439	SER	O-C-N	5.56	132.65	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	439	SER	C-N-CA	-5.56	110.63	122.30
1	E	319	LYS	CB-CA-C	-5.56	99.28	110.40
1	E	527	SER	O-C-N	5.56	131.59	122.70
1	E	578	MET	N-CA-C	-5.56	95.99	111.00
1	F	275	ILE	CG1-CB-CG2	-5.56	99.17	111.40
1	A	431	TYR	CB-CA-C	5.56	121.51	110.40
1	A	460	PHE	CG-CD2-CE2	5.56	126.91	120.80
1	B	568	MET	CA-CB-CG	5.56	122.75	113.30
1	A	429	PHE	N-CA-CB	-5.55	100.60	110.60
1	A	590	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	C	275	ILE	CG1-CB-CG2	-5.55	99.18	111.40
1	D	431	TYR	CB-CA-C	5.55	121.51	110.40
1	E	577	GLY	O-C-N	5.55	131.59	122.70
1	F	429	PHE	N-CA-CB	-5.55	100.60	110.60
1	E	42	ASP	N-CA-C	-5.55	96.01	111.00
1	F	394	HIS	O-C-N	5.55	131.58	122.70
1	A	297	HIS	CA-CB-CG	-5.55	104.16	113.60
1	A	527	SER	O-C-N	5.55	131.58	122.70
1	B	429	PHE	N-CA-CB	-5.55	100.61	110.60
1	D	89	VAL	N-CA-C	-5.55	96.01	111.00
1	F	577	GLY	O-C-N	5.55	131.58	122.70
1	F	578	MET	N-CA-C	-5.55	96.01	111.00
1	C	319	LYS	CB-CA-C	-5.55	99.30	110.40
1	E	590	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	C	431	TYR	CB-CA-C	5.55	121.49	110.40
1	D	578	MET	N-CA-C	-5.55	96.03	111.00
1	F	431	TYR	CB-CA-C	5.55	121.49	110.40
1	B	460	PHE	CG-CD2-CE2	5.54	126.90	120.80
1	B	495	LEU	N-CA-CB	5.54	121.49	110.40
1	B	578	MET	N-CA-C	-5.54	96.03	111.00
1	F	527	SER	O-C-N	5.54	131.57	122.70
1	A	578	MET	N-CA-C	-5.54	96.04	111.00
1	B	297	HIS	CA-CB-CG	-5.54	104.18	113.60
1	B	483	CYS	CA-C-N	5.54	132.62	117.10
1	B	577	GLY	O-C-N	5.54	131.57	122.70
1	C	527	SER	O-C-N	5.54	131.56	122.70
1	D	318	PRO	N-CD-CG	-5.54	94.89	103.20
1	D	429	PHE	N-CA-CB	-5.54	100.62	110.60
1	F	264	TYR	CD1-CE1-CZ	-5.54	114.81	119.80
1	C	578	MET	N-CA-C	-5.54	96.04	111.00
1	C	590	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	577	GLY	O-C-N	5.54	131.56	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	495	LEU	N-CA-CB	5.54	121.47	110.40
1	E	431	TYR	CB-CA-C	5.54	121.47	110.40
1	A	439	SER	O-C-N	5.54	132.61	123.20
1	D	483	CYS	CA-C-N	5.54	132.60	117.10
1	E	429	PHE	N-CA-CB	-5.54	100.64	110.60
1	F	297	HIS	CA-CB-CG	-5.54	104.19	113.60
1	D	45	ILE	CG1-CB-CG2	5.53	123.58	111.40
1	E	439	SER	C-N-CA	-5.53	110.68	122.30
1	E	460	PHE	CG-CD2-CE2	5.53	126.89	120.80
1	D	123	VAL	O-C-N	-5.53	113.85	122.70
1	F	483	CYS	CA-C-N	5.53	132.59	117.10
1	B	496	ASP	CB-CG-OD2	5.53	123.28	118.30
1	E	45	ILE	CG1-CB-CG2	5.53	123.57	111.40
1	E	441	GLU	N-CA-C	5.53	125.93	111.00
1	F	439	SER	O-C-N	5.53	132.60	123.20
1	A	483	CYS	CA-C-N	5.53	132.57	117.10
1	C	577	GLY	O-C-N	5.53	131.54	122.70
1	F	123	VAL	O-C-N	-5.53	113.86	122.70
1	A	45	ILE	CG1-CB-CG2	5.53	123.56	111.40
1	A	441	GLU	N-CA-C	5.53	125.92	111.00
1	B	45	ILE	CG1-CB-CG2	5.53	123.56	111.40
1	C	123	VAL	O-C-N	-5.53	113.86	122.70
1	C	441	GLU	N-CA-C	5.53	125.92	111.00
1	E	483	CYS	CA-C-N	5.53	132.57	117.10
1	F	460	PHE	CG-CD2-CE2	5.53	126.88	120.80
1	E	64	ARG	NH1-CZ-NH2	5.52	125.48	119.40
1	C	439	SER	O-C-N	5.52	132.59	123.20
1	C	483	CYS	CA-C-N	5.52	132.56	117.10
1	E	496	ASP	CB-CG-OD2	5.52	123.27	118.30
1	E	553	LEU	C-N-CA	-5.52	107.89	121.70
1	B	441	GLU	N-CA-C	5.52	125.91	111.00
1	F	45	ILE	CG1-CB-CG2	5.52	123.55	111.40
1	F	215	ARG	CB-CG-CD	5.52	125.96	111.60
1	F	441	GLU	N-CA-C	5.52	125.91	111.00
1	F	474	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	B	123	VAL	O-C-N	-5.52	113.87	122.70
1	D	577	GLY	O-C-N	5.52	131.53	122.70
1	C	264	TYR	CD1-CE1-CZ	-5.52	114.83	119.80
1	C	45	ILE	CG1-CB-CG2	5.51	123.53	111.40
1	D	527	SER	O-C-N	5.51	131.52	122.70
1	D	553	LEU	C-N-CA	-5.51	107.91	121.70
1	A	553	LEU	C-N-CA	-5.51	107.92	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	441	GLU	N-CA-C	5.51	125.88	111.00
1	F	197	TRP	CD1-CG-CD2	-5.51	101.89	106.30
1	B	284	ALA	CB-CA-C	5.51	118.36	110.10
1	C	360	LYS	CD-CE-NZ	-5.51	99.03	111.70
1	F	590	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	215	ARG	CB-CG-CD	5.51	125.92	111.60
1	B	133	VAL	CA-CB-CG2	-5.51	102.64	110.90
1	D	64	ARG	NH1-CZ-NH2	5.51	125.46	119.40
1	A	496	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	360	LYS	CD-CE-NZ	-5.50	99.04	111.70
1	B	262	TYR	CB-CG-CD2	5.50	124.30	121.00
1	C	215	ARG	CB-CG-CD	5.50	125.91	111.60
1	D	360	LYS	CD-CE-NZ	-5.50	99.04	111.70
1	E	262	TYR	CB-CG-CD2	5.50	124.30	121.00
1	A	123	VAL	O-C-N	-5.50	113.90	122.70
1	A	360	LYS	CD-CE-NZ	-5.50	99.05	111.70
1	B	553	LEU	C-N-CA	-5.50	107.94	121.70
1	C	253	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	F	553	LEU	C-N-CA	-5.50	107.94	121.70
1	F	360	LYS	CD-CE-NZ	-5.50	99.05	111.70
1	E	215	ARG	CB-CG-CD	5.50	125.90	111.60
1	F	262	TYR	CB-CG-CD2	5.50	124.30	121.00
1	F	284	ALA	CB-CA-C	5.50	118.35	110.10
1	B	215	ARG	CB-CG-CD	5.50	125.89	111.60
1	D	215	ARG	CB-CG-CD	5.50	125.89	111.60
1	C	553	LEU	C-N-CA	-5.49	107.97	121.70
1	E	434	ILE	O-C-N	5.49	131.49	122.70
1	F	133	VAL	CA-CB-CG2	-5.49	102.66	110.90
1	E	133	VAL	CA-CB-CG2	-5.49	102.66	110.90
1	A	64	ARG	NH1-CZ-NH2	5.49	125.44	119.40
1	A	262	TYR	CB-CG-CD2	5.49	124.29	121.00
1	B	653	LEU	N-CA-CB	-5.49	99.42	110.40
1	D	496	ASP	CB-CG-OD2	5.49	123.24	118.30
1	D	653	LEU	N-CA-CB	-5.49	99.42	110.40
1	E	360	LYS	CD-CE-NZ	-5.49	99.07	111.70
1	E	439	SER	O-C-N	5.49	132.53	123.20
1	F	653	LEU	N-CA-CB	-5.49	99.42	110.40
1	A	284	ALA	CB-CA-C	5.49	118.33	110.10
1	C	133	VAL	CA-CB-CG2	-5.49	102.67	110.90
1	C	64	ARG	NH1-CZ-NH2	5.49	125.44	119.40
1	C	278	GLU	O-C-N	5.49	131.48	122.70
1	A	653	LEU	N-CA-CB	-5.49	99.43	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	197	TRP	CD1-CG-CD2	-5.49	101.91	106.30
1	E	545	ASN	CA-C-N	5.49	129.27	117.20
1	E	123	VAL	O-C-N	-5.48	113.93	122.70
1	C	653	LEU	N-CA-CB	-5.48	99.44	110.40
1	A	197	TRP	CD1-CG-CD2	-5.48	101.92	106.30
1	B	64	ARG	NH1-CZ-NH2	5.48	125.42	119.40
1	C	545	ASN	CA-C-N	5.48	129.25	117.20
1	D	247	HIS	CB-CA-C	-5.48	99.44	110.40
1	D	262	TYR	CB-CG-CD2	5.48	124.29	121.00
1	E	120	TYR	CB-CA-C	-5.48	99.44	110.40
1	F	496	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	152	ASP	CA-CB-CG	5.47	125.44	113.40
1	D	133	VAL	CA-CB-CG2	-5.47	102.69	110.90
1	D	284	ALA	CB-CA-C	5.47	118.31	110.10
1	D	434	ILE	O-C-N	5.47	131.46	122.70
1	D	545	ASN	CA-C-N	5.47	129.24	117.20
1	F	535	SER	O-C-N	5.47	131.46	122.70
1	B	545	ASN	CA-C-N	5.47	129.24	117.20
1	C	262	TYR	CB-CG-CD2	5.47	124.28	121.00
1	C	361	PHE	O-C-N	5.47	131.46	122.70
1	C	434	ILE	O-C-N	5.47	131.46	122.70
1	F	434	ILE	O-C-N	5.47	131.46	122.70
1	B	270	VAL	CA-C-N	5.47	129.24	117.20
1	D	253	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	E	197	TRP	CD1-CG-CD2	-5.47	101.92	106.30
1	E	637	ASP	CB-CA-C	-5.47	99.46	110.40
1	E	653	LEU	N-CA-CB	-5.47	99.46	110.40
1	F	345	ASN	CA-C-N	5.47	129.24	117.20
1	A	133	VAL	CA-CB-CG2	-5.47	102.69	110.90
1	A	545	ASN	CA-C-N	5.47	129.23	117.20
1	B	278	GLU	O-C-N	5.47	131.45	122.70
1	B	535	SER	O-C-N	5.47	131.45	122.70
1	C	197	TRP	CD1-CG-CD2	-5.47	101.92	106.30
1	C	637	ASP	CB-CA-C	-5.47	99.46	110.40
1	B	197	TRP	CD1-CG-CD2	-5.47	101.93	106.30
1	B	247	HIS	CB-CA-C	-5.47	99.47	110.40
1	E	284	ALA	CB-CA-C	5.47	118.30	110.10
1	A	253	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	C	120	TYR	CB-CA-C	-5.47	99.47	110.40
1	C	247	HIS	CB-CA-C	-5.47	99.47	110.40
1	A	278	GLU	O-C-N	5.46	131.44	122.70
1	A	434	ILE	O-C-N	5.46	131.44	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	637	ASP	CB-CA-C	-5.46	99.47	110.40
1	C	284	ALA	CB-CA-C	5.46	118.30	110.10
1	E	535	SER	O-C-N	5.46	131.44	122.70
1	F	361	PHE	O-C-N	5.46	131.44	122.70
1	F	637	ASP	CB-CA-C	-5.46	99.47	110.40
1	A	270	VAL	CA-C-N	5.46	129.22	117.20
1	A	535	SER	O-C-N	5.46	131.44	122.70
1	A	120	TYR	CB-CA-C	-5.46	99.48	110.40
1	A	247	HIS	CB-CA-C	-5.46	99.48	110.40
1	B	142	PRO	N-CD-CG	-5.46	95.01	103.20
1	C	142	PRO	N-CD-CG	-5.46	95.01	103.20
1	D	278	GLU	O-C-N	5.46	131.44	122.70
1	E	383	LEU	CA-C-O	-5.46	108.63	120.10
1	F	278	GLU	O-C-N	5.46	131.44	122.70
1	F	383	LEU	CA-C-O	-5.46	108.63	120.10
1	F	545	ASN	CA-C-N	5.46	129.21	117.20
1	A	361	PHE	O-C-N	5.46	131.44	122.70
1	B	637	ASP	CB-CA-C	-5.46	99.48	110.40
1	E	152	ASP	CA-CB-CG	5.46	125.41	113.40
1	E	247	HIS	CB-CA-C	-5.46	99.48	110.40
1	F	525	ASP	CA-C-N	5.46	129.21	117.20
1	C	505	LEU	N-CA-CB	-5.46	99.49	110.40
1	D	142	PRO	N-CD-CG	-5.46	95.02	103.20
1	E	270	VAL	CA-C-N	5.46	129.20	117.20
1	F	120	TYR	CB-CA-C	-5.46	99.49	110.40
1	F	152	ASP	CA-CB-CG	5.46	125.40	113.40
1	E	391	PHE	CE1-CZ-CE2	5.46	129.82	120.00
1	A	152	ASP	CA-CB-CG	5.45	125.40	113.40
1	B	345	ASN	CA-C-N	5.45	129.20	117.20
1	C	345	ASN	CA-C-N	5.45	129.20	117.20
1	D	120	TYR	CB-CA-C	-5.45	99.49	110.40
1	D	290	GLU	CA-C-N	5.45	129.20	117.20
1	D	383	LEU	CA-C-O	-5.45	108.65	120.10
1	F	64	ARG	NH1-CZ-NH2	5.45	125.40	119.40
1	F	505	LEU	N-CA-CB	-5.45	99.49	110.40
1	A	525	ASP	CA-C-N	5.45	129.19	117.20
1	B	120	TYR	CB-CA-C	-5.45	99.50	110.40
1	D	152	ASP	CA-CB-CG	5.45	125.39	113.40
1	D	345	ASN	CA-C-N	5.45	129.19	117.20
1	F	270	VAL	CA-C-N	5.45	129.19	117.20
1	A	345	ASN	CA-C-N	5.45	129.19	117.20
1	C	64	ARG	NE-CZ-NH1	5.45	123.03	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	152	ASP	CA-CB-CG	5.45	125.39	113.40
1	B	505	LEU	N-CA-CB	-5.45	99.50	110.40
1	D	270	VAL	CA-C-N	5.45	129.19	117.20
1	D	545	ASN	CA-C-O	-5.45	108.66	120.10
1	D	593	THR	N-CA-CB	-5.45	99.95	110.30
1	D	637	ASP	CB-CA-C	-5.45	99.50	110.40
1	E	355	GLY	CA-C-O	-5.45	110.79	120.60
1	F	593	THR	N-CA-CB	-5.45	99.95	110.30
1	C	270	VAL	CA-C-N	5.45	129.18	117.20
1	D	535	SER	O-C-N	5.45	131.41	122.70
1	E	206	GLU	CA-CB-CG	-5.45	101.42	113.40
1	E	389	ASN	CB-CG-ND2	5.45	129.77	116.70
1	A	142	PRO	N-CD-CG	-5.45	95.03	103.20
1	C	290	GLU	CA-C-N	5.45	129.18	117.20
1	D	151	ILE	O-C-N	5.45	131.41	122.70
1	F	247	HIS	CB-CA-C	-5.45	99.51	110.40
1	F	389	ASN	CB-CG-ND2	5.45	129.77	116.70
1	A	206	GLU	CA-CB-CG	-5.44	101.42	113.40
1	A	383	LEU	CA-C-O	-5.44	108.67	120.10
1	A	505	LEU	N-CA-CB	-5.44	99.52	110.40
1	C	525	ASP	CA-C-N	5.44	129.17	117.20
1	C	535	SER	O-C-N	5.44	131.41	122.70
1	C	545	ASN	CA-C-O	-5.44	108.67	120.10
1	D	206	GLU	CA-CB-CG	-5.44	101.43	113.40
1	E	505	LEU	N-CA-CB	-5.44	99.51	110.40
1	F	340	TYR	CE1-CZ-CE2	5.44	128.51	119.80
1	F	348	HIS	N-CA-CB	5.44	120.40	110.60
1	A	290	GLU	CA-C-N	5.44	129.17	117.20
1	A	333	TYR	N-CA-CB	-5.44	100.81	110.60
1	B	581	ASN	CA-C-O	-5.44	108.68	120.10
1	C	206	GLU	CA-CB-CG	-5.44	101.43	113.40
1	D	333	TYR	N-CA-CB	-5.44	100.81	110.60
1	D	525	ASP	CA-C-N	5.44	129.17	117.20
1	E	348	HIS	N-CA-CB	5.44	120.39	110.60
1	E	525	ASP	CA-C-N	5.44	129.17	117.20
1	F	142	PRO	N-CD-CG	-5.44	95.04	103.20
1	F	333	TYR	N-CA-CB	-5.44	100.81	110.60
1	F	417	ALA	CA-C-N	-5.44	105.23	117.20
1	B	290	GLU	CA-C-N	5.44	129.16	117.20
1	A	389	ASN	CB-CG-ND2	5.44	129.75	116.70
1	B	361	PHE	O-C-N	5.44	131.40	122.70
1	B	441	GLU	CA-C-N	-5.44	105.24	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	525	ASP	CA-C-N	5.44	129.16	117.20
1	C	230	ARG	CA-C-O	-5.44	108.68	120.10
1	C	389	ASN	CB-CG-ND2	5.44	129.75	116.70
1	C	496	ASP	CB-CG-OD2	5.44	123.19	118.30
1	D	361	PHE	O-C-N	5.44	131.40	122.70
1	D	581	ASN	CA-C-O	-5.44	108.68	120.10
1	E	278	GLU	O-C-N	5.44	131.40	122.70
1	B	333	TYR	N-CA-CB	-5.44	100.81	110.60
1	B	355	GLY	CA-C-O	-5.44	110.81	120.60
1	B	389	ASN	CB-CG-ND2	5.44	129.75	116.70
1	C	333	TYR	N-CA-CB	-5.44	100.81	110.60
1	C	391	PHE	CE1-CZ-CE2	5.44	129.78	120.00
1	F	403	HIS	CA-C-N	-5.44	105.24	117.20
1	B	151	ILE	O-C-N	5.43	131.39	122.70
1	B	383	LEU	CA-C-O	-5.43	108.69	120.10
1	B	403	HIS	CA-C-N	-5.43	105.25	117.20
1	C	383	LEU	CA-C-O	-5.43	108.69	120.10
1	E	142	PRO	N-CD-CG	-5.43	95.05	103.20
1	F	367	VAL	CA-CB-CG1	5.43	119.05	110.90
1	A	593	THR	N-CA-CB	-5.43	99.98	110.30
1	B	206	GLU	CA-CB-CG	-5.43	101.45	113.40
1	B	253	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	C	355	GLY	CA-C-O	-5.43	110.82	120.60
1	D	389	ASN	CB-CG-ND2	5.43	129.74	116.70
1	E	345	ASN	CA-C-N	5.43	129.15	117.20
1	F	206	GLU	CA-CB-CG	-5.43	101.45	113.40
1	F	581	ASN	CA-C-O	-5.43	108.69	120.10
1	B	377	ASP	CA-C-O	-5.43	108.69	120.10
1	B	417	ALA	CA-C-N	-5.43	105.25	117.20
1	C	151	ILE	O-C-N	5.43	131.39	122.70
1	D	348	HIS	N-CA-CB	5.43	120.38	110.60
1	E	230	ARG	CA-C-O	-5.43	108.70	120.10
1	E	290	GLU	CA-C-N	5.43	129.15	117.20
1	E	367	VAL	CA-CB-CG1	5.43	119.05	110.90
1	A	545	ASN	CA-C-O	-5.43	108.70	120.10
1	C	471	ASP	N-CA-CB	5.43	120.37	110.60
1	D	501	PHE	CZ-CE2-CD2	-5.43	113.58	120.10
1	A	355	GLY	CA-C-O	-5.43	110.83	120.60
1	A	391	PHE	CE1-CZ-CE2	5.43	129.77	120.00
1	E	403	HIS	CA-C-N	-5.43	105.26	117.20
1	A	403	HIS	CA-C-N	-5.43	105.26	117.20
1	B	434	ILE	O-C-N	5.43	131.38	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	377	ASP	CA-C-O	-5.43	108.70	120.10
1	D	505	LEU	N-CA-CB	-5.43	99.55	110.40
1	E	441	GLU	CA-C-N	-5.43	105.26	117.20
1	E	581	ASN	CA-C-O	-5.43	108.70	120.10
1	C	403	HIS	CA-C-N	-5.42	105.26	117.20
1	C	581	ASN	CA-C-O	-5.42	108.71	120.10
1	C	593	THR	N-CA-CB	-5.42	99.99	110.30
1	D	355	GLY	CA-C-O	-5.42	110.84	120.60
1	D	403	HIS	CA-C-N	-5.42	105.27	117.20
1	D	471	ASP	N-CA-CB	5.42	120.36	110.60
1	E	333	TYR	N-CA-CB	-5.42	100.83	110.60
1	E	545	ASN	CA-C-O	-5.42	108.71	120.10
1	F	391	PHE	CE1-CZ-CE2	5.42	129.76	120.00
1	F	545	ASN	CA-C-O	-5.42	108.71	120.10
1	A	471	ASP	N-CA-CB	5.42	120.36	110.60
1	B	391	PHE	CE1-CZ-CE2	5.42	129.76	120.00
1	D	458	ASN	N-CA-CB	-5.42	100.84	110.60
1	D	580	PHE	O-C-N	-5.42	114.02	122.70
1	E	377	ASP	CA-C-O	-5.42	108.71	120.10
1	F	230	ARG	CA-C-O	-5.42	108.71	120.10
1	F	290	GLU	CA-C-N	5.42	129.13	117.20
1	A	348	HIS	N-CA-CB	5.42	120.36	110.60
1	A	417	ALA	CA-C-N	-5.42	105.27	117.20
1	A	441	GLU	CA-C-N	-5.42	105.27	117.20
1	B	593	THR	N-CA-CB	-5.42	100.00	110.30
1	F	183	TYR	CA-C-O	-5.42	108.72	120.10
1	A	367	VAL	CA-CB-CG1	5.42	119.03	110.90
1	A	581	ASN	CA-C-O	-5.42	108.72	120.10
1	C	367	VAL	CA-CB-CG1	5.42	119.03	110.90
1	A	230	ARG	CA-C-O	-5.42	108.72	120.10
1	A	377	ASP	CA-C-O	-5.42	108.72	120.10
1	C	291	ILE	N-CA-CB	5.42	123.26	110.80
1	D	230	ARG	CA-C-O	-5.42	108.72	120.10
1	D	579	GLU	CA-C-O	5.42	131.48	120.10
1	E	417	ALA	CA-C-N	-5.42	105.28	117.20
1	F	253	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	151	ILE	O-C-N	5.42	131.37	122.70
1	A	580	PHE	O-C-N	-5.42	114.03	122.70
1	B	367	VAL	CA-CB-CG1	5.42	119.02	110.90
1	B	474	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	C	340	TYR	CE1-CZ-CE2	5.42	128.47	119.80
1	D	367	VAL	CA-CB-CG1	5.42	119.02	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	441	GLU	CA-C-N	-5.42	105.28	117.20
1	E	183	TYR	CA-C-O	-5.42	108.73	120.10
1	E	361	PHE	O-C-N	5.42	131.37	122.70
1	E	580	PHE	O-C-N	-5.42	114.03	122.70
1	D	441	GLU	CA-CB-CG	-5.42	101.49	113.40
1	F	355	GLY	CA-C-O	-5.42	110.85	120.60
1	F	441	GLU	CA-CB-CG	-5.42	101.49	113.40
1	A	458	ASN	N-CA-CB	-5.41	100.86	110.60
1	B	230	ARG	CA-C-O	-5.41	108.73	120.10
1	B	471	ASP	N-CA-CB	5.41	120.34	110.60
1	B	545	ASN	CA-C-O	-5.41	108.73	120.10
1	C	73	SER	C-N-CA	5.41	135.23	121.70
1	C	580	PHE	O-C-N	-5.41	114.04	122.70
1	E	441	GLU	CA-CB-CG	-5.41	101.49	113.40
1	E	471	ASP	N-CA-CB	5.41	120.34	110.60
1	F	151	ILE	O-C-N	5.41	131.36	122.70
1	F	291	ILE	N-CA-CB	5.41	123.25	110.80
1	F	322	GLU	CA-C-O	-5.41	108.73	120.10
1	F	458	ASN	N-CA-CB	-5.41	100.86	110.60
1	A	340	TYR	CE1-CZ-CE2	5.41	128.46	119.80
1	B	580	PHE	O-C-N	-5.41	114.04	122.70
1	C	417	ALA	CA-C-N	-5.41	105.29	117.20
1	C	458	ASN	N-CA-CB	-5.41	100.86	110.60
1	D	391	PHE	CE1-CZ-CE2	5.41	129.74	120.00
1	E	151	ILE	O-C-N	5.41	131.36	122.70
1	E	596	HIS	CA-C-O	-5.41	108.73	120.10
1	F	580	PHE	O-C-N	-5.41	114.04	122.70
1	A	183	TYR	CA-C-O	-5.41	108.74	120.10
1	B	33	ILE	CA-C-O	5.41	131.46	120.10
1	B	441	GLU	CA-CB-CG	-5.41	101.50	113.40
1	C	377	ASP	CA-C-O	-5.41	108.74	120.10
1	D	358	HIS	CB-CA-C	5.41	121.22	110.40
1	A	291	ILE	N-CA-CB	5.41	123.24	110.80
1	A	441	GLU	CA-CB-CG	-5.41	101.50	113.40
1	C	348	HIS	N-CA-CB	5.41	120.33	110.60
1	C	361	PHE	CA-CB-CG	-5.41	100.92	113.90
1	E	371	PHE	CD1-CG-CD2	-5.41	111.27	118.30
1	E	593	THR	N-CA-CB	-5.41	100.03	110.30
1	F	371	PHE	CD1-CG-CD2	-5.41	111.27	118.30
1	A	73	SER	C-N-CA	5.41	135.22	121.70
1	B	371	PHE	CD1-CG-CD2	-5.41	111.27	118.30
1	D	417	ALA	CA-C-N	-5.41	105.30	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	253	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	A	474	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	C	474	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	D	340	TYR	CE1-CZ-CE2	5.41	128.45	119.80
1	E	458	ASN	N-CA-CB	-5.41	100.87	110.60
1	F	361	PHE	CA-CB-CG	-5.41	100.93	113.90
1	F	441	GLU	CA-C-N	-5.41	105.31	117.20
1	E	73	SER	C-N-CA	5.40	135.21	121.70
1	B	183	TYR	CA-C-O	-5.40	108.76	120.10
1	B	291	ILE	N-CA-CB	5.40	123.22	110.80
1	B	340	TYR	CE1-CZ-CE2	5.40	128.44	119.80
1	B	348	HIS	N-CA-CB	5.40	120.32	110.60
1	B	443	ILE	CA-C-N	5.40	129.09	117.20
1	D	322	GLU	CA-C-O	-5.40	108.75	120.10
1	F	289	LEU	CB-CA-C	5.40	120.46	110.20
1	F	377	ASP	CA-C-O	-5.40	108.75	120.10
1	A	33	ILE	CA-C-O	5.40	131.44	120.10
1	B	322	GLU	CA-C-O	-5.40	108.76	120.10
1	B	361	PHE	CA-CB-CG	-5.40	100.94	113.90
1	D	291	ILE	N-CA-CB	5.40	123.22	110.80
1	D	596	HIS	CA-C-O	-5.40	108.76	120.10
1	E	579	GLU	CA-C-O	5.40	131.44	120.10
1	F	73	SER	C-N-CA	5.40	135.20	121.70
1	C	33	ILE	CA-C-O	5.40	131.44	120.10
1	D	365	PRO	C-N-CA	-5.40	110.96	122.30
1	E	291	ILE	N-CA-CB	5.40	123.22	110.80
1	F	471	ASP	N-CA-CB	5.40	120.32	110.60
1	A	596	HIS	CA-C-O	-5.40	108.76	120.10
1	B	73	SER	C-N-CA	5.40	135.20	121.70
1	B	137	LEU	CB-CG-CD1	-5.40	101.83	111.00
1	B	579	GLU	CA-C-O	5.40	131.44	120.10
1	C	501	PHE	CZ-CE2-CD2	-5.40	113.62	120.10
1	D	371	PHE	CD1-CG-CD2	-5.40	111.28	118.30
1	F	64	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	F	512	VAL	CA-C-O	5.40	131.43	120.10
1	F	596	HIS	CA-C-O	-5.40	108.77	120.10
1	C	441	GLU	CA-C-N	-5.40	105.33	117.20
1	A	289	LEU	CB-CA-C	5.39	120.45	110.20
1	A	322	GLU	CA-C-O	-5.39	108.77	120.10
1	A	358	HIS	CB-CA-C	5.39	121.19	110.40
1	A	579	GLU	CA-C-O	5.39	131.43	120.10
1	B	358	HIS	CB-CA-C	5.39	121.19	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	365	PRO	C-N-CA	-5.39	110.97	122.30
1	B	596	HIS	CA-C-O	-5.39	108.77	120.10
1	C	441	GLU	CA-CB-CG	-5.39	101.53	113.40
1	C	596	HIS	CA-C-O	-5.39	108.77	120.10
1	D	183	TYR	CA-C-O	-5.39	108.77	120.10
1	F	137	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	B	458	ASN	N-CA-CB	-5.39	100.89	110.60
1	B	512	VAL	CA-C-O	5.39	131.42	120.10
1	C	512	VAL	CA-C-O	5.39	131.43	120.10
1	E	289	LEU	CB-CA-C	5.39	120.44	110.20
1	E	361	PHE	CA-CB-CG	-5.39	100.96	113.90
1	E	501	PHE	CZ-CE2-CD2	-5.39	113.63	120.10
1	A	361	PHE	CA-CB-CG	-5.39	100.96	113.90
1	A	512	VAL	CA-C-O	5.39	131.42	120.10
1	D	289	LEU	CB-CA-C	5.39	120.44	110.20
1	D	512	VAL	CA-C-O	5.39	131.42	120.10
1	E	33	ILE	CA-C-O	5.39	131.42	120.10
1	E	322	GLU	CA-C-O	-5.39	108.78	120.10
1	E	548	ASN	N-CA-C	-5.39	96.45	111.00
1	A	501	PHE	CZ-CE2-CD2	-5.39	113.64	120.10
1	A	548	ASN	N-CA-C	-5.39	96.45	111.00
1	D	33	ILE	CA-C-O	5.39	131.41	120.10
1	E	358	HIS	CB-CA-C	5.39	121.18	110.40
1	F	358	HIS	CB-CA-C	5.39	121.18	110.40
1	A	371	PHE	CD1-CG-CD2	-5.39	111.30	118.30
1	B	548	ASN	N-CA-C	-5.39	96.45	111.00
1	C	183	TYR	CA-C-O	-5.39	108.79	120.10
1	D	73	SER	C-N-CA	5.39	135.17	121.70
1	D	137	LEU	CB-CG-CD1	-5.39	101.84	111.00
1	F	416	VAL	CA-C-N	-5.39	105.35	117.20
1	F	548	ASN	N-CA-C	-5.39	96.46	111.00
1	A	64	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	66	LEU	CB-CG-CD2	5.38	120.15	111.00
1	B	407	GLU	CG-CD-OE2	5.38	129.07	118.30
1	C	416	VAL	CA-C-N	-5.38	105.35	117.20
1	D	162	LYS	N-CA-C	-5.38	96.46	111.00
1	D	548	ASN	N-CA-C	-5.38	96.46	111.00
1	F	33	ILE	CA-C-O	5.38	131.41	120.10
1	C	407	GLU	CG-CD-OE2	5.38	129.06	118.30
1	D	512	VAL	CB-CA-C	5.38	121.63	111.40
1	E	340	TYR	CE1-CZ-CE2	5.38	128.41	119.80
1	C	443	ILE	CA-C-N	5.38	129.04	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	548	ASN	N-CA-C	-5.38	96.47	111.00
1	D	361	PHE	CA-CB-CG	-5.38	100.98	113.90
1	E	443	ILE	CA-C-N	5.38	129.04	117.20
1	C	289	LEU	CB-CA-C	5.38	120.42	110.20
1	A	137	LEU	CB-CG-CD1	-5.38	101.86	111.00
1	A	407	GLU	CG-CD-OE2	5.38	129.06	118.30
1	A	443	ILE	CA-C-N	5.38	129.03	117.20
1	B	289	LEU	CB-CA-C	5.38	120.42	110.20
1	B	501	PHE	CZ-CE2-CD2	-5.38	113.64	120.10
1	C	137	LEU	CB-CG-CD1	-5.38	101.86	111.00
1	C	369	GLU	CA-C-O	-5.38	108.80	120.10
1	E	554	ASP	CA-C-N	-5.38	105.37	117.20
1	F	365	PRO	C-N-CA	-5.38	111.01	122.30
1	F	407	GLU	CG-CD-OE2	5.38	129.06	118.30
1	A	162	LYS	N-CA-C	-5.38	96.48	111.00
1	A	365	PRO	C-N-CA	-5.38	111.01	122.30
1	C	162	LYS	N-CA-C	-5.38	96.48	111.00
1	C	358	HIS	CB-CA-C	5.38	121.15	110.40
1	C	371	PHE	CD1-CG-CD2	-5.38	111.31	118.30
1	C	637	ASP	CA-C-N	5.38	126.95	116.20
1	E	40	LEU	CB-CA-C	5.38	120.42	110.20
1	D	637	ASP	CA-C-N	5.38	126.95	116.20
1	C	322	GLU	CA-C-O	-5.37	108.81	120.10
1	A	66	LEU	CB-CG-CD2	5.37	120.13	111.00
1	E	162	LYS	N-CA-C	-5.37	96.50	111.00
1	F	66	LEU	CB-CG-CD2	5.37	120.13	111.00
1	F	443	ILE	CA-C-N	5.37	129.02	117.20
1	F	579	GLU	CA-C-O	5.37	131.38	120.10
1	A	40	LEU	CB-CA-C	5.37	120.40	110.20
1	A	416	VAL	CA-C-N	-5.37	105.39	117.20
1	B	369	GLU	CA-C-O	-5.37	108.82	120.10
1	B	416	VAL	CA-C-N	-5.37	105.39	117.20
1	B	622	LEU	CA-CB-CG	5.37	127.65	115.30
1	C	365	PRO	C-N-CA	-5.37	111.02	122.30
1	D	66	LEU	CB-CG-CD2	5.37	120.13	111.00
1	D	369	GLU	CA-C-O	-5.37	108.82	120.10
1	D	474	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	E	407	GLU	CG-CD-OE2	5.37	129.04	118.30
1	F	61	ASN	CB-CG-ND2	5.37	129.59	116.70
1	C	386	TYR	CA-CB-CG	5.37	123.60	113.40
1	C	488	ASN	N-CA-C	-5.37	96.51	111.00
1	D	28	PRO	N-CD-CG	-5.37	95.15	103.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	LYS	N-CA-C	-5.37	96.52	111.00
1	C	554	ASP	CA-C-N	-5.37	105.40	117.20
1	D	554	ASP	CA-C-N	-5.37	105.39	117.20
1	E	137	LEU	CB-CG-CD1	-5.37	101.88	111.00
1	E	416	VAL	CA-C-N	-5.37	105.39	117.20
1	A	554	ASP	CA-C-N	-5.36	105.40	117.20
1	C	226	GLN	OE1-CD-NE2	5.36	134.24	121.90
1	C	579	GLU	CA-C-O	5.36	131.37	120.10
1	D	40	LEU	CB-CA-C	5.36	120.39	110.20
1	D	443	ILE	CA-C-N	5.36	129.00	117.20
1	E	512	VAL	CA-C-O	5.36	131.37	120.10
1	C	28	PRO	N-CD-CG	-5.36	95.16	103.20
1	F	162	LYS	N-CA-C	-5.36	96.52	111.00
1	C	40	LEU	CB-CA-C	5.36	120.39	110.20
1	C	256	PHE	CB-CG-CD1	5.36	124.55	120.80
1	D	416	VAL	CA-C-N	-5.36	105.41	117.20
1	E	181	VAL	O-C-N	-5.36	114.12	122.70
1	F	190	MET	C-N-CA	-5.36	108.30	121.70
1	F	488	ASN	N-CA-C	-5.36	96.53	111.00
1	A	488	ASN	N-CA-C	-5.36	96.53	111.00
1	B	64	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	C	61	ASN	CB-CG-ND2	5.36	129.56	116.70
1	A	61	ASN	CB-CG-ND2	5.36	129.56	116.70
1	A	369	GLU	CA-C-O	-5.36	108.85	120.10
1	A	637	ASP	CA-C-N	5.36	126.92	116.20
1	C	181	VAL	O-C-N	-5.36	114.13	122.70
1	E	365	PRO	C-N-CA	-5.36	111.05	122.30
1	E	429	PHE	C-N-CA	-5.36	108.31	121.70
1	F	40	LEU	CB-CA-C	5.36	120.38	110.20
1	A	28	PRO	N-CD-CG	-5.36	95.17	103.20
1	A	622	LEU	CA-CB-CG	5.36	127.62	115.30
1	C	190	MET	C-N-CA	-5.36	108.31	121.70
1	D	190	MET	C-N-CA	-5.36	108.31	121.70
1	D	444	GLU	N-CA-CB	5.36	120.24	110.60
1	D	488	ASN	N-CA-C	-5.36	96.54	111.00
1	E	190	MET	C-N-CA	-5.36	108.31	121.70
1	E	285	HIS	N-CA-CB	-5.36	100.96	110.60
1	F	256	PHE	CB-CG-CD1	5.36	124.55	120.80
1	F	429	PHE	C-N-CA	-5.36	108.31	121.70
1	B	190	MET	C-N-CA	-5.35	108.31	121.70
1	D	386	TYR	CA-CB-CG	5.35	123.57	113.40
1	A	190	MET	C-N-CA	-5.35	108.32	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	512	VAL	CB-CA-C	5.35	121.57	111.40
1	B	61	ASN	CB-CG-ND2	5.35	129.54	116.70
1	B	488	ASN	N-CA-C	-5.35	96.55	111.00
1	D	61	ASN	CB-CG-ND2	5.35	129.55	116.70
1	D	256	PHE	CB-CG-CD1	5.35	124.55	120.80
1	E	61	ASN	CB-CG-ND2	5.35	129.55	116.70
1	E	488	ASN	N-CA-C	-5.35	96.55	111.00
1	F	554	ASP	CA-C-N	-5.35	105.42	117.20
1	F	622	LEU	CA-CB-CG	5.35	127.61	115.30
1	C	66	LEU	CB-CG-CD2	5.35	120.10	111.00
1	E	369	GLU	CA-C-O	-5.35	108.86	120.10
1	F	637	ASP	CA-C-N	5.35	126.90	116.20
1	A	431	TYR	CG-CD2-CE2	-5.35	117.02	121.30
1	B	444	GLU	N-CA-CB	5.35	120.23	110.60
1	B	554	ASP	CA-C-N	-5.35	105.43	117.20
1	D	181	VAL	O-C-N	-5.35	114.14	122.70
1	D	285	HIS	N-CA-CB	-5.35	100.97	110.60
1	D	622	LEU	CA-CB-CG	5.35	127.61	115.30
1	E	512	VAL	CB-CA-C	5.35	121.56	111.40
1	E	622	LEU	CA-CB-CG	5.35	127.60	115.30
1	F	501	PHE	CZ-CE2-CD2	-5.35	113.68	120.10
1	A	95	GLU	CB-CG-CD	5.35	128.64	114.20
1	A	256	PHE	CB-CG-CD1	5.35	124.54	120.80
1	A	429	PHE	C-N-CA	-5.35	108.33	121.70
1	B	285	HIS	N-CA-CB	-5.35	100.97	110.60
1	B	429	PHE	C-N-CA	-5.35	108.33	121.70
1	C	512	VAL	CB-CA-C	5.35	121.56	111.40
1	C	536	PHE	N-CA-CB	5.35	120.23	110.60
1	C	573	SER	CA-CB-OG	-5.35	96.76	111.20
1	D	226	GLN	OE1-CD-NE2	5.35	134.20	121.90
1	D	407	GLU	CG-CD-OE2	5.35	128.99	118.30
1	E	66	LEU	CB-CG-CD2	5.35	120.09	111.00
1	E	238	ASN	CB-CG-ND2	5.35	129.54	116.70
1	F	512	VAL	CB-CA-C	5.35	121.56	111.40
1	F	573	SER	CA-CB-OG	-5.35	96.76	111.20
1	D	429	PHE	C-N-CA	-5.35	108.33	121.70
1	E	95	GLU	CB-CG-CD	5.35	128.63	114.20
1	E	637	ASP	CA-C-N	5.35	126.89	116.20
1	F	181	VAL	O-C-N	-5.35	114.15	122.70
1	B	512	VAL	CB-CA-C	5.34	121.56	111.40
1	C	95	GLU	CB-CG-CD	5.34	128.63	114.20
1	D	95	GLU	CB-CG-CD	5.34	128.63	114.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	28	PRO	N-CD-CG	-5.34	95.18	103.20
1	F	28	PRO	N-CD-CG	-5.34	95.18	103.20
1	F	95	GLU	CB-CG-CD	5.34	128.63	114.20
1	F	285	HIS	N-CA-CB	-5.34	100.98	110.60
1	A	181	VAL	O-C-N	-5.34	114.15	122.70
1	B	28	PRO	N-CD-CG	-5.34	95.19	103.20
1	B	40	LEU	CB-CA-C	5.34	120.35	110.20
1	B	386	TYR	CA-CB-CG	5.34	123.55	113.40
1	E	184	PHE	CB-CG-CD2	-5.34	117.06	120.80
1	A	285	HIS	N-CA-CB	-5.34	100.98	110.60
1	C	622	LEU	CA-CB-CG	5.34	127.59	115.30
1	D	451	ARG	CA-CB-CG	5.34	125.15	113.40
1	D	573	SER	CA-CB-OG	-5.34	96.78	111.20
1	E	451	ARG	CA-CB-CG	5.34	125.15	113.40
1	E	573	SER	CA-CB-OG	-5.34	96.78	111.20
1	F	431	TYR	CG-CD2-CE2	-5.34	117.03	121.30
1	A	573	SER	CA-CB-OG	-5.34	96.78	111.20
1	C	429	PHE	C-N-CA	-5.34	108.35	121.70
1	E	386	TYR	CA-CB-CG	5.34	123.54	113.40
1	E	536	PHE	N-CA-CB	5.34	120.21	110.60
1	A	451	ARG	CA-CB-CG	5.34	125.14	113.40
1	B	95	GLU	CB-CG-CD	5.34	128.61	114.20
1	E	431	TYR	CG-CD2-CE2	-5.34	117.03	121.30
1	F	451	ARG	CA-CB-CG	5.34	125.14	113.40
1	A	226	GLN	OE1-CD-NE2	5.34	134.17	121.90
1	B	246	LEU	N-CA-CB	-5.33	99.73	110.40
1	B	573	SER	CA-CB-OG	-5.33	96.80	111.20
1	E	246	LEU	N-CA-CB	-5.33	99.73	110.40
1	A	386	TYR	CA-CB-CG	5.33	123.53	113.40
1	B	451	ARG	CA-CB-CG	5.33	125.13	113.40
1	B	536	PHE	N-CA-CB	5.33	120.20	110.60
1	D	224	HIS	CA-C-O	5.33	131.30	120.10
1	D	431	TYR	CG-CD2-CE2	-5.33	117.03	121.30
1	F	369	GLU	CA-C-O	-5.33	108.90	120.10
1	F	444	GLU	N-CA-CB	5.33	120.20	110.60
1	A	444	GLU	N-CA-CB	5.33	120.19	110.60
1	D	246	LEU	N-CA-CB	-5.33	99.74	110.40
1	E	265	GLY	O-C-N	-5.33	114.14	123.20
1	A	146	THR	OG1-CB-CG2	5.33	122.25	110.00
1	A	184	PHE	CB-CG-CD2	-5.33	117.07	120.80
1	A	246	LEU	N-CA-CB	-5.33	99.74	110.40
1	B	181	VAL	O-C-N	-5.33	114.17	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	184	PHE	CB-CG-CD2	-5.33	117.07	120.80
1	C	238	ASN	CB-CG-ND2	5.33	129.49	116.70
1	D	146	THR	OG1-CB-CG2	5.33	122.25	110.00
1	B	256	PHE	CB-CG-CD1	5.33	124.53	120.80
1	A	238	ASN	CB-CG-ND2	5.33	129.48	116.70
1	B	184	PHE	CB-CG-CD2	-5.33	117.07	120.80
1	B	411	MET	N-CA-CB	-5.33	101.01	110.60
1	C	285	HIS	N-CA-CB	-5.33	101.01	110.60
1	F	411	MET	N-CA-CB	-5.33	101.02	110.60
1	B	226	GLN	OE1-CD-NE2	5.32	134.14	121.90
1	B	431	TYR	CG-CD2-CE2	-5.32	117.04	121.30
1	B	637	ASP	CA-C-N	5.32	126.85	116.20
1	C	18	LEU	CA-C-O	-5.32	108.92	120.10
1	C	224	HIS	CA-C-O	5.32	131.28	120.10
1	C	246	LEU	N-CA-CB	-5.32	99.75	110.40
1	C	451	ARG	CA-CB-CG	5.32	125.11	113.40
1	D	265	GLY	O-C-N	-5.32	114.15	123.20
1	F	226	GLN	OE1-CD-NE2	5.32	134.15	121.90
1	F	238	ASN	CB-CG-ND2	5.32	129.48	116.70
1	F	386	TYR	CA-CB-CG	5.32	123.52	113.40
1	A	536	PHE	N-CA-CB	5.32	120.18	110.60
1	C	444	GLU	N-CA-CB	5.32	120.18	110.60
1	D	536	PHE	N-CA-CB	5.32	120.18	110.60
1	E	224	HIS	CA-C-O	5.32	131.28	120.10
1	B	231	PHE	CE1-CZ-CE2	-5.32	110.42	120.00
1	C	117	TYR	CA-CB-CG	5.32	123.51	113.40
1	C	265	GLY	O-C-N	-5.32	114.16	123.20
1	D	411	MET	N-CA-CB	-5.32	101.02	110.60
1	E	256	PHE	CB-CG-CD1	5.32	124.53	120.80
1	F	146	THR	OG1-CB-CG2	5.32	122.24	110.00
1	A	265	GLY	O-C-N	-5.32	114.16	123.20
1	B	18	LEU	CA-C-O	-5.32	108.93	120.10
1	B	238	ASN	CB-CG-ND2	5.32	129.46	116.70
1	C	431	TYR	CG-CD2-CE2	-5.32	117.05	121.30
1	E	444	GLU	N-CA-CB	5.32	120.17	110.60
1	F	307	ASP	C-N-CA	5.32	135.00	121.70
1	A	231	PHE	CE1-CZ-CE2	-5.32	110.43	120.00
1	B	307	ASP	C-N-CA	5.32	134.99	121.70
1	E	146	THR	OG1-CB-CG2	5.32	122.23	110.00
1	E	226	GLN	OE1-CD-NE2	5.32	134.13	121.90
1	B	146	THR	OG1-CB-CG2	5.31	122.22	110.00
1	D	117	TYR	CA-CB-CG	5.31	123.50	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	262	TYR	CD1-CG-CD2	-5.31	112.06	117.90
1	C	231	PHE	CE1-CZ-CE2	-5.31	110.44	120.00
1	D	18	LEU	CA-C-O	-5.31	108.94	120.10
1	D	307	ASP	C-N-CA	5.31	134.98	121.70
1	E	18	LEU	CA-C-O	-5.31	108.95	120.10
1	F	147	ASN	CA-CB-CG	-5.31	101.71	113.40
1	A	117	TYR	CA-CB-CG	5.31	123.49	113.40
1	A	224	HIS	CA-C-O	5.31	131.25	120.10
1	B	632	ASP	CA-C-O	-5.31	108.95	120.10
1	C	197	TRP	N-CA-CB	5.31	120.16	110.60
1	D	238	ASN	CB-CG-ND2	5.31	129.44	116.70
1	F	246	LEU	N-CA-CB	-5.31	99.78	110.40
1	F	536	PHE	N-CA-CB	5.31	120.16	110.60
1	F	566	ASP	C-N-CA	-5.31	108.43	121.70
1	A	18	LEU	CA-C-O	-5.31	108.95	120.10
1	A	411	MET	N-CA-CB	-5.31	101.05	110.60
1	B	117	TYR	CA-CB-CG	5.31	123.48	113.40
1	E	147	ASN	CA-CB-CG	-5.31	101.72	113.40
1	E	411	MET	N-CA-CB	-5.31	101.05	110.60
1	F	249	ASP	CA-C-O	-5.31	108.95	120.10
1	B	177	ARG	CG-CD-NE	-5.31	100.66	111.80
1	C	146	THR	OG1-CB-CG2	5.31	122.20	110.00
1	D	64	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	D	471	ASP	C-N-CA	-5.31	111.16	122.30
1	E	350	MET	O-C-N	5.31	131.19	122.70
1	E	566	ASP	C-N-CA	-5.31	108.44	121.70
1	A	147	ASN	CA-CB-CG	-5.30	101.73	113.40
1	A	307	ASP	C-N-CA	5.30	134.96	121.70
1	F	177	ARG	CG-CD-NE	-5.30	100.66	111.80
1	F	184	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	F	231	PHE	CE1-CZ-CE2	-5.30	110.45	120.00
1	F	265	GLY	O-C-N	-5.30	114.18	123.20
1	B	224	HIS	CA-C-O	5.30	131.24	120.10
1	B	265	GLY	O-C-N	-5.30	114.19	123.20
1	C	147	ASN	CA-CB-CG	-5.30	101.74	113.40
1	D	249	ASP	CA-C-O	-5.30	108.97	120.10
1	D	457	HIS	CA-C-O	-5.30	108.97	120.10
1	F	18	LEU	CA-C-O	-5.30	108.97	120.10
1	F	117	TYR	CA-CB-CG	5.30	123.47	113.40
1	F	632	ASP	CA-C-O	-5.30	108.97	120.10
1	A	197	TRP	N-CA-CB	5.30	120.14	110.60
1	C	249	ASP	CA-C-O	-5.30	108.97	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	117	TYR	CA-CB-CG	5.30	123.47	113.40
1	E	197	TRP	N-CA-CB	5.30	120.14	110.60
1	A	566	ASP	C-N-CA	-5.30	108.45	121.70
1	B	147	ASN	CA-CB-CG	-5.30	101.74	113.40
1	D	566	ASP	C-N-CA	-5.30	108.45	121.70
1	E	231	PHE	CE1-CZ-CE2	-5.30	110.46	120.00
1	E	561	SER	C-N-CA	5.30	134.94	121.70
1	B	249	ASP	CA-C-O	-5.29	108.98	120.10
1	C	471	ASP	C-N-CA	-5.29	111.18	122.30
1	A	350	MET	O-C-N	5.29	131.17	122.70
1	B	471	ASP	C-N-CA	-5.29	111.18	122.30
1	B	566	ASP	C-N-CA	-5.29	108.47	121.70
1	B	635	VAL	CB-CA-C	-5.29	101.34	111.40
1	C	177	ARG	CG-CD-NE	-5.29	100.68	111.80
1	C	284	ALA	O-C-N	5.29	131.17	122.70
1	C	307	ASP	C-N-CA	5.29	134.94	121.70
1	D	184	PHE	CB-CG-CD2	-5.29	117.09	120.80
1	D	231	PHE	CE1-CZ-CE2	-5.29	110.47	120.00
1	F	197	TRP	N-CA-CB	5.29	120.13	110.60
1	A	177	ARG	CG-CD-NE	-5.29	100.69	111.80
1	A	249	ASP	CA-C-O	-5.29	108.99	120.10
1	E	471	ASP	C-N-CA	-5.29	111.19	122.30
1	F	224	HIS	CA-C-O	5.29	131.21	120.10
1	D	197	TRP	N-CA-CB	5.29	120.12	110.60
1	D	284	ALA	O-C-N	5.29	131.16	122.70
1	D	350	MET	O-C-N	5.29	131.16	122.70
1	F	471	ASP	C-N-CA	-5.29	111.19	122.30
1	A	284	ALA	O-C-N	5.29	131.16	122.70
1	B	197	TRP	N-CA-CB	5.29	120.12	110.60
1	E	64	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	E	177	ARG	CG-CD-NE	-5.29	100.69	111.80
1	F	489	ASN	CB-CG-OD1	-5.29	111.03	121.60
1	B	506	ASP	O-C-N	5.29	131.16	122.70
1	C	561	SER	C-N-CA	5.29	134.92	121.70
1	D	632	ASP	CA-C-O	-5.29	109.00	120.10
1	A	632	ASP	CA-C-O	-5.29	109.00	120.10
1	B	262	TYR	CD1-CG-CD2	-5.29	112.09	117.90
1	B	350	MET	O-C-N	5.28	131.15	122.70
1	C	632	ASP	CA-C-O	-5.28	109.00	120.10
1	D	177	ARG	CG-CD-NE	-5.28	100.71	111.80
1	E	248	TRP	CB-CG-CD2	5.28	133.47	126.60
1	E	307	ASP	C-N-CA	5.28	134.91	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	635	VAL	CB-CA-C	-5.28	101.36	111.40
1	A	471	ASP	C-N-CA	-5.28	111.21	122.30
1	B	457	HIS	CA-C-O	-5.28	109.01	120.10
1	C	350	MET	O-C-N	5.28	131.15	122.70
1	C	457	HIS	CA-C-O	-5.28	109.01	120.10
1	C	566	ASP	C-N-CA	-5.28	108.50	121.70
1	D	147	ASN	CA-CB-CG	-5.28	101.78	113.40
1	E	632	ASP	CA-C-O	-5.28	109.01	120.10
1	F	284	ALA	O-C-N	5.28	131.15	122.70
1	A	262	TYR	CD1-CG-CD2	-5.28	112.09	117.90
1	A	457	HIS	CA-C-O	-5.28	109.02	120.10
1	B	561	SER	C-N-CA	5.28	134.89	121.70
1	A	561	SER	C-N-CA	5.28	134.89	121.70
1	C	411	MET	N-CA-CB	-5.27	101.11	110.60
1	E	249	ASP	CA-C-O	-5.27	109.03	120.10
1	F	248	TRP	CB-CG-CD2	5.27	133.46	126.60
1	A	248	TRP	CB-CG-CD2	5.27	133.45	126.60
1	C	57	MET	O-C-N	5.27	131.14	122.70
1	F	350	MET	O-C-N	5.27	131.13	122.70
1	C	248	TRP	CB-CG-CD2	5.27	133.45	126.60
1	C	526	SER	CB-CA-C	-5.27	100.09	110.10
1	E	474	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	F	506	ASP	O-C-N	5.27	131.13	122.70
1	A	635	VAL	CB-CA-C	-5.27	101.39	111.40
1	B	284	ALA	O-C-N	5.27	131.13	122.70
1	D	262	TYR	CD1-CG-CD2	-5.27	112.11	117.90
1	E	384	HIS	CA-C-O	-5.27	109.04	120.10
1	F	57	MET	O-C-N	5.27	131.13	122.70
1	C	384	HIS	CA-C-O	-5.27	109.04	120.10
1	D	436	ALA	O-C-N	5.26	131.12	122.70
1	D	489	ASN	CB-CG-OD1	-5.26	111.07	121.60
1	D	561	SER	C-N-CA	5.26	134.86	121.70
1	E	436	ALA	O-C-N	5.26	131.12	122.70
1	E	526	SER	CB-CA-C	-5.26	100.10	110.10
1	F	457	HIS	CA-C-O	-5.26	109.05	120.10
1	A	506	ASP	O-C-N	5.26	131.12	122.70
1	D	304	TYR	CG-CD1-CE1	-5.26	117.09	121.30
1	E	306	THR	CA-C-O	-5.26	109.05	120.10
1	C	635	VAL	CB-CA-C	-5.26	101.41	111.40
1	E	57	MET	O-C-N	5.26	131.12	122.70
1	F	384	HIS	CA-C-O	-5.26	109.05	120.10
1	F	629	ARG	NH1-CZ-NH2	-5.26	113.61	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	HIS	CA-C-O	-5.26	109.06	120.10
1	B	306	THR	CA-C-O	-5.26	109.06	120.10
1	C	489	ASN	CB-CG-OD1	-5.26	111.08	121.60
1	A	526	SER	CB-CA-C	-5.26	100.11	110.10
1	B	57	MET	O-C-N	5.26	131.11	122.70
1	B	428	GLU	CG-CD-OE2	-5.26	107.79	118.30
1	D	57	MET	O-C-N	5.26	131.11	122.70
1	D	376	ARG	O-C-N	5.26	131.11	122.70
1	D	384	HIS	CA-C-O	-5.26	109.06	120.10
1	E	457	HIS	CA-C-O	-5.26	109.06	120.10
1	F	526	SER	CB-CA-C	-5.26	100.11	110.10
1	F	561	SER	C-N-CA	5.26	134.84	121.70
1	A	436	ALA	O-C-N	5.25	131.11	122.70
1	E	506	ASP	O-C-N	5.25	131.11	122.70
1	F	428	GLU	CG-CD-OE2	-5.25	107.79	118.30
1	A	216	LYS	CD-CE-NZ	-5.25	99.62	111.70
1	A	306	THR	CA-C-O	-5.25	109.07	120.10
1	A	428	GLU	CG-CD-OE2	-5.25	107.79	118.30
1	C	428	GLU	CG-CD-OE2	-5.25	107.79	118.30
1	C	436	ALA	O-C-N	5.25	131.11	122.70
1	C	525	ASP	CA-C-O	-5.25	109.07	120.10
1	F	216	LYS	CD-CE-NZ	-5.25	99.62	111.70
1	A	57	MET	O-C-N	5.25	131.10	122.70
1	A	489	ASN	CB-CG-OD1	-5.25	111.10	121.60
1	B	248	TRP	CB-CG-CD2	5.25	133.43	126.60
1	D	248	TRP	CB-CG-CD2	5.25	133.43	126.60
1	E	428	GLU	CG-CD-OE2	-5.25	107.80	118.30
1	C	575	PRO	O-C-N	-5.25	114.30	122.70
1	E	216	LYS	CD-CE-NZ	-5.25	99.63	111.70
1	B	436	ALA	O-C-N	5.25	131.10	122.70
1	D	506	ASP	O-C-N	5.25	131.10	122.70
1	D	635	VAL	CB-CA-C	-5.25	101.43	111.40
1	E	284	ALA	O-C-N	5.25	131.10	122.70
1	E	629	ARG	NH1-CZ-NH2	-5.25	113.63	119.40
1	B	69	ARG	CG-CD-NE	5.25	122.82	111.80
1	B	526	SER	CB-CA-C	-5.25	100.13	110.10
1	B	575	PRO	O-C-N	-5.25	114.31	122.70
1	D	119	LEU	CB-CA-C	5.25	120.17	110.20
1	D	216	LYS	CD-CE-NZ	-5.25	99.63	111.70
1	F	119	LEU	CB-CA-C	5.25	120.17	110.20
1	B	489	ASN	CB-CG-OD1	-5.25	111.11	121.60
1	C	119	LEU	CB-CA-C	5.25	120.17	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	187	ASP	CB-CG-OD2	5.25	123.02	118.30
1	D	526	SER	CB-CA-C	-5.25	100.13	110.10
1	B	216	LYS	CD-CE-NZ	-5.24	99.64	111.70
1	C	216	LYS	CD-CE-NZ	-5.24	99.64	111.70
1	E	635	VAL	CB-CA-C	-5.24	101.44	111.40
1	A	575	PRO	O-C-N	-5.24	114.31	122.70
1	C	643	LYS	CB-CG-CD	5.24	125.23	111.60
1	D	306	THR	CA-C-O	-5.24	109.09	120.10
1	F	262	TYR	CD1-CG-CD2	-5.24	112.13	117.90
1	A	376	ARG	O-C-N	5.24	131.08	122.70
1	A	525	ASP	CA-C-O	-5.24	109.09	120.10
1	C	262	TYR	CD1-CG-CD2	-5.24	112.14	117.90
1	D	525	ASP	CA-C-O	-5.24	109.10	120.10
1	F	304	TYR	CG-CD1-CE1	-5.24	117.11	121.30
1	A	69	ARG	CG-CD-NE	5.24	122.80	111.80
1	B	467	SER	N-CA-C	5.24	125.14	111.00
1	D	428	GLU	CG-CD-OE2	-5.24	107.82	118.30
1	F	525	ASP	CA-C-O	-5.24	109.10	120.10
1	C	306	THR	CA-C-O	-5.24	109.10	120.10
1	A	119	LEU	CB-CA-C	5.24	120.15	110.20
1	A	643	LYS	CB-CG-CD	5.24	125.21	111.60
1	B	384	HIS	CA-C-O	-5.24	109.10	120.10
1	B	643	LYS	CB-CG-CD	5.24	125.21	111.60
1	E	489	ASN	CB-CG-OD1	-5.24	111.13	121.60
1	F	436	ALA	O-C-N	5.24	131.08	122.70
1	F	643	LYS	CB-CG-CD	5.24	125.21	111.60
1	E	643	LYS	CB-CG-CD	5.23	125.21	111.60
1	F	306	THR	CA-C-O	-5.23	109.11	120.10
1	B	119	LEU	CB-CA-C	5.23	120.14	110.20
1	E	376	ARG	O-C-N	5.23	131.07	122.70
1	E	525	ASP	CA-C-O	-5.23	109.11	120.10
1	B	455	LEU	CB-CA-C	-5.23	100.26	110.20
1	C	345	ASN	CB-CG-ND2	-5.23	104.15	116.70
1	E	69	ARG	CG-CD-NE	5.23	122.78	111.80
1	F	69	ARG	CG-CD-NE	5.23	122.78	111.80
1	C	304	TYR	CG-CD1-CE1	-5.23	117.12	121.30
1	B	304	TYR	CG-CD1-CE1	-5.23	117.12	121.30
1	B	395	THR	C-N-CA	5.23	134.77	121.70
1	D	69	ARG	CG-CD-NE	5.23	122.78	111.80
1	E	578	MET	N-CA-CB	5.23	120.01	110.60
1	F	288	ASP	OD1-CG-OD2	5.23	133.23	123.30
1	F	470	ASN	O-C-N	5.23	131.06	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	MET	O-C-N	5.23	131.06	122.70
1	C	578	MET	N-CA-CB	5.23	120.01	110.60
1	F	575	PRO	O-C-N	-5.23	114.34	122.70
1	F	578	MET	N-CA-CB	5.23	120.01	110.60
1	A	304	TYR	CG-CD1-CE1	-5.22	117.12	121.30
1	D	643	LYS	CB-CG-CD	5.22	125.19	111.60
1	F	376	ARG	O-C-N	5.22	131.06	122.70
1	F	395	THR	C-N-CA	5.22	134.76	121.70
1	F	405	ASN	O-C-N	5.22	131.06	122.70
1	D	199	MET	O-C-N	5.22	131.06	122.70
1	E	187	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	448	ILE	O-C-N	5.22	131.05	122.70
1	A	578	MET	N-CA-CB	5.22	120.00	110.60
1	C	506	ASP	O-C-N	5.22	131.05	122.70
1	A	629	ARG	NH1-CZ-NH2	-5.22	113.66	119.40
1	B	345	ASN	CB-CG-ND2	-5.22	104.17	116.70
1	D	345	ASN	CB-CG-ND2	-5.22	104.17	116.70
1	D	575	PRO	O-C-N	-5.22	114.35	122.70
1	E	288	ASP	OD1-CG-OD2	5.22	133.22	123.30
1	E	455	LEU	CB-CA-C	-5.22	100.28	110.20
1	E	575	PRO	O-C-N	-5.22	114.35	122.70
1	A	199	MET	O-C-N	5.22	131.05	122.70
1	A	455	LEU	CB-CA-C	-5.22	100.29	110.20
1	B	376	ARG	O-C-N	5.22	131.05	122.70
1	D	448	ILE	O-C-N	5.22	131.05	122.70
1	E	119	LEU	CB-CA-C	5.22	120.11	110.20
1	E	448	ILE	O-C-N	5.22	131.05	122.70
1	F	511	LYS	CA-C-O	5.22	131.05	120.10
1	A	288	ASP	OD1-CG-OD2	5.21	133.21	123.30
1	A	467	SER	N-CA-C	5.21	125.08	111.00
1	B	525	ASP	CA-C-O	-5.21	109.15	120.10
1	B	629	ARG	NH1-CZ-NH2	-5.21	113.67	119.40
1	C	455	LEU	CB-CA-C	-5.21	100.29	110.20
1	F	345	ASN	CB-CG-ND2	-5.21	104.18	116.70
1	F	467	SER	N-CA-C	5.21	125.08	111.00
1	C	69	ARG	CG-CD-NE	5.21	122.75	111.80
1	A	345	ASN	CB-CG-ND2	-5.21	104.19	116.70
1	A	511	LYS	CA-C-O	5.21	131.04	120.10
1	E	304	TYR	CG-CD1-CE1	-5.21	117.13	121.30
1	F	448	ILE	O-C-N	5.21	131.04	122.70
1	C	288	ASP	OD1-CG-OD2	5.21	133.20	123.30
1	D	467	SER	N-CA-C	5.21	125.07	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	455	LEU	CB-CA-C	-5.21	100.30	110.20
1	C	467	SER	N-CA-C	5.21	125.06	111.00
1	C	629	ARG	NH1-CZ-NH2	-5.21	113.67	119.40
1	D	578	MET	N-CA-CB	5.21	119.98	110.60
1	E	345	ASN	CB-CG-ND2	-5.21	104.20	116.70
1	F	199	MET	O-C-N	5.21	131.03	122.70
1	D	46	TYR	CB-CG-CD1	5.21	124.12	121.00
1	F	161	GLN	CG-CD-OE1	-5.21	111.19	121.60
1	C	161	GLN	CG-CD-OE1	-5.21	111.19	121.60
1	D	178	GLU	CA-CB-CG	5.21	124.85	113.40
1	B	289	LEU	O-C-N	5.20	131.03	122.70
1	B	511	LYS	CA-C-O	5.20	131.03	120.10
1	C	395	THR	C-N-CA	5.20	134.71	121.70
1	D	288	ASP	OD1-CG-OD2	5.20	133.19	123.30
1	D	455	LEU	CB-CA-C	-5.20	100.31	110.20
1	E	199	MET	O-C-N	5.20	131.03	122.70
1	E	391	PHE	CD1-CE1-CZ	-5.20	113.86	120.10
1	E	511	LYS	CA-C-O	5.20	131.03	120.10
1	F	19	ASP	CB-CG-OD2	5.20	122.98	118.30
1	E	467	SER	N-CA-C	5.20	125.05	111.00
1	A	395	THR	C-N-CA	5.20	134.70	121.70
1	A	470	ASN	O-C-N	5.20	131.02	122.70
1	B	161	GLN	CG-CD-OE1	-5.20	111.20	121.60
1	B	178	GLU	CA-CB-CG	5.20	124.84	113.40
1	C	199	MET	O-C-N	5.20	131.02	122.70
1	C	511	LYS	CA-C-O	5.20	131.02	120.10
1	D	470	ASN	O-C-N	5.20	131.02	122.70
1	E	395	THR	C-N-CA	5.20	134.70	121.70
1	B	622	LEU	N-CA-CB	-5.20	100.00	110.40
1	D	511	LYS	CA-C-O	5.20	131.02	120.10
1	F	178	GLU	CA-CB-CG	5.20	124.83	113.40
1	A	405	ASN	O-C-N	5.20	131.02	122.70
1	B	578	MET	N-CA-CB	5.20	119.95	110.60
1	C	405	ASN	O-C-N	5.20	131.01	122.70
1	D	395	THR	C-N-CA	5.20	134.69	121.70
1	F	289	LEU	O-C-N	5.20	131.01	122.70
1	A	161	GLN	CG-CD-OE1	-5.19	111.22	121.60
1	B	405	ASN	O-C-N	5.19	131.01	122.70
1	C	289	LEU	O-C-N	5.19	131.01	122.70
1	C	617	PRO	N-CA-C	5.19	125.60	112.10
1	E	617	PRO	N-CA-C	5.19	125.60	112.10
1	F	391	PHE	CD1-CE1-CZ	-5.19	113.87	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	617	PRO	N-CA-C	5.19	125.60	112.10
1	A	178	GLU	CA-CB-CG	5.19	124.82	113.40
1	B	391	PHE	CD1-CE1-CZ	-5.19	113.87	120.10
1	B	470	ASN	O-C-N	5.19	131.01	122.70
1	D	69	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
1	D	617	PRO	N-CA-C	5.19	125.59	112.10
1	B	288	ASP	OD1-CG-OD2	5.19	133.16	123.30
1	C	376	ARG	O-C-N	5.19	131.00	122.70
1	E	622	LEU	N-CA-CB	-5.19	100.02	110.40
1	B	439	SER	N-CA-C	-5.19	97.00	111.00
1	E	178	GLU	CA-CB-CG	5.19	124.81	113.40
1	B	617	PRO	N-CA-C	5.19	125.58	112.10
1	C	435	ASN	CA-CB-CG	5.18	124.81	113.40
1	D	19	ASP	CB-CG-OD2	5.18	122.97	118.30
1	E	470	ASN	O-C-N	5.18	131.00	122.70
1	E	405	ASN	O-C-N	5.18	130.99	122.70
1	A	19	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	622	LEU	N-CA-CB	-5.18	100.04	110.40
1	D	305	ILE	N-CA-C	-5.18	97.01	111.00
1	F	257	ALA	N-CA-C	-5.18	97.01	111.00
1	A	617	PRO	N-CA-C	5.18	125.57	112.10
1	B	448	ILE	O-C-N	5.18	130.99	122.70
1	B	636	ILE	CB-CA-C	5.18	121.96	111.60
1	D	405	ASN	O-C-N	5.18	130.99	122.70
1	D	629	ARG	NH1-CZ-NH2	-5.18	113.70	119.40
1	C	271	ARG	NH1-CZ-NH2	-5.18	113.70	119.40
1	C	448	ILE	O-C-N	5.18	130.99	122.70
1	E	439	SER	N-CA-C	-5.18	97.02	111.00
1	A	523	SER	CB-CA-C	-5.18	100.26	110.10
1	C	305	ILE	N-CA-C	-5.18	97.03	111.00
1	C	523	SER	CB-CA-C	-5.18	100.27	110.10
1	C	622	LEU	N-CA-CB	-5.18	100.05	110.40
1	D	523	SER	CB-CA-C	-5.18	100.26	110.10
1	D	622	LEU	N-CA-CB	-5.18	100.05	110.40
1	A	439	SER	N-CA-C	-5.17	97.03	111.00
1	B	523	SER	CB-CA-C	-5.17	100.27	110.10
1	C	178	GLU	CA-CB-CG	5.17	124.78	113.40
1	D	248	TRP	N-CA-CB	5.17	119.91	110.60
1	D	482	LEU	O-C-N	5.17	130.98	122.70
1	E	69	ARG	NH1-CZ-NH2	-5.17	113.71	119.40
1	E	161	GLN	CG-CD-OE1	-5.17	111.25	121.60
1	F	528	VAL	O-C-N	5.17	130.98	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	439	SER	N-CA-C	-5.17	97.03	111.00
1	A	187	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	69	ARG	NH1-CZ-NH2	-5.17	113.71	119.40
1	D	161	GLN	CG-CD-OE1	-5.17	111.25	121.60
1	D	177	ARG	NH1-CZ-NH2	-5.17	113.71	119.40
1	D	289	LEU	O-C-N	5.17	130.97	122.70
1	D	528	VAL	O-C-N	5.17	130.97	122.70
1	E	305	ILE	N-CA-C	-5.17	97.03	111.00
1	E	584	VAL	N-CA-C	-5.17	97.04	111.00
1	F	69	ARG	NH1-CZ-NH2	-5.17	113.71	119.40
1	A	391	PHE	CD1-CE1-CZ	-5.17	113.90	120.10
1	C	470	ASN	O-C-N	5.17	130.97	122.70
1	D	436	ALA	CA-C-O	-5.17	109.24	120.10
1	E	523	SER	CB-CA-C	-5.17	100.28	110.10
1	F	584	VAL	N-CA-C	-5.17	97.04	111.00
1	A	636	ILE	CB-CA-C	5.17	121.94	111.60
1	B	435	ASN	CA-CB-CG	5.17	124.77	113.40
1	C	19	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	248	TRP	N-CA-CB	5.17	119.90	110.60
1	D	187	ASP	CB-CG-OD2	5.17	122.95	118.30
1	D	435	ASN	CA-CB-CG	5.17	124.77	113.40
1	F	523	SER	CB-CA-C	-5.17	100.28	110.10
1	A	69	ARG	NH1-CZ-NH2	-5.17	113.72	119.40
1	A	289	LEU	O-C-N	5.17	130.97	122.70
1	B	528	VAL	O-C-N	5.17	130.97	122.70
1	D	584	VAL	N-CA-C	-5.17	97.05	111.00
1	E	262	TYR	CG-CD1-CE1	5.17	125.43	121.30
1	E	636	ILE	CB-CA-C	5.17	121.93	111.60
1	F	622	LEU	N-CA-CB	-5.17	100.07	110.40
1	A	257	ALA	N-CA-C	-5.17	97.06	111.00
1	A	305	ILE	N-CA-C	-5.17	97.06	111.00
1	F	305	ILE	N-CA-C	-5.17	97.05	111.00
1	A	528	VAL	O-C-N	5.16	130.96	122.70
1	A	584	VAL	N-CA-C	-5.16	97.06	111.00
1	B	120	TYR	CB-CG-CD1	-5.16	117.90	121.00
1	B	305	ILE	N-CA-C	-5.16	97.06	111.00
1	E	416	VAL	CA-C-O	5.16	130.94	120.10
1	E	435	ASN	CA-CB-CG	5.16	124.76	113.40
1	A	435	ASN	CA-CB-CG	5.16	124.75	113.40
1	C	257	ALA	N-CA-C	-5.16	97.07	111.00
1	C	636	ILE	CB-CA-C	5.16	121.92	111.60
1	E	528	VAL	O-C-N	5.16	130.96	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	187	ASP	CB-CG-OD2	5.16	122.94	118.30
1	F	482	LEU	O-C-N	5.16	130.96	122.70
1	F	636	ILE	CB-CA-C	5.16	121.92	111.60
1	A	248	TRP	N-CA-CB	5.16	119.89	110.60
1	B	416	VAL	CA-C-O	5.16	130.93	120.10
1	B	584	VAL	N-CA-C	-5.16	97.07	111.00
1	C	391	PHE	CD1-CE1-CZ	-5.16	113.91	120.10
1	C	439	SER	N-CA-C	-5.16	97.08	111.00
1	C	584	VAL	N-CA-C	-5.16	97.07	111.00
1	D	504	GLU	O-C-N	5.16	130.95	122.70
1	E	19	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	248	TRP	N-CA-CB	5.16	119.88	110.60
1	B	257	ALA	N-CA-C	-5.16	97.08	111.00
1	E	107	ARG	CA-C-O	5.16	130.93	120.10
1	E	177	ARG	NH1-CZ-NH2	-5.16	113.73	119.40
1	E	257	ALA	N-CA-C	-5.16	97.08	111.00
1	D	146	THR	CB-CA-C	-5.16	97.68	111.60
1	F	416	VAL	CA-C-O	5.16	130.93	120.10
1	C	553	LEU	CB-CG-CD1	-5.15	102.24	111.00
1	D	257	ALA	N-CA-C	-5.15	97.08	111.00
1	F	248	TRP	N-CA-CB	5.15	119.88	110.60
1	B	608	GLN	N-CA-CB	5.15	119.88	110.60
1	C	233	PHE	CZ-CE2-CD2	-5.15	113.92	120.10
1	C	608	GLN	N-CA-CB	5.15	119.87	110.60
1	D	107	ARG	CA-C-O	5.15	130.92	120.10
1	D	416	VAL	CA-C-O	5.15	130.92	120.10
1	D	636	ILE	CA-CB-CG2	5.15	121.20	110.90
1	E	277	PHE	CA-C-N	5.15	128.54	117.20
1	E	289	LEU	O-C-N	5.15	130.94	122.70
1	E	436	ALA	CA-C-O	-5.15	109.28	120.10
1	E	553	LEU	CB-CG-CD1	-5.15	102.24	111.00
1	A	553	LEU	CB-CG-CD1	-5.15	102.25	111.00
1	B	482	LEU	O-C-N	5.15	130.94	122.70
1	C	107	ARG	CA-C-O	5.15	130.92	120.10
1	C	427	ASP	CB-CA-C	-5.15	100.10	110.40
1	E	248	TRP	N-CA-CB	5.15	119.87	110.60
1	E	482	LEU	O-C-N	5.15	130.94	122.70
1	A	416	VAL	CA-C-O	5.15	130.91	120.10
1	C	482	LEU	N-CA-C	-5.15	97.10	111.00
1	C	636	ILE	CA-CB-CG2	5.15	121.20	110.90
1	B	19	ASP	CB-CG-OD2	5.15	122.93	118.30
1	D	391	PHE	CD1-CE1-CZ	-5.15	113.92	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	608	GLN	N-CA-CB	5.15	119.86	110.60
1	D	636	ILE	CB-CA-C	5.15	121.89	111.60
1	E	46	TYR	CB-CG-CD1	5.15	124.09	121.00
1	F	62	ASP	OD1-CG-OD2	-5.15	113.52	123.30
1	F	427	ASP	CB-CA-C	-5.15	100.10	110.40
1	F	439	SER	N-CA-C	-5.15	97.10	111.00
1	F	608	GLN	N-CA-CB	5.15	119.87	110.60
1	A	177	ARG	NH1-CZ-NH2	-5.15	113.74	119.40
1	A	482	LEU	O-C-N	5.15	130.93	122.70
1	A	608	GLN	N-CA-CB	5.14	119.86	110.60
1	B	146	THR	CB-CA-C	-5.14	97.71	111.60
1	C	62	ASP	OD1-CG-OD2	-5.14	113.52	123.30
1	C	146	THR	CB-CA-C	-5.14	97.71	111.60
1	E	146	THR	CB-CA-C	-5.14	97.71	111.60
1	F	504	GLU	O-C-N	5.14	130.93	122.70
1	B	187	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	271	ARG	NH1-CZ-NH2	-5.14	113.74	119.40
1	B	504	GLU	O-C-N	5.14	130.93	122.70
1	C	243	VAL	CA-CB-CG2	-5.14	103.19	110.90
1	C	436	ALA	CA-C-O	-5.14	109.30	120.10
1	E	608	GLN	N-CA-CB	5.14	119.86	110.60
1	A	107	ARG	CA-C-O	5.14	130.90	120.10
1	A	636	ILE	CA-CB-CG2	5.14	121.18	110.90
1	C	528	VAL	O-C-N	5.14	130.93	122.70
1	E	636	ILE	CA-CB-CG2	5.14	121.18	110.90
1	A	436	ALA	CA-C-O	-5.14	109.31	120.10
1	A	504	GLU	O-C-N	5.14	130.93	122.70
1	E	271	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
1	F	435	ASN	CA-CB-CG	5.14	124.70	113.40
1	F	553	LEU	CB-CG-CD1	-5.14	102.26	111.00
1	A	46	TYR	CB-CG-CD1	5.14	124.08	121.00
1	A	482	LEU	N-CA-C	-5.14	97.13	111.00
1	C	323	LEU	CA-C-N	5.14	128.50	117.20
1	C	496	ASP	C-N-CA	-5.14	108.85	121.70
1	F	508	PHE	C-N-CA	-5.14	108.85	121.70
1	A	146	THR	CB-CA-C	-5.14	97.73	111.60
1	B	482	LEU	N-CA-C	-5.14	97.13	111.00
1	B	634	ARG	CB-CA-C	5.14	120.67	110.40
1	B	636	ILE	CA-CB-CG2	5.14	121.17	110.90
1	C	416	VAL	CA-C-O	5.14	130.89	120.10
1	E	62	ASP	OD1-CG-OD2	-5.14	113.54	123.30
1	E	272	PRO	C-N-CA	-5.14	108.86	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	177	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
1	B	553	LEU	CB-CG-CD1	-5.13	102.27	111.00
1	C	177	ARG	NH1-CZ-NH2	-5.13	113.75	119.40
1	C	508	PHE	C-N-CA	-5.13	108.87	121.70
1	D	120	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	D	508	PHE	C-N-CA	-5.13	108.86	121.70
1	D	553	LEU	CB-CG-CD1	-5.13	102.27	111.00
1	D	634	ARG	CB-CA-C	5.13	120.67	110.40
1	F	271	ARG	NH1-CZ-NH2	-5.13	113.75	119.40
1	A	508	PHE	C-N-CA	-5.13	108.87	121.70
1	C	504	GLU	O-C-N	5.13	130.91	122.70
1	D	427	ASP	CB-CA-C	-5.13	100.13	110.40
1	D	482	LEU	N-CA-C	-5.13	97.14	111.00
1	E	508	PHE	C-N-CA	-5.13	108.87	121.70
1	A	62	ASP	OD1-CG-OD2	-5.13	113.55	123.30
1	A	271	ARG	NH1-CZ-NH2	-5.13	113.75	119.40
1	A	427	ASP	CB-CA-C	-5.13	100.14	110.40
1	B	233	PHE	CZ-CE2-CD2	-5.13	113.94	120.10
1	C	634	ARG	CB-CA-C	5.13	120.66	110.40
1	E	634	ARG	CB-CA-C	5.13	120.66	110.40
1	B	46	TYR	CB-CG-CD1	5.13	124.08	121.00
1	B	105	TYR	CA-CB-CG	-5.13	103.65	113.40
1	F	238	ASN	CA-CB-CG	-5.13	102.11	113.40
1	F	636	ILE	CA-CB-CG2	5.13	121.16	110.90
1	A	7	ASN	N-CA-C	-5.13	97.16	111.00
1	B	7	ASN	N-CA-C	-5.13	97.15	111.00
1	E	233	PHE	CZ-CE2-CD2	-5.13	113.95	120.10
1	F	482	LEU	N-CA-C	-5.13	97.15	111.00
1	B	107	ARG	CA-C-O	5.13	130.87	120.10
1	B	508	PHE	C-N-CA	-5.13	108.89	121.70
1	C	238	ASN	CA-CB-CG	-5.13	102.12	113.40
1	C	482	LEU	O-C-N	5.13	130.90	122.70
1	D	277	PHE	CA-C-N	5.13	128.48	117.20
1	F	7	ASN	N-CA-C	-5.13	97.16	111.00
1	F	105	TYR	CA-CB-CG	-5.13	103.66	113.40
1	A	634	ARG	CB-CA-C	5.12	120.65	110.40
1	B	427	ASP	CB-CA-C	-5.12	100.15	110.40
1	C	7	ASN	N-CA-C	-5.12	97.16	111.00
1	D	105	TYR	CA-CB-CG	-5.12	103.66	113.40
1	D	399	PRO	N-CA-CB	-5.12	96.96	102.60
1	F	146	THR	CB-CA-C	-5.12	97.76	111.60
1	A	277	PHE	CA-C-N	5.12	128.47	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	VAL	CA-CB-CG2	-5.12	103.22	110.90
1	B	436	ALA	CA-C-O	-5.12	109.34	120.10
1	D	243	VAL	CA-CB-CG2	-5.12	103.22	110.90
1	E	272	PRO	CA-C-O	-5.12	107.90	120.20
1	E	427	ASP	CB-CA-C	-5.12	100.15	110.40
1	E	482	LEU	N-CA-C	-5.12	97.17	111.00
1	E	487	ASP	N-CA-CB	-5.12	101.38	110.60
1	F	634	ARG	CB-CA-C	5.12	120.65	110.40
1	A	496	ASP	C-N-CA	-5.12	108.90	121.70
1	B	323	LEU	CA-C-N	5.12	128.47	117.20
1	D	7	ASN	N-CA-C	-5.12	97.17	111.00
1	D	62	ASP	OD1-CG-OD2	-5.12	113.57	123.30
1	E	7	ASN	N-CA-C	-5.12	97.17	111.00
1	E	504	GLU	O-C-N	5.12	130.90	122.70
1	F	107	ARG	CA-C-O	5.12	130.86	120.10
1	A	105	TYR	CA-CB-CG	-5.12	103.67	113.40
1	B	177	ARG	NH1-CZ-NH2	-5.12	113.77	119.40
1	E	496	ASP	C-N-CA	-5.12	108.90	121.70
1	F	436	ALA	CA-C-O	-5.12	109.35	120.10
1	A	233	PHE	CZ-CE2-CD2	-5.12	113.96	120.10
1	B	8	ALA	CA-C-N	5.12	128.46	117.20
1	B	496	ASP	C-N-CA	-5.12	108.90	121.70
1	E	243	VAL	CA-CB-CG2	-5.12	103.22	110.90
1	A	487	ASP	N-CA-CB	-5.12	101.39	110.60
1	A	238	ASN	CA-CB-CG	-5.12	102.14	113.40
1	A	243	VAL	CA-CB-CG2	-5.12	103.23	110.90
1	B	69	ARG	NH1-CZ-NH2	-5.12	113.77	119.40
1	B	238	ASN	CA-CB-CG	-5.12	102.15	113.40
1	B	454	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	272	PRO	CA-C-O	-5.12	107.92	120.20
1	D	8	ALA	CA-C-N	5.12	128.45	117.20
1	D	496	ASP	C-N-CA	-5.12	108.91	121.70
1	E	173	THR	CB-CA-C	-5.12	97.79	111.60
1	E	236	LEU	CB-CG-CD1	-5.12	102.30	111.00
1	F	277	PHE	CA-C-N	5.12	128.45	117.20
1	A	262	TYR	CG-CD1-CE1	5.11	125.39	121.30
1	A	323	LEU	CA-C-N	5.11	128.45	117.20
1	B	62	ASP	OD1-CG-OD2	-5.11	113.58	123.30
1	C	105	TYR	CA-CB-CG	-5.11	103.68	113.40
1	C	272	PRO	C-N-CA	-5.11	108.92	121.70
1	D	221	PHE	N-CA-CB	5.11	119.80	110.60
1	D	323	LEU	CA-C-N	5.11	128.45	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	46	TYR	CB-CG-CD1	5.11	124.07	121.00
1	F	221	PHE	N-CA-CB	5.11	119.80	110.60
1	F	323	LEU	CA-C-N	5.11	128.45	117.20
1	D	272	PRO	CA-C-O	-5.11	107.93	120.20
1	E	274	ASN	CB-CG-OD1	-5.11	111.38	121.60
1	C	173	THR	CB-CA-C	-5.11	97.80	111.60
1	C	277	PHE	CA-C-N	5.11	128.44	117.20
1	D	271	ARG	NH1-CZ-NH2	-5.11	113.78	119.40
1	A	272	PRO	CA-C-O	-5.11	107.94	120.20
1	C	399	PRO	N-CA-CB	-5.11	96.98	102.60
1	E	105	TYR	CA-CB-CG	-5.11	103.69	113.40
1	A	272	PRO	C-N-CA	-5.11	108.93	121.70
1	D	238	ASN	CA-CB-CG	-5.11	102.17	113.40
1	F	173	THR	CB-CA-C	-5.11	97.81	111.60
1	C	564	ILE	CB-CG1-CD1	-5.11	99.61	113.90
1	E	238	ASN	CA-CB-CG	-5.11	102.17	113.40
1	E	323	LEU	CA-C-N	5.11	128.43	117.20
1	F	233	PHE	CZ-CE2-CD2	-5.11	113.97	120.10
1	F	496	ASP	C-N-CA	-5.11	108.94	121.70
1	B	274	ASN	CB-CG-OD1	-5.10	111.39	121.60
1	B	277	PHE	CA-C-N	5.10	128.43	117.20
1	B	487	ASP	N-CA-CB	-5.10	101.41	110.60
1	D	173	THR	CB-CA-C	-5.10	97.82	111.60
1	F	487	ASP	N-CA-CB	-5.10	101.41	110.60
1	A	8	ALA	CA-C-N	5.10	128.42	117.20
1	A	173	THR	CB-CA-C	-5.10	97.82	111.60
1	E	399	PRO	N-CA-CB	-5.10	96.99	102.60
1	F	236	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	F	564	ILE	CB-CG1-CD1	-5.10	99.61	113.90
1	D	113	GLY	O-C-N	5.10	130.86	122.70
1	D	272	PRO	C-N-CA	-5.10	108.95	121.70
1	F	272	PRO	C-N-CA	-5.10	108.95	121.70
1	A	221	PHE	N-CA-CB	5.10	119.78	110.60
1	A	634	ARG	CG-CD-NE	5.10	122.51	111.80
1	B	262	TYR	CG-CD1-CE1	5.10	125.38	121.30
1	D	233	PHE	CZ-CE2-CD2	-5.10	113.98	120.10
1	D	262	TYR	CG-CD1-CE1	5.10	125.38	121.30
1	E	564	ILE	CB-CG1-CD1	-5.10	99.62	113.90
1	E	636	ILE	O-C-N	5.10	130.86	122.70
1	B	173	THR	CB-CA-C	-5.10	97.84	111.60
1	B	272	PRO	CA-C-O	-5.10	107.97	120.20
1	C	8	ALA	CA-C-N	5.10	128.41	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	274	ASN	CB-CG-OD1	-5.10	111.41	121.60
1	D	487	ASP	N-CA-CB	-5.10	101.42	110.60
1	F	89	VAL	CA-CB-CG2	-5.10	103.25	110.90
1	A	236	LEU	CB-CG-CD1	-5.10	102.34	111.00
1	E	8	ALA	CA-C-N	5.10	128.41	117.20
1	F	243	VAL	CA-CB-CG2	-5.10	103.25	110.90
1	A	399	PRO	N-CA-CB	-5.09	97.00	102.60
1	C	221	PHE	N-CA-CB	5.09	119.77	110.60
1	D	564	ILE	CB-CG1-CD1	-5.09	99.64	113.90
1	E	237	SER	CB-CA-C	5.09	119.78	110.10
1	F	263	LYS	N-CA-CB	5.09	119.77	110.60
1	F	272	PRO	CA-C-O	-5.09	107.97	120.20
1	F	634	ARG	CG-CD-NE	5.09	122.50	111.80
1	F	8	ALA	CA-C-N	5.09	128.40	117.20
1	F	254	GLU	N-CA-C	5.09	124.75	111.00
1	A	274	ASN	CB-CG-OD1	-5.09	111.42	121.60
1	A	564	ILE	CB-CG1-CD1	-5.09	99.64	113.90
1	B	113	GLY	O-C-N	5.09	130.84	122.70
1	B	237	SER	CB-CA-C	5.09	119.77	110.10
1	B	272	PRO	C-N-CA	-5.09	108.97	121.70
1	E	634	ARG	CG-CD-NE	5.09	122.49	111.80
1	F	274	ASN	CB-CG-OD1	-5.09	111.42	121.60
1	F	399	PRO	N-CA-CB	-5.09	97.00	102.60
1	C	437	VAL	CG1-CB-CG2	-5.09	102.76	110.90
1	C	487	ASP	N-CA-CB	-5.09	101.44	110.60
1	F	120	TYR	CB-CG-CD1	-5.09	117.95	121.00
1	F	496	ASP	CB-CA-C	5.09	120.58	110.40
1	D	236	LEU	CB-CG-CD1	-5.09	102.35	111.00
1	E	113	GLY	O-C-N	5.09	130.84	122.70
1	F	237	SER	CB-CA-C	5.09	119.76	110.10
1	F	399	PRO	CB-CA-C	5.09	124.72	112.00
1	B	89	VAL	CA-CB-CG2	-5.08	103.28	110.90
1	B	564	ILE	CB-CG1-CD1	-5.08	99.67	113.90
1	C	274	ASN	CB-CG-OD1	-5.08	111.43	121.60
1	E	89	VAL	CA-CB-CG2	-5.08	103.28	110.90
1	B	198	HIS	O-C-N	-5.08	114.57	122.70
1	B	263	LYS	CA-CB-CG	5.08	124.58	113.40
1	C	112	GLU	CB-CA-C	-5.08	100.23	110.40
1	D	237	SER	CB-CA-C	5.08	119.75	110.10
1	D	263	LYS	N-CA-CB	5.08	119.75	110.60
1	D	634	ARG	CG-CD-NE	5.08	122.47	111.80
1	E	221	PHE	N-CA-CB	5.08	119.75	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	SER	CB-CA-C	5.08	119.75	110.10
1	C	139	GLN	N-CA-CB	5.08	119.75	110.60
1	E	263	LYS	N-CA-CB	5.08	119.74	110.60
1	E	294	SER	C-N-CA	-5.08	109.00	121.70
1	B	23	GLU	N-CA-CB	5.08	119.74	110.60
1	B	263	LYS	N-CA-CB	5.08	119.74	110.60
1	B	496	ASP	CB-CA-C	5.08	120.56	110.40
1	C	634	ARG	CG-CD-NE	5.08	122.47	111.80
1	F	139	GLN	N-CA-CB	5.08	119.74	110.60
1	F	262	TYR	CG-CD1-CE1	5.08	125.36	121.30
1	A	89	VAL	CA-CB-CG2	-5.08	103.28	110.90
1	A	453	HIS	C-N-CA	-5.08	109.01	121.70
1	B	453	HIS	C-N-CA	-5.08	109.01	121.70
1	B	553	LEU	CB-CA-C	5.08	119.85	110.20
1	C	89	VAL	CA-CB-CG2	-5.08	103.28	110.90
1	D	636	ILE	O-C-N	5.08	130.82	122.70
1	A	120	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	B	221	PHE	N-CA-CB	5.08	119.73	110.60
1	B	236	LEU	CB-CG-CD1	-5.08	102.37	111.00
1	C	237	SER	CA-CB-OG	-5.08	97.50	111.20
1	D	553	LEU	CB-CA-C	5.08	119.84	110.20
1	D	632	ASP	CA-CB-CG	5.08	124.57	113.40
1	E	430	GLN	CA-C-O	5.08	130.76	120.10
1	F	112	GLU	CB-CA-C	-5.08	100.25	110.40
1	A	112	GLU	CB-CA-C	-5.07	100.25	110.40
1	A	254	GLU	N-CA-C	5.07	124.70	111.00
1	A	294	SER	C-N-CA	-5.07	109.02	121.70
1	A	399	PRO	CB-CA-C	5.07	124.68	112.00
1	B	294	SER	C-N-CA	-5.07	109.02	121.70
1	B	430	GLN	CA-C-O	5.07	130.75	120.10
1	B	634	ARG	CG-CD-NE	5.07	122.46	111.80
1	B	636	ILE	O-C-N	5.07	130.82	122.70
1	C	237	SER	CB-CA-C	5.07	119.74	110.10
1	C	399	PRO	CB-CA-C	5.07	124.68	112.00
1	C	453	HIS	C-N-CA	-5.07	109.02	121.70
1	E	453	HIS	C-N-CA	-5.07	109.02	121.70
1	E	632	ASP	CA-CB-CG	5.07	124.56	113.40
1	F	430	GLN	CA-C-O	5.07	130.76	120.10
1	D	203	PHE	CZ-CE2-CD2	-5.07	114.01	120.10
1	D	399	PRO	CB-CA-C	5.07	124.68	112.00
1	E	254	GLU	N-CA-C	5.07	124.70	111.00
1	F	437	VAL	CG1-CB-CG2	-5.07	102.78	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	453	HIS	C-N-CA	-5.07	109.02	121.70
1	A	113	GLY	O-C-N	5.07	130.81	122.70
1	A	263	LYS	N-CA-CB	5.07	119.73	110.60
1	A	496	ASP	CB-CA-C	5.07	120.54	110.40
1	A	636	ILE	O-C-N	5.07	130.81	122.70
1	C	236	LEU	CB-CG-CD1	-5.07	102.38	111.00
1	C	263	LYS	N-CA-CB	5.07	119.73	110.60
1	D	89	VAL	CA-CB-CG2	-5.07	103.29	110.90
1	D	453	HIS	C-N-CA	-5.07	109.02	121.70
1	E	399	PRO	CB-CA-C	5.07	124.68	112.00
1	C	632	ASP	CA-CB-CG	5.07	124.55	113.40
1	E	112	GLU	CB-CA-C	-5.07	100.26	110.40
1	A	23	GLU	N-CA-CB	5.07	119.72	110.60
1	A	139	GLN	N-CA-CB	5.07	119.72	110.60
1	B	399	PRO	CB-CA-C	5.07	124.67	112.00
1	C	254	GLU	N-CA-C	5.07	124.68	111.00
1	C	496	ASP	CB-CA-C	5.07	120.53	110.40
1	D	112	GLU	CB-CA-C	-5.07	100.27	110.40
1	D	139	GLN	N-CA-CB	5.07	119.72	110.60
1	D	496	ASP	CB-CA-C	5.07	120.53	110.40
1	F	23	GLU	N-CA-CB	5.07	119.72	110.60
1	F	113	GLY	O-C-N	5.07	130.81	122.70
1	F	294	SER	C-N-CA	-5.07	109.03	121.70
1	F	632	ASP	CA-CB-CG	5.07	124.55	113.40
1	B	254	GLU	N-CA-C	5.07	124.68	111.00
1	B	497	GLU	CA-C-O	-5.07	109.46	120.10
1	C	198	HIS	O-C-N	-5.07	114.59	122.70
1	C	430	GLN	CA-C-O	5.07	130.74	120.10
1	D	23	GLU	N-CA-CB	5.07	119.72	110.60
1	D	254	GLU	N-CA-C	5.07	124.68	111.00
1	E	139	GLN	N-CA-CB	5.07	119.72	110.60
1	E	203	PHE	CZ-CE2-CD2	-5.07	114.02	120.10
1	F	263	LYS	CA-CB-CG	5.07	124.55	113.40
1	B	139	GLN	N-CA-CB	5.06	119.72	110.60
1	B	399	PRO	N-CA-CB	-5.06	97.03	102.60
1	D	294	SER	C-N-CA	-5.06	109.04	121.70
1	F	237	SER	CA-CB-OG	-5.06	97.53	111.20
1	A	437	VAL	CG1-CB-CG2	-5.06	102.80	110.90
1	A	553	LEU	CB-CA-C	5.06	119.82	110.20
1	A	632	ASP	CA-CB-CG	5.06	124.54	113.40
1	B	112	GLU	CB-CA-C	-5.06	100.27	110.40
1	C	294	SER	C-N-CA	-5.06	109.05	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	218	GLU	CA-C-N	-5.06	106.06	117.20
1	F	636	ILE	O-C-N	5.06	130.80	122.70
1	B	592	ASP	OD1-CG-OD2	5.06	132.91	123.30
1	C	636	ILE	O-C-N	5.06	130.80	122.70
1	A	263	LYS	CA-CB-CG	5.06	124.53	113.40
1	B	632	ASP	CA-CB-CG	5.06	124.53	113.40
1	C	553	LEU	CB-CA-C	5.06	119.81	110.20
1	D	263	LYS	CA-CB-CG	5.06	124.53	113.40
1	E	23	GLU	N-CA-CB	5.06	119.71	110.60
1	E	352	GLY	O-C-N	5.06	130.79	122.70
1	A	218	GLU	CA-C-N	-5.06	106.07	117.20
1	A	237	SER	CA-CB-OG	-5.06	97.54	111.20
1	A	430	GLN	CA-C-O	5.06	130.72	120.10
1	B	237	SER	CA-CB-OG	-5.06	97.55	111.20
1	D	430	GLN	CA-C-O	5.06	130.72	120.10
1	E	496	ASP	CB-CA-C	5.06	120.52	110.40
1	F	203	PHE	CZ-CE2-CD2	-5.06	114.03	120.10
1	B	218	GLU	CA-C-N	-5.05	106.08	117.20
1	C	23	GLU	N-CA-CB	5.05	119.70	110.60
1	C	218	GLU	CA-C-N	-5.05	106.08	117.20
1	D	237	SER	CA-CB-OG	-5.05	97.55	111.20
1	D	639	VAL	N-CA-C	-5.05	97.36	111.00
1	E	263	LYS	CA-CB-CG	5.05	124.52	113.40
1	F	218	GLU	CA-C-N	-5.05	106.08	117.20
1	B	203	PHE	CZ-CE2-CD2	-5.05	114.04	120.10
1	E	218	GLU	CA-C-N	-5.05	106.08	117.20
1	D	497	GLU	CA-C-O	-5.05	109.49	120.10
1	E	237	SER	CA-CB-OG	-5.05	97.56	111.20
1	A	497	GLU	CA-C-O	-5.05	109.50	120.10
1	B	437	VAL	CG1-CB-CG2	-5.05	102.82	110.90
1	C	263	LYS	CA-CB-CG	5.05	124.51	113.40
1	C	497	GLU	CA-C-O	-5.05	109.50	120.10
1	E	553	LEU	CB-CA-C	5.05	119.80	110.20
1	A	198	HIS	O-C-N	-5.05	114.62	122.70
1	B	78	ARG	NH1-CZ-NH2	-5.05	113.85	119.40
1	C	46	TYR	CB-CG-CD1	5.05	124.03	121.00
1	D	437	VAL	CG1-CB-CG2	-5.05	102.83	110.90
1	F	497	GLU	CA-C-O	-5.05	109.50	120.10
1	F	425	PHE	CB-CG-CD2	-5.04	117.27	120.80
1	A	203	PHE	CZ-CE2-CD2	-5.04	114.05	120.10
1	E	198	HIS	O-C-N	-5.04	114.63	122.70
1	F	553	LEU	CB-CA-C	5.04	119.78	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	437	VAL	CG1-CB-CG2	-5.04	102.83	110.90
1	F	352	GLY	O-C-N	5.04	130.77	122.70
1	F	639	VAL	N-CA-C	-5.04	97.39	111.00
1	A	352	GLY	O-C-N	5.04	130.76	122.70
1	A	440	GLY	CA-C-N	-5.04	106.11	117.20
1	C	113	GLY	O-C-N	5.04	130.76	122.70
1	F	57	MET	CB-CA-C	5.04	120.48	110.40
1	A	639	VAL	N-CA-C	-5.04	97.40	111.00
1	C	440	GLY	CA-C-N	-5.04	106.12	117.20
1	D	90	LEU	CB-CG-CD2	-5.04	102.44	111.00
1	E	78	ARG	NH1-CZ-NH2	-5.04	113.86	119.40
1	F	592	ASP	OD1-CG-OD2	5.04	132.87	123.30
1	B	90	LEU	CB-CG-CD2	-5.03	102.44	111.00
1	C	592	ASP	OD1-CG-OD2	5.03	132.86	123.30
1	D	352	GLY	O-C-N	5.03	130.75	122.70
1	D	440	GLY	CA-C-N	-5.03	106.13	117.20
1	F	78	ARG	NH1-CZ-NH2	-5.03	113.86	119.40
1	F	440	GLY	CA-C-N	-5.03	106.13	117.20
1	B	639	VAL	N-CA-C	-5.03	97.41	111.00
1	E	425	PHE	CB-CG-CD2	-5.03	117.28	120.80
1	E	639	VAL	N-CA-C	-5.03	97.41	111.00
1	F	90	LEU	CB-CG-CD2	-5.03	102.44	111.00
1	B	352	GLY	O-C-N	5.03	130.75	122.70
1	D	198	HIS	O-C-N	-5.03	114.65	122.70
1	E	440	GLY	CA-C-N	-5.03	106.13	117.20
1	E	497	GLU	CA-C-O	-5.03	109.54	120.10
1	E	645	VAL	CA-CB-CG2	-5.03	103.35	110.90
1	B	57	MET	CB-CA-C	5.03	120.46	110.40
1	E	57	MET	CB-CA-C	5.03	120.46	110.40
1	A	57	MET	CB-CA-C	5.03	120.46	110.40
1	B	440	GLY	CA-C-N	-5.03	106.14	117.20
1	C	352	GLY	O-C-N	5.03	130.74	122.70
1	D	155	TYR	CB-CA-C	-5.03	100.34	110.40
1	A	592	ASP	OD1-CG-OD2	5.03	132.85	123.30
1	B	155	TYR	CB-CA-C	-5.03	100.35	110.40
1	C	260	THR	CA-CB-CG2	5.03	119.44	112.40
1	C	639	VAL	N-CA-C	-5.03	97.43	111.00
1	E	112	GLU	CG-CD-OE2	-5.03	108.25	118.30
1	F	645	VAL	CA-CB-CG2	-5.03	103.36	110.90
1	B	100	ARG	NH1-CZ-NH2	-5.02	113.87	119.40
1	A	454	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	B	645	VAL	CA-CB-CG2	-5.02	103.37	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	ARG	NH1-CZ-NH2	-5.02	113.88	119.40
1	C	558	TYR	N-CA-CB	-5.02	101.56	110.60
1	F	191	ASN	OD1-CG-ND2	5.02	133.45	121.90
1	C	57	MET	CB-CA-C	5.02	120.44	110.40
1	E	528	VAL	N-CA-CB	-5.02	100.45	111.50
1	A	112	GLU	CG-CD-OE2	-5.02	108.26	118.30
1	A	155	TYR	CB-CA-C	-5.02	100.36	110.40
1	A	425	PHE	CB-CG-CD2	-5.02	117.29	120.80
1	C	191	ASN	OD1-CG-ND2	5.02	133.45	121.90
1	C	262	TYR	CG-CD1-CE1	5.02	125.32	121.30
1	D	592	ASP	OD1-CG-OD2	5.02	132.84	123.30
1	A	90	LEU	CB-CG-CD2	-5.02	102.47	111.00
1	C	120	TYR	CB-CG-CD1	-5.02	117.99	121.00
1	C	203	PHE	CZ-CE2-CD2	-5.02	114.08	120.10
1	E	90	LEU	CB-CG-CD2	-5.02	102.47	111.00
1	F	112	GLU	CG-CD-OE2	-5.02	108.26	118.30
1	F	198	HIS	O-C-N	-5.02	114.67	122.70
1	A	78	ARG	NH1-CZ-NH2	-5.02	113.88	119.40
1	C	155	TYR	CB-CA-C	-5.01	100.37	110.40
1	D	112	GLU	CG-CD-OE2	-5.01	108.27	118.30
1	D	191	ASN	OD1-CG-ND2	5.01	133.43	121.90
1	F	558	TYR	N-CA-CB	-5.01	101.57	110.60
1	C	127	LYS	CB-CA-C	5.01	120.43	110.40
1	F	155	TYR	CB-CA-C	-5.01	100.37	110.40
1	A	191	ASN	OD1-CG-ND2	5.01	133.43	121.90
1	B	260	THR	CA-CB-CG2	5.01	119.42	112.40
1	C	303	GLY	N-CA-C	-5.01	100.57	113.10
1	D	68	GLN	OE1-CD-NE2	-5.01	110.37	121.90
1	E	155	TYR	CB-CA-C	-5.01	100.38	110.40
1	E	191	ASN	OD1-CG-ND2	5.01	133.43	121.90
1	B	350	MET	CB-CG-SD	-5.01	97.37	112.40
1	B	588	ASP	CA-CB-CG	5.01	124.42	113.40
1	C	112	GLU	CG-CD-OE2	-5.01	108.28	118.30
1	C	138	TYR	CZ-CE2-CD2	5.01	124.31	119.80
1	E	68	GLN	OE1-CD-NE2	-5.01	110.38	121.90
1	E	303	GLY	N-CA-C	-5.01	100.58	113.10
1	E	592	ASP	OD1-CG-OD2	5.01	132.82	123.30
1	F	303	GLY	N-CA-C	-5.01	100.58	113.10
1	A	303	GLY	N-CA-C	-5.01	100.58	113.10
1	B	191	ASN	OD1-CG-ND2	5.01	133.42	121.90
1	A	127	LYS	CB-CA-C	5.01	120.41	110.40
1	A	645	VAL	CA-CB-CG2	-5.01	103.39	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	588	ASP	CA-CB-CG	5.01	124.41	113.40
1	D	127	LYS	CB-CA-C	5.01	120.41	110.40
1	D	558	TYR	N-CA-CB	-5.01	101.59	110.60
1	D	645	VAL	CA-CB-CG2	-5.01	103.39	110.90
1	E	177	ARG	CA-C-O	5.01	130.61	120.10
1	F	356	ASP	N-CA-CB	-5.01	101.59	110.60
1	A	558	TYR	N-CA-CB	-5.00	101.59	110.60
1	B	558	TYR	N-CA-CB	-5.00	101.59	110.60
1	A	177	ARG	CA-C-O	5.00	130.61	120.10
1	A	588	ASP	CA-CB-CG	5.00	124.41	113.40
1	C	645	VAL	CA-CB-CG2	-5.00	103.39	110.90
1	D	528	VAL	N-CA-CB	-5.00	100.49	111.50
1	E	350	MET	CB-CG-SD	-5.00	97.39	112.40
1	F	588	ASP	CA-CB-CG	5.00	124.41	113.40
1	A	260	THR	CA-CB-CG2	5.00	119.40	112.40
1	A	528	VAL	N-CA-CB	-5.00	100.50	111.50
1	E	454	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	E	588	ASP	CA-CB-CG	5.00	124.40	113.40

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ARG	Sidechain
1	A	177	ARG	Sidechain
1	A	215	ARG	Sidechain
1	A	454	ARG	Sidechain
1	A	499	ARG	Sidechain
1	A	620	ARG	Sidechain
1	A	628	ARG	Sidechain
1	B	100	ARG	Sidechain
1	B	177	ARG	Sidechain
1	B	215	ARG	Sidechain
1	B	454	ARG	Sidechain
1	B	499	ARG	Sidechain
1	B	620	ARG	Sidechain
1	B	628	ARG	Sidechain
1	C	100	ARG	Sidechain
1	C	177	ARG	Sidechain
1	C	215	ARG	Sidechain
1	C	454	ARG	Sidechain
1	C	499	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	620	ARG	Sidechain
1	C	628	ARG	Sidechain
1	D	100	ARG	Sidechain
1	D	177	ARG	Sidechain
1	D	215	ARG	Sidechain
1	D	454	ARG	Sidechain
1	D	499	ARG	Sidechain
1	D	620	ARG	Sidechain
1	D	628	ARG	Sidechain
1	E	100	ARG	Sidechain
1	E	177	ARG	Sidechain
1	E	215	ARG	Sidechain
1	E	454	ARG	Sidechain
1	E	499	ARG	Sidechain
1	E	620	ARG	Sidechain
1	E	628	ARG	Sidechain
1	F	100	ARG	Sidechain
1	F	177	ARG	Sidechain
1	F	215	ARG	Sidechain
1	F	454	ARG	Sidechain
1	F	499	ARG	Sidechain
1	F	620	ARG	Sidechain
1	F	628	ARG	Sidechain

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	5239	0	4942	566	1
1	B	5239	0	4942	549	0
1	C	5239	0	4942	561	0
1	D	5239	0	4942	580	0
1	E	5239	0	4942	558	1
1	F	5239	0	4943	539	0
2	A	28	0	25	6	0
2	B	28	0	25	6	0
2	C	28	0	25	7	0
2	D	28	0	25	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	28	0	25	6	0
2	F	28	0	25	6	0
3	A	2	0	0	0	0
4	A	176	0	0	31	0
4	B	4	0	0	1	0
4	C	2	0	0	0	0
4	E	3	0	0	1	0
4	F	1	0	0	0	0
All	All	31790	0	29803	3314	1

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 54.

All (3314) 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:B:140:ILE:HG22	1:B:141:THR:HG23	1.20	1.18
1:A:140:ILE:HG22	1:A:141:THR:HG23	1.20	1.17
1:F:140:ILE:HG22	1:F:141:THR:HG23	1.20	1.17
1:E:140:ILE:HG22	1:E:141:THR:HG23	1.20	1.15
1:D:140:ILE:HG22	1:D:141:THR:HG23	1.20	1.15
1:C:140:ILE:HG22	1:C:141:THR:HG23	1.20	1.12
1:E:59:GLU:OE1	1:E:64:ARG:HD3	1.54	1.08
1:D:59:GLU:OE1	1:D:64:ARG:HD3	1.54	1.07
1:F:414:ASN:HD22	1:F:466:MET:HA	1.20	1.07
1:B:59:GLU:OE1	1:B:64:ARG:HD3	1.54	1.06
1:F:59:GLU:OE1	1:F:64:ARG:HD3	1.54	1.05
1:A:59:GLU:OE1	1:A:64:ARG:HD3	1.54	1.05
1:C:59:GLU:OE1	1:C:64:ARG:HD3	1.54	1.05
1:D:634:ARG:HH21	1:F:64:ARG:HD2	1.22	1.05
1:E:513:PRO:HG3	1:E:517:GLU:HB2	1.39	1.05
1:E:414:ASN:HD22	1:E:466:MET:HA	1.20	1.04
1:D:414:ASN:HD22	1:D:466:MET:HA	1.20	1.04
1:F:513:PRO:HG3	1:F:517:GLU:HB2	1.40	1.04
1:A:411:MET:HG2	4:A:834:HOH:O	1.57	1.04
1:D:513:PRO:HG3	1:D:517:GLU:HB2	1.39	1.03
2:E:659:NAG:HN2	2:E:659:NAG:C8	1.72	1.03
2:A:659:NAG:C8	2:A:659:NAG:HN2	1.72	1.03
1:C:414:ASN:HD22	1:C:466:MET:HA	1.20	1.03
1:C:513:PRO:HG3	1:C:517:GLU:HB2	1.40	1.03
2:D:659:NAG:HN2	2:D:659:NAG:C8	1.72	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:659:NAG:HN2	2:B:659:NAG:C8	1.72	1.03
1:C:487:ASP:HB3	1:C:489:ASN:H	1.22	1.03
1:A:414:ASN:HD22	1:A:466:MET:HA	1.20	1.03
1:B:513:PRO:HG3	1:B:517:GLU:HB2	1.39	1.02
1:C:175:LYS:O	1:D:491:ILE:HD11	1.57	1.02
1:F:487:ASP:HB3	1:F:489:ASN:H	1.22	1.02
2:F:659:NAG:HN2	2:F:659:NAG:C8	1.72	1.02
2:C:659:NAG:C8	2:C:659:NAG:HN2	1.72	1.01
1:A:487:ASP:HB3	1:A:489:ASN:H	1.22	1.01
1:A:513:PRO:HG3	1:A:517:GLU:HB2	1.39	1.00
1:B:414:ASN:HD22	1:B:466:MET:HA	1.20	1.00
1:A:273:ASP:OD2	1:B:360:LYS:HE3	1.61	1.00
1:E:487:ASP:HB3	1:E:489:ASN:H	1.22	1.00
1:C:491:ILE:CD1	1:D:175:LYS:HB2	1.93	0.99
1:D:487:ASP:HB3	1:D:489:ASN:H	1.22	0.99
1:B:487:ASP:HB3	1:B:489:ASN:H	1.22	0.98
1:C:252:ILE:HG13	1:C:275:ILE:HG22	1.47	0.97
1:F:252:ILE:HG13	1:F:275:ILE:HG22	1.47	0.96
1:A:360:LYS:HE3	1:B:273:ASP:OD2	1.65	0.96
1:D:252:ILE:HG13	1:D:275:ILE:HG22	1.47	0.96
1:C:175:LYS:HB2	1:D:491:ILE:CD1	1.96	0.96
1:E:585:ALA:HB1	1:E:642:ILE:HG12	1.49	0.95
1:E:252:ILE:HG13	1:E:275:ILE:HG22	1.47	0.94
1:C:585:ALA:HB1	1:C:642:ILE:HG12	1.49	0.94
1:B:585:ALA:HB1	1:B:642:ILE:HG12	1.49	0.94
1:F:585:ALA:HB1	1:F:642:ILE:HG12	1.49	0.93
1:B:252:ILE:HG13	1:B:275:ILE:HG22	1.47	0.93
1:F:634:ARG:HG2	1:F:634:ARG:HH11	1.35	0.92
1:A:585:ALA:HB1	1:A:642:ILE:HG12	1.49	0.92
1:E:634:ARG:HG2	1:E:634:ARG:HH11	1.35	0.92
1:D:585:ALA:HB1	1:D:642:ILE:HG12	1.49	0.92
1:F:165:THR:HG22	1:F:449:ASN:HB2	1.52	0.92
1:A:252:ILE:HG13	1:A:275:ILE:HG22	1.47	0.92
1:E:165:THR:HG22	1:E:449:ASN:HB2	1.52	0.91
1:C:491:ILE:HD11	1:D:175:LYS:HB2	1.53	0.91
1:C:634:ARG:HH11	1:C:634:ARG:HG2	1.34	0.91
1:A:634:ARG:HH11	1:A:634:ARG:HG2	1.35	0.91
1:D:634:ARG:HG2	1:D:634:ARG:HH11	1.35	0.91
1:B:165:THR:HG22	1:B:449:ASN:HB2	1.52	0.91
2:D:658:NDG:C8	2:D:658:NDG:HA	1.84	0.91
1:B:634:ARG:HH11	1:B:634:ARG:HG2	1.35	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:THR:HG22	1:A:449:ASN:HB2	1.52	0.90
2:F:658:NDG:HA	2:F:658:NDG:C8	1.84	0.90
1:C:165:THR:HG22	1:C:449:ASN:HB2	1.52	0.90
2:A:658:NDG:C8	2:A:658:NDG:HA	1.84	0.90
2:E:658:NDG:HA	2:E:658:NDG:C8	1.84	0.90
1:E:272:PRO:O	1:E:273:ASP:HB3	1.71	0.90
2:B:658:NDG:C8	2:B:658:NDG:HA	1.84	0.90
1:D:165:THR:HG22	1:D:449:ASN:HB2	1.52	0.90
2:C:658:NDG:HA	2:C:658:NDG:C8	1.84	0.89
1:E:10:LYS:HG2	1:E:96:TRP:CE2	2.08	0.89
1:D:313:ILE:HD11	1:D:323:LEU:HD13	1.55	0.89
1:B:313:ILE:HD11	1:B:323:LEU:HD13	1.55	0.89
1:C:10:LYS:HG2	1:C:96:TRP:CE2	2.08	0.89
1:A:138:TYR:CE2	1:A:188:ILE:HD12	2.08	0.89
1:A:313:ILE:HD11	1:A:323:LEU:HD13	1.55	0.89
1:B:272:PRO:O	1:B:273:ASP:HB3	1.71	0.88
1:E:138:TYR:CE2	1:E:188:ILE:HD12	2.08	0.88
1:F:313:ILE:HD11	1:F:323:LEU:HD13	1.55	0.88
1:B:138:TYR:CE2	1:B:188:ILE:HD12	2.08	0.88
1:D:606:HIS:HD2	1:D:608:GLN:HG2	1.39	0.88
1:E:313:ILE:HD11	1:E:323:LEU:HD13	1.55	0.88
1:A:10:LYS:HG2	1:A:96:TRP:CE2	2.08	0.88
1:C:313:ILE:HD11	1:C:323:LEU:HD13	1.55	0.88
1:D:272:PRO:O	1:D:273:ASP:HB3	1.71	0.88
1:F:138:TYR:CE2	1:F:188:ILE:HD12	2.08	0.88
1:C:606:HIS:HD2	1:C:608:GLN:HG2	1.39	0.88
1:D:138:TYR:CE2	1:D:188:ILE:HD12	2.08	0.88
1:C:138:TYR:CE2	1:C:188:ILE:HD12	2.08	0.88
1:A:272:PRO:O	1:A:273:ASP:HB3	1.71	0.88
1:B:10:LYS:HG2	1:B:96:TRP:CE2	2.08	0.88
1:C:493:LEU:HD13	1:C:498:ALA:HB2	1.56	0.88
1:E:606:HIS:HD2	1:E:608:GLN:HG2	1.39	0.88
1:D:493:LEU:HD13	1:D:498:ALA:HB2	1.56	0.88
1:F:272:PRO:O	1:F:273:ASP:HB3	1.71	0.87
1:F:493:LEU:HD13	1:F:498:ALA:HB2	1.56	0.87
1:C:272:PRO:O	1:C:273:ASP:HB3	1.71	0.87
1:D:10:LYS:HG2	1:D:96:TRP:CE2	2.08	0.87
1:A:493:LEU:HD13	1:A:498:ALA:HB2	1.56	0.87
1:F:10:LYS:HG2	1:F:96:TRP:CE2	2.08	0.87
1:E:493:LEU:HD13	1:E:498:ALA:HB2	1.56	0.87
1:B:493:LEU:HD13	1:B:498:ALA:HB2	1.56	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:606:HIS:HD2	1:B:608:GLN:HG2	1.39	0.86
1:A:140:ILE:HG22	1:A:141:THR:CG2	2.04	0.86
1:D:272:PRO:HG2	1:E:272:PRO:HG2	1.55	0.86
1:F:606:HIS:HD2	1:F:608:GLN:HG2	1.39	0.86
1:F:76:ASN:HB3	1:F:79:GLN:HB2	1.57	0.86
1:F:239:TRP:CZ2	1:F:574:LYS:HG2	2.11	0.86
1:E:140:ILE:HG22	1:E:141:THR:CG2	2.04	0.86
1:B:76:ASN:HB3	1:B:79:GLN:HB2	1.58	0.85
1:C:239:TRP:CZ2	1:C:574:LYS:HG2	2.10	0.85
1:D:239:TRP:CZ2	1:D:574:LYS:HG2	2.10	0.85
1:A:456:ASN:HD22	1:A:457:HIS:H	1.24	0.85
1:B:239:TRP:CZ2	1:B:574:LYS:HG2	2.10	0.85
1:B:456:ASN:HD22	1:B:457:HIS:H	1.24	0.85
1:C:175:LYS:O	1:D:491:ILE:CD1	2.25	0.85
1:A:239:TRP:CZ2	1:A:574:LYS:HG2	2.10	0.85
1:A:606:HIS:HD2	1:A:608:GLN:HG2	1.39	0.85
1:C:140:ILE:HG22	1:C:141:THR:CG2	2.04	0.85
1:C:76:ASN:HB3	1:C:79:GLN:HB2	1.58	0.85
1:B:140:ILE:HG22	1:B:141:THR:CG2	2.04	0.85
1:E:239:TRP:CZ2	1:E:574:LYS:HG2	2.10	0.85
1:E:76:ASN:HB3	1:E:79:GLN:HB2	1.58	0.84
1:D:140:ILE:HG22	1:D:141:THR:CG2	2.04	0.84
1:A:76:ASN:HB3	1:A:79:GLN:HB2	1.57	0.84
1:E:120:TYR:CD2	1:E:134:LEU:HD13	2.13	0.83
1:C:456:ASN:HD22	1:C:457:HIS:H	1.24	0.83
1:F:456:ASN:HD22	1:F:457:HIS:H	1.24	0.83
1:D:120:TYR:CD2	1:D:134:LEU:HD13	2.13	0.83
1:B:366:GLY:H	1:B:369:GLU:HG3	1.43	0.83
1:E:414:ASN:ND2	1:E:466:MET:HA	1.94	0.83
1:A:120:TYR:CD2	1:A:134:LEU:HD13	2.13	0.83
1:F:366:GLY:H	1:F:369:GLU:HG3	1.43	0.83
1:A:366:GLY:H	1:A:369:GLU:HG3	1.44	0.83
1:D:456:ASN:HD22	1:D:457:HIS:H	1.24	0.83
1:F:140:ILE:HG22	1:F:141:THR:CG2	2.04	0.83
1:D:414:ASN:ND2	1:D:466:MET:HA	1.94	0.83
1:B:414:ASN:ND2	1:B:466:MET:HA	1.94	0.83
1:C:414:ASN:ND2	1:C:466:MET:HA	1.94	0.82
1:F:414:ASN:ND2	1:F:466:MET:HA	1.94	0.82
1:F:120:TYR:CD2	1:F:134:LEU:HD13	2.13	0.82
1:D:366:GLY:H	1:D:369:GLU:HG3	1.43	0.82
1:B:120:TYR:CD2	1:B:134:LEU:HD13	2.13	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:TYR:CD2	1:C:134:LEU:HD13	2.14	0.82
1:F:462:TYR:O	1:F:520:GLU:HA	1.80	0.82
1:C:462:TYR:O	1:C:520:GLU:HA	1.80	0.82
1:D:76:ASN:HB3	1:D:79:GLN:HB2	1.58	0.82
1:D:462:TYR:O	1:D:520:GLU:HA	1.80	0.82
1:C:11:GLN:HG3	1:C:15:ASN:HD21	1.45	0.82
1:E:11:GLN:HG3	1:E:15:ASN:HD21	1.45	0.82
1:E:283:VAL:O	1:E:284:ALA:HB2	1.80	0.81
1:A:462:TYR:O	1:A:520:GLU:HA	1.80	0.81
1:F:11:GLN:HG3	1:F:15:ASN:HD21	1.45	0.81
1:B:462:TYR:O	1:B:520:GLU:HA	1.80	0.81
1:E:462:TYR:O	1:E:520:GLU:HA	1.80	0.81
1:E:366:GLY:H	1:E:369:GLU:HG3	1.43	0.81
1:A:283:VAL:O	1:A:284:ALA:HB2	1.80	0.81
1:E:456:ASN:HD22	1:E:457:HIS:H	1.24	0.81
1:F:606:HIS:HB3	1:F:608:GLN:H	1.46	0.81
1:C:366:GLY:H	1:C:369:GLU:HG3	1.44	0.81
1:C:576:GLU:OE1	1:D:576:GLU:OE1	1.98	0.81
1:A:414:ASN:ND2	1:A:466:MET:HA	1.94	0.81
1:D:559:GLU:O	1:D:560:ARG:HG3	1.81	0.81
1:C:175:LYS:C	1:D:491:ILE:HD11	2.02	0.80
1:E:606:HIS:HB3	1:E:608:GLN:H	1.46	0.80
1:C:283:VAL:O	1:C:284:ALA:HB2	1.80	0.80
1:B:559:GLU:O	1:B:560:ARG:HG3	1.81	0.80
1:C:559:GLU:O	1:C:560:ARG:HG3	1.81	0.80
1:B:606:HIS:HB3	1:B:608:GLN:H	1.46	0.80
1:F:283:VAL:O	1:F:284:ALA:HB2	1.80	0.80
1:B:11:GLN:HG3	1:B:15:ASN:HD21	1.45	0.80
1:D:11:GLN:HG3	1:D:15:ASN:HD21	1.45	0.80
1:E:559:GLU:O	1:E:560:ARG:HG3	1.81	0.79
1:A:639:VAL:HG23	1:A:641:ASN:ND2	1.98	0.79
1:A:559:GLU:O	1:A:560:ARG:HG3	1.81	0.79
1:F:639:VAL:HG23	1:F:641:ASN:ND2	1.98	0.79
1:F:559:GLU:O	1:F:560:ARG:HG3	1.81	0.79
1:C:606:HIS:HB3	1:C:608:GLN:H	1.46	0.79
1:C:272:PRO:HG2	1:F:272:PRO:HG2	1.64	0.79
1:D:283:VAL:O	1:D:284:ALA:HB2	1.80	0.79
1:F:295:ARG:HG2	1:F:339:TYR:CZ	2.18	0.79
1:D:606:HIS:HB3	1:D:608:GLN:H	1.46	0.79
1:E:639:VAL:HG23	1:E:641:ASN:ND2	1.98	0.79
1:B:295:ARG:HG2	1:B:339:TYR:CZ	2.18	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:ASP:OD1	1:E:189:GLY:N	2.16	0.79
1:A:295:ARG:HG2	1:A:339:TYR:CZ	2.18	0.79
1:C:187:ASP:OD1	1:C:189:GLY:N	2.16	0.79
1:A:408:PHE:N	1:A:641:ASN:OD1	2.16	0.78
1:A:316:ARG:HD3	4:A:829:HOH:O	1.81	0.78
1:D:295:ARG:HG2	1:D:339:TYR:CZ	2.18	0.78
1:B:639:VAL:HG23	1:B:641:ASN:ND2	1.98	0.78
1:B:187:ASP:OD1	1:B:189:GLY:N	2.16	0.78
1:D:639:VAL:HG23	1:D:641:ASN:ND2	1.98	0.78
1:E:239:TRP:CH2	1:E:574:LYS:HG2	2.19	0.78
1:E:8:ALA:HA	1:E:553:LEU:HD12	1.66	0.78
1:D:239:TRP:CH2	1:D:574:LYS:HG2	2.19	0.78
1:E:408:PHE:N	1:E:641:ASN:OD1	2.16	0.78
1:E:295:ARG:HG2	1:E:339:TYR:CZ	2.18	0.78
1:E:298:GLU:OE2	4:E:792:HOH:O	2.02	0.78
1:A:11:GLN:HG3	1:A:15:ASN:HD21	1.45	0.78
1:F:239:TRP:CH2	1:F:574:LYS:HG2	2.19	0.78
1:A:606:HIS:HB3	1:A:608:GLN:H	1.46	0.78
1:B:283:VAL:O	1:B:284:ALA:HB2	1.80	0.78
1:C:295:ARG:HG2	1:C:339:TYR:CZ	2.18	0.78
1:D:606:HIS:CD2	1:D:608:GLN:HG2	2.19	0.78
1:C:606:HIS:CD2	1:C:608:GLN:HG2	2.19	0.78
1:C:239:TRP:CH2	1:C:574:LYS:HG2	2.19	0.78
1:A:237:SER:HB3	1:A:573:SER:HA	1.67	0.78
1:B:408:PHE:N	1:B:641:ASN:OD1	2.16	0.78
1:A:551:HIS:CD2	1:A:552:ASP:N	2.52	0.78
1:B:551:HIS:CD2	1:B:552:ASP:N	2.52	0.78
1:C:639:VAL:HG23	1:C:641:ASN:ND2	1.98	0.78
1:D:473:GLU:HA	1:D:512:VAL:O	1.84	0.77
1:F:473:GLU:HA	1:F:512:VAL:O	1.84	0.77
1:F:408:PHE:N	1:F:641:ASN:OD1	2.17	0.77
1:C:8:ALA:HA	1:C:553:LEU:HD12	1.66	0.77
1:B:606:HIS:CD2	1:B:608:GLN:HG2	2.19	0.77
1:B:237:SER:HB3	1:B:573:SER:HA	1.66	0.77
1:A:557:ALA:HB3	1:A:558:TYR:CD1	2.20	0.77
1:A:239:TRP:CH2	1:A:574:LYS:HG2	2.19	0.77
1:B:150:VAL:HG21	1:B:168:VAL:HG12	1.67	0.77
1:E:317:GLN:HB2	1:E:318:PRO:HD2	1.66	0.77
1:B:239:TRP:CH2	1:B:574:LYS:HG2	2.19	0.77
1:C:557:ALA:HB3	1:C:558:TYR:CD1	2.20	0.77
1:D:150:VAL:HG21	1:D:168:VAL:HG12	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:LYS:O	1:C:175:LYS:HG2	1.85	0.77
1:C:175:LYS:HB2	1:D:491:ILE:HG12	1.66	0.77
1:A:606:HIS:CD2	1:A:608:GLN:HG2	2.19	0.77
1:D:551:HIS:CD2	1:D:552:ASP:N	2.52	0.77
1:D:557:ALA:HB3	1:D:558:TYR:CD1	2.20	0.77
1:E:551:HIS:CD2	1:E:552:ASP:N	2.52	0.77
1:F:174:LYS:O	1:F:175:LYS:HG2	1.85	0.77
1:A:174:LYS:O	1:A:175:LYS:HG2	1.85	0.77
1:D:317:GLN:HB2	1:D:318:PRO:HD2	1.66	0.77
1:E:150:VAL:HG21	1:E:168:VAL:HG12	1.67	0.77
1:F:150:VAL:HG21	1:F:168:VAL:HG12	1.67	0.77
1:A:187:ASP:OD1	1:A:189:GLY:N	2.16	0.77
1:B:557:ALA:HB3	1:B:558:TYR:CD1	2.20	0.77
1:A:473:GLU:HA	1:A:512:VAL:O	1.84	0.77
1:D:174:LYS:O	1:D:175:LYS:HG2	1.85	0.77
1:A:150:VAL:HG21	1:A:168:VAL:HG12	1.67	0.77
1:F:237:SER:HB3	1:F:573:SER:HA	1.66	0.77
1:D:408:PHE:N	1:D:641:ASN:OD1	2.16	0.77
1:F:551:HIS:CD2	1:F:552:ASP:N	2.52	0.77
1:C:585:ALA:CB	1:C:642:ILE:HG12	2.15	0.76
1:D:8:ALA:HA	1:D:553:LEU:HD12	1.66	0.76
1:C:237:SER:HB3	1:C:573:SER:HA	1.66	0.76
1:B:317:GLN:HB2	1:B:318:PRO:HD2	1.66	0.76
1:E:473:GLU:HA	1:E:512:VAL:O	1.84	0.76
1:C:408:PHE:N	1:C:641:ASN:OD1	2.17	0.76
1:D:585:ALA:CB	1:D:642:ILE:HG12	2.15	0.76
1:E:606:HIS:CD2	1:E:608:GLN:HG2	2.19	0.76
1:F:8:ALA:HA	1:F:553:LEU:HD12	1.66	0.76
1:A:317:GLN:HB2	1:A:318:PRO:HD2	1.66	0.76
1:E:174:LYS:O	1:E:175:LYS:HG2	1.85	0.76
1:F:187:ASP:OD1	1:F:189:GLY:N	2.16	0.76
1:F:317:GLN:HB2	1:F:318:PRO:HD2	1.66	0.76
1:C:551:HIS:CD2	1:C:552:ASP:N	2.52	0.76
1:B:201:PHE:HB3	1:B:216:LYS:CD	2.16	0.76
1:E:557:ALA:HB3	1:E:558:TYR:CD1	2.20	0.76
1:A:521:ARG:HD3	4:A:864:HOH:O	1.86	0.76
1:D:413:VAL:CG2	1:D:466:MET:HE3	2.16	0.76
1:C:473:GLU:HA	1:C:512:VAL:O	1.84	0.76
1:B:473:GLU:HA	1:B:512:VAL:O	1.84	0.76
1:B:585:ALA:CB	1:B:642:ILE:HG12	2.15	0.76
1:A:8:ALA:HA	1:A:553:LEU:HD12	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:LEU:HD23	1:F:86:LEU:O	1.86	0.76
1:B:174:LYS:O	1:B:175:LYS:HG2	1.85	0.76
1:C:150:VAL:HG21	1:C:168:VAL:HG12	1.67	0.76
1:F:606:HIS:CD2	1:F:608:GLN:HG2	2.19	0.76
1:C:86:LEU:O	1:C:86:LEU:HD23	1.86	0.76
1:D:201:PHE:HB3	1:D:216:LYS:CD	2.16	0.76
1:D:272:PRO:HG2	1:E:272:PRO:CG	2.16	0.76
1:F:557:ALA:HB3	1:F:558:TYR:CD1	2.20	0.76
1:A:201:PHE:HB3	1:A:216:LYS:CD	2.16	0.76
1:B:37:PHE:CE2	1:B:101:SER:HB3	2.21	0.76
1:C:317:GLN:HB2	1:C:318:PRO:HD2	1.66	0.76
1:F:201:PHE:HB3	1:F:216:LYS:CD	2.16	0.76
1:E:585:ALA:CB	1:E:642:ILE:HG12	2.15	0.76
1:E:37:PHE:CE2	1:E:101:SER:HB3	2.21	0.76
1:C:37:PHE:CE2	1:C:101:SER:HB3	2.21	0.76
1:C:201:PHE:HB3	1:C:216:LYS:CD	2.16	0.76
1:A:37:PHE:CE2	1:A:101:SER:HB3	2.21	0.76
1:D:237:SER:HB3	1:D:573:SER:HA	1.66	0.76
1:E:201:PHE:HB3	1:E:216:LYS:CD	2.16	0.76
1:F:585:ALA:CB	1:F:642:ILE:HG12	2.15	0.75
1:A:585:ALA:CB	1:A:642:ILE:HG12	2.15	0.75
1:D:533:MET:HB3	1:D:534:PRO:HD2	1.68	0.75
1:F:533:MET:HB3	1:F:534:PRO:HD2	1.68	0.75
1:D:84:LEU:HD11	1:D:204:TRP:CE2	2.21	0.75
1:A:84:LEU:HD11	1:A:204:TRP:CE2	2.21	0.75
1:D:634:ARG:HE	1:F:64:ARG:NE	1.84	0.75
1:E:237:SER:HB3	1:E:573:SER:HA	1.67	0.75
1:E:533:MET:HB3	1:E:534:PRO:HD2	1.68	0.75
1:B:533:MET:HB3	1:B:534:PRO:HD2	1.68	0.75
1:A:379:SER:HB3	4:A:719:HOH:O	1.85	0.75
1:C:175:LYS:HB2	1:D:491:ILE:CG1	2.16	0.75
1:A:533:MET:HB3	1:A:534:PRO:HD2	1.68	0.75
1:C:220:PHE:CE2	1:C:329:GLU:HB2	2.22	0.75
1:D:408:PHE:HB3	1:D:641:ASN:OD1	1.87	0.75
1:D:495:LEU:HD23	1:D:630:ILE:HG21	1.68	0.75
1:E:408:PHE:HB3	1:E:641:ASN:OD1	1.87	0.75
1:B:220:PHE:CE2	1:B:329:GLU:HB2	2.22	0.75
1:E:84:LEU:HD11	1:E:204:TRP:CE2	2.21	0.75
1:A:392:LYS:O	1:A:396:ASP:HB2	1.87	0.75
1:D:634:ARG:HH21	1:F:64:ARG:CD	1.98	0.75
1:F:408:PHE:HB3	1:F:641:ASN:OD1	1.87	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ALA:HA	1:B:553:LEU:HD12	1.66	0.75
1:D:86:LEU:O	1:D:86:LEU:HD23	1.86	0.75
1:B:86:LEU:HD23	1:B:86:LEU:O	1.86	0.74
1:C:408:PHE:HB3	1:C:641:ASN:OD1	1.87	0.74
1:D:392:LYS:O	1:D:396:ASP:HB2	1.87	0.74
1:E:86:LEU:HD23	1:E:86:LEU:O	1.86	0.74
1:F:392:LYS:O	1:F:396:ASP:HB2	1.87	0.74
1:B:185:GLY:O	1:B:375:THR:HG22	1.87	0.74
1:C:533:MET:HB3	1:C:534:PRO:HD2	1.68	0.74
1:D:185:GLY:O	1:D:375:THR:HG22	1.87	0.74
1:A:220:PHE:CE2	1:A:329:GLU:HB2	2.22	0.74
1:B:392:LYS:O	1:B:396:ASP:HB2	1.87	0.74
1:A:86:LEU:HD23	1:A:86:LEU:O	1.86	0.74
1:F:37:PHE:CE2	1:F:101:SER:HB3	2.21	0.74
1:A:235:ARG:NH2	4:A:705:HOH:O	1.98	0.74
1:C:495:LEU:HD23	1:C:630:ILE:HG21	1.68	0.74
1:D:283:VAL:HG11	1:D:349:VAL:HB	1.70	0.74
1:C:84:LEU:HD11	1:C:204:TRP:CE2	2.21	0.74
1:E:185:GLY:O	1:E:375:THR:HG22	1.87	0.74
1:F:220:PHE:CE2	1:F:329:GLU:HB2	2.22	0.74
1:A:408:PHE:HB3	1:A:641:ASN:OD1	1.87	0.74
1:E:220:PHE:CE2	1:E:329:GLU:HB2	2.22	0.74
1:D:177:ARG:HD2	1:E:360:LYS:HB3	1.68	0.74
1:D:37:PHE:CE2	1:D:101:SER:HB3	2.21	0.74
1:B:408:PHE:HB3	1:B:641:ASN:OD1	1.87	0.74
1:C:392:LYS:O	1:C:396:ASP:HB2	1.87	0.74
1:F:84:LEU:HD11	1:F:204:TRP:CE2	2.21	0.74
1:C:261:SER:OG	1:C:267:GLU:HG2	1.88	0.74
1:B:495:LEU:HD23	1:B:630:ILE:HG21	1.68	0.74
1:E:261:SER:OG	1:E:267:GLU:HG2	1.88	0.74
1:B:84:LEU:HD11	1:B:204:TRP:CE2	2.21	0.74
1:A:261:SER:OG	1:A:267:GLU:HG2	1.88	0.74
1:E:392:LYS:O	1:E:396:ASP:HB2	1.87	0.74
1:A:495:LEU:HD23	1:A:630:ILE:HG21	1.68	0.74
1:D:413:VAL:HG22	1:D:466:MET:HE3	1.70	0.74
1:F:185:GLY:O	1:F:375:THR:HG22	1.87	0.73
1:E:495:LEU:HD23	1:E:630:ILE:HG21	1.68	0.73
1:D:220:PHE:CE2	1:D:329:GLU:HB2	2.22	0.73
1:C:413:VAL:CG2	1:C:466:MET:HE3	2.18	0.73
1:B:283:VAL:HG11	1:B:349:VAL:HB	1.70	0.73
1:C:185:GLY:O	1:C:375:THR:HG22	1.87	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:PRO:CG	1:E:272:PRO:HG2	2.18	0.73
1:E:412:VAL:HG22	1:E:412:VAL:O	1.89	0.73
1:E:207:ASP:OD2	1:E:212:HIS:HB2	1.89	0.73
1:B:207:ASP:OD2	1:B:212:HIS:HB2	1.89	0.73
1:D:634:ARG:HE	1:F:64:ARG:CZ	2.01	0.73
1:F:495:LEU:HD23	1:F:630:ILE:HG21	1.68	0.73
1:D:187:ASP:OD1	1:D:189:GLY:N	2.16	0.73
1:A:412:VAL:O	1:A:412:VAL:HG22	1.89	0.73
1:C:175:LYS:HB2	1:D:491:ILE:HD11	1.71	0.73
1:C:86:LEU:CD2	1:C:90:LEU:HD22	2.19	0.73
1:A:185:GLY:O	1:A:375:THR:HG22	1.87	0.73
1:C:465:THR:HG23	1:C:518:THR:OG1	1.89	0.73
1:A:86:LEU:CD2	1:A:90:LEU:HD22	2.19	0.73
1:A:207:ASP:OD2	1:A:212:HIS:HB2	1.89	0.73
1:A:465:THR:HG23	1:A:518:THR:OG1	1.89	0.73
1:E:86:LEU:CD2	1:E:90:LEU:HD22	2.19	0.73
1:C:533:MET:HE3	1:C:533:MET:H	1.53	0.73
1:F:7:ASN:C	1:F:9:GLN:H	1.93	0.73
1:B:412:VAL:HG22	1:B:412:VAL:O	1.89	0.73
1:D:307:ASP:HA	1:D:336:ASN:HB2	1.71	0.72
1:A:413:VAL:CG2	1:A:466:MET:HE3	2.19	0.72
1:F:261:SER:OG	1:F:267:GLU:HG2	1.88	0.72
1:A:413:VAL:HG22	1:A:466:MET:HE3	1.71	0.72
1:F:307:ASP:HA	1:F:336:ASN:HB2	1.71	0.72
1:D:207:ASP:OD2	1:D:212:HIS:HB2	1.89	0.72
1:A:307:ASP:HA	1:A:336:ASN:HB2	1.71	0.72
1:B:261:SER:OG	1:B:267:GLU:HG2	1.88	0.72
1:D:261:SER:OG	1:D:267:GLU:HG2	1.88	0.72
1:F:465:THR:HG23	1:F:518:THR:OG1	1.89	0.72
1:D:10:LYS:HG2	1:D:96:TRP:CD2	2.25	0.72
1:D:465:THR:HG23	1:D:518:THR:OG1	1.89	0.72
1:C:207:ASP:OD2	1:C:212:HIS:HB2	1.89	0.72
1:F:207:ASP:OD2	1:F:212:HIS:HB2	1.89	0.72
1:B:86:LEU:CD2	1:B:90:LEU:HD22	2.19	0.72
1:B:465:THR:HG23	1:B:518:THR:OG1	1.89	0.72
1:A:10:LYS:HG2	1:A:96:TRP:CD2	2.25	0.72
1:A:283:VAL:HG11	1:A:349:VAL:HB	1.70	0.72
1:F:86:LEU:CD2	1:F:90:LEU:HD22	2.19	0.72
1:D:86:LEU:CD2	1:D:90:LEU:HD22	2.19	0.72
2:D:659:NAG:N2	2:D:659:NAG:C8	2.52	0.72
1:B:10:LYS:HG2	1:B:96:TRP:CD2	2.25	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:LYS:HG2	1:F:96:TRP:CD2	2.25	0.72
1:C:307:ASP:HA	1:C:336:ASN:HB2	1.71	0.72
1:E:10:LYS:HG2	1:E:96:TRP:CD2	2.25	0.72
1:F:283:VAL:HG11	1:F:349:VAL:HB	1.70	0.72
1:D:412:VAL:O	1:D:412:VAL:HG22	1.89	0.72
1:C:283:VAL:HG11	1:C:349:VAL:HB	1.70	0.71
1:B:307:ASP:HA	1:B:336:ASN:HB2	1.71	0.71
1:E:307:ASP:HA	1:E:336:ASN:HB2	1.71	0.71
1:E:465:THR:HG23	1:E:518:THR:OG1	1.89	0.71
1:C:413:VAL:HG22	1:C:466:MET:HE3	1.71	0.71
1:C:10:LYS:HG2	1:C:96:TRP:CD2	2.25	0.71
1:D:537:GLN:O	1:D:540:LYS:N	2.23	0.71
1:C:412:VAL:HG22	1:C:412:VAL:O	1.89	0.71
1:F:565:PRO:HB2	1:F:568:MET:CG	2.21	0.71
1:B:565:PRO:HB2	1:B:568:MET:CG	2.21	0.71
1:F:174:LYS:C	1:F:175:LYS:HG2	2.11	0.71
1:E:174:LYS:C	1:E:175:LYS:HG2	2.11	0.71
1:E:253:ARG:NH1	1:E:274:ASN:OD1	2.24	0.71
1:D:569:LEU:HD23	1:D:570:LEU:HD13	1.73	0.71
1:D:477:THR:HB	1:D:479:ARG:NH1	2.06	0.71
1:B:174:LYS:C	1:B:175:LYS:HG2	2.11	0.71
1:E:477:THR:HB	1:E:479:ARG:NH1	2.06	0.71
1:A:477:THR:HB	1:A:479:ARG:NH1	2.06	0.71
1:C:487:ASP:HB3	1:C:490:GLY:H	1.56	0.71
2:C:659:NAG:C8	2:C:659:NAG:N2	2.52	0.71
1:D:174:LYS:C	1:D:175:LYS:HG2	2.11	0.71
1:B:167:ASN:OD1	1:B:451:ARG:NE	2.24	0.71
1:B:123:VAL:HG11	1:B:134:LEU:HD21	1.73	0.71
1:E:283:VAL:HG11	1:E:349:VAL:HB	1.70	0.71
1:C:477:THR:HB	1:C:479:ARG:NH1	2.06	0.71
1:C:174:LYS:C	1:C:175:LYS:HG2	2.11	0.71
1:A:177:ARG:NH1	1:A:179:GLN:HG3	2.06	0.71
1:C:569:LEU:HD23	1:C:570:LEU:HD13	1.73	0.71
1:A:123:VAL:HG11	1:A:134:LEU:HD21	1.72	0.70
1:E:565:PRO:HB2	1:E:568:MET:HG2	1.74	0.70
1:C:177:ARG:NH1	1:C:179:GLN:HG3	2.06	0.70
1:C:253:ARG:NH1	1:C:274:ASN:OD1	2.24	0.70
1:E:167:ASN:OD1	1:E:451:ARG:NE	2.24	0.70
1:E:487:ASP:HB3	1:E:490:GLY:H	1.56	0.70
1:E:177:ARG:NH1	1:E:179:GLN:HG3	2.06	0.70
1:B:537:GLN:O	1:B:540:LYS:N	2.23	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ARG:NH1	1:B:274:ASN:OD1	2.24	0.70
1:D:167:ASN:OD1	1:D:451:ARG:NE	2.24	0.70
1:F:463:LYS:HG2	1:F:520:GLU:HB2	1.73	0.70
1:F:537:GLN:O	1:F:540:LYS:N	2.23	0.70
1:F:177:ARG:NH1	1:F:179:GLN:HG3	2.06	0.70
1:F:253:ARG:NH1	1:F:274:ASN:OD1	2.24	0.70
1:E:413:VAL:HG22	1:E:466:MET:HE3	1.74	0.70
1:F:295:ARG:HG2	1:F:339:TYR:CE1	2.27	0.70
1:D:565:PRO:HB2	1:D:568:MET:HG2	1.74	0.70
1:A:253:ARG:NH1	1:A:274:ASN:OD1	2.24	0.70
1:D:253:ARG:NH1	1:D:274:ASN:OD1	2.24	0.70
1:E:463:LYS:HG2	1:E:520:GLU:HB2	1.73	0.70
1:D:565:PRO:HB2	1:D:568:MET:CG	2.21	0.70
1:E:569:LEU:HD23	1:E:570:LEU:HD13	1.73	0.70
1:B:177:ARG:NH1	1:B:179:GLN:HG3	2.06	0.70
1:A:487:ASP:HB3	1:A:490:GLY:H	1.56	0.70
1:B:487:ASP:HB3	1:B:490:GLY:H	1.56	0.70
1:E:123:VAL:HG11	1:E:134:LEU:HD21	1.72	0.70
1:E:565:PRO:HB2	1:E:568:MET:CG	2.21	0.70
1:B:152:ASP:OD1	4:B:679:HOH:O	2.10	0.70
1:A:565:PRO:HB2	1:A:568:MET:CG	2.21	0.70
1:A:81:LYS:HD2	4:A:793:HOH:O	1.90	0.70
1:D:123:VAL:HG11	1:D:134:LEU:HD21	1.73	0.70
1:D:295:ARG:HG2	1:D:339:TYR:CE1	2.26	0.70
1:A:174:LYS:C	1:A:175:LYS:HG2	2.11	0.70
1:F:413:VAL:CG2	1:F:466:MET:HE3	2.22	0.70
1:A:411:MET:CG	4:A:834:HOH:O	2.22	0.70
1:A:167:ASN:OD1	1:A:451:ARG:NE	2.24	0.70
1:F:477:THR:HB	1:F:479:ARG:NH1	2.06	0.70
1:D:177:ARG:NH1	1:D:179:GLN:HG3	2.06	0.70
1:D:424:THR:O	1:D:651:HIS:ND1	2.23	0.70
1:C:295:ARG:HG2	1:C:339:TYR:CE1	2.27	0.70
1:F:412:VAL:O	1:F:412:VAL:HG22	1.89	0.70
1:B:569:LEU:HD23	1:B:570:LEU:HD13	1.73	0.70
2:F:658:NDG:N2	2:F:658:NDG:C8	2.55	0.70
2:B:658:NDG:C8	2:B:658:NDG:N2	2.55	0.70
1:B:295:ARG:HG2	1:B:339:TYR:CE1	2.27	0.70
1:B:477:THR:HB	1:B:479:ARG:NH1	2.06	0.70
1:A:569:LEU:HD23	1:A:570:LEU:HD13	1.73	0.70
1:C:565:PRO:HB2	1:C:568:MET:CG	2.21	0.70
1:E:413:VAL:CG2	1:E:466:MET:HE3	2.22	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:487:ASP:HB3	1:F:490:GLY:H	1.56	0.69
1:C:123:VAL:HG11	1:C:134:LEU:HD21	1.73	0.69
1:D:121:VAL:HG23	1:D:199:MET:HG2	1.74	0.69
1:F:569:LEU:HD23	1:F:570:LEU:HD13	1.73	0.69
1:A:463:LYS:HG2	1:A:520:GLU:HB2	1.73	0.69
1:C:167:ASN:OD1	1:C:451:ARG:NE	2.24	0.69
1:A:382:ARG:HD2	4:A:712:HOH:O	1.91	0.69
1:A:59:GLU:OE1	1:A:64:ARG:CD	2.38	0.69
1:B:487:ASP:HB3	1:B:489:ASN:N	2.04	0.69
1:A:295:ARG:HG2	1:A:339:TYR:CE1	2.27	0.69
2:B:659:NAG:N2	2:B:659:NAG:C8	2.52	0.69
1:E:8:ALA:CA	1:E:553:LEU:HD12	2.23	0.69
1:B:424:THR:O	1:B:651:HIS:ND1	2.23	0.69
1:C:463:LYS:HG2	1:C:520:GLU:HB2	1.73	0.69
1:D:89:VAL:O	1:D:91:ASN:N	2.26	0.69
1:E:537:GLN:O	1:E:540:LYS:N	2.23	0.69
1:B:59:GLU:OE1	1:B:64:ARG:CD	2.38	0.69
2:E:658:NDG:N2	2:E:658:NDG:C8	2.55	0.69
1:B:463:LYS:HG2	1:B:520:GLU:HB2	1.73	0.69
1:E:295:ARG:HG2	1:E:339:TYR:CE1	2.27	0.69
1:B:565:PRO:HB2	1:B:568:MET:HG2	1.74	0.69
1:E:121:VAL:HG23	1:E:199:MET:HG2	1.74	0.69
2:D:658:NDG:N2	2:D:658:NDG:C8	2.55	0.69
2:A:658:NDG:C8	2:A:658:NDG:N2	2.55	0.69
1:A:8:ALA:CA	1:A:553:LEU:HD12	2.23	0.69
1:C:89:VAL:O	1:C:91:ASN:N	2.26	0.69
1:B:89:VAL:O	1:B:91:ASN:N	2.26	0.69
1:F:565:PRO:HB2	1:F:568:MET:HG2	1.74	0.69
1:C:565:PRO:HB2	1:C:568:MET:HG2	1.74	0.69
1:E:69:ARG:N	1:E:112:GLU:OE2	2.25	0.69
1:D:487:ASP:HB3	1:D:490:GLY:H	1.56	0.69
1:D:463:LYS:HG2	1:D:520:GLU:HB2	1.73	0.69
1:F:59:GLU:OE1	1:F:64:ARG:CD	2.38	0.69
1:B:8:ALA:CA	1:B:553:LEU:HD12	2.23	0.69
1:B:121:VAL:HG23	1:B:199:MET:HG2	1.74	0.69
1:B:69:ARG:N	1:B:112:GLU:OE2	2.25	0.69
1:B:307:ASP:OD2	1:B:311:HIS:HB2	1.93	0.68
1:C:535:SER:HB3	1:C:538:SER:HB3	1.76	0.68
1:D:522:SER:O	1:D:523:SER:C	2.32	0.68
1:F:121:VAL:HG23	1:F:199:MET:HG2	1.74	0.68
1:F:123:VAL:HG11	1:F:134:LEU:HD21	1.73	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:89:VAL:O	1:F:91:ASN:N	2.26	0.68
1:A:89:VAL:O	1:A:91:ASN:N	2.26	0.68
1:A:565:PRO:HB2	1:A:568:MET:HG2	1.74	0.68
1:F:522:SER:O	1:F:523:SER:C	2.32	0.68
1:C:537:GLN:O	1:C:540:LYS:N	2.24	0.68
1:C:8:ALA:CA	1:C:553:LEU:HD12	2.23	0.68
1:E:535:SER:HB3	1:E:538:SER:HB3	1.76	0.68
1:A:69:ARG:N	1:A:112:GLU:OE2	2.25	0.68
1:D:59:GLU:OE1	1:D:64:ARG:CD	2.38	0.68
1:B:413:VAL:HG22	1:B:466:MET:HE3	1.76	0.68
1:A:522:SER:O	1:A:523:SER:C	2.32	0.68
1:C:121:VAL:HG23	1:C:199:MET:HG2	1.74	0.68
1:F:413:VAL:HG22	1:F:466:MET:HE3	1.74	0.68
1:F:8:ALA:CA	1:F:553:LEU:HD12	2.23	0.68
1:F:307:ASP:OD2	1:F:311:HIS:HB2	1.93	0.68
1:D:535:SER:HB3	1:D:538:SER:HB3	1.76	0.68
1:F:167:ASN:OD1	1:F:451:ARG:NE	2.24	0.68
1:C:59:GLU:OE1	1:C:64:ARG:CD	2.38	0.68
1:D:8:ALA:CA	1:D:553:LEU:HD12	2.23	0.68
1:D:84:LEU:HD11	1:D:204:TRP:CZ2	2.29	0.68
1:C:84:LEU:HD11	1:C:204:TRP:CZ2	2.29	0.68
1:E:89:VAL:O	1:E:91:ASN:N	2.26	0.68
1:E:84:LEU:HD11	1:E:204:TRP:CZ2	2.29	0.68
1:F:69:ARG:N	1:F:112:GLU:OE2	2.26	0.68
1:E:487:ASP:HB3	1:E:489:ASN:N	2.04	0.68
1:A:573:SER:N	4:A:857:HOH:O	2.27	0.68
1:A:84:LEU:HD11	1:A:204:TRP:CZ2	2.29	0.68
1:A:360:LYS:CE	1:B:273:ASP:OD2	2.41	0.68
1:B:414:ASN:ND2	1:B:467:SER:H	1.93	0.67
1:C:7:ASN:O	1:C:9:GLN:N	2.27	0.67
1:F:7:ASN:O	1:F:9:GLN:N	2.28	0.67
1:C:278:GLU:H	1:C:354:GLN:HE22	1.42	0.67
1:C:307:ASP:OD2	1:C:311:HIS:HB2	1.93	0.67
2:E:659:NAG:N2	2:E:659:NAG:C8	2.52	0.67
2:C:658:NDG:C8	2:C:658:NDG:N2	2.55	0.67
1:E:7:ASN:O	1:E:9:GLN:N	2.27	0.67
1:A:7:ASN:O	1:A:9:GLN:N	2.27	0.67
1:F:84:LEU:HD11	1:F:204:TRP:CZ2	2.29	0.67
1:D:278:GLU:H	1:D:354:GLN:HE22	1.42	0.67
1:A:121:VAL:HG23	1:A:199:MET:HG2	1.74	0.67
1:D:639:VAL:HG23	1:D:641:ASN:HD22	1.60	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:ASP:OD2	1:D:311:HIS:HB2	1.93	0.67
1:E:307:ASP:OD2	1:E:311:HIS:HB2	1.93	0.67
1:A:537:GLN:O	1:A:540:LYS:N	2.23	0.67
1:B:76:ASN:O	1:B:77:THR:C	2.32	0.67
2:A:659:NAG:N2	2:A:659:NAG:C8	2.52	0.67
2:F:659:NAG:N2	2:F:659:NAG:C8	2.52	0.67
1:B:413:VAL:CG2	1:B:466:MET:HE3	2.25	0.67
1:D:7:ASN:O	1:D:9:GLN:N	2.28	0.67
1:A:424:THR:O	1:A:651:HIS:ND1	2.23	0.67
1:F:535:SER:HB3	1:F:538:SER:HB3	1.76	0.67
1:E:182:ALA:O	1:E:186:GLU:HB2	1.95	0.67
1:A:182:ALA:O	1:A:186:GLU:HB2	1.95	0.67
1:E:353:ARG:C	1:E:355:GLY:H	1.97	0.67
1:A:572:LYS:N	4:A:857:HOH:O	2.28	0.67
1:B:278:GLU:H	1:B:354:GLN:HE22	1.42	0.67
1:E:414:ASN:ND2	1:E:467:SER:H	1.93	0.67
1:C:424:THR:O	1:C:651:HIS:ND1	2.23	0.67
1:E:639:VAL:HG23	1:E:641:ASN:HD22	1.60	0.67
1:B:535:SER:HB3	1:B:538:SER:HB3	1.76	0.67
1:B:182:ALA:O	1:B:186:GLU:HB2	1.95	0.67
1:C:634:ARG:HH21	1:E:64:ARG:HD2	1.59	0.67
1:B:353:ARG:C	1:B:355:GLY:H	1.97	0.67
1:F:278:GLU:H	1:F:354:GLN:HE22	1.42	0.67
1:A:535:SER:HB3	1:A:538:SER:HB3	1.76	0.67
1:D:414:ASN:ND2	1:D:467:SER:H	1.93	0.67
1:A:353:ARG:C	1:A:355:GLY:N	2.49	0.67
1:C:639:VAL:HG23	1:C:641:ASN:HD22	1.60	0.67
1:A:307:ASP:OD2	1:A:311:HIS:HB2	1.93	0.67
1:C:353:ARG:C	1:C:355:GLY:H	1.97	0.66
1:F:414:ASN:ND2	1:F:467:SER:H	1.93	0.66
1:C:414:ASN:ND2	1:C:467:SER:H	1.93	0.66
1:B:84:LEU:HD11	1:B:204:TRP:CZ2	2.29	0.66
1:D:182:ALA:O	1:D:186:GLU:HB2	1.95	0.66
1:B:551:HIS:O	1:B:552:ASP:HB3	1.96	0.66
1:C:551:HIS:O	1:C:552:ASP:HB3	1.96	0.66
1:F:353:ARG:C	1:F:355:GLY:H	1.97	0.66
1:F:424:THR:O	1:F:651:HIS:ND1	2.23	0.66
1:A:353:ARG:C	1:A:355:GLY:H	1.97	0.66
1:E:424:THR:O	1:E:651:HIS:ND1	2.23	0.66
1:E:522:SER:O	1:E:523:SER:C	2.32	0.66
1:C:182:ALA:O	1:C:186:GLU:HB2	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ASP:OD2	1:B:360:LYS:CE	2.41	0.66
1:D:177:ARG:CD	1:E:360:LYS:HB3	2.25	0.66
1:B:7:ASN:O	1:B:9:GLN:N	2.28	0.66
1:D:551:HIS:O	1:D:552:ASP:HB3	1.96	0.66
1:A:48:ASP:CB	1:A:92:GLN:HE21	2.09	0.66
1:F:182:ALA:O	1:F:186:GLU:HB2	1.95	0.66
1:A:475:LEU:HB2	1:A:590:ASP:OD1	1.96	0.66
1:B:353:ARG:C	1:B:355:GLY:N	2.49	0.66
1:D:353:ARG:C	1:D:355:GLY:H	1.97	0.66
1:D:48:ASP:CB	1:D:92:GLN:HE21	2.09	0.66
1:F:1:ASP:HB2	1:F:4:GLY:H	1.61	0.66
1:C:491:ILE:HD11	1:D:175:LYS:O	1.96	0.66
1:D:487:ASP:HB3	1:D:489:ASN:N	2.04	0.66
1:A:639:VAL:HG23	1:A:641:ASN:HD22	1.60	0.66
1:D:475:LEU:HB2	1:D:590:ASP:OD1	1.96	0.66
1:A:414:ASN:ND2	1:A:467:SER:H	1.93	0.66
1:C:1:ASP:HB2	1:C:4:GLY:H	1.61	0.66
1:C:522:SER:O	1:C:523:SER:C	2.32	0.66
1:C:76:ASN:O	1:C:77:THR:C	2.32	0.66
1:B:48:ASP:CB	1:B:92:GLN:HE21	2.09	0.66
1:C:634:ARG:HH11	1:C:634:ARG:CG	2.09	0.65
1:F:48:ASP:CB	1:F:92:GLN:HE21	2.09	0.65
1:F:475:LEU:HB2	1:F:590:ASP:OD1	1.96	0.65
1:D:76:ASN:O	1:D:77:THR:C	2.32	0.65
1:E:353:ARG:C	1:E:355:GLY:N	2.49	0.65
1:A:533:MET:HE3	1:A:533:MET:H	1.61	0.65
1:A:1:ASP:HB2	1:A:4:GLY:H	1.61	0.65
1:C:475:LEU:HB2	1:C:590:ASP:OD1	1.96	0.65
1:D:1:ASP:HB2	1:D:4:GLY:H	1.61	0.65
1:F:639:VAL:HG23	1:F:641:ASN:HD22	1.60	0.65
1:B:533:MET:H	1:B:533:MET:HE3	1.61	0.65
1:E:59:GLU:OE1	1:E:64:ARG:CD	2.38	0.65
1:B:165:THR:CG2	1:B:449:ASN:HB2	2.27	0.65
1:F:512:VAL:CG1	1:F:513:PRO:HD2	2.27	0.65
1:F:353:ARG:C	1:F:355:GLY:N	2.49	0.65
1:D:353:ARG:C	1:D:355:GLY:N	2.49	0.65
1:C:529:THR:O	1:C:530:VAL:HG23	1.97	0.65
1:D:69:ARG:N	1:D:112:GLU:OE2	2.25	0.65
1:E:512:VAL:CG1	1:E:513:PRO:HD2	2.27	0.65
1:E:414:ASN:HD21	1:E:467:SER:H	1.45	0.65
1:C:414:ASN:HD21	1:C:467:SER:H	1.45	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:ASN:HD21	1:B:467:SER:H	1.45	0.65
1:A:353:ARG:O	1:A:355:GLY:N	2.30	0.65
1:C:48:ASP:CB	1:C:92:GLN:HE21	2.09	0.65
1:C:69:ARG:N	1:C:112:GLU:OE2	2.25	0.65
1:F:446:VAL:HG13	1:F:446:VAL:O	1.97	0.65
1:F:414:ASN:HD21	1:F:467:SER:H	1.45	0.65
1:D:512:VAL:CG1	1:D:513:PRO:HD2	2.27	0.65
1:A:414:ASN:HD21	1:A:467:SER:H	1.45	0.65
1:B:512:VAL:CG1	1:B:513:PRO:HD2	2.27	0.65
1:A:278:GLU:H	1:A:354:GLN:HE22	1.42	0.65
1:B:475:LEU:HB2	1:B:590:ASP:OD1	1.96	0.65
1:B:40:LEU:HD11	1:B:54:GLU:HG3	1.79	0.65
1:E:39:PRO:HB3	1:E:102:ASN:HD21	1.62	0.65
1:B:353:ARG:O	1:B:355:GLY:N	2.30	0.65
1:F:353:ARG:O	1:F:355:GLY:N	2.30	0.65
1:A:551:HIS:O	1:A:552:ASP:HB3	1.96	0.65
1:E:475:LEU:HB2	1:E:590:ASP:OD1	1.96	0.65
1:C:40:LEU:HD11	1:C:54:GLU:HG3	1.79	0.65
1:C:487:ASP:HB3	1:C:489:ASN:N	2.04	0.65
1:E:278:GLU:H	1:E:354:GLN:HE22	1.42	0.65
1:C:551:HIS:HD2	1:C:552:ASP:HA	1.62	0.65
1:A:529:THR:O	1:A:530:VAL:HG23	1.97	0.65
1:E:473:GLU:C	1:E:474:ARG:HG2	2.17	0.65
1:B:46:TYR:CE2	1:B:53:VAL:HG21	2.32	0.65
1:D:39:PRO:HB3	1:D:102:ASN:HD21	1.62	0.65
1:F:529:THR:O	1:F:530:VAL:HG23	1.97	0.65
1:E:466:MET:HG3	1:E:466:MET:O	1.97	0.64
1:B:455:LEU:HG	1:B:456:ASN:N	2.13	0.64
1:E:48:ASP:CB	1:E:92:GLN:HE21	2.09	0.64
1:D:40:LEU:HD11	1:D:54:GLU:HG3	1.79	0.64
1:B:529:THR:O	1:B:530:VAL:HG23	1.97	0.64
1:F:148:SER:HB2	1:F:259:LEU:O	1.97	0.64
1:E:446:VAL:O	1:E:446:VAL:HG13	1.97	0.64
1:C:353:ARG:O	1:C:355:GLY:N	2.30	0.64
1:D:551:HIS:HD2	1:D:552:ASP:HA	1.62	0.64
1:D:533:MET:H	1:D:533:MET:HE3	1.61	0.64
1:B:148:SER:HB2	1:B:259:LEU:O	1.97	0.64
1:E:1:ASP:HB2	1:E:4:GLY:H	1.61	0.64
1:D:529:THR:O	1:D:530:VAL:HG23	1.97	0.64
1:B:473:GLU:C	1:B:474:ARG:HG2	2.18	0.64
1:C:39:PRO:HB3	1:C:102:ASN:HD21	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:ARG:O	1:D:355:GLY:N	2.30	0.64
1:E:353:ARG:O	1:E:355:GLY:N	2.30	0.64
1:B:551:HIS:HD2	1:B:552:ASP:HA	1.62	0.64
1:E:551:HIS:O	1:E:552:ASP:HB3	1.96	0.64
1:B:446:VAL:HG13	1:B:446:VAL:O	1.97	0.64
1:A:39:PRO:HB3	1:A:102:ASN:HD21	1.62	0.64
1:D:455:LEU:HG	1:D:456:ASN:N	2.13	0.64
1:C:353:ARG:C	1:C:355:GLY:N	2.49	0.64
1:A:446:VAL:HG13	1:A:446:VAL:O	1.97	0.64
1:D:466:MET:O	1:D:466:MET:HG3	1.97	0.64
1:D:414:ASN:HD21	1:D:467:SER:H	1.45	0.64
1:A:473:GLU:C	1:A:474:ARG:HG2	2.17	0.64
1:A:512:VAL:CG1	1:A:513:PRO:HD2	2.27	0.64
1:E:165:THR:CG2	1:E:449:ASN:HB2	2.27	0.64
1:A:551:HIS:HD2	1:A:552:ASP:HA	1.62	0.64
1:F:551:HIS:O	1:F:552:ASP:HB3	1.96	0.64
1:B:522:SER:O	1:B:523:SER:C	2.32	0.64
1:C:148:SER:HB2	1:C:259:LEU:O	1.97	0.64
1:A:40:LEU:HD11	1:A:54:GLU:HG3	1.79	0.64
1:B:1:ASP:HB2	1:B:4:GLY:H	1.61	0.64
1:C:512:VAL:CG1	1:C:513:PRO:HD2	2.27	0.64
1:F:165:THR:CG2	1:F:449:ASN:HB2	2.27	0.64
1:F:46:TYR:CE2	1:F:53:VAL:HG21	2.32	0.64
1:F:76:ASN:O	1:F:77:THR:C	2.32	0.64
1:F:40:LEU:HD11	1:F:54:GLU:HG3	1.79	0.64
1:F:487:ASP:HB3	1:F:489:ASN:N	2.04	0.64
1:B:466:MET:O	1:B:466:MET:HG3	1.97	0.64
1:D:46:TYR:CE2	1:D:53:VAL:HG21	2.32	0.64
1:B:639:VAL:HG23	1:B:641:ASN:HD22	1.60	0.64
1:E:46:TYR:CE2	1:E:53:VAL:HG21	2.32	0.64
1:B:39:PRO:HB3	1:B:102:ASN:HD21	1.62	0.64
1:A:148:SER:HB2	1:A:259:LEU:O	1.97	0.64
1:C:473:GLU:C	1:C:474:ARG:HG2	2.17	0.64
1:E:40:LEU:HD11	1:E:54:GLU:HG3	1.79	0.64
1:E:148:SER:HB2	1:E:259:LEU:O	1.97	0.64
1:A:487:ASP:HB3	1:A:489:ASN:N	2.04	0.64
1:C:46:TYR:CE2	1:C:53:VAL:HG21	2.32	0.64
1:A:46:TYR:CE2	1:A:53:VAL:HG21	2.32	0.64
1:A:255:GLY:HA2	1:A:271:ARG:NH1	2.13	0.64
1:F:473:GLU:C	1:F:474:ARG:HG2	2.17	0.63
1:A:466:MET:O	1:A:466:MET:HG3	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:GLY:HA2	1:F:271:ARG:NH1	2.14	0.63
1:F:551:HIS:HD2	1:F:552:ASP:HA	1.62	0.63
1:E:168:VAL:CG2	1:E:452:VAL:HG12	2.29	0.63
1:E:300:ILE:HG12	1:E:324:LEU:HD11	1.81	0.63
1:D:446:VAL:HG13	1:D:446:VAL:O	1.97	0.63
1:D:61:ASN:C	1:D:63:HIS:H	2.02	0.63
1:C:466:MET:O	1:C:466:MET:HG3	1.97	0.63
1:B:168:VAL:CG2	1:B:452:VAL:HG12	2.29	0.63
1:F:300:ILE:HG12	1:F:324:LEU:HD11	1.81	0.63
1:B:255:GLY:HA2	1:B:271:ARG:NH1	2.13	0.63
1:B:29:ASP:N	1:B:29:ASP:OD1	2.31	0.63
1:C:446:VAL:HG13	1:C:446:VAL:O	1.97	0.63
1:F:466:MET:O	1:F:466:MET:HG3	1.97	0.63
1:B:300:ILE:HG12	1:B:324:LEU:HD11	1.81	0.63
1:D:473:GLU:C	1:D:474:ARG:HG2	2.17	0.63
1:F:455:LEU:HG	1:F:456:ASN:N	2.13	0.63
1:E:455:LEU:HG	1:E:456:ASN:N	2.13	0.63
1:E:551:HIS:HD2	1:E:552:ASP:HA	1.62	0.63
1:E:533:MET:CB	1:E:534:PRO:HD2	2.28	0.63
1:E:255:GLY:HA2	1:E:271:ARG:NH1	2.14	0.63
1:B:5:THR:HG23	1:B:10:LYS:HE3	1.81	0.63
1:E:529:THR:O	1:E:530:VAL:HG23	1.97	0.63
1:C:300:ILE:HG12	1:C:324:LEU:HD11	1.81	0.63
1:A:183:TYR:OH	1:A:234:GLU:OE1	2.11	0.63
1:D:148:SER:HB2	1:D:259:LEU:O	1.97	0.63
1:A:5:THR:HG23	1:A:10:LYS:HE3	1.81	0.63
1:A:455:LEU:HG	1:A:456:ASN:N	2.13	0.63
1:F:150:VAL:HG12	1:F:433:LEU:HD11	1.81	0.63
1:D:380:PHE:CE2	1:D:384:HIS:CE1	2.87	0.63
1:D:300:ILE:HG12	1:D:324:LEU:HD11	1.81	0.63
1:D:486:GLU:HA	1:D:492:THR:HA	1.81	0.63
1:E:634:ARG:HH11	1:E:634:ARG:CG	2.09	0.63
1:C:255:GLY:HA2	1:C:271:ARG:NH1	2.14	0.63
1:F:5:THR:HG23	1:F:10:LYS:HE3	1.81	0.63
1:F:39:PRO:HB3	1:F:102:ASN:HD21	1.62	0.63
1:A:239:TRP:CH2	1:A:574:LYS:HE3	2.34	0.63
1:F:402:THR:HG23	1:F:405:ASN:OD1	1.99	0.63
1:B:380:PHE:CE2	1:B:384:HIS:CE1	2.87	0.63
1:A:61:ASN:C	1:A:63:HIS:H	2.02	0.62
1:E:512:VAL:HG13	1:E:513:PRO:HD2	1.81	0.62
1:D:254:GLU:OE2	1:E:360:LYS:NZ	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:TRP:CH2	1:C:574:LYS:HE3	2.34	0.62
1:D:168:VAL:CG2	1:D:452:VAL:HG12	2.28	0.62
1:E:486:GLU:HA	1:E:492:THR:HA	1.81	0.62
1:D:239:TRP:CH2	1:D:574:LYS:HE3	2.34	0.62
1:C:455:LEU:HG	1:C:456:ASN:N	2.13	0.62
1:E:150:VAL:HG12	1:E:433:LEU:HD11	1.81	0.62
1:F:168:VAL:CG2	1:F:452:VAL:HG12	2.29	0.62
1:C:262:TYR:CE1	1:C:268:PHE:CE1	2.88	0.62
1:C:486:GLU:HA	1:C:492:THR:HA	1.81	0.62
1:C:168:VAL:CG2	1:C:452:VAL:HG12	2.28	0.62
1:B:402:THR:HG23	1:B:405:ASN:OD1	1.99	0.62
1:E:380:PHE:CE2	1:E:384:HIS:CE1	2.87	0.62
1:C:183:TYR:OH	1:C:234:GLU:OE1	2.11	0.62
1:D:512:VAL:HG13	1:D:513:PRO:HD2	1.81	0.62
1:A:168:VAL:CG2	1:A:452:VAL:HG12	2.29	0.62
1:E:262:TYR:CE1	1:E:268:PHE:CE1	2.88	0.62
1:A:300:ILE:HG12	1:A:324:LEU:HD11	1.81	0.62
1:E:239:TRP:CH2	1:E:574:LYS:HE3	2.34	0.62
1:D:62:ASP:O	1:D:63:HIS:HD2	1.83	0.62
1:F:512:VAL:HG13	1:F:513:PRO:HD2	1.81	0.62
1:B:512:VAL:HG13	1:B:513:PRO:HD2	1.81	0.62
1:A:76:ASN:O	1:A:77:THR:C	2.32	0.62
1:A:402:THR:HG23	1:A:405:ASN:OD1	1.99	0.62
1:B:486:GLU:HA	1:B:492:THR:HA	1.81	0.62
1:D:402:THR:HG23	1:D:405:ASN:OD1	1.99	0.62
1:C:380:PHE:CE2	1:C:384:HIS:CE1	2.87	0.62
1:E:61:ASN:C	1:E:63:HIS:H	2.02	0.62
1:A:29:ASP:OD1	1:A:29:ASP:N	2.31	0.62
1:E:127:LYS:NZ	1:E:211:TYR:HE2	1.98	0.62
1:E:62:ASP:O	1:E:63:HIS:HD2	1.83	0.62
1:C:62:ASP:O	1:C:63:HIS:HD2	1.83	0.62
1:A:165:THR:CG2	1:A:449:ASN:HB2	2.27	0.62
1:B:239:TRP:CH2	1:B:574:LYS:HE3	2.34	0.62
1:A:150:VAL:HG12	1:A:433:LEU:HD11	1.81	0.62
1:A:380:PHE:CE2	1:A:384:HIS:CE1	2.87	0.62
1:A:486:GLU:HA	1:A:492:THR:HA	1.81	0.62
1:E:5:THR:HG23	1:E:10:LYS:HE3	1.81	0.62
1:F:239:TRP:CH2	1:F:574:LYS:HE3	2.34	0.62
1:A:256:PHE:CD2	1:A:378:PRO:HD3	2.35	0.62
1:F:62:ASP:O	1:F:63:HIS:HD2	1.83	0.62
1:C:61:ASN:C	1:C:63:HIS:H	2.02	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:ARG:HH21	1:F:338:GLN:NE2	1.98	0.62
1:B:256:PHE:CD2	1:B:378:PRO:HD3	2.35	0.62
1:D:127:LYS:NZ	1:D:211:TYR:HE2	1.98	0.62
1:F:380:PHE:CE2	1:F:384:HIS:CE1	2.87	0.62
1:D:262:TYR:CE1	1:D:268:PHE:CE1	2.88	0.62
1:F:487:ASP:HB3	1:F:490:GLY:N	2.15	0.61
1:E:256:PHE:CD2	1:E:378:PRO:HD3	2.35	0.61
1:F:262:TYR:CE1	1:F:268:PHE:CE1	2.88	0.61
1:E:402:THR:HG23	1:E:405:ASN:OD1	1.99	0.61
1:F:486:GLU:HA	1:F:492:THR:HA	1.81	0.61
1:B:61:ASN:C	1:B:63:HIS:H	2.02	0.61
1:A:512:VAL:HG13	1:A:513:PRO:HD2	1.81	0.61
1:F:256:PHE:CD2	1:F:378:PRO:HD3	2.35	0.61
1:D:5:THR:HG23	1:D:10:LYS:HE3	1.81	0.61
1:D:120:TYR:O	1:D:124:ILE:HG13	2.00	0.61
1:C:150:VAL:HG12	1:C:433:LEU:HD11	1.81	0.61
1:D:485:ILE:HD12	1:D:579:GLU:O	2.01	0.61
1:B:127:LYS:NZ	1:B:211:TYR:HE2	1.98	0.61
1:A:485:ILE:HD12	1:A:579:GLU:O	2.01	0.61
1:C:272:PRO:HG2	1:F:272:PRO:CG	2.30	0.61
1:C:256:PHE:CD2	1:C:378:PRO:HD3	2.35	0.61
1:E:76:ASN:O	1:E:77:THR:C	2.32	0.61
1:F:120:TYR:O	1:F:124:ILE:HG13	2.00	0.61
1:C:127:LYS:NZ	1:C:211:TYR:HE2	1.98	0.61
1:C:32:ASP:HB2	1:C:36:ASN:HD22	1.65	0.61
1:D:32:ASP:HB2	1:D:36:ASN:HD22	1.65	0.61
1:F:61:ASN:C	1:F:63:HIS:H	2.02	0.61
1:C:165:THR:CG2	1:C:449:ASN:HB2	2.27	0.61
1:D:255:GLY:HA2	1:D:271:ARG:NH1	2.13	0.61
1:D:256:PHE:CD2	1:D:378:PRO:HD3	2.35	0.61
1:C:5:THR:HG23	1:C:10:LYS:HE3	1.81	0.61
1:B:150:VAL:HG12	1:B:433:LEU:HD11	1.81	0.61
1:D:150:VAL:HG12	1:D:433:LEU:HD11	1.81	0.61
1:F:533:MET:CB	1:F:534:PRO:HD2	2.28	0.61
1:C:533:MET:CB	1:C:534:PRO:HD2	2.28	0.61
1:A:262:TYR:CE1	1:A:268:PHE:CE1	2.88	0.61
1:B:485:ILE:HD12	1:B:579:GLU:O	2.01	0.61
1:F:485:ILE:HD12	1:F:579:GLU:O	2.01	0.61
1:C:512:VAL:HG13	1:C:513:PRO:HD2	1.81	0.61
1:C:177:ARG:HD2	1:F:360:LYS:HB3	1.82	0.61
1:A:256:PHE:CE2	1:A:377:ASP:HA	2.36	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:485:ILE:HD12	1:E:579:GLU:O	2.01	0.61
1:D:634:ARG:NH2	1:F:64:ARG:HD2	2.06	0.61
1:B:487:ASP:HB3	1:B:490:GLY:N	2.15	0.61
1:B:32:ASP:HB2	1:B:36:ASN:HD22	1.65	0.61
1:F:86:LEU:HD22	1:F:90:LEU:HD22	1.83	0.61
1:C:402:THR:HG23	1:C:405:ASN:OD1	1.99	0.61
1:B:62:ASP:O	1:B:63:HIS:HD2	1.83	0.61
1:F:634:ARG:CG	1:F:634:ARG:HH11	2.09	0.61
1:C:256:PHE:CE2	1:C:377:ASP:HA	2.36	0.61
1:A:120:TYR:O	1:A:124:ILE:HG13	2.00	0.61
1:B:262:TYR:CE1	1:B:268:PHE:CE1	2.88	0.61
1:D:634:ARG:HH11	1:D:634:ARG:CG	2.09	0.61
1:D:256:PHE:CE2	1:D:377:ASP:HA	2.36	0.61
1:F:256:PHE:CE2	1:F:377:ASP:HA	2.36	0.61
1:E:86:LEU:HD22	1:E:90:LEU:CD2	2.31	0.61
1:A:62:ASP:O	1:A:63:HIS:HD2	1.83	0.60
1:C:487:ASP:HB3	1:C:490:GLY:N	2.15	0.60
1:E:487:ASP:HB3	1:E:490:GLY:N	2.15	0.60
1:B:634:ARG:HH11	1:B:634:ARG:CG	2.09	0.60
1:C:485:ILE:HD12	1:C:579:GLU:O	2.01	0.60
1:F:32:ASP:HB2	1:F:36:ASN:HD22	1.65	0.60
1:A:127:LYS:NZ	1:A:211:TYR:HE2	1.98	0.60
1:E:183:TYR:OH	1:E:234:GLU:OE1	2.11	0.60
1:D:487:ASP:HB3	1:D:490:GLY:N	2.15	0.60
1:D:7:ASN:C	1:D:9:GLN:N	2.55	0.60
1:A:571:PRO:C	4:A:857:HOH:O	2.39	0.60
1:E:120:TYR:O	1:E:124:ILE:HG13	2.00	0.60
1:C:120:TYR:O	1:C:124:ILE:HG13	2.00	0.60
1:C:86:LEU:HD22	1:C:90:LEU:CD2	2.31	0.60
1:D:86:LEU:HD22	1:D:90:LEU:CD2	2.31	0.60
1:A:86:LEU:HD22	1:A:90:LEU:CD2	2.31	0.60
1:C:535:SER:OG	1:C:536:PHE:N	2.34	0.60
1:B:300:ILE:CD1	1:B:390:ILE:HG22	2.31	0.60
1:A:32:ASP:HB2	1:A:36:ASN:HD22	1.65	0.60
1:D:183:TYR:OH	1:D:234:GLU:OE1	2.11	0.60
1:D:19:ASP:O	1:D:20:LYS:C	2.40	0.60
1:A:487:ASP:HB3	1:A:490:GLY:N	2.15	0.60
1:E:256:PHE:CE2	1:E:377:ASP:HA	2.36	0.60
1:E:121:VAL:CG2	1:E:199:MET:HG2	2.32	0.60
1:B:121:VAL:CG2	1:B:199:MET:HG2	2.32	0.60
1:E:132:ILE:HG22	1:E:133:VAL:N	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:THR:CG2	1:D:449:ASN:HB2	2.27	0.60
1:B:86:LEU:HD22	1:B:90:LEU:CD2	2.31	0.60
1:C:300:ILE:CD1	1:C:390:ILE:HG22	2.31	0.60
1:D:300:ILE:CD1	1:D:390:ILE:HG22	2.31	0.60
1:F:127:LYS:NZ	1:F:211:TYR:HE2	1.98	0.60
1:C:272:PRO:CG	1:F:272:PRO:HG2	2.31	0.60
1:A:283:VAL:O	1:A:284:ALA:CB	2.49	0.60
1:C:86:LEU:HD22	1:C:90:LEU:HD22	1.83	0.60
1:D:479:ARG:NH2	1:D:618:ASP:OD2	2.35	0.60
1:E:479:ARG:NH2	1:E:618:ASP:OD2	2.35	0.60
1:A:479:ARG:NH2	1:A:618:ASP:OD2	2.35	0.60
1:F:300:ILE:CD1	1:F:390:ILE:HG22	2.31	0.60
1:B:132:ILE:HG22	1:B:133:VAL:N	2.16	0.60
1:A:367:VAL:O	1:A:373:THR:HG22	2.02	0.60
1:B:183:TYR:OH	1:B:234:GLU:HB3	2.02	0.60
1:A:19:ASP:O	1:A:20:LYS:C	2.40	0.60
1:D:591:LYS:HA	1:D:594:GLU:HB2	1.84	0.60
1:B:19:ASP:O	1:B:20:LYS:C	2.40	0.60
1:B:56:LEU:HD21	1:B:110:MET:HE1	1.84	0.60
1:E:7:ASN:C	1:E:9:GLN:N	2.55	0.60
1:C:429:PHE:HB3	1:C:452:VAL:HG23	1.84	0.60
1:F:121:VAL:CG2	1:F:199:MET:HG2	2.32	0.60
1:B:535:SER:OG	1:B:536:PHE:N	2.34	0.60
1:B:591:LYS:HA	1:B:594:GLU:HB2	1.84	0.60
1:C:132:ILE:HG22	1:C:133:VAL:N	2.16	0.60
1:E:429:PHE:HB3	1:E:452:VAL:HG23	1.84	0.60
1:F:86:LEU:HD22	1:F:90:LEU:CD2	2.31	0.60
1:A:300:ILE:CD1	1:A:390:ILE:HG22	2.31	0.60
1:F:19:ASP:O	1:F:20:LYS:C	2.40	0.60
1:D:367:VAL:O	1:D:373:THR:HG22	2.02	0.60
1:C:367:VAL:O	1:C:373:THR:HG22	2.02	0.60
1:C:479:ARG:NH2	1:C:618:ASP:OD2	2.34	0.60
1:B:479:ARG:NH2	1:B:618:ASP:OD2	2.35	0.60
1:A:535:SER:OG	1:A:536:PHE:N	2.34	0.60
1:D:183:TYR:OH	1:D:234:GLU:HB3	2.02	0.60
1:E:32:ASP:HB2	1:E:36:ASN:HD22	1.65	0.60
1:B:624:TYR:CE1	1:B:625:PRO:HB3	2.37	0.60
1:E:301:ASP:OD2	1:E:393:LYS:NZ	2.33	0.60
1:D:606:HIS:HD2	1:D:608:GLN:CG	2.14	0.60
1:B:120:TYR:O	1:B:124:ILE:HG13	2.00	0.60
1:B:429:PHE:HB3	1:B:452:VAL:HG23	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:535:SER:OG	1:D:536:PHE:N	2.34	0.60
1:F:535:SER:OG	1:F:536:PHE:N	2.34	0.60
1:A:121:VAL:CG2	1:A:199:MET:HG2	2.32	0.60
1:E:300:ILE:CD1	1:E:390:ILE:HG22	2.31	0.60
1:B:256:PHE:CE2	1:B:377:ASP:HA	2.36	0.60
1:C:260:THR:HG22	1:C:268:PHE:CE2	2.37	0.60
1:E:183:TYR:OH	1:E:234:GLU:HB3	2.02	0.60
1:E:160:THR:O	1:E:161:GLN:HB2	2.02	0.60
1:F:183:TYR:OH	1:F:234:GLU:HB3	2.02	0.60
1:A:591:LYS:HB2	1:A:591:LYS:NZ	2.17	0.60
1:D:86:LEU:HD22	1:D:90:LEU:HD22	1.83	0.59
1:F:479:ARG:NH2	1:F:618:ASP:OD2	2.35	0.59
1:E:535:SER:OG	1:E:536:PHE:N	2.34	0.59
1:C:591:LYS:HA	1:C:594:GLU:HB2	1.84	0.59
1:A:160:THR:O	1:A:161:GLN:HB2	2.02	0.59
1:C:19:ASP:O	1:C:20:LYS:C	2.40	0.59
1:A:575:PRO:HD2	1:A:576:GLU:HG3	1.84	0.59
1:D:624:TYR:CE1	1:D:625:PRO:HB3	2.37	0.59
1:C:575:PRO:HD2	1:C:576:GLU:HG3	1.84	0.59
1:B:86:LEU:HD22	1:B:90:LEU:HD22	1.83	0.59
1:A:86:LEU:HD22	1:A:90:LEU:HD22	1.83	0.59
1:D:496:ASP:OD1	1:D:499:ARG:HD3	2.03	0.59
1:F:591:LYS:HB2	1:F:591:LYS:NZ	2.17	0.59
1:D:76:ASN:HD22	1:D:79:GLN:H	1.51	0.59
1:B:7:ASN:C	1:B:9:GLN:N	2.55	0.59
1:D:168:VAL:HG21	1:D:452:VAL:HG12	1.84	0.59
1:D:121:VAL:CG2	1:D:199:MET:HG2	2.32	0.59
1:D:132:ILE:HG22	1:D:133:VAL:N	2.16	0.59
1:F:367:VAL:O	1:F:373:THR:HG22	2.02	0.59
1:E:367:VAL:O	1:E:373:THR:HG22	2.02	0.59
1:E:86:LEU:HD22	1:E:90:LEU:HD22	1.83	0.59
1:E:491:ILE:O	1:E:491:ILE:HG22	2.03	0.59
1:F:591:LYS:HA	1:F:594:GLU:HB2	1.84	0.59
1:A:132:ILE:HG22	1:A:133:VAL:N	2.16	0.59
1:B:575:PRO:HD2	1:B:576:GLU:HG3	1.84	0.59
1:C:624:TYR:CE1	1:C:625:PRO:HB3	2.37	0.59
1:B:168:VAL:HG21	1:B:452:VAL:HG12	1.84	0.59
1:F:429:PHE:HB3	1:F:452:VAL:HG23	1.84	0.59
1:F:533:MET:H	1:F:533:MET:CE	2.16	0.59
1:A:307:ASP:OD1	1:A:309:ASP:N	2.34	0.59
1:C:121:VAL:CG2	1:C:199:MET:HG2	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ILE:O	1:A:491:ILE:HG22	2.03	0.59
1:C:591:LYS:HB2	1:C:591:LYS:NZ	2.17	0.59
1:C:301:ASP:OD2	1:C:393:LYS:NZ	2.33	0.59
1:B:468:ASN:HD22	1:B:514:SER:HA	1.67	0.59
1:F:76:ASN:HD22	1:F:79:GLN:H	1.51	0.59
1:E:533:MET:H	1:E:533:MET:CE	2.16	0.59
1:C:496:ASP:OD1	1:C:499:ARG:HD3	2.03	0.59
1:C:76:ASN:HD22	1:C:79:GLN:H	1.51	0.59
1:A:7:ASN:C	1:A:9:GLN:N	2.55	0.59
1:B:574:LYS:HD3	1:B:578:MET:SD	2.43	0.59
1:D:429:PHE:HB3	1:D:452:VAL:HG23	1.84	0.59
1:E:168:VAL:HG21	1:E:452:VAL:HG12	1.84	0.59
1:A:168:VAL:HG21	1:A:452:VAL:HG12	1.84	0.59
1:C:168:VAL:HG21	1:C:452:VAL:HG12	1.84	0.59
1:B:89:VAL:O	1:B:90:LEU:C	2.41	0.59
1:A:591:LYS:HA	1:A:594:GLU:HB2	1.84	0.59
1:B:269:PRO:HB3	1:B:363:LEU:HD23	1.85	0.59
1:E:591:LYS:HB2	1:E:591:LYS:NZ	2.17	0.59
1:C:160:THR:O	1:C:161:GLN:HB2	2.02	0.59
1:A:496:ASP:OD1	1:A:499:ARG:HD3	2.03	0.59
1:C:470:ASN:CB	1:C:474:ARG:HD3	2.33	0.59
1:C:491:ILE:O	1:C:491:ILE:HG22	2.03	0.59
1:D:574:LYS:HD3	1:D:578:MET:SD	2.43	0.59
1:C:89:VAL:O	1:C:90:LEU:C	2.41	0.59
1:D:48:ASP:HB3	1:D:92:GLN:NE2	2.18	0.59
1:E:89:VAL:O	1:E:90:LEU:C	2.41	0.59
1:F:593:THR:C	1:F:595:GLY:H	2.06	0.59
1:C:593:THR:C	1:C:595:GLY:H	2.06	0.59
1:A:183:TYR:OH	1:A:234:GLU:HB3	2.02	0.59
1:C:183:TYR:OH	1:C:234:GLU:HB3	2.02	0.59
1:F:260:THR:HG22	1:F:268:PHE:CE2	2.37	0.59
1:D:56:LEU:HD11	1:D:110:MET:CE	2.33	0.59
1:E:207:ASP:OD2	1:E:212:HIS:CB	2.51	0.59
1:B:593:THR:C	1:B:595:GLY:H	2.06	0.59
1:E:575:PRO:HD2	1:E:576:GLU:HG3	1.84	0.59
1:F:301:ASP:OD2	1:F:393:LYS:NZ	2.33	0.59
1:F:132:ILE:HG22	1:F:133:VAL:N	2.16	0.59
1:A:574:LYS:HD3	1:A:578:MET:SD	2.43	0.59
1:E:48:ASP:HB3	1:E:92:GLN:NE2	2.18	0.59
1:D:260:THR:HG22	1:D:268:PHE:CE2	2.37	0.59
1:E:56:LEU:HD11	1:E:110:MET:CE	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:THR:O	1:B:161:GLN:HB2	2.02	0.59
1:E:634:ARG:HG2	1:E:634:ARG:NH1	2.14	0.58
1:F:574:LYS:HD3	1:F:578:MET:SD	2.43	0.58
1:A:76:ASN:HD22	1:A:79:GLN:H	1.51	0.58
1:A:533:MET:HG2	4:A:781:HOH:O	2.02	0.58
1:D:593:THR:C	1:D:595:GLY:H	2.06	0.58
1:A:260:THR:HG22	1:A:268:PHE:CE2	2.37	0.58
1:B:260:THR:HG22	1:B:268:PHE:CE2	2.37	0.58
1:F:269:PRO:HB3	1:F:363:LEU:HD23	1.85	0.58
1:A:624:TYR:CE1	1:A:625:PRO:HB3	2.37	0.58
1:F:468:ASN:HD22	1:F:514:SER:HA	1.67	0.58
1:D:470:ASN:CB	1:D:474:ARG:HD3	2.33	0.58
1:D:491:ILE:HG22	1:D:491:ILE:O	2.03	0.58
1:E:574:LYS:HD3	1:E:578:MET:SD	2.43	0.58
1:D:283:VAL:O	1:D:284:ALA:CB	2.49	0.58
1:F:48:ASP:HB3	1:F:92:GLN:NE2	2.18	0.58
1:C:533:MET:H	1:C:533:MET:CE	2.16	0.58
1:E:19:ASP:O	1:E:20:LYS:C	2.40	0.58
1:C:468:ASN:HD22	1:C:514:SER:HA	1.67	0.58
1:F:624:TYR:CE1	1:F:625:PRO:HB3	2.37	0.58
1:A:269:PRO:HB3	1:A:363:LEU:HD23	1.85	0.58
1:D:634:ARG:HG2	1:D:634:ARG:NH1	2.14	0.58
1:E:470:ASN:CB	1:E:474:ARG:HD3	2.33	0.58
1:D:272:PRO:HG2	1:E:272:PRO:CD	2.33	0.58
1:D:301:ASP:OD2	1:D:393:LYS:NZ	2.33	0.58
1:E:551:HIS:HD2	1:E:552:ASP:CA	2.16	0.58
1:C:48:ASP:HB3	1:C:92:GLN:NE2	2.18	0.58
1:E:593:THR:C	1:E:595:GLY:H	2.06	0.58
1:A:429:PHE:HB3	1:A:452:VAL:HG23	1.84	0.58
1:B:533:MET:H	1:B:533:MET:CE	2.16	0.58
1:A:533:MET:H	1:A:533:MET:CE	2.16	0.58
1:A:48:ASP:HB3	1:A:92:GLN:NE2	2.18	0.58
1:C:207:ASP:OD2	1:C:212:HIS:CB	2.51	0.58
1:E:591:LYS:HA	1:E:594:GLU:HB2	1.84	0.58
1:B:496:ASP:OD1	1:B:499:ARG:HD3	2.03	0.58
1:F:160:THR:O	1:F:161:GLN:HB2	2.02	0.58
1:A:634:ARG:HH11	1:A:634:ARG:CG	2.09	0.58
1:C:7:ASN:C	1:C:9:GLN:N	2.55	0.58
1:C:360:LYS:HE3	1:F:273:ASP:OD2	2.03	0.58
1:B:491:ILE:HG22	1:B:491:ILE:O	2.03	0.58
1:E:624:TYR:CE1	1:E:625:PRO:HB3	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:LEU:HD11	1:C:110:MET:CE	2.33	0.58
1:D:269:PRO:HB3	1:D:363:LEU:HD23	1.85	0.58
1:A:593:THR:C	1:A:595:GLY:H	2.06	0.58
1:D:160:THR:O	1:D:161:GLN:HB2	2.02	0.58
1:E:606:HIS:HD2	1:E:608:GLN:CG	2.14	0.58
1:C:573:SER:HB2	1:C:578:MET:HG3	1.86	0.58
1:C:574:LYS:HD3	1:C:578:MET:SD	2.43	0.58
1:D:591:LYS:HB2	1:D:591:LYS:NZ	2.17	0.58
1:C:56:LEU:HD21	1:C:110:MET:HE1	1.84	0.58
1:D:468:ASN:HD22	1:D:514:SER:HA	1.67	0.58
1:C:629:ARG:HH11	1:C:629:ARG:HG3	1.69	0.58
1:C:269:PRO:HB3	1:C:363:LEU:HD23	1.85	0.58
1:A:470:ASN:CB	1:A:474:ARG:HD3	2.33	0.58
1:B:367:VAL:O	1:B:373:THR:HG22	2.02	0.58
1:D:207:ASP:OD2	1:D:212:HIS:CB	2.51	0.58
1:E:260:THR:HG22	1:E:268:PHE:CE2	2.37	0.58
1:B:301:ASP:OD2	1:B:393:LYS:NZ	2.33	0.58
1:A:56:LEU:HD21	1:A:110:MET:HE1	1.85	0.58
1:B:11:GLN:O	1:B:15:ASN:ND2	2.37	0.58
1:D:46:TYR:CD2	1:D:53:VAL:HG21	2.39	0.58
1:F:56:LEU:HD11	1:F:110:MET:CE	2.33	0.58
1:F:89:VAL:O	1:F:90:LEU:C	2.41	0.58
1:D:89:VAL:O	1:D:90:LEU:C	2.41	0.58
1:A:89:VAL:O	1:A:90:LEU:C	2.41	0.58
1:E:496:ASP:OD1	1:E:499:ARG:HD3	2.03	0.58
1:F:496:ASP:OD1	1:F:499:ARG:HD3	2.03	0.58
1:A:301:ASP:OD2	1:A:393:LYS:NZ	2.33	0.58
1:F:175:LYS:O	1:F:176:ASN:HB2	2.04	0.58
1:F:168:VAL:HG21	1:F:452:VAL:HG12	1.84	0.58
1:F:551:HIS:HD2	1:F:552:ASP:CA	2.16	0.58
1:B:48:ASP:HB3	1:B:92:GLN:NE2	2.18	0.58
1:B:207:ASP:OD2	1:B:212:HIS:CB	2.51	0.58
1:F:491:ILE:HG22	1:F:491:ILE:O	2.03	0.58
1:B:591:LYS:HB2	1:B:591:LYS:NZ	2.17	0.58
1:E:235:ARG:O	1:E:240:LEU:HB2	2.04	0.58
1:C:175:LYS:O	1:C:176:ASN:HB2	2.04	0.58
1:B:573:SER:HB2	1:B:578:MET:HG3	1.86	0.58
1:D:575:PRO:HD2	1:D:576:GLU:HG3	1.84	0.58
1:B:551:HIS:HD2	1:B:552:ASP:CA	2.16	0.58
1:D:533:MET:H	1:D:533:MET:CE	2.16	0.58
1:B:56:LEU:HD11	1:B:110:MET:CE	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:575:PRO:HD2	1:F:576:GLU:HG3	1.84	0.58
1:A:11:GLN:O	1:A:15:ASN:ND2	2.37	0.57
1:D:551:HIS:HD2	1:D:552:ASP:CA	2.16	0.57
1:F:207:ASP:OD2	1:F:212:HIS:CB	2.51	0.57
1:B:183:TYR:OH	1:B:234:GLU:OE1	2.11	0.57
1:E:56:LEU:HD21	1:E:110:MET:HE1	1.86	0.57
1:A:56:LEU:HD11	1:A:110:MET:CE	2.33	0.57
1:D:235:ARG:O	1:D:240:LEU:HB2	2.04	0.57
1:B:76:ASN:HD22	1:B:79:GLN:H	1.51	0.57
1:F:470:ASN:CB	1:F:474:ARG:HD3	2.33	0.57
1:D:522:SER:O	1:D:524:LYS:N	2.38	0.57
1:A:468:ASN:HD22	1:A:514:SER:HA	1.67	0.57
1:A:470:ASN:ND2	1:A:474:ARG:HD3	2.20	0.57
1:E:175:LYS:O	1:E:176:ASN:HB2	2.04	0.57
1:D:48:ASP:HB3	1:D:92:GLN:HE21	1.69	0.57
1:A:629:ARG:HH11	1:A:629:ARG:HG3	1.69	0.57
1:A:95:GLU:HA	1:A:128:LEU:HD21	1.86	0.57
1:E:629:ARG:HG3	1:E:629:ARG:HH11	1.69	0.57
1:E:468:ASN:HD22	1:E:514:SER:HA	1.67	0.57
1:F:470:ASN:ND2	1:F:474:ARG:HD3	2.20	0.57
1:B:470:ASN:CB	1:B:474:ARG:HD3	2.33	0.57
1:A:46:TYR:CD2	1:A:53:VAL:HG21	2.39	0.57
1:D:573:SER:HB2	1:D:578:MET:HG3	1.86	0.57
1:E:573:SER:HB2	1:E:578:MET:HG3	1.86	0.57
1:B:46:TYR:CD2	1:B:53:VAL:HG21	2.39	0.57
1:F:11:GLN:O	1:F:15:ASN:ND2	2.37	0.57
1:F:46:TYR:CD2	1:F:53:VAL:HG21	2.39	0.57
1:F:573:SER:HB2	1:F:578:MET:HG3	1.86	0.57
1:A:551:HIS:HD2	1:A:552:ASP:CA	2.16	0.57
1:C:551:HIS:HD2	1:C:552:ASP:CA	2.16	0.57
1:F:522:SER:O	1:F:524:LYS:N	2.38	0.57
1:E:11:GLN:O	1:E:15:ASN:ND2	2.37	0.57
1:F:606:HIS:HD2	1:F:608:GLN:CG	2.14	0.57
1:E:76:ASN:HD22	1:E:79:GLN:H	1.51	0.57
1:F:629:ARG:HH11	1:F:629:ARG:HG3	1.69	0.57
1:E:269:PRO:HB3	1:E:363:LEU:HD23	1.85	0.57
1:F:235:ARG:O	1:F:240:LEU:HB2	2.04	0.57
1:B:425:PHE:CE1	1:B:456:ASN:HB3	2.40	0.57
1:C:283:VAL:O	1:C:284:ALA:CB	2.49	0.57
1:A:522:SER:O	1:A:524:LYS:N	2.38	0.57
1:A:74:LEU:O	1:A:74:LEU:HG	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:LYS:CB	1:D:491:ILE:HG12	2.34	0.57
1:C:46:TYR:CD2	1:C:53:VAL:HG21	2.39	0.57
1:D:11:GLN:O	1:D:15:ASN:ND2	2.37	0.57
1:E:46:TYR:CD2	1:E:53:VAL:HG21	2.39	0.57
1:A:235:ARG:O	1:A:240:LEU:HB2	2.04	0.57
1:E:522:SER:O	1:E:524:LYS:N	2.38	0.57
1:C:74:LEU:HG	1:C:74:LEU:O	2.05	0.57
1:F:74:LEU:O	1:F:74:LEU:HG	2.05	0.57
1:C:470:ASN:ND2	1:C:474:ARG:HD3	2.20	0.57
1:C:173:THR:HG22	1:C:174:LYS:O	2.05	0.57
1:D:425:PHE:CE1	1:D:456:ASN:HB3	2.40	0.57
1:D:307:ASP:OD1	1:D:309:ASP:N	2.34	0.57
1:F:477:THR:HB	1:F:479:ARG:HH12	1.70	0.57
1:C:522:SER:O	1:C:524:LYS:N	2.38	0.57
1:C:235:ARG:O	1:C:240:LEU:HB2	2.04	0.57
1:D:156:SER:OG	1:E:438:ASP:OD1	2.23	0.57
1:D:413:VAL:HG23	1:D:466:MET:HE3	1.87	0.56
1:D:173:THR:HG22	1:D:174:LYS:O	2.05	0.56
1:C:11:GLN:O	1:C:15:ASN:ND2	2.37	0.56
1:C:425:PHE:CE1	1:C:456:ASN:HB3	2.40	0.56
1:A:354:GLN:HA	1:A:354:GLN:NE2	2.20	0.56
1:A:173:THR:HG22	1:A:174:LYS:O	2.05	0.56
1:A:175:LYS:O	1:A:176:ASN:HB2	2.04	0.56
1:E:173:THR:HG22	1:E:174:LYS:O	2.05	0.56
1:F:48:ASP:HB3	1:F:92:GLN:HE21	1.69	0.56
1:D:533:MET:CB	1:D:534:PRO:HD2	2.28	0.56
1:B:89:VAL:O	1:B:92:GLN:N	2.38	0.56
1:E:48:ASP:HB3	1:E:92:GLN:HE21	1.69	0.56
1:B:629:ARG:HH11	1:B:629:ARG:HG3	1.69	0.56
1:A:207:ASP:OD2	1:A:212:HIS:CB	2.51	0.56
1:D:74:LEU:HG	1:D:74:LEU:O	2.05	0.56
1:A:48:ASP:HB3	1:A:92:GLN:HE21	1.69	0.56
1:B:74:LEU:O	1:B:74:LEU:HG	2.05	0.56
1:D:175:LYS:O	1:D:176:ASN:HB2	2.04	0.56
1:A:101:SER:O	1:A:104:ALA:HB3	2.06	0.56
1:C:271:ARG:NH2	1:C:377:ASP:OD1	2.39	0.56
1:D:101:SER:O	1:D:104:ALA:HB3	2.06	0.56
1:F:101:SER:O	1:F:104:ALA:HB3	2.05	0.56
1:A:425:PHE:CE1	1:A:456:ASN:HB3	2.40	0.56
1:F:354:GLN:NE2	1:F:354:GLN:HA	2.20	0.56
1:F:173:THR:HG22	1:F:174:LYS:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:629:ARG:HH11	1:D:629:ARG:HG3	1.69	0.56
1:D:89:VAL:O	1:D:92:GLN:N	2.38	0.56
1:A:477:THR:HB	1:A:479:ARG:HH12	1.70	0.56
1:C:95:GLU:HA	1:C:128:LEU:HD21	1.86	0.56
1:D:95:GLU:HA	1:D:128:LEU:HD21	1.87	0.56
1:A:271:ARG:NH2	1:A:377:ASP:OD1	2.39	0.56
1:B:235:ARG:O	1:B:240:LEU:HB2	2.04	0.56
1:E:470:ASN:ND2	1:E:474:ARG:HD3	2.20	0.56
1:C:487:ASP:O	1:C:488:ASN:HB3	2.06	0.56
1:B:101:SER:O	1:B:104:ALA:HB3	2.05	0.56
1:E:533:MET:HE3	1:E:533:MET:H	1.70	0.56
1:D:470:ASN:ND2	1:D:474:ARG:HD3	2.20	0.56
1:A:89:VAL:O	1:A:92:GLN:N	2.38	0.56
1:E:307:ASP:OD1	1:E:309:ASP:N	2.34	0.56
1:B:95:GLU:HA	1:B:128:LEU:HD21	1.87	0.56
1:F:237:SER:HB3	1:F:573:SER:CA	2.36	0.56
1:C:354:GLN:NE2	1:C:354:GLN:HA	2.20	0.56
1:B:173:THR:HG22	1:B:174:LYS:O	2.05	0.56
1:C:89:VAL:O	1:C:92:GLN:N	2.38	0.56
1:D:477:THR:HB	1:D:479:ARG:HH12	1.70	0.56
1:B:522:SER:O	1:B:524:LYS:N	2.38	0.56
1:B:482:LEU:HB2	1:B:505:LEU:HD22	1.87	0.56
1:F:237:SER:HA	1:F:574:LYS:HD2	1.88	0.56
1:C:477:THR:HB	1:C:479:ARG:HH12	1.70	0.56
1:B:271:ARG:NH2	1:B:377:ASP:OD1	2.39	0.56
1:D:29:ASP:OD1	1:D:29:ASP:N	2.31	0.56
1:C:634:ARG:HG2	1:C:634:ARG:NH1	2.14	0.56
1:B:470:ASN:ND2	1:B:474:ARG:HD3	2.20	0.56
1:E:271:ARG:NH2	1:E:377:ASP:OD1	2.39	0.56
1:D:237:SER:HA	1:D:574:LYS:HD2	1.88	0.56
1:A:174:LYS:O	1:A:175:LYS:CG	2.54	0.56
1:E:89:VAL:O	1:E:92:GLN:N	2.38	0.56
1:E:412:VAL:HB	1:E:640:SER:HB2	1.88	0.56
1:F:412:VAL:HB	1:F:640:SER:HB2	1.88	0.56
1:B:237:SER:HA	1:B:574:LYS:HD2	1.88	0.56
1:C:576:GLU:CD	1:D:576:GLU:OE1	2.44	0.56
1:F:283:VAL:O	1:F:284:ALA:CB	2.49	0.56
1:E:477:THR:HB	1:E:479:ARG:HH12	1.70	0.56
1:E:29:ASP:O	1:E:33:ILE:HG13	2.06	0.56
1:F:76:ASN:CB	1:F:79:GLN:HB2	2.34	0.56
1:F:95:GLU:HA	1:F:128:LEU:HD21	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ASP:O	1:B:33:ILE:HG13	2.06	0.56
1:F:482:LEU:HB2	1:F:505:LEU:HD22	1.87	0.56
1:F:29:ASP:O	1:F:33:ILE:HG13	2.06	0.56
1:E:74:LEU:O	1:E:74:LEU:HG	2.05	0.56
1:E:403:HIS:C	1:E:405:ASN:N	2.59	0.55
1:C:634:ARG:HE	1:E:64:ARG:NE	2.04	0.55
1:C:414:ASN:ND2	1:C:467:SER:N	2.54	0.55
1:E:101:SER:O	1:E:104:ALA:HB3	2.06	0.55
1:A:573:SER:HB2	1:A:578:MET:HG3	1.86	0.55
1:A:237:SER:HA	1:A:574:LYS:HD2	1.88	0.55
1:E:354:GLN:NE2	1:E:354:GLN:HA	2.20	0.55
1:F:89:VAL:O	1:F:92:GLN:N	2.38	0.55
1:E:95:GLU:HA	1:E:128:LEU:HD21	1.86	0.55
1:A:482:LEU:HB2	1:A:505:LEU:HD22	1.87	0.55
1:F:437:VAL:HG23	1:F:437:VAL:O	2.07	0.55
1:C:174:LYS:O	1:C:175:LYS:CG	2.54	0.55
1:C:101:SER:O	1:C:104:ALA:HB3	2.05	0.55
1:F:463:LYS:HG2	1:F:520:GLU:CB	2.36	0.55
1:E:463:LYS:HG2	1:E:520:GLU:CB	2.36	0.55
1:C:526:SER:OG	1:C:527:SER:N	2.40	0.55
1:A:230:ARG:NE	4:A:751:HOH:O	2.19	0.55
1:F:321:ILE:HG12	1:F:321:ILE:O	2.07	0.55
1:D:414:ASN:ND2	1:D:467:SER:N	2.54	0.55
1:E:237:SER:HB3	1:E:573:SER:CA	2.36	0.55
1:E:425:PHE:CE1	1:E:456:ASN:HB3	2.40	0.55
1:A:551:HIS:O	1:A:552:ASP:CB	2.55	0.55
1:F:529:THR:C	1:F:530:VAL:HG23	2.27	0.55
1:E:624:TYR:CD1	1:E:625:PRO:HB3	2.42	0.55
1:C:321:ILE:HG12	1:C:321:ILE:O	2.07	0.55
1:E:487:ASP:O	1:E:488:ASN:HB3	2.06	0.55
1:D:271:ARG:NH2	1:D:377:ASP:OD1	2.39	0.55
1:F:425:PHE:CE1	1:F:456:ASN:HB3	2.40	0.55
1:B:412:VAL:HB	1:B:640:SER:HB2	1.88	0.55
1:D:68:GLN:HB3	1:D:69:ARG:NH1	2.22	0.55
1:B:529:THR:C	1:B:530:VAL:HG23	2.27	0.55
1:C:482:LEU:HB2	1:C:505:LEU:HD22	1.87	0.55
1:A:634:ARG:HG2	1:A:634:ARG:NH1	2.14	0.55
1:A:606:HIS:HD2	1:A:608:GLN:CG	2.14	0.55
1:E:237:SER:HA	1:E:574:LYS:HD2	1.88	0.55
1:B:354:GLN:HA	1:B:354:GLN:NE2	2.20	0.55
1:B:175:LYS:O	1:B:176:ASN:HB2	2.04	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ASP:HB3	1:B:92:GLN:HE21	1.69	0.55
1:F:66:LEU:HD13	1:F:111:ASN:ND2	2.22	0.55
1:A:66:LEU:HD13	1:A:111:ASN:ND2	2.22	0.55
1:E:321:ILE:HG12	1:E:321:ILE:O	2.07	0.55
1:D:437:VAL:HG23	1:D:437:VAL:O	2.07	0.55
1:D:487:ASP:O	1:D:488:ASN:HB3	2.06	0.55
1:D:237:SER:HB3	1:D:573:SER:CA	2.36	0.55
1:B:237:SER:CB	1:B:573:SER:HA	2.37	0.55
1:D:551:HIS:O	1:D:552:ASP:CB	2.55	0.55
1:A:29:ASP:O	1:A:33:ILE:HG13	2.06	0.55
1:A:127:LYS:NZ	1:A:211:TYR:CE2	2.75	0.55
1:D:29:ASP:O	1:D:33:ILE:HG13	2.06	0.55
1:D:66:LEU:HD13	1:D:111:ASN:ND2	2.22	0.55
1:F:307:ASP:OD1	1:F:309:ASP:N	2.34	0.55
1:C:529:THR:C	1:C:530:VAL:HG23	2.27	0.55
1:F:183:TYR:OH	1:F:234:GLU:OE1	2.11	0.55
1:E:482:LEU:HB2	1:E:505:LEU:HD22	1.87	0.55
1:D:482:LEU:HB2	1:D:505:LEU:HD22	1.87	0.55
1:A:437:VAL:O	1:A:437:VAL:HG23	2.07	0.55
1:D:321:ILE:O	1:D:321:ILE:HG12	2.07	0.55
1:F:414:ASN:ND2	1:F:467:SER:N	2.54	0.55
1:C:76:ASN:CB	1:C:79:GLN:HB2	2.34	0.55
1:A:412:VAL:HB	1:A:640:SER:HB2	1.88	0.55
1:F:487:ASP:O	1:F:488:ASN:HB3	2.06	0.55
1:F:484:PRO:HD2	1:F:498:ALA:HB1	1.89	0.55
1:B:48:ASP:CA	1:B:92:GLN:HE21	2.20	0.55
1:E:529:THR:C	1:E:530:VAL:HG23	2.27	0.55
1:F:127:LYS:NZ	1:F:211:TYR:CE2	2.75	0.55
1:A:624:TYR:CD1	1:A:625:PRO:HB3	2.42	0.55
1:A:321:ILE:O	1:A:321:ILE:HG12	2.07	0.55
1:A:487:ASP:O	1:A:488:ASN:HB3	2.06	0.55
1:C:606:HIS:HD2	1:C:608:GLN:CG	2.14	0.55
1:D:484:PRO:HD2	1:D:498:ALA:HB1	1.89	0.55
1:E:484:PRO:HD2	1:E:498:ALA:HB1	1.89	0.55
1:B:484:PRO:HD2	1:B:498:ALA:HB1	1.89	0.55
1:C:237:SER:HB3	1:C:573:SER:CA	2.36	0.55
1:A:237:SER:HB3	1:A:573:SER:CA	2.36	0.55
1:A:78:ARG:O	1:A:79:GLN:C	2.45	0.55
1:A:76:ASN:CB	1:A:79:GLN:HB2	2.34	0.55
1:D:463:LYS:HG2	1:D:520:GLU:CB	2.36	0.55
1:A:301:ASP:CG	1:A:393:LYS:HZ1	2.11	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:VAL:HB	1:D:640:SER:HB2	1.88	0.55
1:A:68:GLN:HB3	1:A:69:ARG:NH1	2.22	0.55
1:C:38:ASN:C	1:C:40:LEU:H	2.10	0.55
1:D:526:SER:OG	1:D:527:SER:N	2.40	0.55
1:E:66:LEU:HD13	1:E:111:ASN:ND2	2.22	0.55
1:F:271:ARG:NH2	1:F:377:ASP:OD1	2.39	0.54
1:C:463:LYS:HG2	1:C:520:GLU:CB	2.36	0.54
1:E:418:ILE:HD11	1:E:462:TYR:CE1	2.43	0.54
1:C:48:ASP:HB3	1:C:92:GLN:HE21	1.69	0.54
1:C:307:ASP:OD1	1:C:309:ASP:N	2.34	0.54
1:A:26:LYS:NZ	4:A:732:HOH:O	2.28	0.54
1:B:66:LEU:HD13	1:B:111:ASN:ND2	2.22	0.54
1:E:437:VAL:HG23	1:E:437:VAL:O	2.07	0.54
1:B:321:ILE:O	1:B:321:ILE:HG12	2.07	0.54
1:B:437:VAL:HG23	1:B:437:VAL:O	2.07	0.54
1:E:414:ASN:ND2	1:E:467:SER:N	2.54	0.54
1:A:414:ASN:ND2	1:A:467:SER:N	2.54	0.54
2:D:658:NDG:O7	2:D:658:NDG:H3	2.08	0.54
2:B:658:NDG:H3	2:B:658:NDG:O7	2.07	0.54
1:C:237:SER:HA	1:C:574:LYS:HD2	1.88	0.54
1:A:463:LYS:HG2	1:A:520:GLU:CB	2.36	0.54
1:B:283:VAL:O	1:B:284:ALA:CB	2.49	0.54
1:F:48:ASP:CA	1:F:92:GLN:HE21	2.20	0.54
1:C:412:VAL:HB	1:C:640:SER:HB2	1.88	0.54
1:A:529:THR:C	1:A:530:VAL:HG23	2.27	0.54
1:B:403:HIS:C	1:B:405:ASN:N	2.59	0.54
1:B:624:TYR:CD1	1:B:625:PRO:HB3	2.42	0.54
1:B:414:ASN:ND2	1:B:467:SER:N	2.54	0.54
1:B:313:ILE:HG13	1:B:313:ILE:O	2.07	0.54
1:C:484:PRO:HD2	1:C:498:ALA:HB1	1.89	0.54
1:B:237:SER:HB3	1:B:573:SER:CA	2.36	0.54
1:E:574:LYS:HE2	1:E:578:MET:HG2	1.90	0.54
1:C:425:PHE:N	1:C:456:ASN:O	2.39	0.54
1:C:418:ILE:HD11	1:C:462:TYR:CE1	2.43	0.54
1:E:68:GLN:HB3	1:E:69:ARG:NH1	2.22	0.54
1:B:487:ASP:O	1:B:488:ASN:HB3	2.06	0.54
1:F:78:ARG:O	1:F:79:GLN:C	2.45	0.54
1:B:418:ILE:HD11	1:B:462:TYR:CE1	2.43	0.54
1:A:235:ARG:CZ	4:A:705:HOH:O	2.48	0.54
1:D:477:THR:HG23	1:D:509:PHE:CD1	2.43	0.54
1:B:526:SER:OG	1:B:527:SER:N	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:624:TYR:CD1	1:D:625:PRO:HB3	2.42	0.54
1:C:624:TYR:CD1	1:C:625:PRO:HB3	2.42	0.54
1:E:29:ASP:N	1:E:29:ASP:OD1	2.31	0.54
1:A:473:GLU:O	1:A:473:GLU:HG3	2.08	0.54
1:B:174:LYS:O	1:B:175:LYS:CG	2.54	0.54
1:C:477:THR:HG23	1:C:509:PHE:CD1	2.43	0.54
1:F:68:GLN:HB3	1:F:69:ARG:NH1	2.22	0.54
1:C:68:GLN:HB3	1:C:69:ARG:NH1	2.22	0.54
1:D:127:LYS:NZ	1:D:211:TYR:CE2	2.75	0.54
1:C:403:HIS:C	1:C:405:ASN:N	2.59	0.54
1:A:161:GLN:HG3	1:B:443:ILE:HD13	1.90	0.54
1:C:437:VAL:O	1:C:437:VAL:HG23	2.07	0.54
1:D:12:GLN:OE1	1:D:547:VAL:HG21	2.08	0.54
1:A:574:LYS:HE2	1:A:578:MET:HG2	1.90	0.54
1:D:354:GLN:NE2	1:D:354:GLN:HA	2.20	0.54
1:F:418:ILE:HD11	1:F:462:TYR:CE1	2.43	0.54
1:B:463:LYS:HG2	1:B:520:GLU:CB	2.36	0.54
1:E:477:THR:HG23	1:E:509:PHE:CD1	2.43	0.54
1:E:526:SER:OG	1:E:527:SER:N	2.40	0.54
1:C:473:GLU:HG3	1:C:473:GLU:O	2.08	0.54
1:D:301:ASP:CG	1:D:393:LYS:HZ1	2.11	0.54
1:A:551:HIS:HD2	1:A:552:ASP:N	2.05	0.54
1:E:174:LYS:O	1:E:175:LYS:CG	2.54	0.54
1:C:48:ASP:CA	1:C:92:GLN:HE21	2.20	0.54
1:D:220:PHE:CZ	1:D:329:GLU:HB2	2.43	0.54
1:E:521:ARG:HG2	1:E:522:SER:N	2.23	0.54
1:E:127:LYS:NZ	1:E:211:TYR:CE2	2.75	0.54
1:D:126:SER:OG	1:D:127:LYS:N	2.41	0.54
1:C:611:VAL:HG12	1:C:612:HIS:HD2	1.73	0.54
1:D:313:ILE:O	1:D:313:ILE:HG13	2.07	0.54
1:C:12:GLN:OE1	1:C:547:VAL:HG21	2.08	0.54
1:A:138:TYR:CD2	1:A:188:ILE:HD12	2.43	0.54
1:B:12:GLN:OE1	1:B:547:VAL:HG21	2.08	0.54
1:D:37:PHE:CZ	1:D:101:SER:HB3	2.43	0.54
1:C:367:VAL:HG23	1:C:373:THR:O	2.08	0.54
1:A:48:ASP:CA	1:A:92:GLN:HE21	2.20	0.54
1:B:477:THR:HG23	1:B:509:PHE:CD1	2.43	0.54
1:A:570:LEU:N	4:A:858:HOH:O	2.40	0.54
1:E:38:ASN:C	1:E:40:LEU:H	2.10	0.54
1:B:127:LYS:NZ	1:B:211:TYR:CE2	2.75	0.54
1:D:620:ARG:HG3	1:D:624:TYR:CD2	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:620:ARG:HG3	1:C:624:TYR:CD2	2.43	0.54
1:F:624:TYR:CD1	1:F:625:PRO:HB3	2.42	0.54
1:C:66:LEU:HD13	1:C:111:ASN:ND2	2.22	0.54
1:C:78:ARG:O	1:C:79:GLN:C	2.45	0.54
1:F:37:PHE:CZ	1:F:101:SER:HB3	2.43	0.54
1:B:574:LYS:HE2	1:B:578:MET:HG2	1.90	0.54
1:E:283:VAL:O	1:E:284:ALA:CB	2.49	0.54
1:A:418:ILE:HD11	1:A:462:TYR:CE1	2.43	0.54
1:A:521:ARG:HB3	4:A:864:HOH:O	2.07	0.54
1:F:533:MET:H	1:F:533:MET:HE3	1.71	0.54
1:C:220:PHE:CZ	1:C:329:GLU:HB2	2.43	0.54
1:B:68:GLN:HB3	1:B:69:ARG:NH1	2.22	0.54
1:F:526:SER:OG	1:F:527:SER:N	2.40	0.54
1:F:38:ASN:C	1:F:40:LEU:H	2.10	0.54
1:E:324:LEU:O	1:E:328:ILE:HG13	2.08	0.54
1:F:403:HIS:C	1:F:405:ASN:N	2.59	0.54
1:E:611:VAL:HG12	1:E:612:HIS:HD2	1.73	0.54
2:A:658:NDG:H3	2:A:658:NDG:O7	2.08	0.54
1:A:425:PHE:N	1:A:456:ASN:O	2.39	0.54
1:F:367:VAL:HG23	1:F:373:THR:O	2.08	0.54
1:D:38:ASN:C	1:D:40:LEU:H	2.10	0.54
1:C:127:LYS:NZ	1:C:211:TYR:CE2	2.75	0.54
1:F:611:VAL:HG12	1:F:612:HIS:HD2	1.73	0.54
1:B:620:ARG:HG3	1:B:624:TYR:CD2	2.43	0.54
1:A:526:SER:OG	1:A:527:SER:N	2.40	0.54
1:C:37:PHE:CE2	1:C:101:SER:CB	2.92	0.53
1:E:313:ILE:O	1:E:313:ILE:HG13	2.07	0.53
1:F:220:PHE:CZ	1:F:329:GLU:HB2	2.43	0.53
1:A:477:THR:HG23	1:A:509:PHE:CD1	2.43	0.53
1:D:521:ARG:HG2	1:D:522:SER:N	2.23	0.53
1:B:38:ASN:C	1:B:40:LEU:H	2.10	0.53
1:F:324:LEU:O	1:F:328:ILE:HG13	2.08	0.53
1:D:324:LEU:O	1:D:328:ILE:HG13	2.08	0.53
1:A:324:LEU:O	1:A:328:ILE:HG13	2.08	0.53
1:E:126:SER:OG	1:E:127:LYS:N	2.41	0.53
1:D:611:VAL:HG12	1:D:612:HIS:HD2	1.73	0.53
1:B:76:ASN:CB	1:B:79:GLN:HB2	2.34	0.53
1:E:12:GLN:OE1	1:E:547:VAL:HG21	2.08	0.53
1:C:37:PHE:CZ	1:C:101:SER:HB3	2.43	0.53
1:A:484:PRO:HD2	1:A:498:ALA:HB1	1.89	0.53
1:D:367:VAL:HG23	1:D:373:THR:O	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:278:GLU:H	1:E:354:GLN:NE2	2.06	0.53
1:E:551:HIS:O	1:E:552:ASP:CB	2.55	0.53
1:F:174:LYS:O	1:F:175:LYS:CG	2.54	0.53
1:C:551:HIS:O	1:C:552:ASP:CB	2.55	0.53
1:D:48:ASP:CA	1:D:92:GLN:HE21	2.20	0.53
1:D:529:THR:C	1:D:530:VAL:HG23	2.27	0.53
1:A:38:ASN:C	1:A:40:LEU:H	2.10	0.53
1:A:256:PHE:CZ	1:A:258:PRO:HB3	2.44	0.53
1:B:256:PHE:CD1	1:B:256:PHE:C	2.82	0.53
1:B:126:SER:OG	1:B:127:LYS:N	2.41	0.53
2:F:658:NDG:H3	2:F:658:NDG:O7	2.08	0.53
1:E:256:PHE:CD1	1:E:256:PHE:C	2.82	0.53
1:E:256:PHE:CZ	1:E:258:PRO:HB3	2.44	0.53
1:A:12:GLN:OE1	1:A:547:VAL:HG21	2.08	0.53
1:F:237:SER:CB	1:F:573:SER:HA	2.37	0.53
1:B:278:GLU:H	1:B:354:GLN:NE2	2.06	0.53
1:E:48:ASP:CA	1:E:92:GLN:HE21	2.20	0.53
1:C:29:ASP:O	1:C:33:ILE:HG13	2.06	0.53
1:B:78:ARG:O	1:B:79:GLN:C	2.45	0.53
1:C:138:TYR:CD2	1:C:188:ILE:HD12	2.43	0.53
1:C:574:LYS:HE2	1:C:578:MET:HG2	1.90	0.53
1:D:237:SER:CB	1:D:573:SER:HA	2.37	0.53
1:B:367:VAL:HG23	1:B:373:THR:O	2.08	0.53
1:A:278:GLU:H	1:A:354:GLN:NE2	2.06	0.53
1:A:367:VAL:HG23	1:A:373:THR:O	2.08	0.53
1:A:201:PHE:HB3	1:A:216:LYS:HD3	1.90	0.53
1:C:201:PHE:HB3	1:C:216:LYS:HD3	1.90	0.53
1:C:324:LEU:O	1:C:328:ILE:HG13	2.08	0.53
1:F:620:ARG:HG3	1:F:624:TYR:CD2	2.43	0.53
1:E:61:ASN:C	1:E:63:HIS:N	2.62	0.53
2:E:658:NDG:H3	2:E:658:NDG:O7	2.08	0.53
1:F:313:ILE:O	1:F:313:ILE:HG13	2.07	0.53
1:C:256:PHE:CZ	1:C:258:PRO:HB3	2.44	0.53
1:F:256:PHE:C	1:F:256:PHE:CD1	2.82	0.53
1:F:424:THR:HA	1:F:456:ASN:O	2.09	0.53
1:D:418:ILE:HD11	1:D:462:TYR:CE1	2.43	0.53
1:E:201:PHE:HB3	1:E:216:LYS:HD3	1.90	0.53
1:E:220:PHE:CZ	1:E:329:GLU:HB2	2.43	0.53
1:B:256:PHE:CZ	1:B:258:PRO:HB3	2.44	0.53
1:F:403:HIS:O	1:F:405:ASN:N	2.42	0.53
1:D:21:ILE:O	1:D:21:ILE:HG13	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:ILE:HG13	1:F:21:ILE:O	2.09	0.53
1:A:313:ILE:O	1:A:313:ILE:HG13	2.07	0.53
1:F:256:PHE:CZ	1:F:258:PRO:HB3	2.44	0.53
1:F:425:PHE:N	1:F:456:ASN:O	2.39	0.53
1:D:551:HIS:HD2	1:D:552:ASP:N	2.05	0.53
1:B:307:ASP:OD1	1:B:309:ASP:N	2.34	0.53
1:B:477:THR:HB	1:B:479:ARG:HH12	1.70	0.53
1:B:521:ARG:HG2	1:B:522:SER:N	2.23	0.53
1:A:403:HIS:C	1:A:405:ASN:N	2.59	0.53
1:E:197:TRP:NE1	1:E:223:VAL:HG21	2.24	0.53
1:A:21:ILE:HG13	1:A:21:ILE:O	2.09	0.53
1:D:76:ASN:CB	1:D:79:GLN:HB2	2.34	0.53
1:A:338:GLN:NE2	1:E:316:ARG:HH21	2.07	0.53
1:C:424:THR:HA	1:C:456:ASN:O	2.09	0.53
1:B:220:PHE:CZ	1:B:329:GLU:HB2	2.43	0.53
1:F:521:ARG:HG2	1:F:522:SER:N	2.23	0.53
1:C:521:ARG:HG2	1:C:522:SER:N	2.23	0.53
1:B:611:VAL:HG12	1:B:612:HIS:HD2	1.73	0.53
1:E:620:ARG:HG3	1:E:624:TYR:CD2	2.43	0.53
1:B:197:TRP:NE1	1:B:223:VAL:HG21	2.24	0.53
1:F:45:ILE:O	1:F:94:LYS:HD3	2.09	0.53
1:B:61:ASN:C	1:B:63:HIS:N	2.62	0.53
1:F:61:ASN:C	1:F:63:HIS:N	2.62	0.53
1:D:174:LYS:O	1:D:175:LYS:CG	2.54	0.53
1:D:256:PHE:CD1	1:D:256:PHE:C	2.82	0.53
2:C:658:NDG:H3	2:C:658:NDG:O7	2.07	0.53
1:E:37:PHE:CZ	1:E:101:SER:HB3	2.43	0.53
1:B:37:PHE:CZ	1:B:101:SER:HB3	2.43	0.53
1:F:12:GLN:OE1	1:F:547:VAL:HG21	2.08	0.53
1:F:574:LYS:HE2	1:F:578:MET:HG2	1.89	0.53
1:F:477:THR:HG23	1:F:509:PHE:CD1	2.43	0.53
1:C:403:HIS:O	1:C:405:ASN:N	2.42	0.53
1:D:45:ILE:O	1:D:94:LYS:HD3	2.09	0.53
1:A:303:GLY:O	1:A:315:ILE:HG12	2.09	0.53
1:B:248:TRP:CH2	1:B:289:LEU:HD13	2.44	0.53
1:A:248:TRP:CH2	1:A:289:LEU:HD13	2.44	0.53
1:B:45:ILE:O	1:B:94:LYS:HD3	2.09	0.53
1:C:31:LYS:O	1:C:34:ALA:HB3	2.09	0.53
1:E:473:GLU:HG3	1:E:473:GLU:O	2.08	0.53
1:A:37:PHE:CZ	1:A:101:SER:HB3	2.43	0.53
1:D:574:LYS:HE2	1:D:578:MET:HG2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:GLU:H	1:C:354:GLN:NE2	2.06	0.53
1:F:126:SER:OG	1:F:127:LYS:N	2.41	0.53
1:A:620:ARG:HG3	1:A:624:TYR:CD2	2.43	0.53
1:F:17:LEU:HD21	1:F:103:ALA:O	2.09	0.53
1:E:31:LYS:O	1:E:34:ALA:HB3	2.09	0.53
1:D:197:TRP:NE1	1:D:223:VAL:HG21	2.24	0.53
1:C:248:TRP:CH2	1:C:289:LEU:HD13	2.44	0.53
1:A:17:LEU:HD21	1:A:103:ALA:O	2.09	0.53
1:E:17:LEU:HD21	1:E:103:ALA:O	2.09	0.53
1:D:31:LYS:O	1:D:34:ALA:HB3	2.09	0.53
1:C:78:ARG:HD3	1:C:82:GLU:OE2	2.10	0.53
1:D:256:PHE:CZ	1:D:258:PRO:HB3	2.44	0.53
1:B:138:TYR:CD2	1:B:188:ILE:HD12	2.43	0.53
1:C:313:ILE:HG13	1:C:313:ILE:O	2.07	0.53
1:B:424:THR:HA	1:B:456:ASN:O	2.09	0.53
1:B:425:PHE:N	1:B:456:ASN:O	2.39	0.53
1:A:317:GLN:CB	1:A:318:PRO:HD2	2.36	0.53
1:D:201:PHE:HB3	1:D:216:LYS:HD3	1.90	0.53
1:E:479:ARG:HD2	1:E:587:THR:CG2	2.39	0.53
1:A:403:HIS:O	1:A:405:ASN:N	2.42	0.53
1:A:126:SER:OG	1:A:127:LYS:N	2.41	0.53
1:F:197:TRP:NE1	1:F:223:VAL:HG21	2.24	0.53
1:C:303:GLY:O	1:C:315:ILE:HG12	2.09	0.53
1:C:45:ILE:O	1:C:94:LYS:HD3	2.09	0.53
1:A:31:LYS:O	1:A:34:ALA:HB3	2.09	0.53
1:A:45:ILE:O	1:A:94:LYS:HD3	2.09	0.53
1:E:303:GLY:O	1:E:315:ILE:HG12	2.09	0.53
1:E:21:ILE:HG13	1:E:21:ILE:O	2.09	0.53
1:D:473:GLU:O	1:D:473:GLU:HG3	2.08	0.52
1:C:487:ASP:CB	1:C:489:ASN:H	2.10	0.52
1:B:473:GLU:O	1:B:473:GLU:HG3	2.08	0.52
1:E:37:PHE:CE2	1:E:101:SER:CB	2.92	0.52
1:E:78:ARG:O	1:E:79:GLN:C	2.45	0.52
1:E:78:ARG:HD3	1:E:82:GLU:OE2	2.09	0.52
1:F:278:GLU:H	1:F:354:GLN:NE2	2.06	0.52
1:D:557:ALA:HB3	1:D:558:TYR:CE1	2.44	0.52
1:C:479:ARG:HD2	1:C:587:THR:CG2	2.39	0.52
1:C:4:GLY:HA2	1:C:95:GLU:OE1	2.09	0.52
1:C:301:ASP:CG	1:C:393:LYS:HZ1	2.11	0.52
1:A:197:TRP:NE1	1:A:223:VAL:HG21	2.24	0.52
1:E:398:PHE:HB3	1:E:399:PRO:HD2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:303:GLY:O	1:F:315:ILE:HG12	2.09	0.52
1:B:78:ARG:HD3	1:B:82:GLU:OE2	2.09	0.52
1:F:473:GLU:HG3	1:F:473:GLU:O	2.08	0.52
1:E:138:TYR:CD2	1:E:188:ILE:HD12	2.43	0.52
1:E:367:VAL:HG23	1:E:373:THR:O	2.08	0.52
1:E:425:PHE:N	1:E:456:ASN:O	2.39	0.52
1:A:557:ALA:HB3	1:A:558:TYR:CE1	2.44	0.52
1:F:557:ALA:HB3	1:F:558:TYR:CE1	2.44	0.52
1:B:4:GLY:HA2	1:B:95:GLU:OE1	2.09	0.52
1:B:324:LEU:O	1:B:328:ILE:HG13	2.08	0.52
1:F:248:TRP:CH2	1:F:289:LEU:HD13	2.44	0.52
1:E:43:THR:HG23	1:E:49:HIS:C	2.29	0.52
1:F:78:ARG:HD3	1:F:82:GLU:OE2	2.09	0.52
1:A:78:ARG:HD3	1:A:82:GLU:OE2	2.09	0.52
1:C:551:HIS:HD2	1:C:552:ASP:N	2.05	0.52
1:A:256:PHE:CD1	1:A:256:PHE:C	2.82	0.52
1:E:403:HIS:O	1:E:405:ASN:N	2.42	0.52
1:B:17:LEU:HD21	1:B:103:ALA:O	2.09	0.52
1:D:303:GLY:O	1:D:315:ILE:HG12	2.09	0.52
1:C:43:THR:HG23	1:C:49:HIS:C	2.29	0.52
1:A:43:THR:HG23	1:A:49:HIS:C	2.29	0.52
1:F:551:HIS:O	1:F:552:ASP:CB	2.55	0.52
1:F:52:ALA:HB1	1:F:89:VAL:HG23	1.91	0.52
1:B:403:HIS:O	1:B:405:ASN:N	2.42	0.52
1:F:43:THR:HG23	1:F:49:HIS:C	2.29	0.52
1:C:138:TYR:CZ	1:C:188:ILE:HD12	2.45	0.52
1:C:256:PHE:C	1:C:256:PHE:CD1	2.82	0.52
1:A:220:PHE:CZ	1:A:329:GLU:HB2	2.43	0.52
1:C:479:ARG:HD2	1:C:587:THR:HG21	1.92	0.52
1:B:479:ARG:HD2	1:B:587:THR:HG21	1.92	0.52
1:E:4:GLY:HA2	1:E:95:GLU:OE1	2.09	0.52
1:E:248:TRP:CH2	1:E:289:LEU:HD13	2.44	0.52
1:D:248:TRP:CH2	1:D:289:LEU:HD13	2.44	0.52
1:F:337:VAL:HG13	1:F:338:GLN:N	2.25	0.52
1:A:316:ARG:CD	4:A:829:HOH:O	2.48	0.52
1:B:201:PHE:HB3	1:B:216:LYS:HD3	1.90	0.52
1:A:521:ARG:HG2	1:A:522:SER:N	2.23	0.52
1:C:317:GLN:CB	1:C:318:PRO:HD2	2.36	0.52
1:A:533:MET:CB	1:A:534:PRO:HD2	2.28	0.52
1:A:52:ALA:HB1	1:A:89:VAL:HG23	1.91	0.52
1:A:479:ARG:HD2	1:A:587:THR:HG21	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:ILE:O	1:E:94:LYS:HD3	2.09	0.52
1:B:43:THR:HG23	1:B:49:HIS:C	2.29	0.52
1:D:78:ARG:HD3	1:D:82:GLU:OE2	2.09	0.52
1:A:413:VAL:HG23	1:A:466:MET:HE3	1.91	0.52
1:F:138:TYR:CD2	1:F:188:ILE:HD12	2.43	0.52
1:D:4:GLY:HA2	1:D:95:GLU:OE1	2.09	0.52
1:C:17:LEU:HD21	1:C:103:ALA:O	2.09	0.52
1:B:31:LYS:O	1:B:34:ALA:HB3	2.09	0.52
1:D:37:PHE:CE2	1:D:101:SER:CB	2.91	0.52
1:B:557:ALA:HB3	1:B:558:TYR:CE1	2.44	0.52
1:A:479:ARG:HD2	1:A:587:THR:CG2	2.39	0.52
1:F:4:GLY:HA2	1:F:95:GLU:OE1	2.09	0.52
1:A:343:LEU:HD11	4:A:861:HOH:O	2.09	0.52
1:A:424:THR:HA	1:A:456:ASN:O	2.09	0.52
1:F:417:ALA:O	1:F:463:LYS:N	2.37	0.52
1:F:201:PHE:HB3	1:F:216:LYS:HD3	1.90	0.52
1:F:479:ARG:HD2	1:F:587:THR:CG2	2.39	0.52
1:D:403:HIS:O	1:D:405:ASN:N	2.42	0.52
1:C:197:TRP:NE1	1:C:223:VAL:HG21	2.24	0.52
1:A:398:PHE:HB3	1:A:399:PRO:HD2	1.91	0.52
1:B:21:ILE:HG13	1:B:21:ILE:O	2.09	0.52
1:A:61:ASN:C	1:A:63:HIS:N	2.62	0.52
2:A:658:NDG:C7	2:A:658:NDG:C8	2.88	0.52
1:A:138:TYR:CZ	1:A:188:ILE:HD12	2.45	0.52
1:A:337:VAL:HG13	1:A:338:GLN:N	2.25	0.52
1:D:455:LEU:HG	1:D:456:ASN:H	1.75	0.52
1:B:479:ARG:HD2	1:B:587:THR:CG2	2.39	0.52
1:C:398:PHE:HB3	1:C:399:PRO:HD2	1.91	0.52
1:C:21:ILE:O	1:C:21:ILE:HG13	2.09	0.52
1:C:61:ASN:C	1:C:63:HIS:N	2.62	0.51
2:F:658:NDG:C7	2:F:658:NDG:C8	2.88	0.51
1:D:424:THR:HA	1:D:456:ASN:O	2.09	0.51
1:C:557:ALA:HB3	1:C:558:TYR:CE1	2.44	0.51
1:E:430:GLN:HA	1:E:450:ALA:O	2.10	0.51
1:D:89:VAL:C	1:D:91:ASN:N	2.63	0.51
1:E:52:ALA:HB1	1:E:89:VAL:HG23	1.91	0.51
1:D:43:THR:HG23	1:D:49:HIS:C	2.29	0.51
1:B:303:GLY:O	1:B:315:ILE:HG12	2.09	0.51
1:F:398:PHE:HB3	1:F:399:PRO:HD2	1.91	0.51
1:D:61:ASN:C	1:D:63:HIS:N	2.62	0.51
2:D:658:NDG:C7	2:D:658:NDG:C8	2.88	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:PRO:HB2	4:A:857:HOH:O	2.09	0.51
1:E:237:SER:CB	1:E:573:SER:HA	2.37	0.51
1:E:424:THR:HA	1:E:456:ASN:O	2.09	0.51
1:A:430:GLN:HA	1:A:450:ALA:O	2.10	0.51
1:F:551:HIS:HD2	1:F:552:ASP:N	2.05	0.51
1:B:269:PRO:HB3	1:B:363:LEU:CD2	2.41	0.51
1:D:17:LEU:HD21	1:D:103:ALA:O	2.09	0.51
1:F:31:LYS:O	1:F:34:ALA:HB3	2.09	0.51
1:B:280:VAL:HA	1:B:357:PRO:HB3	1.93	0.51
1:A:280:VAL:HA	1:A:357:PRO:HB3	1.93	0.51
1:B:513:PRO:CG	1:B:517:GLU:HB2	2.27	0.51
2:E:658:NDG:C7	2:E:658:NDG:C8	2.88	0.51
2:B:658:NDG:C7	2:B:658:NDG:C8	2.88	0.51
1:D:425:PHE:N	1:D:456:ASN:O	2.39	0.51
1:C:337:VAL:HG13	1:C:338:GLN:N	2.25	0.51
1:D:52:ALA:HB1	1:D:89:VAL:HG23	1.91	0.51
1:F:29:ASP:OD1	1:F:29:ASP:N	2.31	0.51
1:E:337:VAL:HG13	1:E:338:GLN:N	2.25	0.51
1:E:487:ASP:CB	1:E:489:ASN:H	2.09	0.51
1:D:272:PRO:CD	1:E:272:PRO:HG2	2.41	0.51
1:D:366:GLY:N	1:D:369:GLU:HG3	2.21	0.51
1:D:353:ARG:NE	1:D:369:GLU:OE2	2.43	0.51
1:A:4:GLY:HA2	1:A:95:GLU:OE1	2.09	0.51
1:B:301:ASP:CG	1:B:393:LYS:HZ1	2.12	0.51
1:A:156:SER:OG	1:B:438:ASP:OD1	2.27	0.51
1:D:322:GLU:O	1:D:323:LEU:C	2.49	0.51
1:F:138:TYR:CZ	1:F:188:ILE:HD12	2.45	0.51
1:D:8:ALA:HA	1:D:553:LEU:CD1	2.40	0.51
1:B:430:GLN:HA	1:B:450:ALA:O	2.10	0.51
1:D:430:GLN:HA	1:D:450:ALA:O	2.10	0.51
1:B:533:MET:CB	1:B:534:PRO:HD2	2.28	0.51
1:D:48:ASP:OD2	1:D:51:ALA:HB3	2.11	0.51
1:B:411:MET:N	1:B:411:MET:SD	2.83	0.51
1:F:300:ILE:CD1	1:F:390:ILE:CG2	2.89	0.51
1:D:403:HIS:C	1:D:405:ASN:N	2.59	0.51
1:A:269:PRO:HB3	1:A:363:LEU:CD2	2.41	0.51
2:C:658:NDG:C8	2:C:658:NDG:C7	2.88	0.51
1:B:366:GLY:N	1:B:369:GLU:HG3	2.21	0.51
1:B:201:PHE:HB3	1:B:216:LYS:HD2	1.92	0.51
1:C:89:VAL:C	1:C:91:ASN:N	2.63	0.51
1:B:52:ALA:HB1	1:B:89:VAL:HG23	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:VAL:C	1:B:91:ASN:N	2.63	0.51
1:E:48:ASP:OD2	1:E:51:ALA:HB3	2.11	0.51
1:D:479:ARG:HD2	1:D:587:THR:CG2	2.39	0.51
1:C:126:SER:OG	1:C:127:LYS:N	2.41	0.51
1:E:269:PRO:HB3	1:E:363:LEU:CD2	2.41	0.51
1:D:280:VAL:HA	1:D:357:PRO:HB3	1.93	0.51
1:B:106:PHE:O	1:B:107:ARG:C	2.49	0.51
1:D:159:MET:HE2	1:E:155:TYR:CG	2.45	0.51
1:F:634:ARG:HG2	1:F:634:ARG:NH1	2.14	0.51
1:B:322:GLU:O	1:B:323:LEU:C	2.49	0.51
1:D:337:VAL:HG13	1:D:338:GLN:N	2.25	0.51
1:D:138:TYR:CD2	1:D:188:ILE:HD12	2.43	0.51
1:E:76:ASN:HD22	1:E:79:GLN:HG3	1.76	0.51
1:D:353:ARG:O	1:D:354:GLN:C	2.49	0.51
1:D:418:ILE:HD11	1:D:462:TYR:HE1	1.76	0.51
1:F:430:GLN:HA	1:F:450:ALA:O	2.10	0.51
1:E:557:ALA:HB3	1:E:558:TYR:CE1	2.44	0.51
1:E:89:VAL:C	1:E:91:ASN:N	2.63	0.51
1:C:300:ILE:CD1	1:C:390:ILE:CG2	2.89	0.51
1:A:300:ILE:CD1	1:A:390:ILE:CG2	2.89	0.51
1:D:269:PRO:HB3	1:D:363:LEU:CD2	2.41	0.51
1:C:269:PRO:HB3	1:C:363:LEU:CD2	2.41	0.51
1:F:280:VAL:HA	1:F:357:PRO:HB3	1.93	0.51
1:C:280:VAL:HA	1:C:357:PRO:HB3	1.93	0.51
1:B:487:ASP:CB	1:B:489:ASN:H	2.09	0.51
1:E:138:TYR:CZ	1:E:188:ILE:HD12	2.45	0.51
1:A:102:ASN:O	1:A:104:ALA:N	2.44	0.51
1:B:37:PHE:CE2	1:B:101:SER:CB	2.92	0.51
1:B:606:HIS:HD2	1:B:608:GLN:CG	2.14	0.51
1:F:56:LEU:HD21	1:F:110:MET:HE1	1.93	0.51
1:E:13:ASP:CG	1:E:100:ARG:HD2	2.31	0.51
1:F:366:GLY:N	1:F:369:GLU:HG3	2.22	0.51
1:D:278:GLU:H	1:D:354:GLN:NE2	2.06	0.51
1:C:417:ALA:O	1:C:463:LYS:N	2.37	0.51
1:C:430:GLN:HA	1:C:450:ALA:O	2.10	0.51
1:A:611:VAL:HG12	1:A:612:HIS:HD2	1.73	0.51
1:E:280:VAL:HA	1:E:357:PRO:HB3	1.93	0.51
1:B:337:VAL:HG13	1:B:338:GLN:N	2.25	0.51
1:C:413:VAL:HG23	1:C:466:MET:HE3	1.91	0.51
1:D:177:ARG:HD2	1:E:360:LYS:O	2.11	0.51
1:A:37:PHE:CE2	1:A:101:SER:CB	2.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:580:PHE:CD2	1:F:649:ILE:HG13	2.46	0.51
1:C:546:ALA:HB1	1:C:552:ASP:OD1	2.11	0.51
1:C:52:ALA:HB1	1:C:89:VAL:HG23	1.92	0.51
1:A:48:ASP:OD2	1:A:51:ALA:HB3	2.11	0.51
1:D:300:ILE:CD1	1:D:390:ILE:CG2	2.89	0.51
1:B:71:TRP:CZ3	1:B:365:PRO:HG2	2.46	0.51
1:F:13:ASP:CG	1:F:100:ARG:HD2	2.31	0.51
1:B:13:ASP:CG	1:B:100:ARG:HD2	2.31	0.51
1:B:454:ARG:CZ	1:B:567:ARG:HD2	2.41	0.51
1:A:418:ILE:HD11	1:A:462:TYR:HE1	1.76	0.51
1:E:86:LEU:HD23	1:E:86:LEU:C	2.30	0.51
1:A:138:TYR:O	1:A:142:PRO:HG3	2.11	0.50
1:B:138:TYR:O	1:B:142:PRO:HG3	2.11	0.50
1:D:102:ASN:O	1:D:104:ALA:N	2.44	0.50
1:E:580:PHE:CD2	1:E:649:ILE:HG13	2.46	0.50
1:D:479:ARG:HD2	1:D:587:THR:HG21	1.92	0.50
1:F:479:ARG:HD2	1:F:587:THR:HG21	1.92	0.50
1:F:71:TRP:CZ3	1:F:365:PRO:HG2	2.46	0.50
1:C:71:TRP:CZ3	1:C:365:PRO:HG2	2.46	0.50
1:D:398:PHE:HB3	1:D:399:PRO:HD2	1.92	0.50
1:E:454:ARG:CZ	1:E:567:ARG:HD2	2.41	0.50
1:A:454:ARG:CZ	1:A:567:ARG:HD2	2.41	0.50
1:B:398:PHE:HB3	1:B:399:PRO:HD2	1.91	0.50
1:F:455:LEU:HG	1:F:456:ASN:H	1.75	0.50
1:B:417:ALA:O	1:B:463:LYS:N	2.37	0.50
1:E:546:ALA:HB1	1:E:552:ASP:OD1	2.11	0.50
1:F:48:ASP:OD2	1:F:51:ALA:HB3	2.11	0.50
1:B:564:ILE:HB	1:B:565:PRO:CD	2.42	0.50
1:B:300:ILE:CD1	1:B:390:ILE:CG2	2.89	0.50
1:B:402:THR:N	1:B:405:ASN:HB2	2.27	0.50
1:C:13:ASP:CG	1:C:100:ARG:HD2	2.31	0.50
1:D:279:ASP:OD1	1:D:286:VAL:N	2.42	0.50
1:C:454:ARG:CZ	1:C:567:ARG:HD2	2.41	0.50
1:C:491:ILE:HD11	1:D:175:LYS:C	2.32	0.50
1:C:138:TYR:O	1:C:142:PRO:HG3	2.12	0.50
1:C:580:PHE:CD2	1:C:649:ILE:HG13	2.46	0.50
1:A:580:PHE:CD2	1:A:649:ILE:HG13	2.46	0.50
1:A:13:ASP:OD1	1:A:100:ARG:NE	2.43	0.50
1:E:455:LEU:HG	1:E:456:ASN:H	1.75	0.50
1:E:317:GLN:CB	1:E:318:PRO:HD2	2.36	0.50
1:B:479:ARG:HH11	1:B:587:THR:CG2	2.24	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:TRP:CZ3	1:D:365:PRO:HG2	2.47	0.50
1:D:158:LYS:O	1:D:159:MET:C	2.49	0.50
1:A:158:LYS:O	1:A:159:MET:C	2.49	0.50
1:E:106:PHE:O	1:E:107:ARG:C	2.49	0.50
1:C:506:ASP:OD1	1:C:507:LYS:N	2.44	0.50
1:C:158:LYS:O	1:C:159:MET:C	2.49	0.50
1:D:78:ARG:O	1:D:79:GLN:C	2.45	0.50
1:D:632:ASP:O	1:D:635:VAL:HG23	2.12	0.50
1:B:465:THR:O	1:B:466:MET:HB3	2.12	0.50
1:D:138:TYR:O	1:D:142:PRO:HG3	2.11	0.50
1:B:580:PHE:CD2	1:B:649:ILE:HG13	2.46	0.50
1:D:13:ASP:CG	1:D:100:ARG:HD2	2.31	0.50
1:C:48:ASP:OD2	1:C:51:ALA:HB3	2.11	0.50
1:D:564:ILE:HB	1:D:565:PRO:CD	2.42	0.50
1:A:402:THR:N	1:A:405:ASN:HB2	2.27	0.50
1:D:316:ARG:HH21	1:F:338:GLN:HE22	1.58	0.50
1:B:455:LEU:HG	1:B:456:ASN:H	1.75	0.50
1:F:353:ARG:O	1:F:354:GLN:C	2.49	0.50
1:E:479:ARG:HH11	1:E:587:THR:CG2	2.25	0.50
1:E:479:ARG:HD2	1:E:587:THR:HG21	1.92	0.50
1:F:479:ARG:HH11	1:F:587:THR:CG2	2.24	0.50
1:A:403:HIS:C	1:A:405:ASN:H	2.15	0.50
1:D:403:HIS:C	1:D:405:ASN:H	2.15	0.50
1:C:402:THR:N	1:C:405:ASN:HB2	2.27	0.50
1:E:71:TRP:CZ3	1:E:365:PRO:HG2	2.47	0.50
1:A:506:ASP:OD1	1:A:507:LYS:N	2.44	0.50
1:D:454:ARG:CZ	1:D:567:ARG:HD2	2.41	0.50
1:C:8:ALA:CB	1:C:553:LEU:HD12	2.42	0.50
1:D:8:ALA:CB	1:D:553:LEU:HD12	2.42	0.50
1:F:8:ALA:CB	1:F:553:LEU:HD12	2.42	0.50
1:C:455:LEU:HG	1:C:456:ASN:H	1.75	0.50
1:D:13:ASP:OD1	1:D:100:ARG:NE	2.43	0.50
1:E:418:ILE:HD11	1:E:462:TYR:HE1	1.76	0.50
1:A:173:THR:HG22	1:A:176:ASN:HB2	1.94	0.50
1:A:479:ARG:HH11	1:A:587:THR:CG2	2.25	0.50
1:E:564:ILE:HB	1:E:565:PRO:CD	2.42	0.50
1:E:402:THR:N	1:E:405:ASN:HB2	2.27	0.50
1:C:29:ASP:OD1	1:C:29:ASP:N	2.31	0.50
1:D:72:TYR:HA	1:D:79:GLN:OE1	2.12	0.50
1:F:543:ALA:HA	1:F:553:LEU:HD11	1.94	0.50
1:F:76:ASN:HD22	1:F:79:GLN:HG3	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:SER:CB	1:C:573:SER:HA	2.37	0.50
1:C:418:ILE:HD11	1:C:462:TYR:HE1	1.76	0.50
1:D:402:THR:N	1:D:405:ASN:HB2	2.27	0.50
1:F:222:TRP:CH2	1:F:226:GLN:NE2	2.80	0.50
1:B:76:ASN:HD22	1:B:79:GLN:HG3	1.76	0.50
1:E:97:TYR:O	1:E:101:SER:HB2	2.12	0.50
1:C:96:TRP:O	1:C:97:TYR:C	2.50	0.50
1:A:11:GLN:HG3	1:A:15:ASN:ND2	2.22	0.50
1:A:455:LEU:HG	1:A:456:ASN:H	1.75	0.50
1:A:13:ASP:CG	1:A:100:ARG:HD2	2.31	0.50
1:B:551:HIS:O	1:B:552:ASP:CB	2.55	0.50
1:D:546:ALA:HB1	1:D:552:ASP:OD1	2.11	0.50
1:D:555:LEU:HD12	1:D:555:LEU:H	1.77	0.50
1:F:173:THR:HG22	1:F:176:ASN:HB2	1.94	0.50
1:E:555:LEU:O	1:E:557:ALA:N	2.45	0.50
1:F:555:LEU:HD12	1:F:555:LEU:H	1.77	0.50
1:B:86:LEU:C	1:B:86:LEU:HD23	2.30	0.50
1:E:522:SER:C	1:E:524:LYS:N	2.63	0.50
1:E:300:ILE:CD1	1:E:390:ILE:CG2	2.89	0.50
1:F:269:PRO:HB3	1:F:363:LEU:CD2	2.40	0.50
1:D:222:TRP:CZ2	1:D:226:GLN:NE2	2.80	0.50
1:F:454:ARG:CZ	1:F:567:ARG:HD2	2.41	0.50
1:A:106:PHE:O	1:A:107:ARG:C	2.49	0.50
1:E:8:ALA:HA	1:E:553:LEU:CD1	2.40	0.50
1:E:96:TRP:O	1:E:97:TYR:C	2.51	0.50
1:C:97:TYR:O	1:C:101:SER:HB2	2.12	0.50
1:E:138:TYR:O	1:E:142:PRO:HG3	2.11	0.50
1:B:138:TYR:CZ	1:B:188:ILE:HD12	2.45	0.50
1:B:8:ALA:CB	1:B:553:LEU:HD12	2.42	0.50
1:F:72:TYR:HA	1:F:79:GLN:OE1	2.12	0.50
1:F:419:ASP:HB2	1:F:463:LYS:HZ2	1.77	0.50
1:C:353:ARG:O	1:C:354:GLN:C	2.49	0.50
1:F:555:LEU:O	1:F:557:ALA:N	2.45	0.50
1:E:533:MET:CB	1:E:534:PRO:CD	2.90	0.50
1:B:479:ARG:NH1	1:B:587:THR:OG1	2.45	0.50
1:F:428:GLU:HG3	1:F:453:HIS:CD2	2.47	0.50
1:F:632:ASP:O	1:F:635:VAL:HG23	2.12	0.50
1:F:83:ALA:HB2	1:F:114:GLU:HA	1.94	0.50
1:C:76:ASN:HD22	1:C:79:GLN:HG3	1.76	0.49
1:E:632:ASP:O	1:E:635:VAL:HG23	2.12	0.49
1:E:543:ALA:HA	1:E:553:LEU:HD11	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ASN:O	1:C:104:ALA:N	2.44	0.49
1:B:96:TRP:O	1:B:97:TYR:C	2.50	0.49
1:A:237:SER:CB	1:A:573:SER:HA	2.37	0.49
1:A:72:TYR:HA	1:A:79:GLN:OE1	2.12	0.49
1:F:424:THR:HA	1:F:457:HIS:HA	1.94	0.49
1:A:173:THR:CG2	1:A:176:ASN:HB2	2.42	0.49
1:D:201:PHE:HB3	1:D:216:LYS:HD2	1.92	0.49
1:D:533:MET:CB	1:D:534:PRO:CD	2.90	0.49
1:A:89:VAL:C	1:A:91:ASN:N	2.63	0.49
1:F:13:ASP:OD1	1:F:100:ARG:NE	2.43	0.49
1:E:285:HIS:O	1:E:288:ASP:HB2	2.12	0.49
1:C:83:ALA:HB2	1:C:114:GLU:HA	1.94	0.49
1:C:222:TRP:CZ2	1:C:226:GLN:NE2	2.80	0.49
1:F:106:PHE:O	1:F:107:ARG:C	2.49	0.49
1:D:506:ASP:OD1	1:D:507:LYS:N	2.44	0.49
1:D:428:GLU:HG3	1:D:453:HIS:CD2	2.47	0.49
1:B:227:LEU:CD1	1:B:227:LEU:N	2.75	0.49
1:B:83:ALA:HB2	1:B:114:GLU:HA	1.94	0.49
1:D:633:GLU:C	1:D:635:VAL:N	2.66	0.49
1:C:72:TYR:HA	1:C:79:GLN:OE1	2.12	0.49
1:C:173:THR:HG22	1:C:176:ASN:HB2	1.94	0.49
1:C:8:ALA:HA	1:C:553:LEU:CD1	2.40	0.49
1:F:138:TYR:O	1:F:142:PRO:HG3	2.12	0.49
1:D:11:GLN:HG3	1:D:15:ASN:ND2	2.22	0.49
1:F:560:ARG:NH1	1:F:606:HIS:N	2.60	0.49
1:F:239:TRP:CZ3	1:F:574:LYS:NZ	2.79	0.49
1:E:72:TYR:HA	1:E:79:GLN:OE1	2.12	0.49
1:C:424:THR:HA	1:C:457:HIS:HA	1.94	0.49
1:F:546:ALA:HB1	1:F:552:ASP:OD1	2.11	0.49
1:E:555:LEU:H	1:E:555:LEU:HD12	1.77	0.49
1:B:533:MET:CB	1:B:534:PRO:CD	2.90	0.49
1:B:48:ASP:OD2	1:B:51:ALA:HB3	2.11	0.49
1:A:71:TRP:CZ3	1:A:365:PRO:HG2	2.46	0.49
1:B:70:HIS:ND1	1:B:71:TRP:N	2.60	0.49
1:B:222:TRP:CH2	1:B:226:GLN:NE2	2.80	0.49
1:B:632:ASP:O	1:B:635:VAL:HG23	2.12	0.49
1:E:506:ASP:OD1	1:E:507:LYS:N	2.44	0.49
1:D:173:THR:CG2	1:D:176:ASN:HB2	2.42	0.49
1:E:8:ALA:CB	1:E:553:LEU:HD12	2.42	0.49
1:C:560:ARG:NH1	1:C:606:HIS:N	2.60	0.49
1:D:580:PHE:CD2	1:D:649:ILE:HG13	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ARG:HH21	1:C:338:GLN:NE2	2.11	0.49
1:B:551:HIS:HD2	1:B:552:ASP:N	2.05	0.49
1:F:533:MET:CB	1:F:534:PRO:CD	2.90	0.49
1:A:533:MET:CB	1:A:534:PRO:CD	2.90	0.49
1:C:533:MET:CB	1:C:534:PRO:CD	2.90	0.49
1:D:479:ARG:HH11	1:D:587:THR:CG2	2.25	0.49
1:C:70:HIS:ND1	1:C:71:TRP:N	2.60	0.49
1:B:222:TRP:CZ2	1:B:226:GLN:NE2	2.80	0.49
1:D:222:TRP:CH2	1:D:226:GLN:NE2	2.80	0.49
1:A:222:TRP:CH2	1:A:226:GLN:NE2	2.80	0.49
1:D:285:HIS:O	1:D:288:ASP:HB2	2.12	0.49
1:F:506:ASP:OD1	1:F:507:LYS:N	2.44	0.49
1:A:428:GLU:HG3	1:A:453:HIS:CD2	2.47	0.49
1:D:76:ASN:HD22	1:D:79:GLN:HG3	1.76	0.49
1:B:72:TYR:HA	1:B:79:GLN:OE1	2.12	0.49
1:A:8:ALA:CB	1:A:553:LEU:HD12	2.42	0.49
1:F:37:PHE:CE2	1:F:101:SER:CB	2.91	0.49
1:F:353:ARG:NE	1:F:369:GLU:OE2	2.43	0.49
1:B:555:LEU:H	1:B:555:LEU:HD12	1.77	0.49
1:F:89:VAL:C	1:F:91:ASN:N	2.63	0.49
1:B:175:LYS:O	1:B:176:ASN:CB	2.60	0.49
1:C:201:PHE:HB3	1:C:216:LYS:HD2	1.92	0.49
1:A:479:ARG:NH1	1:A:587:THR:OG1	2.45	0.49
1:C:564:ILE:HB	1:C:565:PRO:CD	2.42	0.49
1:F:522:SER:C	1:F:524:LYS:N	2.63	0.49
1:F:403:HIS:C	1:F:405:ASN:H	2.15	0.49
1:D:402:THR:O	1:D:405:ASN:HB2	2.13	0.49
1:A:589:GLY:O	1:A:593:THR:OG1	2.30	0.49
1:C:222:TRP:CH2	1:C:226:GLN:NE2	2.80	0.49
1:F:279:ASP:OD1	1:F:286:VAL:N	2.42	0.49
1:D:83:ALA:HB2	1:D:114:GLU:HA	1.94	0.49
1:E:158:LYS:O	1:E:159:MET:C	2.49	0.49
1:C:428:GLU:HG3	1:C:453:HIS:CD2	2.47	0.49
1:C:173:THR:CG2	1:C:176:ASN:HB2	2.42	0.49
1:B:97:TYR:O	1:B:101:SER:HB2	2.12	0.49
1:B:102:ASN:O	1:B:104:ALA:N	2.44	0.49
1:D:543:ALA:HA	1:D:553:LEU:HD11	1.94	0.49
1:A:424:THR:HA	1:A:457:HIS:HA	1.94	0.49
1:A:353:ARG:O	1:A:354:GLN:C	2.49	0.49
1:E:424:THR:HA	1:E:457:HIS:HA	1.94	0.49
1:A:546:ALA:HB1	1:A:552:ASP:OD1	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:ALA:HB1	1:B:552:ASP:OD1	2.11	0.49
1:B:173:THR:HG22	1:B:176:ASN:HB2	1.94	0.49
1:B:307:ASP:C	1:B:336:ASN:HD22	2.16	0.49
1:F:564:ILE:HB	1:F:565:PRO:CD	2.42	0.49
1:C:479:ARG:HH11	1:C:587:THR:CG2	2.25	0.49
1:A:564:ILE:HB	1:A:565:PRO:CD	2.42	0.49
1:F:69:ARG:HA	1:F:264:TYR:CD2	2.48	0.49
1:F:402:THR:N	1:F:405:ASN:HB2	2.27	0.49
1:F:301:ASP:CG	1:F:393:LYS:HZ1	2.15	0.49
1:E:16:HIS:CD2	1:E:27:TYR:CE2	3.01	0.49
1:F:108:GLU:HA	1:F:108:GLU:OE1	2.13	0.49
1:B:227:LEU:N	1:B:227:LEU:HD12	2.27	0.49
1:F:285:HIS:O	1:F:288:ASP:HB2	2.12	0.49
1:C:434:ILE:C	1:C:436:ALA:H	2.16	0.49
1:B:428:GLU:HG3	1:B:453:HIS:CD2	2.47	0.49
1:B:285:HIS:O	1:B:288:ASP:HB2	2.12	0.49
1:C:633:GLU:C	1:C:635:VAL:N	2.66	0.49
1:C:227:LEU:CD1	1:C:227:LEU:N	2.75	0.49
1:D:560:ARG:NH1	1:D:606:HIS:N	2.60	0.49
1:F:96:TRP:O	1:F:97:TYR:C	2.51	0.49
1:A:555:LEU:H	1:A:555:LEU:HD12	1.77	0.49
1:E:173:THR:HG22	1:E:176:ASN:HB2	1.94	0.49
1:B:217:GLY:H	1:B:220:PHE:H	1.61	0.49
1:A:628:ARG:O	1:A:629:ARG:C	2.50	0.49
1:C:589:GLY:O	1:C:593:THR:OG1	2.30	0.49
1:B:16:HIS:CD2	1:B:27:TYR:CE2	3.01	0.49
1:E:402:THR:O	1:E:405:ASN:HB2	2.13	0.49
1:A:592:ASP:C	1:A:594:GLU:H	2.16	0.49
1:E:594:GLU:HG2	1:E:594:GLU:O	2.13	0.49
1:F:70:HIS:ND1	1:F:71:TRP:N	2.60	0.49
1:F:158:LYS:O	1:F:159:MET:C	2.49	0.49
1:D:195:VAL:HG22	1:D:196:THR:N	2.28	0.49
1:C:285:HIS:O	1:C:288:ASP:HB2	2.12	0.49
1:E:83:ALA:HB2	1:E:114:GLU:HA	1.94	0.49
1:D:227:LEU:N	1:D:227:LEU:CD1	2.75	0.49
1:E:633:GLU:C	1:E:635:VAL:N	2.66	0.49
1:C:11:GLN:HG3	1:C:15:ASN:ND2	2.22	0.49
1:A:543:ALA:HA	1:A:553:LEU:HD11	1.94	0.49
1:D:138:TYR:CZ	1:D:188:ILE:HD12	2.45	0.49
1:C:463:LYS:CG	1:C:520:GLU:HG3	2.43	0.49
1:D:463:LYS:CG	1:D:520:GLU:HG3	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:173:THR:CG2	1:F:176:ASN:HB2	2.42	0.49
1:D:479:ARG:NH1	1:D:587:THR:OG1	2.45	0.49
1:D:190:MET:HG3	1:D:568:MET:HE2	1.95	0.49
1:F:479:ARG:NH1	1:F:587:THR:OG1	2.45	0.49
1:E:538:SER:O	1:E:542:GLN:HG3	2.13	0.49
1:B:538:SER:O	1:B:542:GLN:HG3	2.13	0.49
1:C:69:ARG:HA	1:C:264:TYR:CD2	2.48	0.49
1:D:443:ILE:HD13	1:E:161:GLN:HG3	1.95	0.49
1:F:357:PRO:HB2	1:F:358:HIS:CE1	2.48	0.49
1:C:13:ASP:OD1	1:C:100:ARG:NE	2.43	0.49
1:E:108:GLU:OE1	1:E:108:GLU:HA	2.13	0.49
1:C:632:ASP:O	1:C:635:VAL:HG23	2.12	0.49
1:D:106:PHE:O	1:D:107:ARG:C	2.49	0.49
1:B:506:ASP:OD1	1:B:507:LYS:N	2.44	0.49
1:E:222:TRP:CZ2	1:E:226:GLN:NE2	2.80	0.49
1:D:16:HIS:CD2	1:D:27:TYR:CE2	3.01	0.49
1:E:227:LEU:CD1	1:E:227:LEU:N	2.75	0.49
1:A:487:ASP:CB	1:A:489:ASN:H	2.09	0.49
1:A:585:ALA:HA	1:A:642:ILE:HA	1.95	0.49
1:B:313:ILE:HD12	1:B:314:ASP:O	2.13	0.49
1:A:188:ILE:HG23	4:A:720:HOH:O	2.12	0.49
1:A:313:ILE:HD12	1:A:314:ASP:O	2.13	0.49
1:A:560:ARG:NH1	1:A:606:HIS:N	2.60	0.49
1:E:76:ASN:ND2	1:E:79:GLN:HG3	2.28	0.49
1:F:418:ILE:HD11	1:F:462:TYR:HE1	1.76	0.49
1:A:555:LEU:O	1:A:557:ALA:N	2.45	0.49
1:B:555:LEU:O	1:B:557:ALA:N	2.45	0.49
1:B:173:THR:CG2	1:B:176:ASN:HB2	2.42	0.49
1:C:479:ARG:NH1	1:C:587:THR:OG1	2.45	0.49
1:F:402:THR:O	1:F:405:ASN:HB2	2.13	0.49
1:A:402:THR:O	1:A:405:ASN:HB2	2.13	0.49
1:D:592:ASP:C	1:D:594:GLU:H	2.16	0.49
1:E:301:ASP:CG	1:E:393:LYS:HZ1	2.15	0.49
1:F:592:ASP:C	1:F:594:GLU:H	2.16	0.49
1:A:357:PRO:HB2	1:A:358:HIS:CE1	2.48	0.49
1:E:357:PRO:HB2	1:E:358:HIS:CE1	2.48	0.49
1:A:222:TRP:CZ2	1:A:226:GLN:NE2	2.80	0.49
1:A:16:HIS:CD2	1:A:27:TYR:CE2	3.01	0.49
1:B:434:ILE:C	1:B:436:ALA:H	2.16	0.49
1:A:632:ASP:O	1:A:635:VAL:HG23	2.12	0.49
1:C:543:ALA:HA	1:C:553:LEU:HD11	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:GLU:O	1:A:323:LEU:C	2.49	0.49
1:E:322:GLU:O	1:E:323:LEU:C	2.49	0.49
1:A:96:TRP:O	1:A:97:TYR:C	2.51	0.49
1:C:313:ILE:HD12	1:C:314:ASP:O	2.13	0.49
1:B:8:ALA:HA	1:B:553:LEU:CD1	2.40	0.49
1:A:76:ASN:HD22	1:A:79:GLN:HG3	1.76	0.49
1:B:353:ARG:NE	1:B:369:GLU:OE2	2.43	0.49
1:D:424:THR:HA	1:D:457:HIS:HA	1.94	0.49
1:C:86:LEU:HD23	1:C:86:LEU:C	2.30	0.49
1:E:217:GLY:H	1:E:220:PHE:H	1.61	0.49
1:D:589:GLY:O	1:D:593:THR:OG1	2.30	0.49
1:D:594:GLU:O	1:D:594:GLU:HG2	2.13	0.49
1:A:70:HIS:ND1	1:A:71:TRP:N	2.60	0.49
1:F:222:TRP:CZ2	1:F:226:GLN:NE2	2.80	0.49
1:E:222:TRP:CH2	1:E:226:GLN:NE2	2.80	0.49
1:F:16:HIS:CD2	1:F:27:TYR:CE2	3.01	0.49
1:E:428:GLU:HG3	1:E:453:HIS:CD2	2.47	0.49
1:D:270:VAL:HG13	1:E:270:VAL:HG13	1.94	0.49
1:F:227:LEU:N	1:F:227:LEU:CD1	2.75	0.49
1:A:465:THR:O	1:A:466:MET:HB3	2.12	0.49
1:E:642:ILE:HG21	1:E:642:ILE:HD13	1.63	0.49
1:E:102:ASN:O	1:E:104:ALA:N	2.44	0.49
1:D:313:ILE:HD12	1:D:314:ASP:O	2.13	0.49
1:F:322:GLU:O	1:F:323:LEU:C	2.49	0.49
1:F:102:ASN:O	1:F:104:ALA:N	2.44	0.49
1:F:76:ASN:O	1:F:78:ARG:N	2.46	0.49
1:A:76:ASN:ND2	1:A:79:GLN:HG3	2.28	0.49
1:B:418:ILE:HD11	1:B:462:TYR:HE1	1.76	0.49
1:C:555:LEU:HD12	1:C:555:LEU:H	1.77	0.49
1:C:555:LEU:O	1:C:557:ALA:N	2.45	0.49
1:A:178:GLU:OE1	4:A:705:HOH:O	2.19	0.49
1:E:479:ARG:NH1	1:E:587:THR:OG1	2.45	0.49
1:B:594:GLU:HG2	1:B:594:GLU:O	2.13	0.49
1:E:70:HIS:ND1	1:E:71:TRP:N	2.60	0.49
1:B:357:PRO:HB2	1:B:358:HIS:CE1	2.48	0.49
1:B:434:ILE:C	1:B:436:ALA:N	2.66	0.49
1:F:434:ILE:C	1:F:436:ALA:N	2.66	0.49
1:C:414:ASN:HD21	1:C:467:SER:N	2.10	0.48
1:D:173:THR:HG22	1:D:176:ASN:HB2	1.94	0.48
1:C:491:ILE:CG1	1:D:175:LYS:HB2	2.42	0.48
1:E:313:ILE:HD12	1:E:314:ASP:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:ASP:C	1:D:187:ASP:OD1	2.52	0.48
1:D:538:SER:O	1:D:542:GLN:HG3	2.13	0.48
1:B:69:ARG:HA	1:B:264:TYR:CD2	2.48	0.48
1:D:522:SER:C	1:D:524:LYS:N	2.63	0.48
1:F:41:GLY:O	1:F:42:ASP:HB2	2.13	0.48
1:A:108:GLU:OE1	1:A:108:GLU:HA	2.13	0.48
1:A:285:HIS:O	1:A:288:ASP:HB2	2.12	0.48
1:D:76:ASN:O	1:D:78:ARG:N	2.46	0.48
1:A:57:MET:O	1:A:61:ASN:HB2	2.13	0.48
1:B:560:ARG:NH1	1:B:606:HIS:N	2.60	0.48
1:E:76:ASN:CB	1:E:79:GLN:HB2	2.34	0.48
1:A:76:ASN:O	1:A:78:ARG:N	2.46	0.48
1:B:353:ARG:O	1:B:354:GLN:C	2.49	0.48
1:C:353:ARG:NE	1:C:369:GLU:OE2	2.43	0.48
1:E:173:THR:CG2	1:E:176:ASN:HB2	2.42	0.48
1:F:201:PHE:HB3	1:F:216:LYS:HD2	1.92	0.48
1:D:628:ARG:O	1:D:629:ARG:C	2.50	0.48
1:F:217:GLY:H	1:F:220:PHE:H	1.61	0.48
1:B:411:MET:C	1:B:412:VAL:HG12	2.34	0.48
1:A:69:ARG:HA	1:A:264:TYR:CD2	2.48	0.48
1:A:538:SER:O	1:A:542:GLN:HG3	2.13	0.48
1:F:609:CYS:C	1:F:611:VAL:H	2.17	0.48
1:F:594:GLU:O	1:F:594:GLU:HG2	2.13	0.48
1:D:70:HIS:ND1	1:D:71:TRP:N	2.61	0.48
1:E:227:LEU:HD12	1:E:227:LEU:N	2.27	0.48
1:B:195:VAL:HG22	1:B:196:THR:N	2.28	0.48
1:A:83:ALA:HB2	1:A:114:GLU:HA	1.94	0.48
1:A:227:LEU:N	1:A:227:LEU:CD1	2.75	0.48
1:C:76:ASN:O	1:C:78:ARG:N	2.46	0.48
1:E:313:ILE:C	1:E:313:ILE:HD12	2.34	0.48
1:F:97:TYR:O	1:F:101:SER:HB2	2.12	0.48
1:F:544:ASP:O	1:F:547:VAL:HG23	2.14	0.48
1:F:76:ASN:ND2	1:F:79:GLN:HG3	2.28	0.48
1:E:76:ASN:O	1:E:78:ARG:N	2.46	0.48
1:D:300:ILE:HD11	1:D:390:ILE:HG22	1.95	0.48
1:E:403:HIS:C	1:E:405:ASN:H	2.15	0.48
1:C:357:PRO:HB2	1:C:358:HIS:CE1	2.48	0.48
1:F:227:LEU:N	1:F:227:LEU:HD12	2.27	0.48
1:C:106:PHE:O	1:C:107:ARG:C	2.49	0.48
1:D:57:MET:O	1:D:61:ASN:HB2	2.13	0.48
1:B:57:MET:O	1:B:61:ASN:HB2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ASN:O	1:B:78:ARG:N	2.46	0.48
1:D:175:LYS:O	1:D:176:ASN:CB	2.60	0.48
1:D:555:LEU:O	1:D:557:ALA:N	2.45	0.48
1:C:217:GLY:H	1:C:220:PHE:H	1.61	0.48
1:F:307:ASP:C	1:F:336:ASN:HD22	2.16	0.48
1:E:69:ARG:HA	1:E:264:TYR:CD2	2.48	0.48
1:A:300:ILE:HD11	1:A:390:ILE:HG22	1.95	0.48
1:C:592:ASP:C	1:C:594:GLU:H	2.16	0.48
1:C:443:ILE:HD13	1:F:161:GLN:HG3	1.95	0.48
1:C:434:ILE:C	1:C:436:ALA:N	2.66	0.48
1:E:195:VAL:HG22	1:E:196:THR:N	2.28	0.48
1:C:195:VAL:HG22	1:C:196:THR:N	2.28	0.48
1:C:16:HIS:CD2	1:C:27:TYR:CE2	3.01	0.48
1:B:296:ILE:HG23	1:B:296:ILE:HD12	1.42	0.48
1:E:57:MET:O	1:E:61:ASN:HB2	2.13	0.48
1:D:513:PRO:CG	1:D:517:GLU:HB2	2.27	0.48
1:B:585:ALA:HA	1:B:642:ILE:HA	1.95	0.48
1:F:313:ILE:HD12	1:F:314:ASP:O	2.13	0.48
1:B:543:ALA:HA	1:B:553:LEU:HD11	1.94	0.48
1:B:7:ASN:O	1:B:8:ALA:C	2.51	0.48
1:C:493:LEU:HA	1:C:497:GLU:OE1	2.14	0.48
1:E:560:ARG:NH1	1:E:606:HIS:N	2.60	0.48
1:D:97:TYR:O	1:D:101:SER:HB2	2.12	0.48
1:F:7:ASN:C	1:F:9:GLN:N	2.55	0.48
1:E:493:LEU:HA	1:E:497:GLU:OE1	2.14	0.48
1:B:493:LEU:HA	1:B:497:GLU:OE1	2.14	0.48
1:F:463:LYS:CG	1:F:520:GLU:HG3	2.43	0.48
1:D:86:LEU:C	1:D:86:LEU:HD23	2.30	0.48
1:E:307:ASP:C	1:E:336:ASN:HD22	2.16	0.48
1:F:38:ASN:C	1:F:40:LEU:N	2.67	0.48
1:B:403:HIS:C	1:B:405:ASN:H	2.15	0.48
1:B:402:THR:O	1:B:405:ASN:HB2	2.13	0.48
1:C:609:CYS:C	1:C:611:VAL:H	2.17	0.48
1:B:108:GLU:OE1	1:B:108:GLU:HA	2.13	0.48
1:E:434:ILE:C	1:E:436:ALA:N	2.66	0.48
1:F:57:MET:O	1:F:61:ASN:HB2	2.13	0.48
1:C:57:MET:O	1:C:61:ASN:HB2	2.13	0.48
1:C:175:LYS:O	1:C:176:ASN:CB	2.60	0.48
1:A:487:ASP:O	1:A:488:ASN:CB	2.62	0.48
1:D:487:ASP:O	1:D:488:ASN:CB	2.62	0.48
1:B:487:ASP:O	1:B:488:ASN:CB	2.62	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:THR:HA	1:B:449:ASN:O	2.14	0.48
1:F:313:ILE:HD12	1:F:313:ILE:C	2.34	0.48
1:A:97:TYR:O	1:A:101:SER:HB2	2.12	0.48
1:E:175:LYS:O	1:E:176:ASN:CB	2.60	0.48
1:C:433:LEU:HD23	1:C:433:LEU:HA	1.56	0.48
1:A:307:ASP:C	1:A:336:ASN:HD22	2.16	0.48
1:D:564:ILE:HB	1:D:565:PRO:HD2	1.96	0.48
1:D:69:ARG:HA	1:D:264:TYR:CD2	2.48	0.48
1:C:38:ASN:C	1:C:40:LEU:N	2.67	0.48
1:C:402:THR:O	1:C:405:ASN:HB2	2.13	0.48
1:A:227:LEU:N	1:A:227:LEU:HD12	2.27	0.48
1:C:225:HIS:HD2	1:C:388:ASP:OD2	1.97	0.48
1:A:434:ILE:C	1:A:436:ALA:H	2.16	0.48
1:C:487:ASP:O	1:C:488:ASN:CB	2.62	0.48
1:F:585:ALA:HA	1:F:642:ILE:HA	1.95	0.48
1:D:585:ALA:HA	1:D:642:ILE:HA	1.95	0.48
1:D:313:ILE:C	1:D:313:ILE:HD12	2.34	0.48
1:A:544:ASP:O	1:A:547:VAL:HG23	2.14	0.48
1:F:493:LEU:HA	1:F:497:GLU:OE1	2.14	0.48
1:A:493:LEU:HA	1:A:497:GLU:OE1	2.14	0.48
1:F:7:ASN:O	1:F:8:ALA:C	2.51	0.48
1:A:239:TRP:CZ3	1:A:574:LYS:NZ	2.79	0.48
1:D:123:VAL:CG1	1:D:134:LEU:HD21	2.43	0.48
1:B:463:LYS:CG	1:B:520:GLU:HG3	2.43	0.48
1:D:307:ASP:C	1:D:336:ASN:HD22	2.16	0.48
1:C:307:ASP:C	1:C:336:ASN:HD22	2.16	0.48
1:B:38:ASN:C	1:B:40:LEU:N	2.67	0.48
1:E:38:ASN:C	1:E:40:LEU:N	2.67	0.48
1:B:56:LEU:HD21	1:B:110:MET:CE	2.44	0.48
1:B:592:ASP:C	1:B:594:GLU:H	2.16	0.48
1:E:592:ASP:C	1:E:594:GLU:H	2.16	0.48
1:D:227:LEU:HD12	1:D:227:LEU:N	2.28	0.48
1:C:108:GLU:OE1	1:C:108:GLU:HA	2.13	0.48
1:E:279:ASP:OD1	1:E:286:VAL:N	2.42	0.48
1:E:225:HIS:HD2	1:E:388:ASP:OD2	1.97	0.48
1:D:56:LEU:HD21	1:D:110:MET:HE1	1.94	0.48
1:F:465:THR:O	1:F:466:MET:HB3	2.12	0.48
1:A:487:ASP:OD2	1:A:489:ASN:HB2	2.14	0.48
1:E:585:ALA:HA	1:E:642:ILE:HA	1.95	0.48
1:D:165:THR:HA	1:D:449:ASN:O	2.14	0.48
1:C:313:ILE:HD12	1:C:313:ILE:C	2.34	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:THR:HG22	1:D:6:GLY:O	2.14	0.48
1:B:424:THR:HA	1:B:457:HIS:HA	1.94	0.48
1:E:201:PHE:HB3	1:E:216:LYS:HD2	1.92	0.48
1:A:86:LEU:C	1:A:86:LEU:HD23	2.30	0.48
1:B:628:ARG:O	1:B:629:ARG:C	2.50	0.48
1:E:564:ILE:HB	1:E:565:PRO:HD2	1.96	0.48
1:D:508:PHE:CE2	1:D:521:ARG:CD	2.97	0.48
1:E:508:PHE:CE2	1:E:521:ARG:CD	2.97	0.48
1:E:589:GLY:O	1:E:593:THR:OG1	2.30	0.48
1:E:491:ILE:O	1:E:492:THR:CG2	2.62	0.48
1:C:594:GLU:O	1:C:594:GLU:HG2	2.13	0.48
1:D:357:PRO:HB2	1:D:358:HIS:CE1	2.48	0.48
1:D:108:GLU:OE1	1:D:108:GLU:HA	2.13	0.48
1:B:296:ILE:HD13	1:B:296:ILE:HA	1.38	0.48
1:D:76:ASN:ND2	1:D:79:GLN:HG3	2.28	0.48
1:C:487:ASP:OD2	1:C:489:ASN:HB2	2.14	0.48
1:C:491:ILE:O	1:C:492:THR:CG2	2.62	0.48
1:D:487:ASP:CB	1:D:489:ASN:H	2.09	0.48
1:C:585:ALA:HA	1:C:642:ILE:HA	1.95	0.48
1:F:165:THR:HA	1:F:449:ASN:O	2.14	0.48
1:C:544:ASP:O	1:C:547:VAL:HG23	2.14	0.48
1:B:5:THR:HG22	1:B:6:GLY:O	2.14	0.48
1:A:608:GLN:NE2	4:A:820:HOH:O	2.31	0.48
1:C:564:ILE:HB	1:C:565:PRO:HD2	1.96	0.48
1:B:522:SER:C	1:B:524:LYS:N	2.63	0.48
1:B:300:ILE:HD11	1:B:390:ILE:HG22	1.95	0.48
1:C:403:HIS:C	1:C:405:ASN:H	2.15	0.48
1:D:41:GLY:O	1:D:42:ASP:HB2	2.13	0.48
1:B:633:GLU:C	1:B:635:VAL:N	2.66	0.48
1:A:434:ILE:C	1:A:436:ALA:N	2.66	0.48
1:A:224:HIS:O	1:A:228:THR:OG1	2.30	0.48
1:D:478:PHE:CZ	1:D:519:ILE:HD12	2.49	0.48
1:F:195:VAL:HG22	1:F:196:THR:N	2.28	0.48
1:C:76:ASN:ND2	1:C:79:GLN:HG3	2.28	0.48
1:E:487:ASP:O	1:E:488:ASN:CB	2.62	0.48
1:E:578:MET:SD	1:E:580:PHE:CZ	3.07	0.48
1:C:187:ASP:C	1:C:187:ASP:OD1	2.52	0.48
1:A:187:ASP:C	1:A:187:ASP:OD1	2.52	0.48
1:E:392:LYS:HA	1:E:395:THR:HB	1.96	0.48
1:E:411:MET:C	1:E:412:VAL:HG12	2.34	0.48
1:C:411:MET:SD	1:C:411:MET:N	2.83	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522:SER:C	1:C:524:LYS:N	2.63	0.48
1:A:38:ASN:C	1:A:40:LEU:N	2.67	0.48
1:F:300:ILE:HD11	1:F:390:ILE:HG22	1.95	0.48
1:A:609:CYS:C	1:A:611:VAL:H	2.17	0.48
1:A:594:GLU:HG2	1:A:594:GLU:O	2.13	0.48
1:B:589:GLY:O	1:B:593:THR:OG1	2.30	0.48
1:A:41:GLY:O	1:A:42:ASP:HB2	2.13	0.48
1:E:434:ILE:HD11	1:E:447:GLU:HA	1.96	0.48
1:E:513:PRO:CG	1:E:517:GLU:HB2	2.27	0.47
1:D:177:ARG:NH1	1:E:361:PHE:HE1	2.12	0.47
1:D:544:ASP:O	1:D:547:VAL:HG23	2.14	0.47
1:C:239:TRP:CZ3	1:C:574:LYS:NZ	2.79	0.47
1:B:578:MET:SD	1:B:580:PHE:CZ	3.07	0.47
1:B:187:ASP:OD1	1:B:187:ASP:C	2.52	0.47
1:D:150:VAL:CG2	1:D:168:VAL:HG12	2.42	0.47
1:F:187:ASP:C	1:F:187:ASP:OD1	2.52	0.47
1:F:392:LYS:HA	1:F:395:THR:HB	1.96	0.47
1:A:217:GLY:H	1:A:220:PHE:H	1.61	0.47
1:D:217:GLY:H	1:D:220:PHE:H	1.61	0.47
1:F:628:ARG:O	1:F:629:ARG:C	2.50	0.47
1:B:307:ASP:OD1	1:B:307:ASP:C	2.53	0.47
1:C:538:SER:O	1:C:542:GLN:HG3	2.13	0.47
1:F:589:GLY:O	1:F:593:THR:OG1	2.30	0.47
1:B:508:PHE:CE2	1:B:521:ARG:CD	2.97	0.47
1:B:41:GLY:O	1:B:42:ASP:HB2	2.13	0.47
1:D:56:LEU:HD21	1:D:110:MET:CE	2.44	0.47
1:C:513:PRO:CG	1:C:517:GLU:HB2	2.27	0.47
1:D:491:ILE:O	1:D:492:THR:CG2	2.62	0.47
1:E:165:THR:HA	1:E:449:ASN:O	2.14	0.47
1:E:544:ASP:O	1:E:547:VAL:HG23	2.14	0.47
1:A:313:ILE:C	1:A:313:ILE:HD12	2.34	0.47
1:D:96:TRP:O	1:D:97:TYR:C	2.51	0.47
1:F:56:LEU:HD21	1:F:110:MET:CE	2.44	0.47
1:A:366:GLY:N	1:A:369:GLU:HG3	2.22	0.47
1:A:463:LYS:CG	1:A:520:GLU:HG3	2.43	0.47
1:F:317:GLN:CB	1:F:318:PRO:HD2	2.36	0.47
1:D:392:LYS:HA	1:D:395:THR:HB	1.96	0.47
1:C:392:LYS:HA	1:C:395:THR:HB	1.96	0.47
1:D:40:LEU:HA	1:D:40:LEU:HD12	1.52	0.47
1:C:56:LEU:HD21	1:C:110:MET:CE	2.44	0.47
1:A:56:LEU:HD21	1:A:110:MET:CE	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:434:ILE:HD11	1:F:447:GLU:HA	1.96	0.47
1:E:296:ILE:HD12	1:E:296:ILE:HG23	1.42	0.47
1:D:487:ASP:OD2	1:D:489:ASN:HB2	2.14	0.47
1:C:165:THR:HA	1:C:449:ASN:O	2.14	0.47
1:E:7:ASN:O	1:E:8:ALA:C	2.51	0.47
1:E:463:LYS:CG	1:E:520:GLU:HG3	2.43	0.47
1:A:175:LYS:O	1:A:176:ASN:CB	2.60	0.47
1:A:522:SER:C	1:A:524:LYS:N	2.63	0.47
1:F:538:SER:O	1:F:542:GLN:HG3	2.13	0.47
1:F:451:ARG:HH11	1:F:451:ARG:HD3	1.47	0.47
1:D:609:CYS:C	1:D:611:VAL:H	2.17	0.47
1:F:491:ILE:O	1:F:492:THR:CG2	2.62	0.47
1:B:609:CYS:C	1:B:611:VAL:H	2.17	0.47
1:E:30:LEU:HD23	1:E:30:LEU:HA	1.55	0.47
1:E:41:GLY:O	1:E:42:ASP:HB2	2.13	0.47
1:A:633:GLU:C	1:A:635:VAL:N	2.66	0.47
1:F:434:ILE:C	1:F:436:ALA:H	2.16	0.47
1:B:279:ASP:OD1	1:B:286:VAL:N	2.42	0.47
1:D:434:ILE:C	1:D:436:ALA:H	2.16	0.47
1:A:275:ILE:HG21	1:A:275:ILE:HD13	1.54	0.47
1:A:553:LEU:HA	1:A:553:LEU:HD23	1.55	0.47
1:C:322:GLU:O	1:C:323:LEU:C	2.49	0.47
1:D:493:LEU:HA	1:D:497:GLU:OE1	2.14	0.47
1:D:578:MET:SD	1:D:580:PHE:CZ	3.07	0.47
1:B:564:ILE:HB	1:B:565:PRO:HD2	1.96	0.47
1:F:508:PHE:CE2	1:F:521:ARG:CD	2.97	0.47
1:E:40:LEU:HD12	1:E:40:LEU:HA	1.52	0.47
1:F:315:ILE:HG13	1:F:315:ILE:O	2.15	0.47
1:D:315:ILE:HG13	1:D:315:ILE:O	2.15	0.47
1:B:434:ILE:HD11	1:B:447:GLU:HA	1.96	0.47
1:A:434:ILE:HD11	1:A:447:GLU:HA	1.96	0.47
1:A:225:HIS:HD2	1:A:388:ASP:OD2	1.97	0.47
1:D:225:HIS:HD2	1:D:388:ASP:OD2	1.97	0.47
1:A:195:VAL:HG22	1:A:196:THR:N	2.28	0.47
1:C:62:ASP:HB2	1:C:64:ARG:HG2	1.97	0.47
1:A:165:THR:HA	1:A:449:ASN:O	2.14	0.47
1:E:11:GLN:HG3	1:E:15:ASN:ND2	2.22	0.47
1:E:5:THR:HG22	1:E:6:GLY:O	2.14	0.47
1:A:5:THR:HG22	1:A:6:GLY:O	2.14	0.47
1:B:11:GLN:HG3	1:B:15:ASN:ND2	2.21	0.47
1:F:11:GLN:HG3	1:F:15:ASN:ND2	2.22	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:MET:SD	1:C:580:PHE:CZ	3.07	0.47
1:E:417:ALA:O	1:E:463:LYS:N	2.37	0.47
1:E:307:ASP:C	1:E:307:ASP:OD1	2.53	0.47
1:F:411:MET:SD	1:F:411:MET:N	2.83	0.47
1:E:405:ASN:HD22	1:E:405:ASN:HA	1.45	0.47
1:B:13:ASP:OD1	1:B:100:ARG:NE	2.43	0.47
1:C:227:LEU:N	1:C:227:LEU:HD12	2.27	0.47
1:A:290:GLU:HG2	4:A:749:HOH:O	2.14	0.47
1:D:316:ARG:HE	1:F:338:GLN:HE22	1.63	0.47
1:F:553:LEU:HD23	1:F:553:LEU:HA	1.55	0.47
1:F:578:MET:SD	1:F:580:PHE:CZ	3.07	0.47
1:E:187:ASP:OD1	1:E:187:ASP:C	2.52	0.47
1:C:586:VAL:O	1:C:641:ASN:HB2	2.15	0.47
1:B:533:MET:HB3	1:B:534:PRO:CD	2.43	0.47
1:C:508:PHE:CE2	1:C:521:ARG:CD	2.97	0.47
1:C:593:THR:C	1:C:595:GLY:N	2.68	0.47
1:E:609:CYS:C	1:E:611:VAL:H	2.17	0.47
1:E:56:LEU:HD21	1:E:110:MET:CE	2.44	0.47
1:E:106:PHE:O	1:E:109:ARG:N	2.43	0.47
1:C:434:ILE:HD11	1:C:447:GLU:HA	1.96	0.47
1:F:478:PHE:CZ	1:F:519:ILE:HD12	2.49	0.47
1:B:225:HIS:HD2	1:B:388:ASP:OD2	1.97	0.47
1:B:478:PHE:CZ	1:B:519:ILE:HD12	2.49	0.47
1:C:478:PHE:CZ	1:C:519:ILE:HD12	2.49	0.47
1:E:62:ASP:HB2	1:E:64:ARG:HG2	1.97	0.47
1:D:62:ASP:HB2	1:D:64:ARG:HG2	1.97	0.47
1:B:76:ASN:ND2	1:B:79:GLN:HG3	2.28	0.47
1:A:62:ASP:HB2	1:A:64:ARG:HG2	1.97	0.47
1:D:414:ASN:HD21	1:D:467:SER:N	2.10	0.47
1:B:487:ASP:OD2	1:B:489:ASN:HB2	2.14	0.47
1:C:5:THR:HG22	1:C:6:GLY:O	2.14	0.47
1:B:239:TRP:CZ3	1:B:574:LYS:NZ	2.79	0.47
1:A:78:ARG:HD3	1:A:78:ARG:HH11	1.31	0.47
1:A:586:VAL:O	1:A:641:ASN:HB2	2.15	0.47
1:E:586:VAL:O	1:E:641:ASN:HB2	2.15	0.47
1:A:551:HIS:CD2	1:A:551:HIS:C	2.88	0.47
1:D:551:HIS:CD2	1:D:551:HIS:C	2.88	0.47
1:A:508:PHE:CE2	1:A:521:ARG:CD	2.97	0.47
1:A:201:PHE:HB3	1:A:216:LYS:HD2	1.92	0.47
1:D:533:MET:HB3	1:D:534:PRO:CD	2.43	0.47
1:C:307:ASP:OD1	1:C:307:ASP:C	2.53	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:ARG:HD3	1:C:451:ARG:HH11	1.47	0.47
1:D:38:ASN:C	1:D:40:LEU:N	2.67	0.47
1:A:491:ILE:O	1:A:492:THR:CG2	2.62	0.47
1:C:592:ASP:O	1:C:594:GLU:N	2.45	0.47
1:A:593:THR:C	1:A:595:GLY:N	2.68	0.47
1:A:154:ALA:O	1:A:157:ALA:HB3	2.15	0.47
1:B:158:LYS:O	1:B:159:MET:C	2.49	0.47
1:D:106:PHE:O	1:D:109:ARG:N	2.43	0.47
1:E:434:ILE:C	1:E:436:ALA:H	2.16	0.47
1:E:319:LYS:O	1:E:320:GLY:C	2.53	0.47
1:F:225:HIS:HD2	1:F:388:ASP:OD2	1.97	0.47
1:E:154:ALA:HB1	1:E:448:ILE:HG21	1.97	0.47
1:C:653:LEU:HA	1:C:653:LEU:HD12	1.47	0.47
1:D:653:LEU:HA	1:D:653:LEU:HD12	1.47	0.47
1:F:296:ILE:HD13	1:F:296:ILE:HA	1.38	0.47
1:F:414:ASN:HD21	1:F:467:SER:N	2.10	0.47
1:F:586:VAL:O	1:F:641:ASN:HB2	2.15	0.47
1:D:307:ASP:C	1:D:307:ASP:OD1	2.53	0.47
1:A:307:ASP:C	1:A:307:ASP:OD1	2.53	0.47
1:D:593:THR:C	1:D:595:GLY:N	2.68	0.47
1:B:491:ILE:O	1:B:492:THR:CG2	2.62	0.47
1:B:620:ARG:HG3	1:B:624:TYR:CG	2.50	0.47
1:B:593:THR:C	1:B:595:GLY:N	2.68	0.47
1:F:197:TRP:CD1	1:F:223:VAL:HG21	2.50	0.47
1:E:315:ILE:O	1:E:315:ILE:HG13	2.15	0.47
1:A:222:TRP:CD1	1:A:622:LEU:HD23	2.50	0.47
1:E:222:TRP:CD1	1:E:622:LEU:HD23	2.50	0.47
1:E:465:THR:O	1:E:466:MET:HB3	2.12	0.47
1:F:487:ASP:OD2	1:F:489:ASN:HB2	2.14	0.47
1:B:313:ILE:HD12	1:B:313:ILE:C	2.34	0.47
1:A:392:LYS:HA	1:A:395:THR:HB	1.96	0.47
1:F:620:ARG:HG3	1:F:624:TYR:CG	2.50	0.47
1:B:197:TRP:CD1	1:B:223:VAL:HG21	2.50	0.47
1:C:41:GLY:O	1:C:42:ASP:HB2	2.13	0.47
1:C:30:LEU:HD23	1:C:30:LEU:HA	1.55	0.47
1:D:434:ILE:HD11	1:D:447:GLU:HA	1.96	0.47
1:E:478:PHE:CZ	1:E:519:ILE:HD12	2.49	0.47
1:D:154:ALA:O	1:D:157:ALA:HB3	2.15	0.47
1:A:8:ALA:HA	1:A:553:LEU:CD1	2.40	0.47
1:F:5:THR:HG22	1:F:6:GLY:O	2.14	0.47
1:F:8:ALA:HA	1:F:553:LEU:CD1	2.40	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:MET:SD	1:A:580:PHE:CZ	3.07	0.47
1:E:65:LEU:HA	1:E:65:LEU:HD12	1.72	0.47
1:A:353:ARG:NE	1:A:369:GLU:OE2	2.43	0.47
1:F:123:VAL:CG1	1:F:134:LEU:HD21	2.43	0.47
1:C:576:GLU:OE1	1:D:576:GLU:CD	2.53	0.47
1:E:150:VAL:CG2	1:E:168:VAL:HG12	2.42	0.47
1:E:300:ILE:HD11	1:E:390:ILE:HG22	1.95	0.47
1:D:623:GLY:O	1:D:626:LEU:N	2.39	0.47
1:E:620:ARG:HG3	1:E:624:TYR:CG	2.50	0.47
1:B:222:TRP:CD1	1:B:622:LEU:HD23	2.50	0.47
1:C:319:LYS:O	1:C:320:GLY:C	2.53	0.47
1:C:154:ALA:O	1:C:157:ALA:HB3	2.15	0.47
1:A:478:PHE:CZ	1:A:519:ILE:HD12	2.49	0.47
1:D:170:PHE:HD1	1:D:170:PHE:HA	1.53	0.47
1:B:123:VAL:CG1	1:B:134:LEU:HD21	2.43	0.46
1:E:551:HIS:CD2	1:E:551:HIS:C	2.88	0.46
1:E:86:LEU:HD21	1:E:90:LEU:HD22	1.97	0.46
1:F:564:ILE:HB	1:F:565:PRO:HD2	1.96	0.46
1:A:564:ILE:HB	1:A:565:PRO:HD2	1.96	0.46
1:D:620:ARG:HG3	1:D:624:TYR:CG	2.50	0.46
1:A:625:PRO:C	1:A:626:LEU:HD23	2.36	0.46
1:E:623:GLY:O	1:E:626:LEU:N	2.39	0.46
1:F:222:TRP:CD1	1:F:622:LEU:CD2	2.98	0.46
1:C:399:PRO:HA	1:C:400:PRO:HD3	1.59	0.46
1:C:222:TRP:CD1	1:C:622:LEU:CD2	2.98	0.46
1:B:154:ALA:HB1	1:B:448:ILE:HG21	1.97	0.46
1:F:614:GLU:HG3	1:F:614:GLU:H	1.15	0.46
1:F:413:VAL:HG23	1:F:466:MET:HE3	1.95	0.46
1:E:239:TRP:CZ3	1:E:574:LYS:NZ	2.79	0.46
1:A:295:ARG:HH11	1:A:295:ARG:HD2	1.31	0.46
1:B:586:VAL:O	1:B:641:ASN:HB2	2.15	0.46
1:B:317:GLN:CB	1:B:318:PRO:HD2	2.36	0.46
1:F:86:LEU:C	1:F:86:LEU:HD23	2.30	0.46
1:B:392:LYS:HA	1:B:395:THR:HB	1.96	0.46
1:F:411:MET:C	1:F:412:VAL:HG12	2.34	0.46
1:C:40:LEU:HA	1:C:40:LEU:HD12	1.52	0.46
1:C:628:ARG:O	1:C:629:ARG:C	2.50	0.46
1:B:42:ASP:O	1:B:45:ILE:HG12	2.16	0.46
1:F:222:TRP:CD1	1:F:622:LEU:HD23	2.50	0.46
1:F:633:GLU:C	1:F:635:VAL:N	2.66	0.46
1:E:222:TRP:CD1	1:E:622:LEU:CD2	2.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:PHE:HD1	1:B:170:PHE:HA	1.53	0.46
1:D:465:THR:O	1:D:466:MET:HB3	2.12	0.46
1:E:487:ASP:OD2	1:E:489:ASN:HB2	2.14	0.46
1:B:544:ASP:O	1:B:547:VAL:HG23	2.14	0.46
1:E:353:ARG:O	1:E:354:GLN:C	2.49	0.46
1:E:353:ARG:NE	1:E:369:GLU:OE2	2.43	0.46
1:F:593:THR:C	1:F:595:GLY:N	2.68	0.46
1:C:300:ILE:HD11	1:C:390:ILE:HG22	1.95	0.46
1:E:260:THR:HG22	1:E:268:PHE:CD2	2.51	0.46
1:E:625:PRO:C	1:E:626:LEU:HD23	2.36	0.46
1:E:42:ASP:O	1:E:45:ILE:HG12	2.16	0.46
1:C:222:TRP:CD1	1:C:622:LEU:HD23	2.50	0.46
1:B:285:HIS:HB2	1:B:288:ASP:CG	2.36	0.46
1:A:285:HIS:HB2	1:A:288:ASP:CG	2.36	0.46
1:A:279:ASP:OD1	1:A:286:VAL:N	2.42	0.46
1:F:642:ILE:HG21	1:F:642:ILE:HD13	1.63	0.46
1:D:642:ILE:HG21	1:D:642:ILE:HD13	1.63	0.46
1:B:419:ASP:HB2	1:B:463:LYS:HZ2	1.80	0.46
1:C:411:MET:C	1:C:412:VAL:HG12	2.34	0.46
1:C:405:ASN:HA	1:C:405:ASN:HD22	1.45	0.46
1:B:260:THR:HG22	1:B:268:PHE:CD2	2.51	0.46
1:C:441:GLU:C	1:C:443:ILE:H	2.18	0.46
1:E:628:ARG:O	1:E:629:ARG:C	2.50	0.46
1:E:16:HIS:HB3	1:E:30:LEU:CD1	2.46	0.46
1:C:42:ASP:O	1:C:45:ILE:HG12	2.16	0.46
1:F:30:LEU:HD23	1:F:30:LEU:HA	1.55	0.46
1:D:434:ILE:C	1:D:436:ALA:N	2.66	0.46
1:D:319:LYS:O	1:D:320:GLY:C	2.53	0.46
1:C:80:ARG:HD2	1:C:80:ARG:HH11	1.24	0.46
1:B:62:ASP:HB2	1:B:64:ARG:HG2	1.97	0.46
1:F:62:ASP:HB2	1:F:64:ARG:HG2	1.97	0.46
1:A:414:ASN:HD21	1:A:467:SER:N	2.10	0.46
1:F:175:LYS:O	1:F:176:ASN:CB	2.60	0.46
1:A:150:VAL:CG2	1:A:168:VAL:HG12	2.42	0.46
1:F:307:ASP:C	1:F:307:ASP:OD1	2.53	0.46
1:B:16:HIS:HB3	1:B:30:LEU:CD1	2.46	0.46
1:B:625:PRO:C	1:B:626:LEU:HD23	2.36	0.46
1:C:625:PRO:C	1:C:626:LEU:HD23	2.36	0.46
1:F:625:PRO:C	1:F:626:LEU:HD23	2.36	0.46
1:A:315:ILE:HG13	1:A:315:ILE:O	2.15	0.46
1:D:222:TRP:CD1	1:D:622:LEU:CD2	2.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:TRP:CD1	1:C:223:VAL:HG21	2.50	0.46
1:E:285:HIS:HB2	1:E:288:ASP:CG	2.36	0.46
1:F:154:ALA:HB1	1:F:448:ILE:HG21	1.97	0.46
1:D:7:ASN:O	1:D:8:ALA:C	2.51	0.46
1:D:586:VAL:O	1:D:641:ASN:HB2	2.15	0.46
1:A:86:LEU:HD21	1:A:90:LEU:HD22	1.98	0.46
1:F:260:THR:HG22	1:F:268:PHE:CD2	2.51	0.46
1:D:159:MET:HE1	1:E:155:TYR:CD1	2.50	0.46
1:C:285:HIS:HB2	1:C:288:ASP:CG	2.36	0.46
1:F:319:LYS:O	1:F:320:GLY:C	2.53	0.46
1:D:12:GLN:HA	1:D:15:ASN:HD22	1.81	0.46
1:A:417:ALA:O	1:A:463:LYS:N	2.37	0.46
1:A:641:ASN:H	1:A:641:ASN:ND2	2.14	0.46
1:E:451:ARG:HH11	1:E:451:ARG:HD3	1.47	0.46
1:F:42:ASP:O	1:F:45:ILE:HG12	2.16	0.46
1:D:222:TRP:CD1	1:D:622:LEU:HD23	2.50	0.46
1:D:197:TRP:CD1	1:D:223:VAL:HG21	2.50	0.46
1:D:159:MET:CE	1:E:155:TYR:CD1	2.99	0.46
1:D:285:HIS:HB2	1:D:288:ASP:CG	2.36	0.46
1:D:16:HIS:HB3	1:D:30:LEU:CD1	2.46	0.46
1:C:512:VAL:HA	1:C:513:PRO:HD2	1.59	0.46
1:D:271:ARG:HA	1:D:272:PRO:HD3	1.69	0.46
1:A:260:THR:HG22	1:A:268:PHE:CD2	2.51	0.46
1:A:620:ARG:HG3	1:A:624:TYR:CG	2.50	0.46
1:D:42:ASP:O	1:D:45:ILE:HG12	2.16	0.46
1:C:315:ILE:O	1:C:315:ILE:HG13	2.15	0.46
1:A:42:ASP:O	1:A:45:ILE:HG12	2.16	0.46
1:A:16:HIS:HB3	1:A:30:LEU:CD1	2.46	0.46
1:B:469:ASN:HA	1:B:469:ASN:HD22	1.40	0.46
1:E:413:VAL:HG23	1:E:466:MET:HE3	1.95	0.46
1:C:275:ILE:HD13	1:C:275:ILE:HG21	1.54	0.46
1:C:12:GLN:HA	1:C:15:ASN:HD22	1.81	0.46
1:E:239:TRP:HH2	1:E:574:LYS:HE3	1.81	0.46
1:E:13:ASP:OD1	1:E:100:ARG:NE	2.43	0.46
1:B:408:PHE:CD1	1:B:588:ASP:HB2	2.51	0.46
1:C:408:PHE:CD1	1:C:588:ASP:HB2	2.51	0.46
1:B:433:LEU:HA	1:B:433:LEU:HD23	1.56	0.46
1:F:551:HIS:C	1:F:551:HIS:CD2	2.88	0.46
1:A:190:MET:HG3	1:A:568:MET:HE2	1.97	0.46
1:D:260:THR:HG22	1:D:268:PHE:CD2	2.51	0.46
1:A:197:TRP:CD1	1:A:223:VAL:HG21	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:HIS:HB3	1:C:30:LEU:CD1	2.46	0.46
1:E:154:ALA:O	1:E:157:ALA:HB3	2.15	0.46
1:B:154:ALA:O	1:B:157:ALA:HB3	2.15	0.46
1:B:319:LYS:O	1:B:320:GLY:C	2.53	0.46
1:C:465:THR:O	1:C:466:MET:HB3	2.12	0.46
1:D:275:ILE:HD13	1:D:275:ILE:HG21	1.54	0.46
1:A:65:LEU:HD12	1:A:65:LEU:HA	1.71	0.46
1:B:551:HIS:CD2	1:B:551:HIS:C	2.88	0.46
1:B:86:LEU:HD21	1:B:90:LEU:HD22	1.97	0.46
1:D:451:ARG:HH11	1:D:451:ARG:HD3	1.47	0.46
1:B:592:ASP:C	1:B:594:GLU:N	2.70	0.46
1:A:592:ASP:O	1:A:594:GLU:N	2.45	0.46
1:C:620:ARG:HG3	1:C:624:TYR:CG	2.50	0.46
1:E:197:TRP:CD1	1:E:223:VAL:HG21	2.50	0.46
1:B:315:ILE:O	1:B:315:ILE:HG13	2.15	0.46
1:A:154:ALA:HB1	1:A:448:ILE:HG21	1.97	0.46
1:A:222:TRP:CD1	1:A:622:LEU:CD2	2.98	0.46
1:F:285:HIS:HB2	1:F:288:ASP:CG	2.36	0.46
1:F:16:HIS:HB3	1:F:30:LEU:CD1	2.46	0.46
1:D:154:ALA:HB1	1:D:448:ILE:HG21	1.97	0.46
1:B:251:ILE:HG12	1:B:251:ILE:H	1.45	0.46
1:E:219:LEU:HD12	1:E:219:LEU:HA	1.81	0.46
1:F:12:GLN:HA	1:F:15:ASN:HD22	1.81	0.45
1:F:543:ALA:O	1:F:547:VAL:HG22	2.16	0.45
1:C:239:TRP:HH2	1:C:574:LYS:HE3	1.81	0.45
1:D:417:ALA:O	1:D:463:LYS:N	2.37	0.45
1:E:32:ASP:O	1:E:36:ASN:HB2	2.16	0.45
1:C:154:ALA:HB1	1:C:448:ILE:HG21	1.97	0.45
1:A:312:THR:O	1:A:312:THR:OG1	2.33	0.45
1:F:528:VAL:HG13	1:F:528:VAL:H	1.51	0.45
1:E:414:ASN:HD21	1:E:467:SER:N	2.10	0.45
1:A:411:MET:C	1:A:412:VAL:HG12	2.34	0.45
1:E:275:ILE:HD13	1:E:275:ILE:HG21	1.54	0.45
1:E:12:GLN:HA	1:E:15:ASN:HD22	1.81	0.45
1:A:543:ALA:O	1:A:547:VAL:HG22	2.16	0.45
1:B:577:GLY:CA	1:B:650:VAL:HG13	2.47	0.45
1:D:577:GLY:CA	1:D:650:VAL:HG13	2.47	0.45
1:C:366:GLY:N	1:C:369:GLU:HG3	2.22	0.45
1:A:408:PHE:CD1	1:A:588:ASP:HB2	2.51	0.45
1:D:641:ASN:ND2	1:D:641:ASN:H	2.14	0.45
1:B:32:ASP:O	1:B:36:ASN:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:592:ASP:C	1:F:594:GLU:N	2.70	0.45
1:D:567:ARG:HD3	1:D:567:ARG:HH11	1.42	0.45
1:C:279:ASP:OD1	1:C:286:VAL:N	2.42	0.45
1:A:192:ILE:HD13	1:A:192:ILE:HA	1.48	0.45
1:A:7:ASN:O	1:A:8:ALA:C	2.51	0.45
1:A:577:GLY:CA	1:A:650:VAL:HG13	2.47	0.45
1:D:86:LEU:HD21	1:D:90:LEU:HD22	1.98	0.45
1:A:68:GLN:HB3	1:A:69:ARG:HH11	1.82	0.45
1:F:127:LYS:HG2	1:F:127:LYS:H	0.97	0.45
1:B:222:TRP:CD1	1:B:622:LEU:CD2	2.98	0.45
1:C:105:TYR:O	1:C:109:ARG:NE	2.46	0.45
1:F:154:ALA:O	1:F:157:ALA:HB3	2.15	0.45
1:C:224:HIS:O	1:C:228:THR:OG1	2.30	0.45
1:F:224:HIS:O	1:F:228:THR:OG1	2.30	0.45
1:B:80:ARG:HD2	1:B:80:ARG:HH11	1.24	0.45
1:A:272:PRO:HG2	1:B:272:PRO:HG2	1.99	0.45
1:D:543:ALA:O	1:D:547:VAL:HG22	2.16	0.45
1:F:577:GLY:CA	1:F:650:VAL:HG13	2.47	0.45
1:E:408:PHE:CD1	1:E:588:ASP:HB2	2.51	0.45
1:D:68:GLN:HB3	1:D:69:ARG:HH11	1.81	0.45
1:B:30:LEU:HA	1:B:30:LEU:HD23	1.55	0.45
1:D:32:ASP:O	1:D:36:ASN:HB2	2.16	0.45
1:A:32:ASP:O	1:A:36:ASN:HB2	2.16	0.45
1:E:132:ILE:HG13	1:E:132:ILE:H	1.46	0.45
1:D:625:PRO:C	1:D:626:LEU:HD23	2.36	0.45
1:A:251:ILE:H	1:A:251:ILE:HG12	1.45	0.45
1:A:411:MET:N	1:A:411:MET:SD	2.83	0.45
1:D:360:LYS:HE3	1:E:273:ASP:OD2	2.16	0.45
1:C:271:ARG:HA	1:C:272:PRO:HD3	1.69	0.45
1:E:78:ARG:HH11	1:E:78:ARG:HD3	1.31	0.45
1:D:411:MET:N	1:D:411:MET:SD	2.83	0.45
1:E:593:THR:C	1:E:595:GLY:N	2.68	0.45
1:B:27:TYR:HA	1:B:28:PRO:HD2	1.60	0.45
1:C:32:ASP:HB2	1:C:36:ASN:ND2	2.32	0.45
1:A:567:ARG:HD3	1:A:567:ARG:HH11	1.42	0.45
1:C:106:PHE:O	1:C:108:GLU:N	2.50	0.45
1:F:275:ILE:HG21	1:F:275:ILE:HD13	1.54	0.45
1:E:543:ALA:O	1:E:547:VAL:HG22	2.16	0.45
1:A:12:GLN:HA	1:A:15:ASN:HD22	1.81	0.45
1:D:39:PRO:HB2	1:D:53:VAL:CG1	2.47	0.45
1:D:411:MET:C	1:D:412:VAL:HG12	2.34	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40:LEU:HA	1:F:40:LEU:HD12	1.52	0.45
1:D:592:ASP:C	1:D:594:GLU:N	2.70	0.45
1:C:56:LEU:HD11	1:C:110:MET:HE3	1.99	0.45
1:D:437:VAL:HG22	1:D:437:VAL:H	1.44	0.45
1:D:106:PHE:O	1:D:108:GLU:N	2.50	0.45
1:B:12:GLN:HA	1:B:15:ASN:HD22	1.81	0.45
1:D:580:PHE:HD2	1:D:649:ILE:HG13	1.82	0.45
1:C:551:HIS:CD2	1:C:551:HIS:C	2.88	0.45
1:C:533:MET:HB3	1:C:534:PRO:CD	2.43	0.45
1:B:495:LEU:HD13	1:B:583:TYR:OH	2.17	0.45
1:C:260:THR:HG22	1:C:268:PHE:CD2	2.51	0.45
1:F:32:ASP:HB2	1:F:36:ASN:ND2	2.32	0.45
1:E:105:TYR:O	1:E:109:ARG:NE	2.46	0.45
1:B:478:PHE:CZ	1:B:519:ILE:CD1	3.00	0.45
1:D:374:ALA:C	1:D:376:ARG:N	2.70	0.45
1:F:374:ALA:C	1:F:376:ARG:N	2.70	0.45
1:B:374:ALA:C	1:B:376:ARG:N	2.69	0.45
1:F:192:ILE:HD12	1:F:192:ILE:HG23	1.72	0.45
1:D:65:LEU:HD21	1:D:110:MET:HE2	1.99	0.45
1:E:512:VAL:HA	1:E:513:PRO:HD2	1.59	0.45
1:B:543:ALA:O	1:B:547:VAL:HG22	2.16	0.45
1:B:641:ASN:ND2	1:B:641:ASN:H	2.14	0.45
1:F:86:LEU:HD21	1:F:90:LEU:HD22	1.98	0.45
1:A:533:MET:HB3	1:A:534:PRO:CD	2.43	0.45
1:A:311:HIS:HA	1:A:311:HIS:HD2	1.65	0.45
1:C:177:ARG:HB3	1:C:177:ARG:HE	1.41	0.45
1:E:127:LYS:H	1:E:127:LYS:HG2	0.97	0.45
1:B:20:LYS:HG3	1:B:20:LYS:HZ1	1.74	0.45
1:F:106:PHE:O	1:F:108:GLU:N	2.50	0.45
1:D:478:PHE:CZ	1:D:519:ILE:CD1	3.00	0.45
1:E:302:HIS:CE1	1:E:304:TYR:HH	2.35	0.45
1:F:487:ASP:O	1:F:488:ASN:CB	2.62	0.45
1:C:491:ILE:CD1	1:D:175:LYS:O	2.63	0.45
1:A:39:PRO:HB2	1:A:53:VAL:CG1	2.47	0.45
1:F:78:ARG:HD3	1:F:78:ARG:HH11	1.31	0.45
1:D:239:TRP:CZ3	1:D:574:LYS:NZ	2.79	0.45
1:C:577:GLY:CA	1:C:650:VAL:HG13	2.47	0.45
1:A:419:ASP:HB2	1:A:463:LYS:HZ2	1.82	0.45
1:C:576:GLU:H	1:C:576:GLU:HG3	1.20	0.45
1:F:408:PHE:CD1	1:F:588:ASP:HB2	2.51	0.45
1:C:68:GLN:HB3	1:C:69:ARG:HH11	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:405:ASN:HA	1:F:405:ASN:HD22	1.45	0.45
1:C:32:ASP:O	1:C:36:ASN:HB2	2.16	0.45
1:F:32:ASP:O	1:F:36:ASN:HB2	2.16	0.45
1:A:56:LEU:HD11	1:A:110:MET:HE3	1.99	0.45
1:E:567:ARG:HH11	1:E:567:ARG:HD3	1.42	0.45
1:E:106:PHE:O	1:E:108:GLU:N	2.50	0.45
1:A:319:LYS:O	1:A:320:GLY:C	2.53	0.45
1:E:224:HIS:O	1:E:228:THR:OG1	2.30	0.45
1:E:10:LYS:HA	1:E:96:TRP:CE2	2.52	0.45
1:B:316:ARG:HH21	1:D:338:GLN:NE2	2.15	0.45
1:C:39:PRO:HB2	1:C:53:VAL:CG1	2.47	0.45
1:A:301:ASP:CB	1:C:295:ARG:NH2	2.80	0.45
1:F:533:MET:HB3	1:F:534:PRO:CD	2.43	0.45
1:D:139:GLN:OE1	1:D:536:PHE:N	2.40	0.45
1:B:56:LEU:HD11	1:B:110:MET:HE3	1.99	0.45
1:B:576:GLU:H	1:B:576:GLU:HG3	1.20	0.45
1:D:43:THR:O	1:D:44:SER:CB	2.63	0.45
1:A:374:ALA:C	1:A:376:ARG:N	2.70	0.45
1:C:192:ILE:HA	1:C:192:ILE:HD13	1.48	0.45
1:B:414:ASN:HD21	1:B:467:SER:N	2.10	0.44
1:E:39:PRO:HB2	1:E:53:VAL:CG1	2.47	0.44
1:E:580:PHE:HD2	1:E:649:ILE:HG13	1.82	0.44
1:C:123:VAL:CG1	1:C:134:LEU:HD21	2.43	0.44
1:B:630:ILE:HG21	1:B:630:ILE:HD13	1.71	0.44
1:A:139:GLN:OE1	1:A:536:PHE:N	2.40	0.44
1:E:592:ASP:C	1:E:594:GLU:N	2.70	0.44
1:B:105:TYR:O	1:B:109:ARG:NE	2.46	0.44
1:A:192:ILE:HG23	1:A:192:ILE:HD12	1.72	0.44
1:E:469:ASN:HD22	1:E:469:ASN:HA	1.40	0.44
1:B:39:PRO:HB2	1:B:53:VAL:CG1	2.47	0.44
1:C:580:PHE:HD2	1:C:649:ILE:HG13	1.82	0.44
1:E:123:VAL:CG1	1:E:134:LEU:HD21	2.43	0.44
1:F:641:ASN:H	1:F:641:ASN:ND2	2.14	0.44
1:E:641:ASN:H	1:E:641:ASN:ND2	2.14	0.44
1:D:295:ARG:HD2	1:D:295:ARG:HH11	1.31	0.44
1:F:150:VAL:CG2	1:F:168:VAL:HG12	2.42	0.44
1:C:592:ASP:O	1:C:619:ASN:ND2	2.40	0.44
1:B:399:PRO:HA	1:B:400:PRO:HD3	1.59	0.44
1:A:106:PHE:O	1:A:108:GLU:N	2.50	0.44
1:C:27:TYR:HA	1:C:28:PRO:HD2	1.60	0.44
1:A:296:ILE:HA	1:A:296:ILE:HD13	1.38	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:GLN:HE21	1:E:11:GLN:HB2	1.21	0.44
1:A:338:GLN:HE22	1:E:316:ARG:HE	1.65	0.44
1:E:239:TRP:CH2	1:E:574:LYS:CE	3.01	0.44
1:E:577:GLY:CA	1:E:650:VAL:HG13	2.47	0.44
1:D:495:LEU:HD13	1:D:583:TYR:OH	2.17	0.44
1:A:40:LEU:HA	1:A:40:LEU:HD12	1.52	0.44
1:D:27:TYR:HA	1:D:28:PRO:HD2	1.60	0.44
1:A:447:GLU:HG3	4:A:726:HOH:O	2.16	0.44
1:A:653:LEU:HA	1:A:653:LEU:HD12	1.47	0.44
1:B:291:ILE:HG21	1:B:291:ILE:HD12	1.77	0.44
1:C:543:ALA:O	1:C:547:VAL:HG22	2.16	0.44
1:B:150:VAL:CG2	1:B:168:VAL:HG12	2.42	0.44
1:B:139:GLN:OE1	1:B:536:PHE:N	2.40	0.44
1:E:592:ASP:O	1:E:619:ASN:ND2	2.41	0.44
1:D:78:ARG:HD3	1:D:78:ARG:HH11	1.31	0.44
1:C:491:ILE:HD13	1:D:175:LYS:HB2	1.92	0.44
1:B:642:ILE:HG21	1:B:642:ILE:HD13	1.63	0.44
1:A:10:LYS:HA	1:A:96:TRP:CE2	2.52	0.44
1:F:39:PRO:HB2	1:F:53:VAL:CG1	2.47	0.44
1:D:419:ASP:HB2	1:D:463:LYS:HZ2	1.81	0.44
1:D:408:PHE:CD1	1:D:588:ASP:HB2	2.51	0.44
1:B:68:GLN:HB3	1:B:69:ARG:HH11	1.81	0.44
1:E:139:GLN:OE1	1:E:536:PHE:N	2.40	0.44
1:B:624:TYR:HA	1:B:625:PRO:HA	1.77	0.44
1:C:592:ASP:C	1:C:594:GLU:N	2.70	0.44
1:B:106:PHE:O	1:B:108:GLU:N	2.50	0.44
1:E:478:PHE:CZ	1:E:519:ILE:CD1	3.00	0.44
1:E:614:GLU:HG3	1:E:614:GLU:H	1.15	0.44
1:D:553:LEU:HD23	1:D:553:LEU:HA	1.55	0.44
1:F:10:LYS:HA	1:F:96:TRP:CE2	2.53	0.44
1:F:580:PHE:HD2	1:F:649:ILE:HG13	1.82	0.44
1:A:173:THR:O	1:A:176:ASN:HB2	2.18	0.44
1:E:173:THR:O	1:E:176:ASN:HB2	2.18	0.44
1:F:68:GLN:HB3	1:F:69:ARG:HH11	1.82	0.44
1:A:43:THR:O	1:A:44:SER:CB	2.63	0.44
1:A:399:PRO:HA	1:A:400:PRO:HD3	1.59	0.44
1:C:173:THR:O	1:C:176:ASN:HB2	2.18	0.44
1:B:634:ARG:HG2	1:B:634:ARG:NH1	2.14	0.44
1:C:10:LYS:HA	1:C:96:TRP:CE2	2.52	0.44
1:D:10:LYS:HA	1:D:96:TRP:CE2	2.53	0.44
1:E:295:ARG:NE	1:E:339:TYR:CE1	2.86	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:LEU:HD13	1:C:583:TYR:OH	2.17	0.44
1:F:495:LEU:HD13	1:F:583:TYR:OH	2.17	0.44
1:E:68:GLN:HB3	1:E:69:ARG:HH11	1.82	0.44
1:A:30:LEU:HD23	1:A:30:LEU:HA	1.55	0.44
1:A:478:PHE:CZ	1:A:519:ILE:CD1	3.00	0.44
1:D:178:GLU:HG3	1:D:178:GLU:O	2.18	0.44
1:F:513:PRO:CG	1:F:517:GLU:HB2	2.27	0.44
1:A:513:PRO:CG	1:A:517:GLU:HB2	2.27	0.44
1:E:275:ILE:HG23	1:E:276:HIS:N	2.33	0.44
1:D:256:PHE:HA	1:E:361:PHE:CE1	2.52	0.44
1:F:239:TRP:CH2	1:F:574:LYS:CE	3.00	0.44
1:A:239:TRP:CH2	1:A:574:LYS:CE	3.01	0.44
1:E:433:LEU:HD23	1:E:433:LEU:HA	1.55	0.44
1:E:411:MET:N	1:E:411:MET:SD	2.83	0.44
1:B:405:ASN:HD22	1:B:405:ASN:HA	1.45	0.44
1:D:127:LYS:HG2	1:D:127:LYS:H	0.97	0.44
1:F:478:PHE:CZ	1:F:519:ILE:CD1	3.00	0.44
1:F:178:GLU:O	1:F:178:GLU:HG3	2.18	0.44
1:C:275:ILE:HG23	1:C:276:HIS:N	2.33	0.44
1:D:177:ARG:CG	1:E:360:LYS:HB3	2.48	0.44
1:B:239:TRP:CH2	1:B:574:LYS:CE	3.01	0.44
1:A:551:HIS:C	1:A:552:ASP:OD1	2.57	0.44
1:C:555:LEU:O	1:C:556:SER:C	2.54	0.44
1:D:551:HIS:C	1:D:552:ASP:OD1	2.57	0.44
1:B:555:LEU:O	1:B:556:SER:C	2.54	0.44
1:A:32:ASP:HB2	1:A:36:ASN:ND2	2.32	0.44
1:E:56:LEU:HD11	1:E:110:MET:HE3	1.99	0.44
1:C:478:PHE:CZ	1:C:519:ILE:CD1	3.00	0.44
1:F:441:GLU:C	1:F:443:ILE:H	2.18	0.44
1:D:296:ILE:HD12	1:D:296:ILE:HG23	1.42	0.44
1:F:295:ARG:NE	1:F:339:TYR:CE1	2.86	0.43
1:C:295:ARG:NE	1:C:339:TYR:CE1	2.86	0.43
1:C:641:ASN:H	1:C:641:ASN:ND2	2.14	0.43
1:C:48:ASP:OD1	1:C:92:GLN:HG3	2.18	0.43
1:A:495:LEU:HD13	1:A:583:TYR:OH	2.17	0.43
1:E:495:LEU:HD13	1:E:583:TYR:OH	2.17	0.43
1:C:300:ILE:H	1:C:300:ILE:HG13	1.60	0.43
1:E:624:TYR:HA	1:E:625:PRO:HA	1.77	0.43
1:D:374:ALA:C	1:D:376:ARG:H	2.22	0.43
1:E:374:ALA:C	1:E:376:ARG:N	2.69	0.43
1:C:374:ALA:C	1:C:376:ARG:N	2.69	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:CYS:HB3	4:A:763:HOH:O	2.18	0.43
1:B:178:GLU:HG3	1:B:178:GLU:O	2.18	0.43
1:C:78:ARG:HD3	1:C:78:ARG:HH11	1.32	0.43
1:B:10:LYS:HA	1:B:96:TRP:CE2	2.53	0.43
1:E:366:GLY:O	1:E:367:VAL:C	2.57	0.43
1:F:48:ASP:OD1	1:F:92:GLN:HG3	2.18	0.43
1:D:48:ASP:OD1	1:D:92:GLN:HG3	2.18	0.43
1:B:40:LEU:HD12	1:B:40:LEU:HA	1.52	0.43
1:B:32:ASP:HB2	1:B:36:ASN:ND2	2.32	0.43
1:A:211:TYR:CE1	1:A:612:HIS:HA	2.53	0.43
1:B:591:LYS:HB2	1:B:591:LYS:HZ2	1.82	0.43
1:A:441:GLU:C	1:A:443:ILE:H	2.18	0.43
1:C:215:ARG:NE	1:C:218:GLU:OE2	2.45	0.43
1:B:65:LEU:HD12	1:B:82:GLU:HG2	2.00	0.43
2:D:658:NDG:H8C3	2:D:658:NDG:HA	1.78	0.43
1:E:271:ARG:HA	1:E:272:PRO:HD3	1.69	0.43
1:E:65:LEU:HD12	1:E:82:GLU:HG2	2.00	0.43
1:D:295:ARG:NE	1:D:339:TYR:CE1	2.86	0.43
1:F:551:HIS:C	1:F:552:ASP:OD1	2.57	0.43
1:C:551:HIS:C	1:C:552:ASP:OD1	2.57	0.43
1:D:84:LEU:HD11	1:D:204:TRP:CD2	2.54	0.43
1:E:48:ASP:OD1	1:E:92:GLN:HG3	2.18	0.43
1:E:211:TYR:CE1	1:E:612:HIS:HA	2.53	0.43
1:E:32:ASP:HB2	1:E:36:ASN:ND2	2.32	0.43
1:A:105:TYR:O	1:A:109:ARG:NE	2.46	0.43
1:F:374:ALA:C	1:F:376:ARG:H	2.22	0.43
1:E:374:ALA:C	1:E:376:ARG:H	2.22	0.43
1:D:239:TRP:CH2	1:D:574:LYS:CE	3.01	0.43
1:C:366:GLY:O	1:C:367:VAL:C	2.57	0.43
1:F:551:HIS:CD2	1:F:552:ASP:CA	2.99	0.43
1:B:403:HIS:O	1:B:404:ASP:C	2.57	0.43
1:A:300:ILE:HG12	1:A:324:LEU:CD1	2.48	0.43
1:B:132:ILE:HG13	1:B:132:ILE:H	1.46	0.43
1:A:592:ASP:C	1:A:594:GLU:N	2.70	0.43
1:C:66:LEU:HD21	1:C:70:HIS:ND1	2.34	0.43
1:B:374:ALA:C	1:B:376:ARG:H	2.21	0.43
1:C:312:THR:O	1:C:312:THR:OG1	2.33	0.43
1:A:642:ILE:HG21	1:A:642:ILE:HD13	1.63	0.43
1:A:275:ILE:HG23	1:A:276:HIS:N	2.33	0.43
1:C:239:TRP:CH2	1:C:574:LYS:CE	3.01	0.43
1:A:580:PHE:HD2	1:A:649:ILE:HG13	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:TYR:CE1	4:A:861:HOH:O	2.72	0.43
1:A:576:GLU:H	1:A:576:GLU:HG3	1.20	0.43
1:A:106:PHE:O	1:A:109:ARG:N	2.43	0.43
1:E:458:ASN:O	1:E:459:GLU:C	2.56	0.43
1:A:469:ASN:HA	1:A:469:ASN:HD22	1.40	0.43
1:C:553:LEU:HA	1:C:553:LEU:HD23	1.55	0.43
1:F:271:ARG:NH2	1:F:377:ASP:OD2	2.52	0.43
1:B:84:LEU:HD11	1:B:204:TRP:CD2	2.54	0.43
1:B:324:LEU:HA	1:B:324:LEU:HD23	1.82	0.43
1:E:486:GLU:HA	1:E:492:THR:H	1.84	0.43
1:B:127:LYS:H	1:B:127:LYS:HG2	0.97	0.43
1:B:43:THR:O	1:B:44:SER:CB	2.63	0.43
1:C:374:ALA:C	1:C:376:ARG:H	2.22	0.43
1:B:224:HIS:O	1:B:228:THR:OG1	2.30	0.43
1:C:458:ASN:O	1:C:459:GLU:C	2.56	0.43
1:C:614:GLU:HG3	1:C:614:GLU:H	1.15	0.43
1:D:78:ARG:NH1	1:D:82:GLU:OE2	2.52	0.43
1:C:367:VAL:HA	1:C:373:THR:CG2	2.49	0.43
1:A:295:ARG:NE	1:A:339:TYR:CE1	2.86	0.43
1:B:551:HIS:C	1:B:552:ASP:OD1	2.57	0.43
1:E:533:MET:HB3	1:E:534:PRO:CD	2.43	0.43
1:A:300:ILE:HG13	1:A:300:ILE:H	1.60	0.43
1:D:32:ASP:HB2	1:D:36:ASN:ND2	2.32	0.43
1:B:441:GLU:C	1:B:443:ILE:H	2.18	0.43
1:E:399:PRO:HA	1:E:400:PRO:HD3	1.59	0.43
1:A:296:ILE:HG23	1:A:296:ILE:HD12	1.42	0.43
1:E:441:GLU:C	1:E:443:ILE:H	2.18	0.43
1:D:486:GLU:HA	1:D:492:THR:H	1.84	0.43
1:F:65:LEU:HD12	1:F:82:GLU:HG2	2.00	0.43
1:F:239:TRP:HH2	1:F:574:LYS:HE3	1.81	0.43
1:A:650:VAL:HG12	1:A:651:HIS:H	1.84	0.43
1:B:173:THR:O	1:B:176:ASN:HB2	2.18	0.43
1:F:555:LEU:O	1:F:556:SER:C	2.54	0.43
1:A:48:ASP:OD1	1:A:92:GLN:HG3	2.18	0.43
1:A:178:GLU:HG3	1:A:178:GLU:O	2.18	0.43
1:E:311:HIS:HA	1:E:311:HIS:HD2	1.65	0.43
1:D:190:MET:HG3	1:D:568:MET:CE	2.49	0.43
1:B:158:LYS:HD3	1:B:158:LYS:HA	1.72	0.43
1:A:458:ASN:O	1:A:459:GLU:C	2.56	0.43
1:F:469:ASN:HD22	1:F:469:ASN:HA	1.40	0.43
1:B:192:ILE:HA	1:B:192:ILE:HD13	1.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:275:ILE:HG23	1:F:276:HIS:N	2.33	0.43
1:B:275:ILE:HG23	1:B:276:HIS:N	2.33	0.43
1:B:295:ARG:NE	1:B:339:TYR:CE1	2.86	0.43
1:D:630:ILE:HG21	1:D:630:ILE:HD13	1.71	0.43
1:D:300:ILE:HG12	1:D:324:LEU:CD1	2.48	0.43
1:C:211:TYR:CE1	1:C:612:HIS:HA	2.53	0.43
1:A:66:LEU:HD21	1:A:70:HIS:ND1	2.34	0.43
1:F:458:ASN:O	1:F:459:GLU:C	2.56	0.43
1:E:178:GLU:O	1:E:178:GLU:HG3	2.18	0.43
1:D:192:ILE:HD12	1:D:192:ILE:HG23	1.72	0.43
1:F:62:ASP:O	1:F:63:HIS:C	2.57	0.43
1:C:65:LEU:HD12	1:C:65:LEU:HA	1.71	0.43
1:D:173:THR:O	1:D:176:ASN:HB2	2.18	0.43
1:A:65:LEU:HD12	1:A:82:GLU:HG2	2.00	0.43
1:B:366:GLY:O	1:B:367:VAL:C	2.57	0.43
1:F:367:VAL:HA	1:F:373:THR:CG2	2.49	0.43
1:C:630:ILE:HD13	1:C:630:ILE:HG21	1.71	0.43
1:F:190:MET:HG3	1:F:568:MET:CE	2.49	0.43
1:B:300:ILE:H	1:B:300:ILE:HG13	1.60	0.43
1:A:405:ASN:HA	1:A:405:ASN:HD22	1.45	0.43
1:D:403:HIS:O	1:D:404:ASP:C	2.57	0.43
1:C:403:HIS:O	1:C:404:ASP:C	2.57	0.43
1:F:66:LEU:HD21	1:F:70:HIS:ND1	2.34	0.43
1:B:236:LEU:HA	1:B:236:LEU:HD12	1.83	0.43
1:F:291:ILE:HD12	1:F:291:ILE:HG21	1.77	0.43
1:E:271:ARG:NH2	1:E:377:ASP:OD2	2.52	0.42
1:B:650:VAL:HG12	1:B:651:HIS:H	1.84	0.42
1:A:123:VAL:CG1	1:A:134:LEU:HD21	2.43	0.42
1:A:367:VAL:HA	1:A:373:THR:CG2	2.49	0.42
1:E:650:VAL:HG12	1:E:651:HIS:H	1.84	0.42
1:C:150:VAL:CG2	1:C:168:VAL:HG12	2.41	0.42
1:A:390:ILE:HD11	4:A:861:HOH:O	2.19	0.42
1:D:211:TYR:CE1	1:D:612:HIS:HA	2.53	0.42
1:E:403:HIS:O	1:E:404:ASP:C	2.57	0.42
1:B:211:TYR:CE1	1:B:612:HIS:HA	2.53	0.42
1:A:443:ILE:HD13	1:B:161:GLN:HG3	2.00	0.42
1:E:70:HIS:CG	1:E:71:TRP:N	2.87	0.42
1:D:215:ARG:NE	1:D:218:GLU:OE2	2.44	0.42
1:D:80:ARG:HD2	1:D:80:ARG:HH11	1.24	0.42
1:C:65:LEU:HD12	1:C:82:GLU:HG2	2.00	0.42
1:B:466:MET:HE3	1:B:466:MET:HB2	1.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:ILE:HG23	1:D:276:HIS:N	2.33	0.42
1:A:338:GLN:HE22	1:E:316:ARG:HH21	1.66	0.42
1:B:580:PHE:HD2	1:B:649:ILE:HG13	1.82	0.42
1:E:419:ASP:HB2	1:E:463:LYS:HZ2	1.84	0.42
1:E:367:VAL:HA	1:E:373:THR:CG2	2.49	0.42
1:D:576:GLU:HG3	1:D:576:GLU:H	1.20	0.42
1:D:555:LEU:O	1:D:556:SER:C	2.54	0.42
1:F:173:THR:O	1:F:176:ASN:HB2	2.18	0.42
1:F:433:LEU:HD23	1:F:433:LEU:HA	1.55	0.42
1:C:329:GLU:HA	1:C:344:HIS:HB3	2.01	0.42
1:B:569:LEU:CD2	1:B:570:LEU:HD13	2.46	0.42
1:D:324:LEU:HA	1:D:324:LEU:HD23	1.82	0.42
1:A:624:TYR:HA	1:A:625:PRO:HA	1.77	0.42
1:F:623:GLY:O	1:F:626:LEU:N	2.39	0.42
1:D:285:HIS:HB2	1:D:288:ASP:OD2	2.19	0.42
1:D:192:ILE:HA	1:D:192:ILE:HD13	1.48	0.42
1:D:224:HIS:O	1:D:228:THR:OG1	2.30	0.42
1:C:178:GLU:HG3	1:C:178:GLU:O	2.18	0.42
1:B:653:LEU:HA	1:B:653:LEU:HD12	1.46	0.42
1:C:634:ARG:HE	1:E:64:ARG:CZ	2.31	0.42
1:D:65:LEU:HD12	1:D:82:GLU:HG2	2.00	0.42
1:B:65:LEU:HA	1:B:65:LEU:HD12	1.71	0.42
1:F:314:ASP:OD1	1:F:316:ARG:N	2.48	0.42
1:B:39:PRO:HB2	1:B:53:VAL:HG12	2.01	0.42
1:D:39:PRO:HB2	1:D:53:VAL:HG12	2.01	0.42
1:A:366:GLY:O	1:A:367:VAL:C	2.57	0.42
1:E:551:HIS:C	1:E:552:ASP:OD1	2.57	0.42
1:E:48:ASP:OD2	1:E:52:ALA:N	2.52	0.42
1:C:495:LEU:HD13	1:C:583:TYR:CZ	2.55	0.42
1:C:185:GLY:HA2	1:C:375:THR:HG23	2.01	0.42
1:E:190:MET:HG3	1:E:568:MET:CE	2.49	0.42
1:A:271:ARG:NH2	1:A:377:ASP:OD2	2.52	0.42
1:F:211:TYR:CE1	1:F:612:HIS:HA	2.53	0.42
1:B:592:ASP:O	1:B:594:GLU:N	2.45	0.42
1:E:27:TYR:HA	1:E:28:PRO:HD2	1.60	0.42
1:D:66:LEU:HD21	1:D:70:HIS:ND1	2.34	0.42
1:B:66:LEU:HD21	1:B:70:HIS:ND1	2.34	0.42
1:A:45:ILE:C	1:A:94:LYS:HD3	2.40	0.42
1:E:43:THR:O	1:E:44:SER:CB	2.63	0.42
1:B:285:HIS:HB2	1:B:288:ASP:OD2	2.19	0.42
1:B:458:ASN:O	1:B:459:GLU:C	2.56	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:GLU:H	1:B:372:GLU:HG2	1.02	0.42
1:B:314:ASP:OD1	1:B:316:ARG:N	2.48	0.42
1:B:9:GLN:O	1:B:10:LYS:C	2.58	0.42
1:C:650:VAL:HG12	1:C:651:HIS:H	1.84	0.42
1:D:329:GLU:HA	1:D:344:HIS:HB3	2.01	0.42
1:B:564:ILE:HD13	1:B:564:ILE:HG21	1.87	0.42
1:F:540:LYS:O	1:F:541:GLU:C	2.58	0.42
1:C:259:LEU:HA	1:C:259:LEU:HD12	1.80	0.42
1:B:486:GLU:HA	1:B:492:THR:H	1.84	0.42
1:A:486:GLU:HA	1:A:492:THR:H	1.84	0.42
1:D:592:ASP:O	1:D:594:GLU:N	2.45	0.42
1:F:45:ILE:C	1:F:94:LYS:HD3	2.40	0.42
1:F:296:ILE:HG23	1:F:296:ILE:HD12	1.42	0.42
1:D:296:ILE:HD13	1:D:296:ILE:HA	1.38	0.42
1:E:115:PHE:O	1:E:116:VAL:C	2.57	0.42
1:D:239:TRP:HH2	1:D:574:LYS:HE3	1.81	0.42
1:F:185:GLY:HA2	1:F:375:THR:HG23	2.01	0.42
1:E:495:LEU:HD13	1:E:583:TYR:CZ	2.55	0.42
1:F:495:LEU:HD13	1:F:583:TYR:CZ	2.55	0.42
1:F:569:LEU:CD2	1:F:570:LEU:HD13	2.46	0.42
1:E:540:LYS:O	1:E:541:GLU:C	2.58	0.42
1:A:256:PHE:HA	1:B:361:PHE:CE1	2.54	0.42
1:C:324:LEU:HD23	1:C:324:LEU:HA	1.82	0.42
1:E:132:ILE:CG2	1:E:133:VAL:N	2.83	0.42
1:C:624:TYR:HA	1:C:625:PRO:HA	1.77	0.42
1:A:70:HIS:CG	1:A:71:TRP:N	2.87	0.42
1:C:70:HIS:CG	1:C:71:TRP:N	2.87	0.42
1:D:105:TYR:O	1:D:109:ARG:NE	2.46	0.42
1:D:30:LEU:HA	1:D:30:LEU:HD23	1.55	0.42
1:C:143:HIS:CE1	1:C:151:ILE:HG13	2.55	0.42
2:C:658:NDG:HA	2:C:658:NDG:H8C3	1.78	0.42
1:A:337:VAL:H	1:A:337:VAL:HG12	1.70	0.42
1:F:56:LEU:HD11	1:F:110:MET:HE3	2.01	0.42
1:E:78:ARG:NH1	1:E:82:GLU:OE2	2.52	0.42
1:B:329:GLU:HA	1:B:344:HIS:HB3	2.01	0.42
1:B:48:ASP:OD1	1:B:92:GLN:HG3	2.18	0.42
1:B:185:GLY:HA2	1:B:375:THR:HG23	2.01	0.42
1:F:329:GLU:HA	1:F:344:HIS:HB3	2.01	0.42
1:A:495:LEU:HD13	1:A:583:TYR:CZ	2.55	0.42
1:A:190:MET:HG3	1:A:568:MET:CE	2.49	0.42
1:A:569:LEU:CD2	1:A:570:LEU:HD13	2.46	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:MET:HG3	1:C:568:MET:CE	2.49	0.42
1:F:592:ASP:O	1:F:594:GLU:N	2.45	0.42
1:C:45:ILE:C	1:C:94:LYS:HD3	2.40	0.42
1:B:106:PHE:O	1:B:109:ARG:N	2.43	0.42
1:F:285:HIS:HB2	1:F:288:ASP:OD2	2.19	0.42
1:B:195:VAL:CG2	1:B:196:THR:N	2.81	0.42
1:B:115:PHE:O	1:B:116:VAL:C	2.57	0.42
1:E:140:ILE:CG2	1:E:141:THR:HG23	2.14	0.42
1:D:62:ASP:O	1:D:63:HIS:C	2.57	0.42
1:D:65:LEU:HA	1:D:65:LEU:HD12	1.71	0.42
1:C:62:ASP:O	1:C:63:HIS:C	2.57	0.42
1:D:271:ARG:NH2	1:D:377:ASP:OD2	2.52	0.42
1:C:12:GLN:NE2	1:C:544:ASP:OD1	2.52	0.42
1:A:39:PRO:HB2	1:A:53:VAL:HG12	2.01	0.42
1:F:65:LEU:HA	1:F:65:LEU:HD12	1.71	0.42
1:C:367:VAL:HB	1:C:373:THR:HG23	2.02	0.42
1:E:433:LEU:HG	1:E:450:ALA:HB2	2.02	0.42
1:F:48:ASP:OD2	1:F:52:ALA:N	2.53	0.42
1:E:84:LEU:HD11	1:E:204:TRP:CD2	2.54	0.42
1:B:540:LYS:O	1:B:541:GLU:C	2.58	0.42
1:C:540:LYS:O	1:C:541:GLU:C	2.58	0.42
1:A:540:LYS:O	1:A:541:GLU:C	2.58	0.42
1:D:132:ILE:CG2	1:D:133:VAL:N	2.83	0.42
1:C:623:GLY:O	1:C:626:LEU:N	2.39	0.42
1:F:399:PRO:HA	1:F:400:PRO:HD3	1.59	0.42
1:C:195:VAL:CG2	1:C:196:THR:N	2.81	0.42
1:A:374:ALA:C	1:A:376:ARG:H	2.22	0.42
1:A:143:HIS:CE1	1:A:151:ILE:HG13	2.55	0.42
1:D:162:LYS:HA	1:D:163:PRO:HD3	1.67	0.42
1:A:155:TYR:HD1	1:A:155:TYR:HA	1.74	0.42
1:F:653:LEU:HA	1:F:653:LEU:HD12	1.47	0.42
1:B:78:ARG:NH1	1:B:82:GLU:OE2	2.52	0.42
1:B:413:VAL:HG23	1:B:466:MET:HE3	1.98	0.42
1:C:486:GLU:HA	1:C:492:THR:H	1.84	0.42
1:C:7:ASN:O	1:C:8:ALA:C	2.51	0.42
1:D:9:GLN:O	1:D:10:LYS:C	2.58	0.42
1:F:39:PRO:HB2	1:F:53:VAL:HG12	2.01	0.42
1:A:433:LEU:HG	1:A:450:ALA:HB2	2.02	0.42
1:B:177:ARG:HE	1:B:177:ARG:HB3	1.42	0.42
1:F:403:HIS:O	1:F:404:ASP:C	2.57	0.42
1:F:486:GLU:HA	1:F:492:THR:H	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:ILE:C	1:E:94:LYS:HD3	2.40	0.42
1:E:285:HIS:HB2	1:E:288:ASP:OD2	2.19	0.42
1:A:285:HIS:HB2	1:A:288:ASP:OD2	2.19	0.42
1:C:156:SER:O	1:C:157:ALA:C	2.58	0.42
1:E:244:ASP:OD1	1:E:382:ARG:NH1	2.53	0.42
1:D:56:LEU:HD11	1:D:110:MET:HE3	2.02	0.42
1:A:78:ARG:NH1	1:A:82:GLU:OE2	2.52	0.42
1:B:433:LEU:HG	1:B:450:ALA:HB2	2.02	0.42
1:E:555:LEU:O	1:E:556:SER:C	2.54	0.42
1:E:300:ILE:HG12	1:E:324:LEU:CD1	2.48	0.42
1:F:300:ILE:HG12	1:F:324:LEU:CD1	2.48	0.42
1:B:271:ARG:NH2	1:B:377:ASP:OD2	2.52	0.42
1:A:403:HIS:O	1:A:404:ASP:C	2.57	0.42
1:E:66:LEU:HD21	1:E:70:HIS:ND1	2.34	0.42
1:B:45:ILE:C	1:B:94:LYS:HD3	2.40	0.42
1:F:43:THR:O	1:F:44:SER:CB	2.63	0.42
1:C:158:LYS:HD3	1:C:158:LYS:HA	1.72	0.42
1:C:106:PHE:O	1:C:109:ARG:N	2.43	0.42
1:F:125:HIS:CE1	1:F:200:ASP:O	2.73	0.42
1:D:469:ASN:HD22	1:D:469:ASN:HA	1.40	0.42
1:A:291:ILE:HD12	1:A:291:ILE:HG21	1.77	0.42
1:C:271:ARG:NH2	1:C:377:ASP:OD2	2.52	0.42
1:F:9:GLN:O	1:F:10:LYS:C	2.58	0.42
1:F:65:LEU:HD21	1:F:110:MET:HE2	2.00	0.42
1:F:78:ARG:NH1	1:F:82:GLU:OE2	2.52	0.42
1:C:456:ASN:ND2	1:C:457:HIS:H	2.05	0.42
1:F:426:PHE:CD1	1:F:455:LEU:HA	2.55	0.42
1:A:367:VAL:HB	1:A:373:THR:HG23	2.02	0.42
1:D:367:VAL:HA	1:D:373:THR:CG2	2.49	0.42
1:E:366:GLY:N	1:E:369:GLU:HG3	2.22	0.42
1:A:555:LEU:O	1:A:556:SER:C	2.54	0.42
1:E:551:HIS:CD2	1:E:552:ASP:CA	2.99	0.42
1:C:84:LEU:HD11	1:C:204:TRP:CD2	2.54	0.42
1:F:329:GLU:HA	1:F:344:HIS:CB	2.50	0.42
1:B:190:MET:HG3	1:B:568:MET:CE	2.49	0.42
1:C:300:ILE:HG12	1:C:324:LEU:CD1	2.48	0.42
1:C:238:ASN:C	1:C:240:LEU:N	2.73	0.42
1:A:195:VAL:CG2	1:A:196:THR:N	2.81	0.42
1:A:387:MET:HB2	1:A:387:MET:HE2	1.99	0.42
1:A:470:ASN:HB3	1:A:474:ARG:HD3	2.02	0.41
1:E:553:LEU:HD23	1:E:553:LEU:HA	1.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:314:ASP:OD1	1:E:316:ARG:N	2.48	0.41
1:D:301:ASP:CB	1:F:295:ARG:NH2	2.83	0.41
1:C:329:GLU:HA	1:C:344:HIS:CB	2.50	0.41
1:D:48:ASP:C	1:D:50:GLY:N	2.70	0.41
1:A:329:GLU:HA	1:A:344:HIS:HB3	2.01	0.41
1:E:185:GLY:HA2	1:E:375:THR:HG23	2.01	0.41
1:F:537:GLN:O	1:F:538:SER:C	2.59	0.41
1:B:256:PHE:CZ	1:B:377:ASP:HA	2.55	0.41
1:F:70:HIS:CG	1:F:71:TRP:N	2.88	0.41
1:D:158:LYS:HD3	1:D:158:LYS:HA	1.72	0.41
1:F:158:LYS:HA	1:F:158:LYS:HD3	1.72	0.41
1:C:285:HIS:HB2	1:C:288:ASP:OD2	2.19	0.41
1:E:296:ILE:HA	1:E:296:ILE:HD13	1.38	0.41
1:D:23:GLU:HA	1:D:24:PRO:HD2	1.87	0.41
1:C:241:ASP:HA	1:C:242:PRO:HD3	1.93	0.41
1:F:105:TYR:O	1:F:109:ARG:NE	2.46	0.41
1:C:296:ILE:HA	1:C:296:ILE:HD13	1.38	0.41
1:C:244:ASP:OD1	1:C:382:ARG:NH1	2.53	0.41
1:A:62:ASP:O	1:A:63:HIS:C	2.57	0.41
1:E:99:PHE:CZ	1:E:123:VAL:HG23	2.55	0.41
1:F:650:VAL:HG12	1:F:651:HIS:H	1.84	0.41
1:D:650:VAL:HG12	1:D:651:HIS:H	1.84	0.41
1:D:367:VAL:HB	1:D:373:THR:HG23	2.02	0.41
1:F:176:ASN:HD22	1:F:176:ASN:HA	1.74	0.41
1:F:433:LEU:HG	1:F:450:ALA:HB2	2.02	0.41
1:B:495:LEU:HD13	1:B:583:TYR:CZ	2.55	0.41
1:C:526:SER:HB3	1:C:529:THR:HB	2.02	0.41
1:E:526:SER:HB3	1:E:529:THR:HB	2.02	0.41
1:A:591:LYS:HB2	1:A:591:LYS:HZ2	1.85	0.41
1:C:45:ILE:HG12	1:C:45:ILE:H	1.49	0.41
1:B:156:SER:O	1:B:157:ALA:C	2.58	0.41
1:F:143:HIS:CE1	1:F:151:ILE:HG13	2.55	0.41
1:C:125:HIS:CE1	1:C:200:ASP:O	2.73	0.41
1:E:653:LEU:HA	1:E:653:LEU:HD12	1.46	0.41
1:D:634:ARG:HE	1:F:64:ARG:NH2	2.18	0.41
1:B:470:ASN:HB3	1:B:474:ARG:HD3	2.03	0.41
1:D:256:PHE:CZ	1:D:377:ASP:HA	2.55	0.41
1:F:456:ASN:ND2	1:F:457:HIS:H	2.05	0.41
1:B:367:VAL:HA	1:B:373:THR:CG2	2.49	0.41
1:D:366:GLY:O	1:D:367:VAL:C	2.57	0.41
1:B:295:ARG:HD2	1:B:295:ARG:HH11	1.31	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:VAL:CG1	1:F:433:LEU:HD11	2.50	0.41
1:E:630:ILE:HD13	1:E:630:ILE:HG21	1.71	0.41
1:D:540:LYS:O	1:D:541:GLU:C	2.58	0.41
1:C:591:LYS:HB2	1:C:591:LYS:HZ2	1.85	0.41
1:A:440:GLY:O	1:A:441:GLU:HG3	2.20	0.41
1:D:70:HIS:CG	1:D:71:TRP:N	2.87	0.41
1:B:70:HIS:CG	1:B:71:TRP:N	2.88	0.41
1:D:45:ILE:C	1:D:94:LYS:HD3	2.40	0.41
1:A:248:TRP:HD1	4:A:753:HOH:O	2.03	0.41
1:C:398:PHE:HD1	1:C:398:PHE:HA	1.70	0.41
1:A:427:ASP:HB3	1:A:567:ARG:HH12	1.86	0.41
1:F:427:ASP:HB3	1:F:567:ARG:HH12	1.86	0.41
1:B:244:ASP:OD1	1:B:382:ARG:NH1	2.53	0.41
1:B:143:HIS:CE1	1:B:151:ILE:HG13	2.55	0.41
1:D:143:HIS:CE1	1:D:151:ILE:HG13	2.55	0.41
1:E:241:ASP:HA	1:E:242:PRO:HD3	1.93	0.41
1:E:143:HIS:CE1	1:E:151:ILE:HG13	2.55	0.41
1:E:62:ASP:O	1:E:63:HIS:C	2.57	0.41
1:E:470:ASN:CG	1:E:474:ARG:HD3	2.41	0.41
1:A:470:ASN:CG	1:A:474:ARG:HD3	2.41	0.41
1:D:314:ASP:OD1	1:D:316:ARG:N	2.48	0.41
1:C:39:PRO:HB2	1:C:53:VAL:HG12	2.01	0.41
1:A:99:PHE:CZ	1:A:123:VAL:HG23	2.55	0.41
1:F:366:GLY:O	1:F:367:VAL:C	2.57	0.41
1:B:99:PHE:CZ	1:B:123:VAL:HG23	2.55	0.41
1:A:185:GLY:HA2	1:A:375:THR:HG23	2.01	0.41
1:B:132:ILE:CG2	1:B:133:VAL:N	2.83	0.41
1:B:440:GLY:O	1:B:441:GLU:HG3	2.20	0.41
1:E:592:ASP:O	1:E:594:GLU:N	2.45	0.41
1:E:156:SER:O	1:E:157:ALA:C	2.58	0.41
1:B:125:HIS:CE1	1:B:200:ASP:O	2.73	0.41
1:D:125:HIS:CE1	1:D:200:ASP:O	2.73	0.41
1:B:62:ASP:O	1:B:63:HIS:C	2.57	0.41
1:C:9:GLN:O	1:C:10:LYS:C	2.58	0.41
1:C:426:PHE:CD1	1:C:455:LEU:HA	2.55	0.41
1:B:367:VAL:HB	1:B:373:THR:HG23	2.02	0.41
1:A:355:GLY:N	4:A:707:HOH:O	2.54	0.41
1:D:433:LEU:HD23	1:D:433:LEU:HA	1.55	0.41
1:D:433:LEU:HG	1:D:450:ALA:HB2	2.02	0.41
1:D:495:LEU:HD13	1:D:583:TYR:CZ	2.55	0.41
1:D:628:ARG:O	1:D:630:ILE:HG13	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:324:LEU:HA	1:F:324:LEU:HD23	1.82	0.41
1:F:241:ASP:HA	1:F:242:PRO:HD3	1.93	0.41
1:A:614:GLU:HG3	1:A:614:GLU:H	1.15	0.41
1:D:458:ASN:O	1:D:459:GLU:C	2.56	0.41
1:C:470:ASN:CG	1:C:474:ARG:HD3	2.41	0.41
1:E:256:PHE:CD1	1:E:256:PHE:O	2.74	0.41
1:C:256:PHE:CD1	1:C:256:PHE:O	2.74	0.41
1:F:48:ASP:C	1:F:50:GLY:N	2.70	0.41
1:D:185:GLY:HA2	1:D:375:THR:HG23	2.01	0.41
1:E:329:GLU:HA	1:E:344:HIS:CB	2.50	0.41
1:D:329:GLU:HA	1:D:344:HIS:CB	2.50	0.41
1:A:177:ARG:HB3	1:A:177:ARG:HE	1.42	0.41
1:A:244:ASP:OD1	1:A:382:ARG:NH1	2.53	0.41
1:B:256:PHE:CD1	1:B:256:PHE:O	2.74	0.41
1:D:626:LEU:HD23	1:D:626:LEU:N	2.36	0.41
1:B:363:LEU:HA	1:B:363:LEU:HD12	1.79	0.41
1:D:238:ASN:C	1:D:240:LEU:N	2.73	0.41
1:C:427:ASP:HB3	1:C:567:ARG:HH12	1.86	0.41
1:F:244:ASP:OD1	1:F:382:ARG:NH1	2.53	0.41
1:D:244:ASP:OD1	1:D:382:ARG:NH1	2.53	0.41
1:A:302:HIS:CE1	1:A:304:TYR:HH	2.38	0.41
1:E:230:ARG:HD2	1:E:230:ARG:HH11	1.64	0.41
1:D:528:VAL:HG13	1:D:528:VAL:H	1.51	0.41
1:C:78:ARG:NH1	1:C:82:GLU:OE2	2.52	0.41
1:D:177:ARG:HE	1:D:177:ARG:HB3	1.41	0.41
1:E:39:PRO:HB2	1:E:53:VAL:HG12	2.01	0.41
1:A:9:GLN:O	1:A:10:LYS:C	2.58	0.41
1:B:12:GLN:NE2	1:B:544:ASP:OD1	2.51	0.41
1:A:426:PHE:CD1	1:A:455:LEU:HA	2.55	0.41
1:E:99:PHE:O	1:E:100:ARG:C	2.59	0.41
1:D:425:PHE:O	1:D:456:ASN:N	2.54	0.41
1:D:456:ASN:ND2	1:D:457:HIS:H	2.05	0.41
1:C:99:PHE:CZ	1:C:123:VAL:HG23	2.55	0.41
1:F:551:HIS:CG	1:F:552:ASP:N	2.89	0.41
1:C:433:LEU:HG	1:C:450:ALA:HB2	2.02	0.41
1:C:48:ASP:C	1:C:50:GLY:N	2.69	0.41
1:B:329:GLU:HA	1:B:344:HIS:CB	2.50	0.41
1:B:190:MET:HG3	1:B:568:MET:HE2	2.03	0.41
1:D:475:LEU:HB3	1:D:589:GLY:HA3	2.03	0.41
1:C:475:LEU:HD23	1:C:475:LEU:HA	1.88	0.41
1:A:256:PHE:CZ	1:A:377:ASP:HA	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ILE:HG12	1:B:324:LEU:CD1	2.48	0.41
1:C:43:THR:O	1:C:44:SER:CB	2.63	0.41
1:A:156:SER:O	1:A:157:ALA:C	2.58	0.41
1:E:427:ASP:HB3	1:E:567:ARG:HH12	1.85	0.41
1:F:319:LYS:HA	1:F:319:LYS:HD3	1.85	0.41
1:E:440:GLY:O	1:E:441:GLU:HG3	2.20	0.41
1:C:115:PHE:O	1:C:116:VAL:C	2.57	0.41
1:C:291:ILE:HD12	1:C:291:ILE:HG21	1.77	0.41
1:D:614:GLU:HG3	1:D:614:GLU:H	1.15	0.41
1:F:470:ASN:HB3	1:F:474:ARG:HD3	2.03	0.41
1:D:256:PHE:O	1:D:256:PHE:CD1	2.74	0.41
1:E:256:PHE:CZ	1:E:377:ASP:HA	2.56	0.41
1:E:9:GLN:O	1:E:10:LYS:C	2.58	0.41
1:B:426:PHE:CD1	1:B:455:LEU:HA	2.55	0.41
1:D:99:PHE:O	1:D:100:ARG:C	2.59	0.41
1:D:426:PHE:CD1	1:D:455:LEU:HA	2.55	0.41
1:E:426:PHE:CD1	1:E:455:LEU:HA	2.55	0.41
1:E:329:GLU:HA	1:E:344:HIS:HB3	2.01	0.41
1:E:139:GLN:NE2	1:E:432:SER:H	2.19	0.41
1:F:475:LEU:HB3	1:F:589:GLY:HA3	2.03	0.41
1:D:526:SER:HB3	1:D:529:THR:HB	2.02	0.41
1:F:38:ASN:O	1:F:40:LEU:N	2.54	0.41
1:C:132:ILE:CG2	1:C:133:VAL:N	2.83	0.41
1:F:626:LEU:HD23	1:F:626:LEU:N	2.36	0.41
1:A:363:LEU:HA	1:A:363:LEU:HD12	1.79	0.41
1:F:567:ARG:HH11	1:F:567:ARG:HD3	1.42	0.41
1:E:125:HIS:CE1	1:E:200:ASP:O	2.73	0.41
1:D:251:ILE:H	1:D:251:ILE:HG12	1.45	0.41
1:E:474:ARG:NH1	1:E:474:ARG:HB3	2.36	0.41
1:D:470:ASN:CG	1:D:474:ARG:HD3	2.41	0.41
1:B:470:ASN:CG	1:B:474:ARG:HD3	2.41	0.41
1:C:560:ARG:HH12	1:C:606:HIS:N	2.19	0.41
1:C:272:PRO:HG2	1:F:272:PRO:CD	2.50	0.41
1:C:256:PHE:CZ	1:C:377:ASP:HA	2.56	0.41
1:F:256:PHE:O	1:F:256:PHE:CD1	2.74	0.41
1:B:560:ARG:HH12	1:B:606:HIS:N	2.19	0.41
1:B:425:PHE:O	1:B:456:ASN:N	2.54	0.41
1:E:150:VAL:CG1	1:E:433:LEU:HD11	2.50	0.41
1:A:433:LEU:HD23	1:A:433:LEU:HA	1.56	0.41
1:D:52:ALA:CB	1:D:89:VAL:HG23	2.51	0.41
1:B:52:ALA:CB	1:B:89:VAL:HG23	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:630:ILE:HD13	1:F:630:ILE:HG21	1.71	0.41
1:F:628:ARG:O	1:F:630:ILE:HG13	2.21	0.41
1:A:564:ILE:HD13	1:A:564:ILE:HG21	1.87	0.41
1:B:87:PHE:CD1	1:B:121:VAL:HG12	2.56	0.41
1:C:87:PHE:CD1	1:C:121:VAL:HG12	2.56	0.41
1:B:29:ASP:O	1:B:30:LEU:C	2.59	0.41
1:C:233:PHE:O	1:C:234:GLU:C	2.59	0.41
1:D:441:GLU:C	1:D:443:ILE:H	2.18	0.41
1:A:132:ILE:CG2	1:A:133:VAL:N	2.83	0.41
1:C:626:LEU:N	1:C:626:LEU:HD23	2.36	0.41
1:E:591:LYS:HZ2	1:E:591:LYS:HB2	1.84	0.41
1:E:238:ASN:C	1:E:240:LEU:N	2.73	0.41
1:F:238:ASN:C	1:F:240:LEU:N	2.73	0.41
1:E:29:ASP:O	1:E:30:LEU:C	2.59	0.41
1:B:222:TRP:O	1:B:223:VAL:C	2.59	0.41
1:D:222:TRP:O	1:D:223:VAL:C	2.59	0.41
1:F:528:VAL:HG23	1:F:528:VAL:O	2.21	0.41
1:C:528:VAL:O	1:C:528:VAL:HG23	2.21	0.41
1:F:139:GLN:NE2	1:F:432:SER:H	2.19	0.41
1:A:23:GLU:HA	1:A:24:PRO:HD2	1.87	0.41
1:C:162:LYS:HA	1:C:163:PRO:HD3	1.67	0.41
1:C:169:SER:O	1:C:170:PHE:HB2	2.21	0.41
1:E:291:ILE:HD12	1:E:291:ILE:HG21	1.77	0.41
1:B:140:ILE:C	1:B:141:THR:HG23	2.42	0.41
1:B:62:ASP:O	1:B:63:HIS:CD2	2.70	0.41
1:D:256:PHE:HA	1:E:361:PHE:CZ	2.56	0.41
1:C:425:PHE:O	1:C:456:ASN:N	2.54	0.41
1:A:99:PHE:O	1:A:100:ARG:C	2.59	0.41
1:C:86:LEU:HD21	1:C:90:LEU:HD22	1.98	0.41
1:A:84:LEU:HD11	1:A:204:TRP:CD2	2.54	0.41
1:F:526:SER:HB3	1:F:529:THR:HB	2.02	0.41
1:F:624:TYR:HA	1:F:625:PRO:HA	1.77	0.41
1:F:398:PHE:HD1	1:F:398:PHE:HA	1.70	0.41
1:C:316:ARG:HE	1:E:338:GLN:HE22	1.69	0.41
1:B:567:ARG:HD3	1:B:567:ARG:HH11	1.42	0.41
1:B:169:SER:O	1:B:170:PHE:HB2	2.21	0.41
1:B:302:HIS:CE1	1:B:304:TYR:HH	2.38	0.41
1:D:236:LEU:HD12	1:D:236:LEU:HA	1.83	0.41
1:C:140:ILE:C	1:C:141:THR:HG23	2.41	0.40
1:E:632:ASP:C	1:E:634:ARG:N	2.73	0.40
1:C:39:PRO:O	1:C:53:VAL:HG11	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PRO:O	1:A:53:VAL:HG11	2.22	0.40
1:F:256:PHE:O	1:F:256:PHE:HD1	2.04	0.40
1:E:367:VAL:HB	1:E:373:THR:HG23	2.02	0.40
1:D:551:HIS:CG	1:D:552:ASP:N	2.89	0.40
1:A:329:GLU:HA	1:A:344:HIS:CB	2.50	0.40
1:B:629:ARG:NH1	1:B:629:ARG:HG3	2.36	0.40
1:C:177:ARG:CD	1:F:360:LYS:HB3	2.48	0.40
1:D:87:PHE:CD1	1:D:121:VAL:HG12	2.56	0.40
1:E:87:PHE:CD1	1:E:121:VAL:HG12	2.56	0.40
1:D:38:ASN:O	1:D:40:LEU:N	2.54	0.40
1:E:38:ASN:O	1:E:40:LEU:N	2.54	0.40
1:A:256:PHE:O	1:A:256:PHE:CD1	2.74	0.40
1:F:132:ILE:CG2	1:F:133:VAL:N	2.83	0.40
1:D:111:ASN:C	1:D:111:ASN:OD1	2.59	0.40
1:B:319:LYS:HD3	1:B:319:LYS:HA	1.85	0.40
1:F:440:GLY:O	1:F:441:GLU:HG3	2.20	0.40
1:C:139:GLN:NE2	1:C:432:SER:H	2.19	0.40
1:A:125:HIS:CE1	1:A:200:ASP:O	2.73	0.40
1:E:528:VAL:HG13	1:E:528:VAL:H	1.51	0.40
1:D:64:ARG:O	1:D:78:ARG:NH1	2.55	0.40
1:B:64:ARG:O	1:B:78:ARG:NH1	2.55	0.40
1:B:275:ILE:HG21	1:B:275:ILE:HD13	1.54	0.40
1:D:39:PRO:O	1:D:53:VAL:HG11	2.22	0.40
1:E:48:ASP:C	1:E:50:GLY:N	2.69	0.40
1:A:238:ASN:C	1:A:240:LEU:N	2.73	0.40
1:D:537:GLN:O	1:D:538:SER:C	2.59	0.40
1:E:190:MET:HG3	1:E:568:MET:HE2	2.02	0.40
1:A:87:PHE:CD1	1:A:121:VAL:HG12	2.56	0.40
1:A:537:GLN:O	1:A:538:SER:C	2.59	0.40
1:B:626:LEU:N	1:B:626:LEU:HD23	2.36	0.40
1:D:624:TYR:HA	1:D:625:PRO:HA	1.77	0.40
1:B:427:ASP:HB3	1:B:567:ARG:HH12	1.86	0.40
1:B:157:ALA:HB1	1:B:448:ILE:HG12	2.03	0.40
1:D:596:HIS:N	1:D:596:HIS:ND1	2.69	0.40
1:B:528:VAL:HG13	1:B:528:VAL:H	1.51	0.40
1:C:470:ASN:HB3	1:C:474:ARG:HD3	2.02	0.40
1:A:474:ARG:HB3	1:A:474:ARG:NH1	2.36	0.40
1:F:271:ARG:HA	1:F:272:PRO:HD3	1.69	0.40
1:D:99:PHE:CZ	1:D:123:VAL:HG23	2.55	0.40
1:F:367:VAL:HB	1:F:373:THR:HG23	2.02	0.40
1:A:523:SER:OG	1:A:524:LYS:HG3	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:569:LEU:CD2	1:C:570:LEU:HD13	2.46	0.40
1:C:475:LEU:HB3	1:C:589:GLY:HA3	2.03	0.40
1:D:440:GLY:O	1:D:441:GLU:HG3	2.20	0.40
1:D:399:PRO:HA	1:D:400:PRO:HD3	1.59	0.40
1:E:169:SER:O	1:E:170:PHE:HB2	2.21	0.40
1:A:631:PRO:HD2	4:A:818:HOH:O	2.20	0.40
1:B:162:LYS:HA	1:B:163:PRO:HD3	1.67	0.40
1:D:632:ASP:C	1:D:634:ARG:N	2.73	0.40
1:B:239:TRP:HH2	1:B:574:LYS:HE3	1.81	0.40
1:F:99:PHE:CZ	1:F:123:VAL:HG23	2.55	0.40
1:B:124:ILE:HG21	1:B:124:ILE:HD13	1.73	0.40
1:E:569:LEU:CD2	1:E:570:LEU:HD13	2.46	0.40
1:B:38:ASN:O	1:B:40:LEU:N	2.54	0.40
1:C:38:ASN:O	1:C:40:LEU:N	2.54	0.40
1:A:132:ILE:HG13	1:A:132:ILE:H	1.46	0.40
1:C:111:ASN:C	1:C:111:ASN:OD1	2.60	0.40
1:A:157:ALA:HB1	1:A:448:ILE:HG12	2.04	0.40
1:F:192:ILE:HD13	1:F:192:ILE:HA	1.48	0.40
1:E:423:ILE:HG23	1:E:458:ASN:CG	2.41	0.40
1:A:423:ILE:HG23	1:A:458:ASN:CG	2.41	0.40
1:B:25:THR:HG22	1:B:26:LYS:H	1.87	0.40
1:C:64:ARG:O	1:C:78:ARG:NH1	2.54	0.40
1:E:470:ASN:HB3	1:E:474:ARG:HD3	2.02	0.40
1:D:474:ARG:HB3	1:D:474:ARG:NH1	2.36	0.40
1:C:465:THR:HG23	1:C:518:THR:HG1	1.84	0.40
1:D:256:PHE:O	1:D:256:PHE:HD1	2.04	0.40
1:B:316:ARG:HH21	1:D:338:GLN:HE22	1.68	0.40
1:F:560:ARG:HH12	1:F:606:HIS:N	2.19	0.40
1:F:425:PHE:O	1:F:456:ASN:N	2.54	0.40
1:E:462:TYR:O	1:E:520:GLU:CA	2.62	0.40
1:E:551:HIS:CG	1:E:552:ASP:N	2.89	0.40
1:B:628:ARG:O	1:B:630:ILE:HG13	2.21	0.40
1:A:628:ARG:O	1:A:630:ILE:HG13	2.21	0.40
1:C:311:HIS:HD2	1:C:311:HIS:HA	1.65	0.40
1:F:87:PHE:CD1	1:F:121:VAL:HG12	2.56	0.40
1:F:523:SER:OG	1:F:524:LYS:HG3	2.22	0.40
1:E:475:LEU:HB3	1:E:589:GLY:HA3	2.03	0.40
1:B:526:SER:HB3	1:B:529:THR:HB	2.02	0.40
1:A:38:ASN:O	1:A:40:LEU:N	2.54	0.40
1:E:390:ILE:HD13	1:E:390:ILE:HA	1.92	0.40
1:B:160:THR:O	1:B:161:GLN:CB	2.66	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:626:LEU:HD23	1:E:626:LEU:N	2.36	0.40
1:A:230:ARG:HH11	1:A:230:ARG:HD2	1.64	0.40
1:F:222:TRP:O	1:F:223:VAL:C	2.59	0.40
1:D:17:LEU:HA	1:D:17:LEU:HD23	1.89	0.40
1:A:159:MET:HB3	1:B:158:LYS:HG3	2.04	0.40
1:F:156:SER:O	1:F:157:ALA:C	2.58	0.40
1:C:423:ILE:HG23	1:C:458:ASN:CG	2.41	0.40
1:E:162:LYS:HA	1:E:163:PRO:HD3	1.67	0.40
1:B:219:LEU:HA	1:B:219:LEU:HD12	1.82	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ASP:OD2	1:E:547:VAL:O[1_556]	1.86	0.34

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	640/657 (97%)	524 (82%)	88 (14%)	28 (4%)	3	24
1	B	640/657 (97%)	523 (82%)	89 (14%)	28 (4%)	3	24
1	C	640/657 (97%)	523 (82%)	89 (14%)	28 (4%)	3	24
1	D	640/657 (97%)	523 (82%)	89 (14%)	28 (4%)	3	24
1	E	640/657 (97%)	524 (82%)	88 (14%)	28 (4%)	3	24
1	F	640/657 (97%)	523 (82%)	89 (14%)	28 (4%)	3	24
All	All	3840/3942 (97%)	3140 (82%)	532 (14%)	168 (4%)	3	24

All (168) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	147	ASN
1	A	176	ASN
1	A	473	GLU
1	A	552	ASP
1	B	7	ASN
1	B	147	ASN
1	B	176	ASN
1	B	473	GLU
1	B	552	ASP
1	C	7	ASN
1	C	147	ASN
1	C	176	ASN
1	C	473	GLU
1	C	552	ASP
1	D	7	ASN
1	D	147	ASN
1	D	176	ASN
1	D	473	GLU
1	D	552	ASP
1	E	7	ASN
1	E	147	ASN
1	E	176	ASN
1	E	473	GLU
1	E	552	ASP
1	F	7	ASN
1	F	147	ASN
1	F	176	ASN
1	F	473	GLU
1	F	552	ASP
1	A	8	ALA
1	A	20	LYS
1	A	42	ASP
1	A	44	SER
1	A	90	LEU
1	A	170	PHE
1	A	171	THR
1	A	320	GLY
1	A	427	ASP
1	A	516	PRO
1	A	557	ALA
1	A	561	SER
1	B	8	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	20	LYS
1	B	42	ASP
1	B	44	SER
1	B	90	LEU
1	B	170	PHE
1	B	171	THR
1	B	320	GLY
1	B	427	ASP
1	B	516	PRO
1	B	557	ALA
1	B	561	SER
1	C	8	ALA
1	C	20	LYS
1	C	42	ASP
1	C	44	SER
1	C	90	LEU
1	C	170	PHE
1	C	171	THR
1	C	320	GLY
1	C	427	ASP
1	C	516	PRO
1	C	557	ALA
1	C	561	SER
1	D	8	ALA
1	D	20	LYS
1	D	42	ASP
1	D	44	SER
1	D	90	LEU
1	D	170	PHE
1	D	171	THR
1	D	320	GLY
1	D	427	ASP
1	D	516	PRO
1	D	557	ALA
1	D	561	SER
1	E	8	ALA
1	E	20	LYS
1	E	42	ASP
1	E	44	SER
1	E	90	LEU
1	E	170	PHE
1	E	171	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	320	GLY
1	E	427	ASP
1	E	516	PRO
1	E	557	ALA
1	E	561	SER
1	F	8	ALA
1	F	20	LYS
1	F	42	ASP
1	F	44	SER
1	F	90	LEU
1	F	170	PHE
1	F	171	THR
1	F	320	GLY
1	F	427	ASP
1	F	516	PRO
1	F	557	ALA
1	F	561	SER
1	A	5	THR
1	A	104	ALA
1	A	242	PRO
1	A	560	ARG
1	A	569	LEU
1	A	595	GLY
1	B	5	THR
1	B	104	ALA
1	B	242	PRO
1	B	560	ARG
1	B	569	LEU
1	B	595	GLY
1	C	5	THR
1	C	104	ALA
1	C	242	PRO
1	C	560	ARG
1	C	569	LEU
1	C	595	GLY
1	D	5	THR
1	D	104	ALA
1	D	242	PRO
1	D	560	ARG
1	D	569	LEU
1	D	595	GLY
1	E	5	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	104	ALA
1	E	242	PRO
1	E	560	ARG
1	E	569	LEU
1	E	595	GLY
1	F	5	THR
1	F	104	ALA
1	F	242	PRO
1	F	560	ARG
1	F	569	LEU
1	F	595	GLY
1	A	63	HIS
1	A	273	ASP
1	B	63	HIS
1	B	273	ASP
1	C	63	HIS
1	C	273	ASP
1	D	63	HIS
1	D	273	ASP
1	E	63	HIS
1	E	273	ASP
1	F	63	HIS
1	F	273	ASP
1	A	496	ASP
1	B	496	ASP
1	C	496	ASP
1	D	496	ASP
1	E	496	ASP
1	F	496	ASP
1	A	549	GLY
1	B	549	GLY
1	C	549	GLY
1	D	549	GLY
1	E	549	GLY
1	F	549	GLY
1	A	24	PRO
1	B	24	PRO
1	C	24	PRO
1	D	24	PRO
1	E	24	PRO
1	F	24	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	570/580 (98%)	416 (73%)	154 (27%)	0	2
1	B	570/580 (98%)	416 (73%)	154 (27%)	0	2
1	C	570/580 (98%)	416 (73%)	154 (27%)	0	2
1	D	570/580 (98%)	416 (73%)	154 (27%)	0	2
1	E	570/580 (98%)	416 (73%)	154 (27%)	0	2
1	F	570/580 (98%)	416 (73%)	154 (27%)	0	2
All	All	3420/3480 (98%)	2496 (73%)	924 (27%)	0	2

All (924) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	15	ASN
1	A	18	LEU
1	A	25	THR
1	A	31	LYS
1	A	44	SER
1	A	48	ASP
1	A	53	VAL
1	A	58	LYS
1	A	63	HIS
1	A	64	ARG
1	A	66	LEU
1	A	67	GLU
1	A	69	ARG
1	A	72	TYR
1	A	77	THR
1	A	85	MET
1	A	86	LEU
1	A	94	LYS
1	A	95	GLU
1	A	107	ARG
1	A	108	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	110	MET
1	A	111	ASN
1	A	112	GLU
1	A	127	LYS
1	A	128	LEU
1	A	145	PHE
1	A	148	SER
1	A	151	ILE
1	A	153	LYS
1	A	156	SER
1	A	158	LYS
1	A	165	THR
1	A	166	PHE
1	A	175	LYS
1	A	176	ASN
1	A	179	GLN
1	A	180	ARG
1	A	181	VAL
1	A	216	LYS
1	A	219	LEU
1	A	221	PHE
1	A	233	PHE
1	A	235	ARG
1	A	241	ASP
1	A	242	PRO
1	A	243	VAL
1	A	244	ASP
1	A	246	LEU
1	A	249	ASP
1	A	250	ARG
1	A	251	ILE
1	A	252	ILE
1	A	256	PHE
1	A	259	LEU
1	A	270	VAL
1	A	272	PRO
1	A	275	ILE
1	A	280	VAL
1	A	281	ASP
1	A	291	ILE
1	A	292	THR
1	A	294	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	297	HIS
1	A	306	THR
1	A	313	ILE
1	A	316	ARG
1	A	318	PRO
1	A	319	LYS
1	A	322	GLU
1	A	323	LEU
1	A	329	GLU
1	A	332	LYS
1	A	334	SER
1	A	335	SER
1	A	342	SER
1	A	343	LEU
1	A	351	LEU
1	A	362	ASN
1	A	367	VAL
1	A	372	GLU
1	A	373	THR
1	A	375	THR
1	A	376	ARG
1	A	382	ARG
1	A	389	ASN
1	A	395	THR
1	A	396	ASP
1	A	397	SER
1	A	399	PRO
1	A	402	THR
1	A	405	ASN
1	A	411	MET
1	A	412	VAL
1	A	416	VAL
1	A	418	ILE
1	A	423	ILE
1	A	427	ASP
1	A	435	ASN
1	A	438	ASP
1	A	439	SER
1	A	452	VAL
1	A	453	HIS
1	A	456	ASN
1	A	461	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	466	MET
1	A	467	SER
1	A	473	GLU
1	A	474	ARG
1	A	475	LEU
1	A	482	LEU
1	A	487	ASP
1	A	491	ILE
1	A	493	LEU
1	A	501	PHE
1	A	502	CYS
1	A	503	ILE
1	A	511	LYS
1	A	519	ILE
1	A	523	SER
1	A	525	ASP
1	A	529	THR
1	A	532	ASP
1	A	533	MET
1	A	535	SER
1	A	539	LEU
1	A	547	VAL
1	A	552	ASP
1	A	554	ASP
1	A	555	LEU
1	A	559	GLU
1	A	565	PRO
1	A	567	ARG
1	A	570	LEU
1	A	574	LYS
1	A	578	MET
1	A	579	GLU
1	A	586	VAL
1	A	587	THR
1	A	591	LYS
1	A	596	HIS
1	A	606	HIS
1	A	609	CYS
1	A	620	ARG
1	A	622	LEU
1	A	625	PRO
1	A	634	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	636	ILE
1	A	639	VAL
1	A	641	ASN
1	A	643	LYS
1	A	645	VAL
1	A	650	VAL
1	B	12	GLN
1	B	15	ASN
1	B	18	LEU
1	B	25	THR
1	B	31	LYS
1	B	44	SER
1	B	48	ASP
1	B	53	VAL
1	B	58	LYS
1	B	63	HIS
1	B	64	ARG
1	B	66	LEU
1	B	67	GLU
1	B	69	ARG
1	B	72	TYR
1	B	77	THR
1	B	85	MET
1	B	86	LEU
1	B	94	LYS
1	B	95	GLU
1	B	107	ARG
1	B	108	GLU
1	B	110	MET
1	B	111	ASN
1	B	112	GLU
1	B	127	LYS
1	B	128	LEU
1	B	145	PHE
1	B	148	SER
1	B	151	ILE
1	B	153	LYS
1	B	156	SER
1	B	158	LYS
1	B	165	THR
1	B	166	PHE
1	B	175	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	176	ASN
1	B	179	GLN
1	B	180	ARG
1	B	181	VAL
1	B	216	LYS
1	B	219	LEU
1	B	221	PHE
1	B	233	PHE
1	B	235	ARG
1	B	241	ASP
1	B	242	PRO
1	B	243	VAL
1	B	244	ASP
1	B	246	LEU
1	B	249	ASP
1	B	250	ARG
1	B	251	ILE
1	B	252	ILE
1	B	256	PHE
1	B	259	LEU
1	B	270	VAL
1	B	272	PRO
1	B	275	ILE
1	B	280	VAL
1	B	281	ASP
1	B	291	ILE
1	B	292	THR
1	B	294	SER
1	B	297	HIS
1	B	306	THR
1	B	313	ILE
1	B	316	ARG
1	B	318	PRO
1	B	319	LYS
1	B	322	GLU
1	B	323	LEU
1	B	329	GLU
1	B	332	LYS
1	B	334	SER
1	B	335	SER
1	B	342	SER
1	B	343	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	351	LEU
1	B	362	ASN
1	B	367	VAL
1	B	372	GLU
1	B	373	THR
1	B	375	THR
1	B	376	ARG
1	B	382	ARG
1	B	389	ASN
1	B	395	THR
1	B	396	ASP
1	B	397	SER
1	B	399	PRO
1	B	402	THR
1	B	405	ASN
1	B	411	MET
1	B	412	VAL
1	B	416	VAL
1	B	418	ILE
1	B	423	ILE
1	B	427	ASP
1	B	435	ASN
1	B	438	ASP
1	B	439	SER
1	B	452	VAL
1	B	453	HIS
1	B	456	ASN
1	B	461	THR
1	B	466	MET
1	B	467	SER
1	B	473	GLU
1	B	474	ARG
1	B	475	LEU
1	B	482	LEU
1	B	487	ASP
1	B	491	ILE
1	B	493	LEU
1	B	501	PHE
1	B	502	CYS
1	B	503	ILE
1	B	511	LYS
1	B	519	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	523	SER
1	B	525	ASP
1	B	529	THR
1	B	532	ASP
1	B	533	MET
1	B	535	SER
1	B	539	LEU
1	B	547	VAL
1	B	552	ASP
1	B	554	ASP
1	B	555	LEU
1	B	559	GLU
1	B	565	PRO
1	B	567	ARG
1	B	570	LEU
1	B	574	LYS
1	B	578	MET
1	B	579	GLU
1	B	586	VAL
1	B	587	THR
1	B	591	LYS
1	B	596	HIS
1	B	606	HIS
1	B	609	CYS
1	B	620	ARG
1	B	622	LEU
1	B	625	PRO
1	B	634	ARG
1	B	636	ILE
1	B	639	VAL
1	B	641	ASN
1	B	643	LYS
1	B	645	VAL
1	B	650	VAL
1	C	12	GLN
1	C	15	ASN
1	C	18	LEU
1	C	25	THR
1	C	31	LYS
1	C	44	SER
1	C	48	ASP
1	C	53	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	58	LYS
1	C	63	HIS
1	C	64	ARG
1	C	66	LEU
1	C	67	GLU
1	C	69	ARG
1	C	72	TYR
1	C	77	THR
1	C	85	MET
1	C	86	LEU
1	C	94	LYS
1	C	95	GLU
1	C	107	ARG
1	C	108	GLU
1	C	110	MET
1	C	111	ASN
1	C	112	GLU
1	C	127	LYS
1	C	128	LEU
1	C	145	PHE
1	C	148	SER
1	C	151	ILE
1	C	153	LYS
1	C	156	SER
1	C	158	LYS
1	C	165	THR
1	C	166	PHE
1	C	175	LYS
1	C	176	ASN
1	C	179	GLN
1	C	180	ARG
1	C	181	VAL
1	C	216	LYS
1	C	219	LEU
1	C	221	PHE
1	C	233	PHE
1	C	235	ARG
1	C	241	ASP
1	C	242	PRO
1	C	243	VAL
1	C	244	ASP
1	C	246	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	249	ASP
1	C	250	ARG
1	C	251	ILE
1	C	252	ILE
1	C	256	PHE
1	C	259	LEU
1	C	270	VAL
1	C	272	PRO
1	C	275	ILE
1	C	280	VAL
1	C	281	ASP
1	C	291	ILE
1	C	292	THR
1	C	294	SER
1	C	297	HIS
1	C	306	THR
1	C	313	ILE
1	C	316	ARG
1	C	318	PRO
1	C	319	LYS
1	C	322	GLU
1	C	323	LEU
1	C	329	GLU
1	C	332	LYS
1	C	334	SER
1	C	335	SER
1	C	342	SER
1	C	343	LEU
1	C	351	LEU
1	C	362	ASN
1	C	367	VAL
1	C	372	GLU
1	C	373	THR
1	C	375	THR
1	C	376	ARG
1	C	382	ARG
1	C	389	ASN
1	C	395	THR
1	C	396	ASP
1	C	397	SER
1	C	399	PRO
1	C	402	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	405	ASN
1	C	411	MET
1	C	412	VAL
1	C	416	VAL
1	C	418	ILE
1	C	423	ILE
1	C	427	ASP
1	C	435	ASN
1	C	438	ASP
1	C	439	SER
1	C	452	VAL
1	C	453	HIS
1	C	456	ASN
1	C	461	THR
1	C	466	MET
1	C	467	SER
1	C	473	GLU
1	C	474	ARG
1	C	475	LEU
1	C	482	LEU
1	C	487	ASP
1	C	491	ILE
1	C	493	LEU
1	C	501	PHE
1	C	502	CYS
1	C	503	ILE
1	C	511	LYS
1	C	519	ILE
1	C	523	SER
1	C	525	ASP
1	C	529	THR
1	C	532	ASP
1	C	533	MET
1	C	535	SER
1	C	539	LEU
1	C	547	VAL
1	C	552	ASP
1	C	554	ASP
1	C	555	LEU
1	C	559	GLU
1	C	565	PRO
1	C	567	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	570	LEU
1	C	574	LYS
1	C	578	MET
1	C	579	GLU
1	C	586	VAL
1	C	587	THR
1	C	591	LYS
1	C	596	HIS
1	C	606	HIS
1	C	609	CYS
1	C	620	ARG
1	C	622	LEU
1	C	625	PRO
1	C	634	ARG
1	C	636	ILE
1	C	639	VAL
1	C	641	ASN
1	C	643	LYS
1	C	645	VAL
1	C	650	VAL
1	D	12	GLN
1	D	15	ASN
1	D	18	LEU
1	D	25	THR
1	D	31	LYS
1	D	44	SER
1	D	48	ASP
1	D	53	VAL
1	D	58	LYS
1	D	63	HIS
1	D	64	ARG
1	D	66	LEU
1	D	67	GLU
1	D	69	ARG
1	D	72	TYR
1	D	77	THR
1	D	85	MET
1	D	86	LEU
1	D	94	LYS
1	D	95	GLU
1	D	107	ARG
1	D	108	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	110	MET
1	D	111	ASN
1	D	112	GLU
1	D	127	LYS
1	D	128	LEU
1	D	145	PHE
1	D	148	SER
1	D	151	ILE
1	D	153	LYS
1	D	156	SER
1	D	158	LYS
1	D	165	THR
1	D	166	PHE
1	D	175	LYS
1	D	176	ASN
1	D	179	GLN
1	D	180	ARG
1	D	181	VAL
1	D	216	LYS
1	D	219	LEU
1	D	221	PHE
1	D	233	PHE
1	D	235	ARG
1	D	241	ASP
1	D	242	PRO
1	D	243	VAL
1	D	244	ASP
1	D	246	LEU
1	D	249	ASP
1	D	250	ARG
1	D	251	ILE
1	D	252	ILE
1	D	256	PHE
1	D	259	LEU
1	D	270	VAL
1	D	272	PRO
1	D	275	ILE
1	D	280	VAL
1	D	281	ASP
1	D	291	ILE
1	D	292	THR
1	D	294	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	297	HIS
1	D	306	THR
1	D	313	ILE
1	D	316	ARG
1	D	318	PRO
1	D	319	LYS
1	D	322	GLU
1	D	323	LEU
1	D	329	GLU
1	D	332	LYS
1	D	334	SER
1	D	335	SER
1	D	342	SER
1	D	343	LEU
1	D	351	LEU
1	D	362	ASN
1	D	367	VAL
1	D	372	GLU
1	D	373	THR
1	D	375	THR
1	D	376	ARG
1	D	382	ARG
1	D	389	ASN
1	D	395	THR
1	D	396	ASP
1	D	397	SER
1	D	399	PRO
1	D	402	THR
1	D	405	ASN
1	D	411	MET
1	D	412	VAL
1	D	416	VAL
1	D	418	ILE
1	D	423	ILE
1	D	427	ASP
1	D	435	ASN
1	D	438	ASP
1	D	439	SER
1	D	452	VAL
1	D	453	HIS
1	D	456	ASN
1	D	461	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	466	MET
1	D	467	SER
1	D	473	GLU
1	D	474	ARG
1	D	475	LEU
1	D	482	LEU
1	D	487	ASP
1	D	491	ILE
1	D	493	LEU
1	D	501	PHE
1	D	502	CYS
1	D	503	ILE
1	D	511	LYS
1	D	519	ILE
1	D	523	SER
1	D	525	ASP
1	D	529	THR
1	D	532	ASP
1	D	533	MET
1	D	535	SER
1	D	539	LEU
1	D	547	VAL
1	D	552	ASP
1	D	554	ASP
1	D	555	LEU
1	D	559	GLU
1	D	565	PRO
1	D	567	ARG
1	D	570	LEU
1	D	574	LYS
1	D	578	MET
1	D	579	GLU
1	D	586	VAL
1	D	587	THR
1	D	591	LYS
1	D	596	HIS
1	D	606	HIS
1	D	609	CYS
1	D	620	ARG
1	D	622	LEU
1	D	625	PRO
1	D	634	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	636	ILE
1	D	639	VAL
1	D	641	ASN
1	D	643	LYS
1	D	645	VAL
1	D	650	VAL
1	E	12	GLN
1	E	15	ASN
1	E	18	LEU
1	E	25	THR
1	E	31	LYS
1	E	44	SER
1	E	48	ASP
1	E	53	VAL
1	E	58	LYS
1	E	63	HIS
1	E	64	ARG
1	E	66	LEU
1	E	67	GLU
1	E	69	ARG
1	E	72	TYR
1	E	77	THR
1	E	85	MET
1	E	86	LEU
1	E	94	LYS
1	E	95	GLU
1	E	107	ARG
1	E	108	GLU
1	E	110	MET
1	E	111	ASN
1	E	112	GLU
1	E	127	LYS
1	E	128	LEU
1	E	145	PHE
1	E	148	SER
1	E	151	ILE
1	E	153	LYS
1	E	156	SER
1	E	158	LYS
1	E	165	THR
1	E	166	PHE
1	E	175	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	176	ASN
1	E	179	GLN
1	E	180	ARG
1	E	181	VAL
1	E	216	LYS
1	E	219	LEU
1	E	221	PHE
1	E	233	PHE
1	E	235	ARG
1	E	241	ASP
1	E	242	PRO
1	E	243	VAL
1	E	244	ASP
1	E	246	LEU
1	E	249	ASP
1	E	250	ARG
1	E	251	ILE
1	E	252	ILE
1	E	256	PHE
1	E	259	LEU
1	E	270	VAL
1	E	272	PRO
1	E	275	ILE
1	E	280	VAL
1	E	281	ASP
1	E	291	ILE
1	E	292	THR
1	E	294	SER
1	E	297	HIS
1	E	306	THR
1	E	313	ILE
1	E	316	ARG
1	E	318	PRO
1	E	319	LYS
1	E	322	GLU
1	E	323	LEU
1	E	329	GLU
1	E	332	LYS
1	E	334	SER
1	E	335	SER
1	E	342	SER
1	E	343	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	351	LEU
1	E	362	ASN
1	E	367	VAL
1	E	372	GLU
1	E	373	THR
1	E	375	THR
1	E	376	ARG
1	E	382	ARG
1	E	389	ASN
1	E	395	THR
1	E	396	ASP
1	E	397	SER
1	E	399	PRO
1	E	402	THR
1	E	405	ASN
1	E	411	MET
1	E	412	VAL
1	E	416	VAL
1	E	418	ILE
1	E	423	ILE
1	E	427	ASP
1	E	435	ASN
1	E	438	ASP
1	E	439	SER
1	E	452	VAL
1	E	453	HIS
1	E	456	ASN
1	E	461	THR
1	E	466	MET
1	E	467	SER
1	E	473	GLU
1	E	474	ARG
1	E	475	LEU
1	E	482	LEU
1	E	487	ASP
1	E	491	ILE
1	E	493	LEU
1	E	501	PHE
1	E	502	CYS
1	E	503	ILE
1	E	511	LYS
1	E	519	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	523	SER
1	E	525	ASP
1	E	529	THR
1	E	532	ASP
1	E	533	MET
1	E	535	SER
1	E	539	LEU
1	E	547	VAL
1	E	552	ASP
1	E	554	ASP
1	E	555	LEU
1	E	559	GLU
1	E	565	PRO
1	E	567	ARG
1	E	570	LEU
1	E	574	LYS
1	E	578	MET
1	E	579	GLU
1	E	586	VAL
1	E	587	THR
1	E	591	LYS
1	E	596	HIS
1	E	606	HIS
1	E	609	CYS
1	E	620	ARG
1	E	622	LEU
1	E	625	PRO
1	E	634	ARG
1	E	636	ILE
1	E	639	VAL
1	E	641	ASN
1	E	643	LYS
1	E	645	VAL
1	E	650	VAL
1	F	12	GLN
1	F	15	ASN
1	F	18	LEU
1	F	25	THR
1	F	31	LYS
1	F	44	SER
1	F	48	ASP
1	F	53	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	58	LYS
1	F	63	HIS
1	F	64	ARG
1	F	66	LEU
1	F	67	GLU
1	F	69	ARG
1	F	72	TYR
1	F	77	THR
1	F	85	MET
1	F	86	LEU
1	F	94	LYS
1	F	95	GLU
1	F	107	ARG
1	F	108	GLU
1	F	110	MET
1	F	111	ASN
1	F	112	GLU
1	F	127	LYS
1	F	128	LEU
1	F	145	PHE
1	F	148	SER
1	F	151	ILE
1	F	153	LYS
1	F	156	SER
1	F	158	LYS
1	F	165	THR
1	F	166	PHE
1	F	175	LYS
1	F	176	ASN
1	F	179	GLN
1	F	180	ARG
1	F	181	VAL
1	F	216	LYS
1	F	219	LEU
1	F	221	PHE
1	F	233	PHE
1	F	235	ARG
1	F	241	ASP
1	F	242	PRO
1	F	243	VAL
1	F	244	ASP
1	F	246	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	249	ASP
1	F	250	ARG
1	F	251	ILE
1	F	252	ILE
1	F	256	PHE
1	F	259	LEU
1	F	270	VAL
1	F	272	PRO
1	F	275	ILE
1	F	280	VAL
1	F	281	ASP
1	F	291	ILE
1	F	292	THR
1	F	294	SER
1	F	297	HIS
1	F	306	THR
1	F	313	ILE
1	F	316	ARG
1	F	318	PRO
1	F	319	LYS
1	F	322	GLU
1	F	323	LEU
1	F	329	GLU
1	F	332	LYS
1	F	334	SER
1	F	335	SER
1	F	342	SER
1	F	343	LEU
1	F	351	LEU
1	F	362	ASN
1	F	367	VAL
1	F	372	GLU
1	F	373	THR
1	F	375	THR
1	F	376	ARG
1	F	382	ARG
1	F	389	ASN
1	F	395	THR
1	F	396	ASP
1	F	397	SER
1	F	399	PRO
1	F	402	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	405	ASN
1	F	411	MET
1	F	412	VAL
1	F	416	VAL
1	F	418	ILE
1	F	423	ILE
1	F	427	ASP
1	F	435	ASN
1	F	438	ASP
1	F	439	SER
1	F	452	VAL
1	F	453	HIS
1	F	456	ASN
1	F	461	THR
1	F	466	MET
1	F	467	SER
1	F	473	GLU
1	F	474	ARG
1	F	475	LEU
1	F	482	LEU
1	F	487	ASP
1	F	491	ILE
1	F	493	LEU
1	F	501	PHE
1	F	502	CYS
1	F	503	ILE
1	F	511	LYS
1	F	519	ILE
1	F	523	SER
1	F	525	ASP
1	F	529	THR
1	F	532	ASP
1	F	533	MET
1	F	535	SER
1	F	539	LEU
1	F	547	VAL
1	F	552	ASP
1	F	554	ASP
1	F	555	LEU
1	F	559	GLU
1	F	565	PRO
1	F	567	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	570	LEU
1	F	574	LYS
1	F	578	MET
1	F	579	GLU
1	F	586	VAL
1	F	587	THR
1	F	591	LYS
1	F	596	HIS
1	F	606	HIS
1	F	609	CYS
1	F	620	ARG
1	F	622	LEU
1	F	625	PRO
1	F	634	ARG
1	F	636	ILE
1	F	639	VAL
1	F	641	ASN
1	F	643	LYS
1	F	645	VAL
1	F	650	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	15	ASN
1	A	36	ASN
1	A	47	ASN
1	A	63	HIS
1	A	76	ASN
1	A	92	GLN
1	A	102	ASN
1	A	225	HIS
1	A	336	ASN
1	A	338	GLN
1	A	354	GLN
1	A	389	ASN
1	A	414	ASN
1	A	449	ASN
1	A	453	HIS
1	A	456	ASN
1	A	469	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	470	ASN
1	A	551	HIS
1	A	606	HIS
1	A	608	GLN
1	A	612	HIS
1	B	11	GLN
1	B	15	ASN
1	B	36	ASN
1	B	47	ASN
1	B	63	HIS
1	B	76	ASN
1	B	92	GLN
1	B	102	ASN
1	B	225	HIS
1	B	336	ASN
1	B	338	GLN
1	B	354	GLN
1	B	394	HIS
1	B	414	ASN
1	B	449	ASN
1	B	453	HIS
1	B	456	ASN
1	B	469	ASN
1	B	551	HIS
1	B	606	HIS
1	B	612	HIS
1	C	11	GLN
1	C	15	ASN
1	C	16	HIS
1	C	36	ASN
1	C	47	ASN
1	C	63	HIS
1	C	76	ASN
1	C	92	GLN
1	C	102	ASN
1	C	225	HIS
1	C	336	ASN
1	C	338	GLN
1	C	354	GLN
1	C	394	HIS
1	C	414	ASN
1	C	449	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	453	HIS
1	C	456	ASN
1	C	469	ASN
1	C	470	ASN
1	C	551	HIS
1	C	606	HIS
1	C	612	HIS
1	D	11	GLN
1	D	15	ASN
1	D	36	ASN
1	D	47	ASN
1	D	63	HIS
1	D	76	ASN
1	D	92	GLN
1	D	102	ASN
1	D	225	HIS
1	D	311	HIS
1	D	336	ASN
1	D	338	GLN
1	D	354	GLN
1	D	394	HIS
1	D	414	ASN
1	D	449	ASN
1	D	453	HIS
1	D	456	ASN
1	D	469	ASN
1	D	551	HIS
1	D	606	HIS
1	D	612	HIS
1	E	11	GLN
1	E	15	ASN
1	E	36	ASN
1	E	47	ASN
1	E	61	ASN
1	E	63	HIS
1	E	76	ASN
1	E	92	GLN
1	E	102	ASN
1	E	225	HIS
1	E	336	ASN
1	E	338	GLN
1	E	354	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	394	HIS
1	E	414	ASN
1	E	449	ASN
1	E	453	HIS
1	E	456	ASN
1	E	469	ASN
1	E	470	ASN
1	E	551	HIS
1	E	606	HIS
1	E	612	HIS
1	F	11	GLN
1	F	15	ASN
1	F	16	HIS
1	F	36	ASN
1	F	47	ASN
1	F	63	HIS
1	F	76	ASN
1	F	92	GLN
1	F	102	ASN
1	F	225	HIS
1	F	336	ASN
1	F	338	GLN
1	F	354	GLN
1	F	394	HIS
1	F	414	ASN
1	F	449	ASN
1	F	453	HIS
1	F	456	ASN
1	F	469	ASN
1	F	551	HIS
1	F	606	HIS
1	F	612	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

12 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NDG	A	658	1,2	14,14,15	18.67	3 (21%)	15,19,21	10.79	11 (73%)
2	NAG	A	659	2	14,14,15	22.22	4 (28%)	15,19,21	10.60	6 (40%)
2	NDG	B	658	1,2	14,14,15	18.67	3 (21%)	15,19,21	10.79	11 (73%)
2	NAG	B	659	2	14,14,15	22.22	4 (28%)	15,19,21	10.60	6 (40%)
2	NDG	C	658	1,2	14,14,15	18.67	3 (21%)	15,19,21	10.79	11 (73%)
2	NAG	C	659	2	14,14,15	22.23	4 (28%)	15,19,21	10.60	6 (40%)
2	NDG	D	658	1,2	14,14,15	18.66	3 (21%)	15,19,21	10.79	11 (73%)
2	NAG	D	659	2	14,14,15	22.22	4 (28%)	15,19,21	10.60	6 (40%)
2	NDG	E	658	1,2	14,14,15	18.66	3 (21%)	15,19,21	10.79	11 (73%)
2	NAG	E	659	2	14,14,15	22.22	4 (28%)	15,19,21	10.60	6 (40%)
2	NDG	F	658	1,2	14,14,15	18.68	3 (21%)	15,19,21	10.79	11 (73%)
2	NAG	F	659	2	14,14,15	22.21	4 (28%)	15,19,21	10.60	6 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDG	A	658	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	659	2	-	0/6/23/26	0/1/1/1
2	NDG	B	658	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	659	2	-	0/6/23/26	0/1/1/1
2	NDG	C	658	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	659	2	-	0/6/23/26	0/1/1/1
2	NDG	D	658	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	659	2	-	0/6/23/26	0/1/1/1
2	NDG	E	658	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	659	2	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDG	F	658	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	659	2	-	0/6/23/26	0/1/1/1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	659	NAG	O5-C1	2.63	1.48	1.43
2	B	659	NAG	O5-C1	2.64	1.48	1.43
2	C	659	NAG	O5-C1	2.65	1.48	1.43
2	A	659	NAG	O5-C1	2.66	1.48	1.43
2	E	659	NAG	O5-C1	2.68	1.48	1.43
2	F	659	NAG	O5-C1	2.69	1.48	1.43
2	F	659	NAG	O5-C5	2.70	1.49	1.43
2	C	659	NAG	O5-C5	2.71	1.49	1.43
2	B	659	NAG	O5-C5	2.71	1.49	1.43
2	A	659	NAG	O5-C5	2.72	1.49	1.43
2	D	659	NAG	O5-C5	2.72	1.49	1.43
2	E	659	NAG	O5-C5	2.74	1.49	1.43
2	E	658	NDG	O-C1	3.17	1.49	1.43
2	B	658	NDG	O-C1	3.17	1.49	1.43
2	F	658	NDG	O-C1	3.18	1.49	1.43
2	C	658	NDG	O-C1	3.20	1.49	1.43
2	A	658	NDG	O-C1	3.20	1.49	1.43
2	D	658	NDG	O-C1	3.23	1.49	1.43
2	F	658	NDG	O7-C7	10.84	1.48	1.23
2	C	658	NDG	O7-C7	10.85	1.48	1.23
2	A	658	NDG	O7-C7	10.89	1.48	1.23
2	B	658	NDG	O7-C7	10.89	1.48	1.23
2	E	658	NDG	O7-C7	10.89	1.48	1.23
2	D	658	NDG	O7-C7	10.90	1.48	1.23
2	D	659	NAG	O7-C7	15.35	1.58	1.23
2	C	659	NAG	O7-C7	15.35	1.58	1.23
2	B	659	NAG	O7-C7	15.37	1.58	1.23
2	E	659	NAG	O7-C7	15.38	1.58	1.23
2	A	659	NAG	O7-C7	15.38	1.58	1.23
2	F	659	NAG	O7-C7	15.40	1.58	1.23
2	D	658	NDG	C8-C7	68.80	2.88	1.50
2	E	658	NDG	C8-C7	68.81	2.88	1.50
2	A	658	NDG	C8-C7	68.82	2.88	1.50
2	B	658	NDG	C8-C7	68.82	2.88	1.50
2	C	658	NDG	C8-C7	68.84	2.88	1.50
2	F	658	NDG	C8-C7	68.86	2.88	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	659	NAG	C8-C7	81.50	3.14	1.50
2	A	659	NAG	C8-C7	81.54	3.14	1.50
2	E	659	NAG	C8-C7	81.54	3.14	1.50
2	D	659	NAG	C8-C7	81.56	3.14	1.50
2	B	659	NAG	C8-C7	81.56	3.14	1.50
2	C	659	NAG	C8-C7	81.59	3.14	1.50

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	659	NAG	C8-C7-N2	-33.86	51.30	116.11
2	D	659	NAG	C8-C7-N2	-33.85	51.33	116.11
2	A	659	NAG	C8-C7-N2	-33.85	51.33	116.11
2	F	659	NAG	C8-C7-N2	-33.85	51.34	116.11
2	E	659	NAG	C8-C7-N2	-33.84	51.34	116.11
2	B	659	NAG	C8-C7-N2	-33.84	51.35	116.11
2	B	658	NDG	C8-C7-N2	-28.13	62.27	116.11
2	C	658	NDG	C8-C7-N2	-28.13	62.28	116.11
2	F	658	NDG	C8-C7-N2	-28.12	62.29	116.11
2	A	658	NDG	C8-C7-N2	-28.11	62.31	116.11
2	D	658	NDG	C8-C7-N2	-28.11	62.31	116.11
2	E	658	NDG	C8-C7-N2	-28.10	62.34	116.11
2	B	659	NAG	O7-C7-N2	-5.89	109.86	121.86
2	A	659	NAG	O7-C7-N2	-5.89	109.86	121.86
2	D	659	NAG	O7-C7-N2	-5.88	109.87	121.86
2	E	659	NAG	O7-C7-N2	-5.88	109.88	121.86
2	F	659	NAG	O7-C7-N2	-5.87	109.89	121.86
2	C	659	NAG	O7-C7-N2	-5.86	109.91	121.86
2	E	659	NAG	C1-O5-C5	-5.45	105.33	112.25
2	B	659	NAG	C1-O5-C5	-5.44	105.34	112.25
2	A	659	NAG	C1-O5-C5	-5.44	105.34	112.25
2	C	659	NAG	C1-O5-C5	-5.43	105.36	112.25
2	F	659	NAG	C1-O5-C5	-5.41	105.38	112.25
2	D	659	NAG	C1-O5-C5	-5.41	105.38	112.25
2	E	658	NDG	C1-O-C5	-3.75	107.50	112.25
2	B	658	NDG	C1-O-C5	-3.73	107.51	112.25
2	A	658	NDG	C1-O-C5	-3.72	107.52	112.25
2	D	658	NDG	C1-O-C5	-3.72	107.53	112.25
2	F	658	NDG	C1-O-C5	-3.70	107.55	112.25
2	C	658	NDG	C1-O-C5	-3.70	107.56	112.25
2	D	659	NAG	O3-C3-C4	-3.03	103.51	110.34
2	A	659	NAG	O3-C3-C4	-3.03	103.51	110.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	659	NAG	O3-C3-C4	-3.03	103.52	110.34
2	C	659	NAG	O3-C3-C4	-3.03	103.52	110.34
2	E	658	NDG	O4-C4-C3	-3.03	103.52	110.34
2	F	659	NAG	O3-C3-C4	-3.03	103.53	110.34
2	B	659	NAG	O3-C3-C4	-3.02	103.53	110.34
2	C	658	NDG	O4-C4-C3	-3.02	103.53	110.34
2	F	658	NDG	O4-C4-C3	-3.02	103.53	110.34
2	D	658	NDG	O4-C4-C3	-3.02	103.55	110.34
2	A	658	NDG	O4-C4-C3	-3.01	103.55	110.34
2	B	658	NDG	O4-C4-C3	-3.01	103.57	110.34
2	C	658	NDG	O6-C6-C5	-2.90	101.74	111.33
2	B	658	NDG	O6-C6-C5	-2.90	101.75	111.33
2	A	658	NDG	O6-C6-C5	-2.90	101.76	111.33
2	D	658	NDG	O6-C6-C5	-2.90	101.76	111.33
2	F	658	NDG	O6-C6-C5	-2.90	101.76	111.33
2	E	658	NDG	O6-C6-C5	-2.89	101.79	111.33
2	D	658	NDG	O7-C7-N2	-2.71	116.34	121.86
2	E	658	NDG	O7-C7-N2	-2.71	116.34	121.86
2	A	658	NDG	O7-C7-N2	-2.70	116.36	121.86
2	F	658	NDG	O7-C7-N2	-2.69	116.38	121.86
2	B	658	NDG	O7-C7-N2	-2.68	116.40	121.86
2	C	658	NDG	O7-C7-N2	-2.67	116.41	121.86
2	D	658	NDG	C3-C2-N2	-2.57	104.40	110.56
2	A	658	NDG	C3-C2-N2	-2.57	104.41	110.56
2	C	658	NDG	C3-C2-N2	-2.56	104.43	110.56
2	B	658	NDG	C3-C2-N2	-2.56	104.43	110.56
2	F	658	NDG	C3-C2-N2	-2.56	104.44	110.56
2	E	658	NDG	C3-C2-N2	-2.55	104.45	110.56
2	E	659	NAG	O6-C6-C5	-2.04	104.59	111.33
2	A	659	NAG	O6-C6-C5	-2.04	104.60	111.33
2	B	659	NAG	O6-C6-C5	-2.04	104.60	111.33
2	F	659	NAG	O6-C6-C5	-2.04	104.60	111.33
2	D	659	NAG	O6-C6-C5	-2.03	104.63	111.33
2	C	659	NAG	O6-C6-C5	-2.03	104.63	111.33
2	C	658	NDG	C6-C5-C4	2.44	119.03	113.02
2	A	658	NDG	C6-C5-C4	2.45	119.05	113.02
2	C	658	NDG	C4-C3-C2	2.45	115.04	111.23
2	F	658	NDG	C6-C5-C4	2.45	119.06	113.02
2	D	658	NDG	C6-C5-C4	2.45	119.06	113.02
2	D	658	NDG	C4-C3-C2	2.45	115.04	111.23
2	B	658	NDG	C6-C5-C4	2.46	119.08	113.02
2	A	658	NDG	C4-C3-C2	2.46	115.06	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	658	NDG	C4-C3-C2	2.46	115.06	111.23
2	E	658	NDG	C6-C5-C4	2.46	119.09	113.02
2	B	658	NDG	C4-C3-C2	2.48	115.08	111.23
2	E	658	NDG	C4-C3-C2	2.48	115.09	111.23
2	C	658	NDG	C2-N2-C7	2.94	126.81	123.04
2	B	658	NDG	C2-N2-C7	2.94	126.81	123.04
2	F	658	NDG	C2-N2-C7	2.96	126.84	123.04
2	A	658	NDG	C2-N2-C7	2.98	126.87	123.04
2	D	658	NDG	C2-N2-C7	3.00	126.89	123.04
2	E	658	NDG	C2-N2-C7	3.01	126.91	123.04
2	B	658	NDG	C3-C4-C5	4.56	118.15	110.20
2	D	658	NDG	C3-C4-C5	4.56	118.15	110.20
2	E	658	NDG	C3-C4-C5	4.57	118.16	110.20
2	A	658	NDG	C3-C4-C5	4.57	118.16	110.20
2	C	658	NDG	C3-C4-C5	4.58	118.18	110.20
2	F	658	NDG	C3-C4-C5	4.59	118.19	110.20
2	A	659	NAG	O7-C7-C8	21.30	161.14	122.06
2	D	659	NAG	O7-C7-C8	21.30	161.15	122.06
2	C	659	NAG	O7-C7-C8	21.30	161.16	122.06
2	B	659	NAG	O7-C7-C8	21.30	161.16	122.06
2	F	659	NAG	O7-C7-C8	21.31	161.17	122.06
2	E	659	NAG	O7-C7-C8	21.31	161.17	122.06
2	D	658	NDG	O7-C7-C8	29.43	176.07	122.06
2	B	658	NDG	O7-C7-C8	29.43	176.08	122.06
2	A	658	NDG	O7-C7-C8	29.44	176.08	122.06
2	F	658	NDG	O7-C7-C8	29.44	176.09	122.06
2	E	658	NDG	O7-C7-C8	29.44	176.10	122.06
2	C	658	NDG	O7-C7-C8	29.45	176.10	122.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	658	NDG	4	0
2	A	659	NAG	2	0
2	B	658	NDG	4	0
2	B	659	NAG	2	0
2	C	658	NDG	5	0
2	C	659	NAG	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	658	NDG	5	0
2	D	659	NAG	2	0
2	E	658	NDG	4	0
2	E	659	NAG	2	0
2	F	658	NDG	4	0
2	F	659	NAG	2	0

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	644/657 (98%)	-0.62	6 (0%) 85 78	2, 11, 53, 85	0
1	B	644/657 (98%)	-0.57	5 (0%) 87 80	2, 11, 53, 85	0
1	C	644/657 (98%)	-0.55	6 (0%) 85 78	2, 11, 53, 85	0
1	D	644/657 (98%)	-0.53	9 (1%) 78 65	2, 11, 53, 85	0
1	E	644/657 (98%)	-0.53	7 (1%) 82 72	2, 11, 53, 85	0
1	F	644/657 (98%)	-0.49	7 (1%) 82 72	2, 11, 53, 85	0
All	All	3864/3942 (98%)	-0.55	40 (1%) 84 75	2, 11, 54, 85	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	6.0
1	B	2	ALA	4.2
1	F	2	ALA	4.2
1	A	3	LEU	4.2
1	D	4	GLY	4.0
1	D	442	ASN	4.0
1	C	1	ASP	3.9
1	F	554	ASP	3.9
1	D	554	ASP	3.6
1	B	554	ASP	3.5
1	A	554	ASP	3.4
1	C	2	ALA	3.2
1	E	3	LEU	3.0
1	D	550	GLY	3.0
1	E	551	HIS	2.9
1	D	551	HIS	2.8
1	C	551	HIS	2.8
1	A	1	ASP	2.7
1	E	1	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	551	HIS	2.7
1	F	1	ASP	2.7
1	F	548	ASN	2.6
1	C	608	GLN	2.6
1	D	559	GLU	2.6
1	A	551	HIS	2.5
1	B	3	LEU	2.5
1	E	554	ASP	2.4
1	C	554	ASP	2.4
1	D	1	ASP	2.4
1	F	3	LEU	2.4
1	E	606	HIS	2.4
1	C	606	HIS	2.3
1	D	3	LEU	2.3
1	E	559	GLU	2.2
1	B	441	GLU	2.2
1	A	607	ALA	2.2
1	F	608	GLN	2.2
1	E	172	GLY	2.1
1	D	2	ALA	2.1
1	B	442	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	F	659	14/15	0.68	0.47	-	73,82,87,89	0
2	NAG	E	659	14/15	0.70	0.49	-	73,82,87,89	0
2	NAG	B	659	14/15	0.72	0.42	-	73,82,87,89	0
2	NAG	A	659	14/15	0.77	0.39	-	73,82,87,89	0
2	NDG	E	658	14/15	0.79	0.36	-	52,57,68,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NDG	C	658	14/15	0.82	0.31	-	52,57,68,70	0
2	NDG	A	658	14/15	0.80	0.34	-	52,57,68,70	0
2	NDG	F	658	14/15	0.82	0.33	-	52,57,68,70	0
2	NDG	D	658	14/15	0.74	0.36	-	52,57,68,70	0
2	NDG	B	658	14/15	0.79	0.33	-	52,57,68,70	0
2	NAG	D	659	14/15	0.48	0.56	-	73,82,87,89	0
2	NAG	C	659	14/15	0.44	0.68	-	73,82,87,89	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CU	A	665	1/1	0.97	0.06	-1.78	9,9,9,9	0
3	CU	A	666	1/1	0.97	0.05	-2.30	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.