



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:50 AM GMT

PDB ID : 2V16  
Title : CRYSTAL STRUCTURE OF RENIN WITH INHIBITOR 3  
Authors : Rahuel, J.; Rasetti, V.; Maibaum, J.; Rueger, H.; Goschke, R.; Cohen, N.C.;  
Stutz, S.; Cumin, F.; Fuhrer, W.; Wood, J.M.; Grutter, M.G.  
Deposited on : 2007-05-22  
Resolution : 2.80 Å(reported)

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

---

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

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

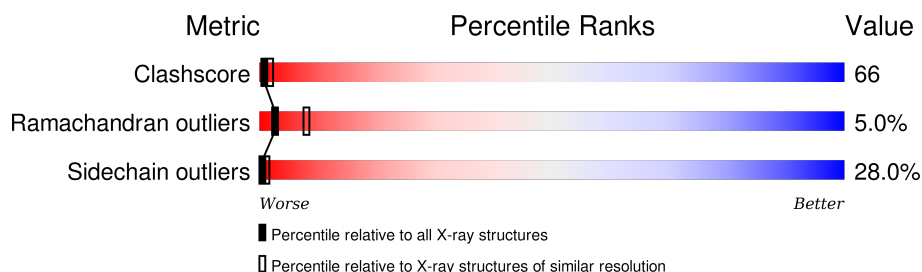
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	340	
1	O	340	

## 2 Entry composition [i](#)

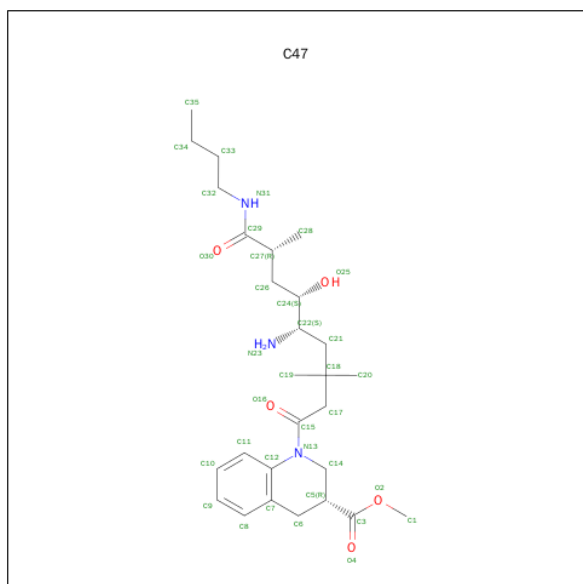
There are 3 unique types of molecules in this entry. The entry contains 5216 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RENIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	334	Total	C	N	O	S	0	0	1
			2567	1639	416	498	14			
1	O	332	Total	C	N	O	S	0	0	1
			2557	1634	414	495	14			

- Molecule 2 is METHYL (3R)-1-[(5S,6S,8R)-5-AMINO-9-BUTYLAMINO-6-HYDROXY-3,3,8-TRIMETHYL-9-OXO-NONANOYL]-3,4-DIHYDRO-2H-QUINOLINE-3-CARBOXYLATE (three-letter code: C47) (formula: C<sub>27</sub>H<sub>43</sub>N<sub>3</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			35	27	3	5		
2	O	1	Total	C	N	O	0	0
			35	27	3	5		

- Molecule 3 is water.

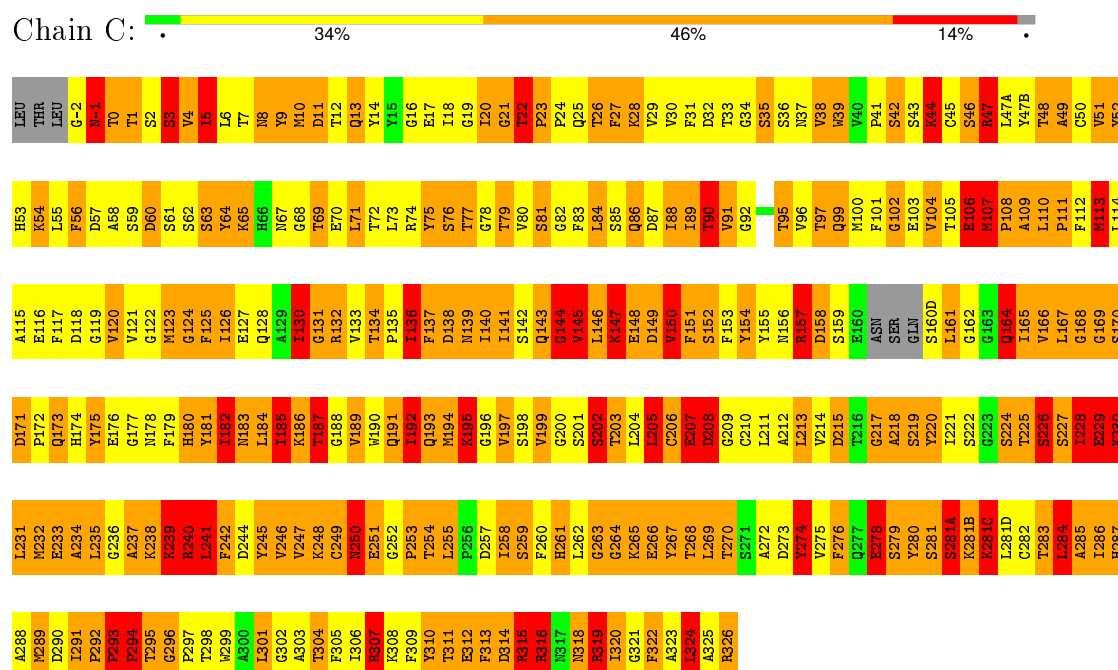
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	15	Total 15	O 15	0	0
3	O	7	Total 7	O 7	0	0

### 3 Residue-property plots

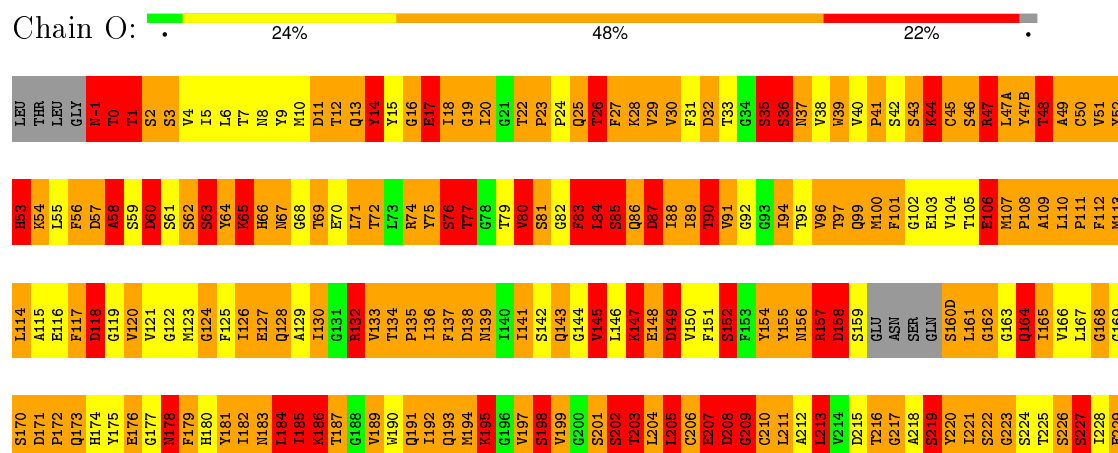
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

#### • Molecule 1: RENIN



#### • Molecule 1: RENIN



K230	L231	M232	E233	A234	L235	G236	A237	K238	K239	R240	L241	F242	D244	Y245	V246	V247	K248	C249	N250	E251	G252	P253	T254	L255	P256	D257	I258	S259	F260	H261	L262	G263	G264	K265	E266	Y267	T268	L269	I270	S271	A272	D273	Y274	V275	F276	Q277	E278	S279	Y280	S281	S281A	K281B	K281C	L281D	C282	T283	L284	A285	I286
H287	A288	M289	D290	L291	P292	P293	F294	T295	G296	P297	T298	H299	A300	I301	G302	A303	T304	F305	I306	R307	K308	F309	Y310	T311	E312	F313	D314	R315	R316	I317	I318	R319	I320	G321	F322	A323	L324	A325	R326																				

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.90 Å   142.90 Å   142.90 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.80)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.214 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5216	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: C47

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	C	4.39	458/2626 (17.4%)	3.84	531/3560 (14.9%)
1	O	4.37	424/2616 (16.2%)	4.21	596/3547 (16.8%)
All	All	4.38	882/5242 (16.8%)	4.03	1127/7107 (15.9%)

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	C	2	2
1	O	5	3
All	All	7	5

All (882) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	266	GLU	CD-OE2	33.99	1.63	1.25
1	O	207	GLU	CD-OE2	32.74	1.61	1.25
1	C	233	GLU	CD-OE1	31.09	1.59	1.25
1	O	316	ARG	CZ-NH1	30.09	1.72	1.33
1	C	266	GLU	CD-OE2	29.57	1.58	1.25
1	C	148	GLU	CD-OE2	29.12	1.57	1.25
1	O	70	GLU	CD-OE2	28.93	1.57	1.25
1	C	240	ARG	CZ-NH2	25.84	1.66	1.33
1	O	233	GLU	CD-OE2	25.61	1.53	1.25
1	C	278	GLU	CD-OE2	25.12	1.53	1.25
1	C	251	GLU	CD-OE2	24.65	1.52	1.25
1	O	202	SER	CB-OG	24.63	1.74	1.42
1	C	316	ARG	CZ-NH2	24.48	1.64	1.33
1	O	176	GLU	CD-OE2	24.06	1.52	1.25

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	229	GLU	CD-OE2	23.73	1.51	1.25
1	C	157	ARG	CZ-NH1	23.12	1.63	1.33
1	C	233	GLU	CD-OE2	23.00	1.50	1.25
1	C	70	GLU	CD-OE2	22.79	1.50	1.25
1	C	278	GLU	CD-OE1	22.68	1.50	1.25
1	O	17	GLU	CD-OE2	22.65	1.50	1.25
1	C	74	ARG	CZ-NH2	22.32	1.62	1.33
1	C	157	ARG	NE-CZ	22.05	1.61	1.33
1	O	278	GLU	CD-OE2	22.01	1.49	1.25
1	C	70	GLU	CD-OE1	21.91	1.49	1.25
1	O	74	ARG	NE-CZ	21.55	1.61	1.33
1	C	240	ARG	NE-CZ	21.48	1.60	1.33
1	O	251	GLU	CD-OE2	20.78	1.48	1.25
1	O	229	GLU	CD-OE1	20.24	1.48	1.25
1	O	176	GLU	CD-OE1	20.16	1.47	1.25
1	C	315	ARG	CZ-NH1	19.94	1.58	1.33
1	C	240	ARG	CZ-NH1	19.62	1.58	1.33
1	O	132	ARG	CZ-NH2	19.26	1.58	1.33
1	C	-2	GLY	C-O	19.14	1.54	1.23
1	O	116	GLU	CD-OE2	19.03	1.46	1.25
1	C	207	GLU	CD-OE2	18.78	1.46	1.25
1	C	116	GLU	CD-OE1	18.32	1.45	1.25
1	O	17	GLU	CD-OE1	18.31	1.45	1.25
1	O	132	ARG	NE-CZ	18.20	1.56	1.33
1	C	74	ARG	CZ-NH1	18.14	1.56	1.33
1	C	207	GLU	CD-OE1	17.81	1.45	1.25
1	O	148	GLU	CD-OE1	17.68	1.45	1.25
1	C	229	GLU	CD-OE2	17.56	1.45	1.25
1	C	176	GLU	CD-OE1	-17.55	1.06	1.25
1	O	106	GLU	CD-OE1	17.52	1.45	1.25
1	C	47	ARG	CZ-NH1	17.49	1.55	1.33
1	O	233	GLU	CD-OE1	17.37	1.44	1.25
1	O	251	GLU	CG-CD	16.85	1.77	1.51
1	C	226	SER	CB-OG	16.84	1.64	1.42
1	O	240	ARG	NE-CZ	16.71	1.54	1.33
1	O	158	ASP	CG-OD1	16.68	1.63	1.25
1	C	157	ARG	CZ-NH2	16.61	1.54	1.33
1	C	224	SER	CB-OG	16.59	1.63	1.42
1	O	70	GLU	CD-OE1	16.32	1.43	1.25
1	O	157	ARG	CZ-NH1	16.04	1.53	1.33
1	C	293	PRO	C-O	15.83	1.54	1.23
1	C	39	TRP	NE1-CE2	-15.63	1.17	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	74	ARG	CZ-NH2	15.59	1.53	1.33
1	O	207	GLU	CD-OE1	15.51	1.42	1.25
1	O	106	GLU	CD-OE2	15.47	1.42	1.25
1	O	103	GLU	CD-OE2	15.42	1.42	1.25
1	O	132	ARG	CZ-NH1	15.40	1.53	1.33
1	C	278	GLU	CG-CD	15.37	1.75	1.51
1	O	158	ASP	CG-OD2	15.37	1.60	1.25
1	O	47	ARG	CZ-NH2	14.84	1.52	1.33
1	C	281(A)	SER	CB-OG	14.80	1.61	1.42
1	O	173	GLN	CG-CD	14.65	1.84	1.51
1	C	312	GLU	CD-OE2	14.55	1.41	1.25
1	O	240	ARG	C-O	14.51	1.50	1.23
1	O	326	ARG	CZ-NH2	14.50	1.51	1.33
1	O	244	ASP	CG-OD1	14.45	1.58	1.25
1	C	-1	ASN	CG-OD1	14.43	1.55	1.24
1	C	64	TYR	CB-CG	-14.43	1.30	1.51
1	O	158	ASP	C-O	14.38	1.50	1.23
1	C	312	GLU	CD-OE1	14.20	1.41	1.25
1	O	173	GLN	CD-NE2	14.18	1.68	1.32
1	C	132	ARG	CZ-NH2	14.18	1.51	1.33
1	O	157	ARG	NE-CZ	13.98	1.51	1.33
1	C	132	ARG	CZ-NH1	13.88	1.51	1.33
1	O	148	GLU	CD-OE2	13.86	1.40	1.25
1	O	156	ASN	CG-OD1	13.81	1.54	1.24
1	C	-2	GLY	N-CA	13.76	1.66	1.46
1	C	159	SER	C-O	13.61	1.49	1.23
1	O	47	ARG	NE-CZ	13.56	1.50	1.33
1	C	173	GLN	CD-NE2	13.40	1.66	1.32
1	O	193	GLN	CD-OE1	13.31	1.53	1.24
1	C	173	GLN	CD-OE1	13.27	1.53	1.24
1	O	201	SER	C-O	13.12	1.48	1.23
1	C	315	ARG	NE-CZ	13.06	1.50	1.33
1	C	250	ASN	CG-OD1	13.04	1.52	1.24
1	O	173	GLN	CD-OE1	12.96	1.52	1.24
1	C	264	GLY	C-O	12.78	1.44	1.23
1	O	36	SER	CB-OG	12.77	1.58	1.42
1	O	158	ASP	CB-CG	12.71	1.78	1.51
1	C	229	GLU	CG-CD	12.69	1.71	1.51
1	C	116	GLU	CD-OE2	12.68	1.39	1.25
1	C	263	GLY	C-O	12.67	1.44	1.23
1	O	139	ASN	CG-OD1	12.55	1.51	1.24
1	O	230	LYS	CE-NZ	12.50	1.80	1.49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	44	LYS	CD-CE	12.48	1.82	1.51
1	C	201	SER	C-O	12.44	1.47	1.23
1	O	-1	ASN	C-O	12.37	1.46	1.23
1	O	250	ASN	CG-OD1	12.32	1.51	1.24
1	C	148	GLU	CD-OE1	12.32	1.39	1.25
1	O	33	THR	C-O	12.30	1.46	1.23
1	O	70	GLU	CG-CD	12.22	1.70	1.51
1	O	201	SER	CB-OG	12.18	1.58	1.42
1	C	39	TRP	CD2-CE2	-12.06	1.26	1.41
1	C	160(D)	SER	CB-OG	12.03	1.57	1.42
1	O	280	TYR	CB-CG	12.03	1.69	1.51
1	C	64	TYR	C-O	-12.03	1.00	1.23
1	C	64	TYR	C-N	-12.00	1.06	1.34
1	O	294	PRO	C-O	11.98	1.47	1.23
1	O	251	GLU	CA-CB	11.96	1.80	1.53
1	O	201	SER	CA-CB	11.84	1.70	1.52
1	O	45	CYS	C-O	11.80	1.45	1.23
1	C	263	GLY	CA-C	11.71	1.70	1.51
1	O	15	TYR	CZ-OH	-11.67	1.18	1.37
1	C	238	LYS	CE-NZ	11.59	1.78	1.49
1	C	144	GLY	C-O	11.58	1.42	1.23
1	O	25	GLN	CD-OE1	11.51	1.49	1.24
1	O	53	HIS	C-O	11.49	1.45	1.23
1	O	230	LYS	CD-CE	11.49	1.79	1.51
1	O	160(D)	SER	N-CA	11.43	1.69	1.46
1	O	312	GLU	CD-OE2	-11.35	1.13	1.25
1	C	314	ASP	CG-OD2	11.31	1.51	1.25
1	O	76	SER	C-O	11.23	1.44	1.23
1	O	186	LYS	CB-CG	11.21	1.82	1.52
1	O	207	GLU	CG-CD	11.20	1.68	1.51
1	C	316	ARG	CZ-NH1	11.19	1.47	1.33
1	O	229	GLU	CG-CD	11.18	1.68	1.51
1	O	47	ARG	CZ-NH1	11.16	1.47	1.33
1	C	208	ASP	N-CA	11.08	1.68	1.46
1	C	207	GLU	C-O	11.07	1.44	1.23
1	O	294	PRO	N-CD	11.05	1.63	1.47
1	C	70	GLU	CG-CD	11.04	1.68	1.51
1	O	39	TRP	CD2-CE3	-11.00	1.23	1.40
1	C	-1	ASN	CG-ND2	10.91	1.60	1.32
1	O	178	ASN	CB-CG	10.88	1.76	1.51
1	O	257	ASP	CG-OD2	10.87	1.50	1.25
1	O	256	PRO	C-O	-10.77	1.01	1.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	269	LEU	C-O	-10.76	1.02	1.23
1	O	44	LYS	CE-NZ	10.73	1.75	1.49
1	C	105	THR	CB-OG1	-10.71	1.21	1.43
1	C	61	SER	CB-OG	-10.68	1.28	1.42
1	C	190	TRP	CZ3-CH2	-10.57	1.23	1.40
1	C	274	TYR	CB-CG	-10.55	1.35	1.51
1	C	17	GLU	CD-OE2	10.46	1.37	1.25
1	C	103	GLU	CD-OE2	10.41	1.37	1.25
1	O	81	SER	CB-OG	10.40	1.55	1.42
1	C	266	GLU	CD-OE1	10.34	1.37	1.25
1	C	294	PRO	N-CD	10.34	1.62	1.47
1	O	59	SER	CA-CB	-10.32	1.37	1.52
1	O	58	ALA	C-O	10.27	1.42	1.23
1	O	180	HIS	CG-ND1	10.25	1.61	1.38
1	C	47	ARG	CZ-NH2	10.21	1.46	1.33
1	C	207	GLU	CB-CG	10.21	1.71	1.52
1	C	119	GLY	C-O	-10.18	1.07	1.23
1	C	159	SER	CB-OG	10.15	1.55	1.42
1	O	161	LEU	C-O	10.15	1.42	1.23
1	C	281(C)	LYS	CD-CE	10.15	1.76	1.51
1	O	315	ARG	CZ-NH2	10.12	1.46	1.33
1	O	239	LYS	CD-CE	10.12	1.76	1.51
1	C	233	GLU	CG-CD	10.11	1.67	1.51
1	C	103	GLU	C-O	-9.94	1.04	1.23
1	C	162	GLY	C-O	-9.93	1.07	1.23
1	C	287	HIS	ND1-CE1	9.91	1.59	1.34
1	C	149	ASP	CG-OD2	9.91	1.48	1.25
1	C	55	LEU	C-O	9.83	1.42	1.23
1	C	186	LYS	CD-CE	9.82	1.75	1.51
1	C	90	THR	CB-OG1	9.82	1.62	1.43
1	O	281(B)	LYS	CE-NZ	9.81	1.73	1.49
1	C	186	LYS	CA-CB	9.78	1.75	1.53
1	O	252	GLY	CA-C	-9.72	1.36	1.51
1	C	319	ARG	NE-CZ	9.71	1.45	1.33
1	C	294	PRO	C-O	9.69	1.42	1.23
1	O	294	PRO	C-N	9.65	1.56	1.34
1	C	193	GLN	CD-OE1	9.65	1.45	1.24
1	O	326	ARG	CD-NE	9.59	1.62	1.46
1	C	39	TRP	CE2-CZ2	-9.58	1.23	1.39
1	O	281	SER	CB-OG	9.58	1.54	1.42
1	O	52	TYR	CZ-OH	9.57	1.54	1.37
1	O	46	SER	CB-OG	9.56	1.54	1.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	190	TRP	CG-CD2	9.54	1.59	1.43
1	O	240	ARG	CZ-NH2	9.49	1.45	1.33
1	C	278	GLU	CB-CG	9.43	1.70	1.52
1	C	44	LYS	CE-NZ	9.41	1.72	1.49
1	C	33	THR	N-CA	-9.39	1.27	1.46
1	O	315	ARG	NE-CZ	9.38	1.45	1.33
1	C	27	PHE	C-O	-9.35	1.05	1.23
1	O	47	ARG	C-O	9.35	1.41	1.23
1	O	204	LEU	CB-CG	9.34	1.79	1.52
1	O	238	LYS	CE-NZ	9.34	1.72	1.49
1	O	155	TYR	C-N	9.32	1.55	1.34
1	O	74	ARG	CD-NE	9.32	1.62	1.46
1	C	42	SER	C-N	-9.27	1.12	1.34
1	O	207	GLU	C-O	9.22	1.40	1.23
1	O	143	GLN	C-O	9.22	1.40	1.23
1	C	27	PHE	N-CA	-9.21	1.27	1.46
1	C	281(C)	LYS	CE-NZ	9.19	1.72	1.49
1	C	244	ASP	CG-OD1	9.15	1.46	1.25
1	O	197	VAL	C-O	9.14	1.40	1.23
1	O	181	TYR	CE2-CZ	-9.14	1.26	1.38
1	C	159	SER	N-CA	9.14	1.64	1.46
1	O	259	SER	CB-OG	9.12	1.54	1.42
1	O	99	GLN	C-O	9.11	1.40	1.23
1	O	43	SER	CB-OG	9.10	1.54	1.42
1	C	115	ALA	C-O	-9.07	1.06	1.23
1	C	67	ASN	CG-ND2	9.05	1.55	1.32
1	O	107	MET	C-O	9.04	1.40	1.23
1	O	216	THR	C-O	9.02	1.40	1.23
1	C	294	PRO	CA-CB	9.02	1.71	1.53
1	O	79	THR	CB-OG1	8.98	1.61	1.43
1	C	39	TRP	CG-CD1	-8.98	1.24	1.36
1	C	220	TYR	CZ-OH	8.97	1.53	1.37
1	O	30	VAL	CB-CG2	-8.94	1.34	1.52
1	C	177	GLY	C-O	8.93	1.38	1.23
1	O	202	SER	CA-CB	8.91	1.66	1.52
1	C	134	THR	N-CA	8.90	1.64	1.46
1	O	60	ASP	CG-OD2	8.90	1.45	1.25
1	O	272	ALA	C-O	-8.89	1.06	1.23
1	O	280	TYR	CZ-OH	8.88	1.52	1.37
1	C	7	THR	C-O	-8.87	1.06	1.23
1	O	238	LYS	CD-CE	8.87	1.73	1.51
1	C	16	GLY	N-CA	-8.86	1.32	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	219	SER	CA-CB	-8.86	1.39	1.52
1	C	132	ARG	CD-NE	8.83	1.61	1.46
1	C	251	GLU	C-O	8.82	1.40	1.23
1	O	84	LEU	C-O	8.81	1.40	1.23
1	O	190	TRP	CB-CG	-8.81	1.34	1.50
1	C	78	GLY	C-O	-8.76	1.09	1.23
1	O	173	GLN	CB-CG	8.76	1.76	1.52
1	O	41	PRO	N-CD	8.75	1.60	1.47
1	O	171	ASP	N-CA	-8.75	1.28	1.46
1	O	190	TRP	CZ3-CH2	-8.74	1.26	1.40
1	C	207	GLU	CG-CD	8.69	1.65	1.51
1	C	315	ARG	CG-CD	8.68	1.73	1.51
1	O	252	GLY	N-CA	-8.65	1.33	1.46
1	C	251	GLU	CD-OE1	8.64	1.35	1.25
1	O	147	LYS	CG-CD	8.64	1.81	1.52
1	C	111	PRO	N-CA	-8.62	1.32	1.47
1	C	318	ASN	CG-OD1	8.59	1.42	1.24
1	O	-1	ASN	CG-OD1	8.58	1.42	1.24
1	O	74	ARG	CZ-NH1	8.57	1.44	1.33
1	O	305	PHE	C-O	-8.57	1.07	1.23
1	C	215	ASP	C-O	-8.56	1.07	1.23
1	C	170	SER	C-O	-8.54	1.07	1.23
1	O	178	ASN	CG-ND2	8.53	1.54	1.32
1	O	-1	ASN	CG-ND2	8.51	1.54	1.32
1	O	182	ILE	N-CA	-8.49	1.29	1.46
1	C	47	ARG	NE-CZ	8.49	1.44	1.33
1	C	251	GLU	CG-CD	8.47	1.64	1.51
1	C	222	SER	CA-CB	-8.45	1.40	1.52
1	C	85	SER	CB-OG	-8.44	1.31	1.42
1	O	47	ARG	CD-NE	8.43	1.60	1.46
1	O	16	GLY	C-O	-8.43	1.10	1.23
1	O	124	GLY	CA-C	8.39	1.65	1.51
1	O	122	GLY	C-O	8.37	1.37	1.23
1	C	138	ASP	CA-CB	-8.34	1.35	1.53
1	O	278	GLU	CD-OE1	8.33	1.34	1.25
1	O	317	ASN	CG-OD1	-8.33	1.05	1.24
1	C	257	ASP	C-O	-8.32	1.07	1.23
1	O	129	ALA	C-O	-8.32	1.07	1.23
1	C	47	ARG	C-O	-8.30	1.07	1.23
1	C	158	ASP	CG-OD1	8.30	1.44	1.25
1	C	326	ARG	CZ-NH1	8.30	1.43	1.33
1	C	266	GLU	C-O	8.29	1.39	1.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	194	MET	CA-CB	-8.29	1.35	1.53
1	C	39	TRP	CG-CD2	-8.23	1.29	1.43
1	O	152	SER	CB-OG	-8.23	1.31	1.42
1	C	156	ASN	CG-OD1	-8.21	1.05	1.24
1	C	180	HIS	CG-CD2	8.20	1.49	1.35
1	C	208	ASP	CG-OD2	8.19	1.44	1.25
1	C	208	ASP	CG-OD1	8.18	1.44	1.25
1	O	171	ASP	CA-CB	-8.16	1.35	1.53
1	O	181	TYR	CZ-OH	-8.16	1.24	1.37
1	O	191	GLN	CD-NE2	8.16	1.53	1.32
1	O	154	TYR	CB-CG	-8.12	1.39	1.51
1	O	204	LEU	CG-CD2	8.12	1.81	1.51
1	O	155	TYR	CA-C	8.12	1.74	1.52
1	C	295	THR	C-O	-8.11	1.07	1.23
1	O	219	SER	N-CA	-8.10	1.30	1.46
1	C	305	PHE	C-O	-8.09	1.07	1.23
1	C	266	GLU	C-N	8.02	1.52	1.34
1	C	4	VAL	CB-CG1	8.01	1.69	1.52
1	O	276	PHE	C-O	8.01	1.38	1.23
1	O	180	HIS	CD2-NE2	8.00	1.58	1.42
1	C	316	ARG	NE-CZ	7.99	1.43	1.33
1	O	225	THR	C-N	-7.99	1.15	1.34
1	C	74	ARG	NE-CZ	7.98	1.43	1.33
1	O	152	SER	CA-CB	-7.97	1.41	1.52
1	O	127	GLU	CD-OE1	7.96	1.34	1.25
1	C	180	HIS	C-O	7.95	1.38	1.23
1	C	248	LYS	CA-CB	-7.95	1.36	1.53
1	C	307	ARG	CA-CB	-7.92	1.36	1.53
1	C	160(D)	SER	C-O	7.92	1.38	1.23
1	C	247	VAL	CA-CB	-7.91	1.38	1.54
1	O	281(A)	SER	CB-OG	7.90	1.52	1.42
1	C	313	PHE	N-CA	-7.89	1.30	1.46
1	O	128	GLN	CD-NE2	7.89	1.52	1.32
1	O	67	ASN	CG-ND2	7.89	1.52	1.32
1	O	72	THR	CB-OG1	7.87	1.58	1.43
1	C	202	SER	CB-OG	7.87	1.52	1.42
1	C	181	TYR	CA-CB	-7.86	1.36	1.53
1	O	24	PRO	CA-C	-7.86	1.37	1.52
1	C	76	SER	CA-CB	7.85	1.64	1.52
1	O	280	TYR	C-O	7.85	1.38	1.23
1	C	0	THR	C-O	7.83	1.38	1.23
1	O	242	PHE	CB-CG	7.78	1.64	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	267	TYR	CZ-OH	-7.78	1.24	1.37
1	C	159	SER	C-N	7.78	1.51	1.34
1	O	39	TRP	CB-CG	-7.78	1.36	1.50
1	O	202	SER	C-O	7.77	1.38	1.23
1	O	251	GLU	CB-CG	7.77	1.67	1.52
1	O	144	GLY	N-CA	7.75	1.57	1.46
1	C	281(B)	LYS	CG-CD	7.74	1.78	1.52
1	O	195	LYS	CD-CE	7.73	1.70	1.51
1	O	181	TYR	N-CA	-7.73	1.30	1.46
1	C	62	SER	C-O	7.73	1.38	1.23
1	O	120	VAL	CB-CG2	-7.72	1.36	1.52
1	C	156	ASN	CG-ND2	-7.71	1.13	1.32
1	O	62	SER	C-O	-7.71	1.08	1.23
1	C	244	ASP	CG-OD2	7.70	1.43	1.25
1	O	44	LYS	CD-CE	7.69	1.70	1.51
1	C	190	TRP	CE3-CZ3	-7.68	1.25	1.38
1	C	191	GLN	CD-OE1	7.68	1.40	1.24
1	O	87	ASP	CG-OD2	7.66	1.43	1.25
1	O	163	GLY	C-O	-7.64	1.11	1.23
1	C	64	TYR	CA-C	-7.62	1.33	1.52
1	O	163	GLY	CA-C	-7.61	1.39	1.51
1	C	299	TRP	CD2-CE3	-7.61	1.28	1.40
1	O	297	PRO	N-CA	-7.60	1.34	1.47
1	C	49	ALA	C-O	-7.59	1.08	1.23
1	C	58	ALA	N-CA	-7.58	1.31	1.46
1	O	144	GLY	C-O	-7.57	1.11	1.23
1	C	92	GLY	N-CA	-7.55	1.34	1.46
1	O	48	THR	C-O	7.54	1.37	1.23
1	C	53	HIS	N-CA	-7.53	1.31	1.46
1	O	228	ILE	C-O	7.53	1.37	1.23
1	O	83	PHE	CB-CG	7.53	1.64	1.51
1	C	248	LYS	CE-NZ	7.52	1.67	1.49
1	C	33	THR	C-O	-7.51	1.09	1.23
1	C	42	SER	CA-C	-7.51	1.33	1.52
1	C	230	LYS	CD-CE	7.50	1.70	1.51
1	C	245	TYR	CB-CG	-7.50	1.40	1.51
1	C	237	ALA	N-CA	7.49	1.61	1.46
1	C	249	CYS	C-O	-7.48	1.09	1.23
1	O	139	ASN	C-O	-7.48	1.09	1.23
1	O	162	GLY	CA-C	-7.48	1.39	1.51
1	C	112	PHE	C-O	-7.47	1.09	1.23
1	C	241	LEU	C-O	-7.47	1.09	1.23

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	265	LYS	CE-NZ	7.47	1.67	1.49
1	O	32	ASP	N-CA	7.46	1.61	1.46
1	O	254	THR	N-CA	7.45	1.61	1.46
1	C	68	GLY	N-CA	-7.44	1.34	1.46
1	C	187	THR	CB-OG1	7.44	1.58	1.43
1	O	156	ASN	CA-CB	7.43	1.72	1.53
1	O	273	ASP	N-CA	-7.43	1.31	1.46
1	O	261	HIS	CG-CD2	7.42	1.48	1.35
1	O	128	GLN	CD-OE1	7.42	1.40	1.24
1	O	85	SER	CA-CB	7.42	1.64	1.52
1	O	187	THR	CB-OG1	7.41	1.58	1.43
1	O	178	ASN	CG-OD1	7.40	1.40	1.24
1	O	43	SER	C-O	7.39	1.37	1.23
1	C	42	SER	C-O	-7.39	1.09	1.23
1	C	240	ARG	CD-NE	7.38	1.58	1.46
1	O	251	GLU	CD-OE1	7.37	1.33	1.25
1	C	200	GLY	C-N	-7.37	1.17	1.34
1	O	171	ASP	CG-OD2	7.36	1.42	1.25
1	O	56	PHE	C-N	-7.35	1.17	1.34
1	O	207	GLU	CB-CG	7.34	1.66	1.52
1	C	26	THR	C-O	-7.34	1.09	1.23
1	C	4	VAL	CA-CB	-7.33	1.39	1.54
1	C	315	ARG	CZ-NH2	7.33	1.42	1.33
1	O	114	LEU	C-O	-7.33	1.09	1.23
1	C	307	ARG	CB-CG	-7.32	1.32	1.52
1	O	309	PHE	N-CA	-7.29	1.31	1.46
1	O	315	ARG	N-CA	-7.29	1.31	1.46
1	C	187	THR	CA-C	7.28	1.71	1.52
1	O	38	VAL	CB-CG1	-7.26	1.37	1.52
1	C	60	ASP	C-O	-7.25	1.09	1.23
1	C	326	ARG	C-O	-7.22	1.09	1.23
1	O	40	VAL	C-N	7.22	1.48	1.34
1	C	-2	GLY	CA-C	7.21	1.63	1.51
1	C	124	GLY	C-O	-7.21	1.12	1.23
1	O	275	VAL	CA-CB	-7.20	1.39	1.54
1	C	199	VAL	N-CA	-7.19	1.31	1.46
1	O	11	ASP	N-CA	-7.18	1.31	1.46
1	O	297	PRO	CA-CB	7.18	1.68	1.53
1	O	220	TYR	N-CA	-7.16	1.32	1.46
1	C	190	TRP	C-O	-7.15	1.09	1.23
1	O	107	MET	CA-C	7.15	1.71	1.52
1	C	281(B)	LYS	CE-NZ	7.14	1.66	1.49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	186	LYS	CG-CD	7.13	1.76	1.52
1	O	276	PHE	CB-CG	-7.13	1.39	1.51
1	C	47	ARG	CD-NE	7.13	1.58	1.46
1	C	92	GLY	CA-C	-7.13	1.40	1.51
1	C	181	TYR	C-O	-7.12	1.09	1.23
1	C	47	ARG	CA-C	-7.10	1.34	1.52
1	C	44	LYS	CA-C	7.09	1.71	1.52
1	C	316	ARG	CA-C	-7.09	1.34	1.52
1	O	261	HIS	CB-CG	7.08	1.62	1.50
1	O	135	PRO	N-CD	7.08	1.57	1.47
1	C	75	TYR	CZ-OH	-7.06	1.25	1.37
1	O	7	THR	C-O	-7.06	1.09	1.23
1	O	316	ARG	NE-CZ	7.05	1.42	1.33
1	C	307	ARG	CZ-NH1	7.02	1.42	1.33
1	O	250	ASN	CA-C	7.02	1.71	1.52
1	O	209	GLY	C-O	7.01	1.34	1.23
1	C	196	GLY	CA-C	7.01	1.63	1.51
1	C	39	TRP	CD1-NE1	-7.01	1.26	1.38
1	C	201	SER	C-N	7.01	1.50	1.34
1	O	121	VAL	C-O	-7.01	1.10	1.23
1	O	164	GLN	CD-NE2	7.00	1.50	1.32
1	O	242	PHE	CA-CB	6.99	1.69	1.53
1	C	287	HIS	CG-CD2	6.98	1.47	1.35
1	O	322	PHE	C-O	-6.97	1.10	1.23
1	O	66	HIS	CG-ND1	6.97	1.54	1.38
1	O	172	PRO	CA-C	-6.96	1.39	1.52
1	C	37	ASN	CG-OD1	-6.95	1.08	1.24
1	O	2	SER	CB-OG	-6.95	1.33	1.42
1	C	58	ALA	C-N	-6.95	1.18	1.34
1	C	25	GLN	C-O	-6.93	1.10	1.23
1	C	58	ALA	CA-CB	-6.92	1.38	1.52
1	O	253	PRO	C-N	6.92	1.50	1.34
1	C	164	GLN	CD-NE2	6.91	1.50	1.32
1	C	54	LYS	CE-NZ	6.91	1.66	1.49
1	O	240	ARG	CA-CB	-6.90	1.38	1.53
1	O	61	SER	CB-OG	6.90	1.51	1.42
1	C	17	GLU	CD-OE1	-6.89	1.18	1.25
1	C	228	ILE	N-CA	6.89	1.60	1.46
1	O	227	SER	CB-OG	-6.89	1.33	1.42
1	C	71	LEU	N-CA	-6.88	1.32	1.46
1	C	97	THR	C-O	6.87	1.36	1.23
1	C	22	THR	CA-C	-6.86	1.35	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	75	TYR	C-O	-6.85	1.10	1.23
1	C	267	TYR	C-O	-6.85	1.10	1.23
1	O	270	THR	CB-OG1	-6.83	1.29	1.43
1	C	149	ASP	CA-C	-6.83	1.35	1.52
1	O	272	ALA	CA-C	-6.82	1.35	1.52
1	O	80	VAL	CB-CG1	6.81	1.67	1.52
1	O	111	PRO	CA-C	-6.81	1.39	1.52
1	C	318	ASN	C-N	-6.80	1.18	1.34
1	C	325	ALA	N-CA	-6.80	1.32	1.46
1	O	232	MET	N-CA	-6.79	1.32	1.46
1	O	52	TYR	CB-CG	6.79	1.61	1.51
1	O	238	LYS	CG-CD	6.75	1.75	1.52
1	O	168	GLY	CA-C	-6.75	1.41	1.51
1	C	58	ALA	CA-C	-6.74	1.35	1.52
1	O	190	TRP	CE3-CZ3	-6.74	1.26	1.38
1	O	47(A)	LEU	CB-CG	6.74	1.72	1.52
1	C	34	GLY	N-CA	-6.73	1.35	1.46
1	C	197	VAL	C-O	6.73	1.36	1.23
1	C	160(D)	SER	CA-C	6.73	1.70	1.52
1	O	326	ARG	CZ-NH1	-6.72	1.24	1.33
1	C	253	PRO	N-CD	6.72	1.57	1.47
1	C	111	PRO	CA-C	-6.72	1.39	1.52
1	O	86	GLN	CD-OE1	6.71	1.38	1.24
1	O	15	TYR	C-N	-6.71	1.21	1.33
1	O	171	ASP	CA-C	-6.71	1.35	1.52
1	O	120	VAL	C-O	-6.71	1.10	1.23
1	O	293	PRO	C-N	6.70	1.47	1.34
1	C	35	SER	CB-OG	-6.69	1.33	1.42
1	C	106	GLU	CD-OE1	6.69	1.33	1.25
1	C	69	THR	CB-OG1	-6.69	1.29	1.43
1	C	197	VAL	CB-CG2	-6.69	1.38	1.52
1	C	289	MET	CG-SD	6.69	1.98	1.81
1	C	148	GLU	CA-CB	-6.68	1.39	1.53
1	C	171	ASP	CB-CG	-6.66	1.37	1.51
1	C	237	ALA	C-O	6.66	1.35	1.23
1	O	31	PHE	CB-CG	-6.65	1.40	1.51
1	O	195	LYS	CE-NZ	6.65	1.65	1.49
1	C	128	GLN	CD-OE1	6.64	1.38	1.24
1	C	240	ARG	CA-C	6.64	1.70	1.52
1	O	217	GLY	N-CA	-6.63	1.36	1.46
1	C	201	SER	CB-OG	6.63	1.50	1.42
1	O	170	SER	C-O	-6.62	1.10	1.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	SER	CB-OG	6.62	1.50	1.42
1	C	47(A)	LEU	C-O	-6.61	1.10	1.23
1	O	39	TRP	CA-CB	-6.61	1.39	1.53
1	C	280	TYR	CZ-OH	-6.61	1.26	1.37
1	C	230	LYS	CA-CB	-6.61	1.39	1.53
1	O	201	SER	C-N	6.59	1.49	1.34
1	C	313	PHE	CB-CG	-6.58	1.40	1.51
1	O	250	ASN	CA-CB	6.58	1.70	1.53
1	O	0	THR	N-CA	6.58	1.59	1.46
1	O	127	GLU	C-O	-6.57	1.10	1.23
1	C	8	ASN	CG-OD1	-6.57	1.09	1.24
1	O	315	ARG	CA-CB	-6.56	1.39	1.53
1	C	230	LYS	CE-NZ	6.55	1.65	1.49
1	C	273	ASP	C-O	6.54	1.35	1.23
1	C	188	GLY	C-O	-6.54	1.13	1.23
1	C	268	THR	C-N	-6.53	1.19	1.34
1	C	199	VAL	C-O	-6.51	1.10	1.23
1	O	240	ARG	CD-NE	6.50	1.57	1.46
1	C	113	MET	C-O	-6.50	1.11	1.23
1	C	205	LEU	C-O	-6.49	1.11	1.23
1	O	115	ALA	C-O	-6.49	1.11	1.23
1	O	195	LYS	CB-CG	6.49	1.70	1.52
1	O	202	SER	C-N	6.49	1.49	1.34
1	O	218	ALA	CA-CB	-6.49	1.38	1.52
1	C	132	ARG	NE-CZ	6.48	1.41	1.33
1	O	35	SER	CB-OG	-6.48	1.33	1.42
1	O	150	VAL	CB-CG1	-6.48	1.39	1.52
1	C	199	VAL	CA-CB	-6.47	1.41	1.54
1	O	67	ASN	C-O	-6.47	1.11	1.23
1	C	116	GLU	C-O	-6.47	1.11	1.23
1	O	117	PHE	CD1-CE1	-6.47	1.26	1.39
1	O	242	PHE	C-O	6.47	1.35	1.23
1	C	82	GLY	C-O	-6.46	1.13	1.23
1	C	181	TYR	CD2-CE2	6.46	1.49	1.39
1	O	318	ASN	CG-ND2	6.46	1.49	1.32
1	O	9	TYR	CB-CG	-6.45	1.42	1.51
1	C	176	GLU	C-O	6.44	1.35	1.23
1	C	263	GLY	N-CA	-6.44	1.36	1.46
1	C	178	ASN	CG-ND2	6.44	1.49	1.32
1	O	192	ILE	N-CA	-6.43	1.33	1.46
1	C	281	SER	CA-CB	6.42	1.62	1.52
1	O	266	GLU	CD-OE1	6.42	1.32	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	180	HIS	CE1-NE2	6.41	1.47	1.32
1	C	171	ASP	CG-OD1	-6.40	1.10	1.25
1	C	210	CYS	C-O	6.39	1.35	1.23
1	C	74	ARG	CA-CB	-6.39	1.39	1.53
1	O	133	VAL	C-N	-6.39	1.19	1.34
1	O	-1	ASN	CB-CG	6.38	1.65	1.51
1	C	46	SER	CA-CB	-6.38	1.43	1.52
1	C	138	ASP	CG-OD2	6.38	1.40	1.25
1	O	9	TYR	CA-CB	-6.38	1.40	1.53
1	O	298	THR	C-O	6.38	1.35	1.23
1	C	121	VAL	C-O	-6.37	1.11	1.23
1	C	226	SER	CA-C	-6.37	1.36	1.52
1	C	176	GLU	CG-CD	-6.36	1.42	1.51
1	C	279	SER	CB-OG	6.36	1.50	1.42
1	C	133	VAL	N-CA	6.36	1.59	1.46
1	C	101	PHE	CB-CG	6.35	1.62	1.51
1	O	246	VAL	CB-CG1	6.34	1.66	1.52
1	C	281(B)	LYS	CD-CE	6.34	1.67	1.51
1	C	274	TYR	C-N	-6.34	1.19	1.34
1	O	29	VAL	CB-CG2	-6.33	1.39	1.52
1	C	60	ASP	N-CA	-6.33	1.33	1.46
1	O	155	TYR	N-CA	-6.32	1.33	1.46
1	C	311	THR	C-O	-6.31	1.11	1.23
1	C	32	ASP	CG-OD1	-6.30	1.10	1.25
1	O	89	ILE	CA-CB	-6.30	1.40	1.54
1	C	186	LYS	CE-NZ	6.30	1.64	1.49
1	O	182	ILE	CA-CB	-6.29	1.40	1.54
1	C	106	GLU	CG-CD	6.29	1.61	1.51
1	C	282	CYS	CA-CB	-6.28	1.40	1.53
1	O	190	TRP	CD2-CE2	-6.28	1.33	1.41
1	C	80	VAL	N-CA	-6.27	1.33	1.46
1	C	39	TRP	CZ2-CH2	-6.27	1.25	1.37
1	O	178	ASN	N-CA	-6.27	1.33	1.46
1	O	195	LYS	CG-CD	6.25	1.73	1.52
1	C	47	ARG	C-N	-6.25	1.19	1.34
1	O	274	TYR	CA-CB	-6.25	1.40	1.53
1	O	317	ASN	N-CA	-6.24	1.33	1.46
1	C	43	SER	N-CA	-6.22	1.33	1.46
1	C	111	PRO	C-N	-6.22	1.19	1.34
1	C	229	GLU	C-O	6.22	1.35	1.23
1	O	208	ASP	CG-OD1	6.21	1.39	1.25
1	C	80	VAL	C-O	-6.20	1.11	1.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	281(C)	LYS	CE-NZ	6.19	1.64	1.49
1	C	96	VAL	C-N	6.19	1.48	1.34
1	C	187	THR	N-CA	6.18	1.58	1.46
1	C	10	MET	N-CA	-6.17	1.34	1.46
1	C	297	PRO	CA-C	-6.17	1.40	1.52
1	O	208	ASP	C-N	6.17	1.44	1.33
1	C	281(A)	SER	C-N	6.16	1.48	1.34
1	O	147	LYS	CE-NZ	-6.15	1.33	1.49
1	C	141	ILE	C-O	-6.15	1.11	1.23
1	C	131	GLY	N-CA	6.14	1.55	1.46
1	O	65	LYS	CE-NZ	6.14	1.64	1.49
1	O	193	GLN	CG-CD	6.13	1.65	1.51
1	O	220	TYR	CB-CG	-6.13	1.42	1.51
1	C	89	ILE	N-CA	-6.13	1.34	1.46
1	O	65	LYS	C-O	6.13	1.34	1.23
1	O	315	ARG	CZ-NH1	6.13	1.41	1.33
1	O	111	PRO	N-CD	6.12	1.56	1.47
1	C	32	ASP	CG-OD2	6.12	1.39	1.25
1	C	43	SER	C-O	-6.12	1.11	1.23
1	C	51	VAL	CA-CB	6.12	1.67	1.54
1	O	119	GLY	CA-C	-6.11	1.42	1.51
1	O	193	GLN	CD-NE2	6.11	1.48	1.32
1	C	6	LEU	N-CA	6.11	1.58	1.46
1	O	149	ASP	CG-OD1	6.11	1.39	1.25
1	C	190	TRP	CE2-CZ2	-6.10	1.29	1.39
1	O	258	ILE	C-N	-6.09	1.20	1.34
1	C	23	PRO	CA-C	-6.09	1.40	1.52
1	O	30	VAL	N-CA	-6.08	1.34	1.46
1	C	53	HIS	CA-CB	-6.08	1.40	1.53
1	O	281(A)	SER	CA-CB	6.07	1.62	1.52
1	C	67	ASN	CG-OD1	6.07	1.37	1.24
1	C	302	GLY	CA-C	-6.07	1.42	1.51
1	C	287	HIS	C-O	6.06	1.34	1.23
1	C	294	PRO	CA-C	6.06	1.65	1.52
1	C	240	ARG	C-O	6.06	1.34	1.23
1	C	274	TYR	CZ-OH	6.06	1.48	1.37
1	O	310	TYR	CZ-OH	6.06	1.48	1.37
1	C	137	PHE	C-O	6.04	1.34	1.23
1	C	120	VAL	N-CA	-6.04	1.34	1.46
1	C	125	PHE	CA-CB	-6.04	1.40	1.53
1	C	127	GLU	CD-OE2	-6.02	1.19	1.25
1	C	214	VAL	CB-CG1	-6.02	1.40	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	266	GLU	CG-CD	6.02	1.60	1.51
1	O	226	SER	C-O	6.00	1.34	1.23
1	C	196	GLY	C-O	-6.00	1.14	1.23
1	C	26	THR	CB-OG1	-6.00	1.31	1.43
1	C	186	LYS	CB-CG	5.99	1.68	1.52
1	C	197	VAL	N-CA	-5.99	1.34	1.46
1	C	156	ASN	CA-C	-5.99	1.37	1.52
1	C	14	TYR	C-O	-5.98	1.11	1.23
1	C	127	GLU	N-CA	-5.97	1.34	1.46
1	O	307	ARG	CZ-NH1	-5.97	1.25	1.33
1	O	117	PHE	CB-CG	5.97	1.61	1.51
1	C	56	PHE	C-O	-5.97	1.12	1.23
1	O	102	GLY	N-CA	-5.97	1.37	1.46
1	C	28	LYS	CA-CB	-5.96	1.40	1.53
1	C	208	ASP	C-O	5.96	1.34	1.23
1	O	194	MET	C-N	-5.96	1.20	1.34
1	C	26	THR	N-CA	-5.95	1.34	1.46
1	O	266	GLU	CB-CG	5.95	1.63	1.52
1	C	326	ARG	NE-CZ	5.95	1.40	1.33
1	O	106	GLU	CG-CD	5.95	1.60	1.51
1	O	257	ASP	C-O	-5.95	1.12	1.23
1	O	1	THR	CB-OG1	-5.94	1.31	1.43
1	C	190	TRP	CZ2-CH2	-5.94	1.26	1.37
1	C	88	ILE	C-O	-5.93	1.12	1.23
1	C	170	SER	CA-C	-5.93	1.37	1.52
1	C	59	SER	N-CA	5.92	1.58	1.46
1	C	42	SER	CB-OG	-5.92	1.34	1.42
1	C	149	ASP	N-CA	-5.92	1.34	1.46
1	C	325	ALA	CA-CB	-5.91	1.40	1.52
1	O	83	PHE	C-O	-5.91	1.12	1.23
1	O	215	ASP	CG-OD1	-5.91	1.11	1.25
1	C	117	PHE	N-CA	-5.91	1.34	1.46
1	O	123	MET	C-O	-5.90	1.12	1.23
1	C	250	ASN	C-O	-5.90	1.12	1.23
1	C	242	PHE	CG-CD2	5.90	1.47	1.38
1	O	9	TYR	C-O	-5.90	1.12	1.23
1	O	142	SER	CB-OG	-5.90	1.34	1.42
1	C	219	SER	N-CA	-5.89	1.34	1.46
1	C	244	ASP	CB-CG	5.89	1.64	1.51
1	C	270	THR	C-N	-5.88	1.20	1.34
1	O	129	ALA	CA-C	-5.88	1.37	1.52
1	C	44	LYS	CG-CD	5.87	1.72	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	68	GLY	C-O	5.87	1.33	1.23
1	O	47(A)	LEU	CA-C	5.86	1.68	1.52
1	C	53	HIS	CB-CG	-5.86	1.39	1.50
1	C	186	LYS	N-CA	5.85	1.58	1.46
1	O	52	TYR	CA-CB	5.85	1.66	1.53
1	O	110	LEU	N-CA	-5.84	1.34	1.46
1	C	226	SER	C-O	-5.83	1.12	1.23
1	O	64	TYR	CZ-OH	5.83	1.47	1.37
1	C	305	PHE	N-CA	-5.83	1.34	1.46
1	O	244	ASP	CG-OD2	5.83	1.38	1.25
1	O	294	PRO	CA-C	5.82	1.64	1.52
1	C	106	GLU	CD-OE2	5.82	1.32	1.25
1	O	54	LYS	CA-CB	-5.80	1.41	1.53
1	C	16	GLY	C-O	-5.79	1.14	1.23
1	O	166	VAL	CA-CB	-5.79	1.42	1.54
1	C	60	ASP	CA-C	-5.78	1.38	1.52
1	C	76	SER	CB-OG	5.78	1.49	1.42
1	C	108	PRO	CA-CB	-5.78	1.42	1.53
1	C	238	LYS	C-O	5.78	1.34	1.23
1	C	106	GLU	C-O	-5.77	1.12	1.23
1	O	246	VAL	CB-CG2	5.77	1.65	1.52
1	C	19	GLY	C-O	-5.76	1.14	1.23
1	O	193	GLN	C-O	-5.75	1.12	1.23
1	O	279	SER	CA-CB	5.75	1.61	1.52
1	C	193	GLN	C-O	5.73	1.34	1.23
1	O	220	TYR	CZ-OH	5.72	1.47	1.37
1	O	217	GLY	C-O	-5.72	1.14	1.23
1	O	177	GLY	C-O	-5.72	1.14	1.23
1	O	33	THR	C-N	5.71	1.43	1.33
1	O	109	ALA	CA-C	-5.70	1.38	1.52
1	O	255	LEU	C-N	5.69	1.45	1.34
1	C	169	GLY	CA-C	5.69	1.60	1.51
1	C	65	LYS	CB-CG	-5.66	1.37	1.52
1	C	42	SER	CA-CB	5.66	1.61	1.52
1	C	84	LEU	N-CA	-5.65	1.35	1.46
1	C	160(D)	SER	N-CA	5.64	1.57	1.46
1	C	292	PRO	CA-C	-5.64	1.41	1.52
1	C	281(A)	SER	C-O	5.64	1.34	1.23
1	C	62	SER	CA-CB	5.63	1.61	1.52
1	O	108	PRO	C-N	-5.63	1.21	1.34
1	O	305	PHE	CA-CB	-5.63	1.41	1.53
1	O	258	ILE	CA-C	-5.62	1.38	1.52

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	67	ASN	CB-CG	5.62	1.64	1.51
1	C	296	GLY	C-O	5.62	1.32	1.23
1	O	9	TYR	N-CA	-5.62	1.35	1.46
1	O	128	GLN	C-O	-5.62	1.12	1.23
1	O	142	SER	C-O	-5.61	1.12	1.23
1	O	64	TYR	C-O	5.61	1.34	1.23
1	C	316	ARG	CG-CD	5.61	1.66	1.51
1	C	101	PHE	CA-CB	5.60	1.66	1.53
1	C	86	GLN	CA-C	-5.59	1.38	1.52
1	O	314	ASP	N-CA	-5.59	1.35	1.46
1	C	153	PHE	CB-CG	-5.58	1.41	1.51
1	C	287	HIS	CA-CB	-5.58	1.41	1.53
1	C	306	ILE	C-N	-5.58	1.21	1.34
1	O	127	GLU	CD-OE2	5.58	1.31	1.25
1	O	321	GLY	C-O	5.58	1.32	1.23
1	O	276	PHE	CA-CB	-5.57	1.41	1.53
1	O	156	ASN	CG-ND2	5.57	1.46	1.32
1	O	63	SER	CA-CB	5.56	1.61	1.52
1	O	180	HIS	CA-C	5.55	1.67	1.52
1	O	257	ASP	CA-CB	-5.55	1.41	1.53
1	C	142	SER	CB-OG	5.55	1.49	1.42
1	C	316	ARG	N-CA	-5.55	1.35	1.46
1	O	6	LEU	N-CA	-5.54	1.35	1.46
1	O	190	TRP	CG-CD1	-5.54	1.28	1.36
1	O	210	CYS	CA-CB	-5.54	1.41	1.53
1	C	32	ASP	C-O	-5.54	1.12	1.23
1	O	59	SER	CB-OG	-5.53	1.35	1.42
1	O	0	THR	C-O	5.52	1.33	1.23
1	C	189	VAL	N-CA	5.52	1.57	1.46
1	O	52	TYR	CG-CD2	5.52	1.46	1.39
1	O	181	TYR	CD2-CE2	5.52	1.47	1.39
1	O	220	TYR	CE1-CZ	5.50	1.45	1.38
1	O	211	LEU	C-O	-5.49	1.12	1.23
1	C	319	ARG	CG-CD	-5.49	1.38	1.51
1	O	273	ASP	CA-CB	-5.48	1.41	1.53
1	C	289	MET	C-O	5.48	1.33	1.23
1	C	22	THR	N-CA	-5.47	1.35	1.46
1	C	39	TRP	C-O	-5.47	1.12	1.23
1	C	190	TRP	CD1-NE1	5.47	1.47	1.38
1	O	314	ASP	CA-C	-5.47	1.38	1.52
1	C	10	MET	CG-SD	5.47	1.95	1.81
1	C	262	LEU	C-O	5.47	1.33	1.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	284	LEU	C-N	5.47	1.46	1.34
1	C	261	HIS	CD2-NE2	5.46	1.53	1.42
1	O	210	CYS	N-CA	-5.46	1.35	1.46
1	O	223	GLY	C-O	5.46	1.32	1.23
1	O	138	ASP	CG-OD2	5.45	1.37	1.25
1	O	169	GLY	C-N	5.45	1.46	1.34
1	O	67	ASN	CA-C	-5.44	1.38	1.52
1	C	1	THR	N-CA	-5.44	1.35	1.46
1	C	281(B)	LYS	CB-CG	5.44	1.67	1.52
1	O	204	LEU	CG-CD1	5.43	1.72	1.51
1	C	31	PHE	C-O	-5.43	1.13	1.23
1	C	168	GLY	C-N	5.42	1.42	1.33
1	C	155	TYR	CB-CG	-5.42	1.43	1.51
1	C	318	ASN	N-CA	-5.42	1.35	1.46
1	C	238	LYS	N-CA	5.42	1.57	1.46
1	C	313	PHE	C-O	-5.42	1.13	1.23
1	C	70	GLU	CA-C	-5.41	1.38	1.52
1	C	229	GLU	CD-OE1	5.40	1.31	1.25
1	C	99	GLN	CA-C	-5.40	1.39	1.52
1	C	299	TRP	CD2-CE2	5.40	1.47	1.41
1	O	150	VAL	CB-CG2	-5.40	1.41	1.52
1	C	90	THR	CA-CB	5.40	1.67	1.53
1	O	20	ILE	N-CA	-5.40	1.35	1.46
1	O	250	ASN	CB-CG	5.40	1.63	1.51
1	C	193	GLN	CD-NE2	5.39	1.46	1.32
1	C	174	HIS	CG-ND1	5.39	1.50	1.38
1	O	273	ASP	C-O	-5.39	1.13	1.23
1	C	251	GLU	CA-CB	5.38	1.65	1.53
1	O	70	GLU	C-O	5.38	1.33	1.23
1	O	161	LEU	CA-CB	-5.38	1.41	1.53
1	C	47	ARG	CG-CD	5.38	1.65	1.51
1	C	184	LEU	CA-C	-5.37	1.39	1.52
1	C	51	VAL	CB-CG2	-5.36	1.41	1.52
1	C	21	GLY	C-O	-5.36	1.15	1.23
1	C	218	ALA	C-N	-5.36	1.21	1.34
1	C	157	ARG	CG-CD	5.36	1.65	1.51
1	O	290	ASP	C-N	5.35	1.46	1.34
1	C	209	GLY	N-CA	5.35	1.54	1.46
1	O	40	VAL	CA-CB	-5.35	1.43	1.54
1	C	247	VAL	CB-CG2	-5.35	1.41	1.52
1	C	195	LYS	N-CA	5.34	1.57	1.46
1	O	47(A)	LEU	CA-CB	5.34	1.66	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	147	LYS	CA-CB	-5.33	1.42	1.53
1	O	39	TRP	CG-CD1	-5.33	1.29	1.36
1	C	57	ASP	N-CA	-5.33	1.35	1.46
1	C	155	TYR	N-CA	-5.33	1.35	1.46
1	C	306	ILE	C-O	-5.32	1.13	1.23
1	C	217	GLY	C-O	-5.31	1.15	1.23
1	C	156	ASN	N-CA	-5.31	1.35	1.46
1	O	296	GLY	CA-C	-5.30	1.43	1.51
1	C	113	MET	C-N	-5.30	1.21	1.34
1	O	58	ALA	CA-CB	-5.30	1.41	1.52
1	O	110	LEU	CB-CG	5.30	1.68	1.52
1	C	161	LEU	N-CA	-5.29	1.35	1.46
1	O	104	VAL	CB-CG1	-5.29	1.41	1.52
1	O	123	MET	CG-SD	-5.29	1.67	1.81
1	O	92	GLY	C-N	-5.29	1.23	1.33
1	C	265	LYS	CD-CE	5.29	1.64	1.51
1	C	180	HIS	ND1-CE1	5.28	1.48	1.34
1	C	237	ALA	CA-CB	5.28	1.63	1.52
1	O	161	LEU	N-CA	-5.28	1.35	1.46
1	O	26	THR	CA-CB	5.28	1.67	1.53
1	O	290	ASP	CG-OD1	5.28	1.37	1.25
1	O	169	GLY	CA-C	5.27	1.60	1.51
1	O	261	HIS	CG-ND1	5.27	1.50	1.38
1	O	273	ASP	CA-C	-5.26	1.39	1.52
1	O	139	ASN	CA-C	-5.26	1.39	1.52
1	O	286	ILE	CA-CB	-5.26	1.42	1.54
1	O	171	ASP	CG-OD1	5.26	1.37	1.25
1	C	195	LYS	CD-CE	5.25	1.64	1.51
1	O	248	LYS	C-O	5.25	1.33	1.23
1	C	96	VAL	N-CA	-5.25	1.35	1.46
1	O	129	ALA	C-N	-5.24	1.22	1.34
1	O	242	PHE	C-N	5.24	1.46	1.34
1	C	287	HIS	CB-CG	-5.23	1.40	1.50
1	O	306	ILE	C-O	5.23	1.33	1.23
1	C	322	PHE	N-CA	5.23	1.56	1.46
1	C	326	ARG	CZ-NH2	5.23	1.39	1.33
1	C	185	ILE	CB-CG2	5.23	1.69	1.52
1	C	96	VAL	CA-CB	-5.23	1.43	1.54
1	C	114	LEU	N-CA	-5.23	1.35	1.46
1	O	247	VAL	N-CA	-5.22	1.35	1.46
1	O	291	ILE	C-O	5.22	1.33	1.23
1	O	125	PHE	CE2-CZ	-5.21	1.27	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	-1	ASN	CB-CG	5.21	1.63	1.51
1	C	135	PRO	C-O	-5.21	1.12	1.23
1	C	319	ARG	CZ-NH1	5.21	1.39	1.33
1	C	128	GLN	CD-NE2	5.20	1.45	1.32
1	O	176	GLU	CA-CB	-5.20	1.42	1.53
1	O	230	LYS	CG-CD	5.20	1.70	1.52
1	O	138	ASP	CB-CG	5.20	1.62	1.51
1	C	250	ASN	CB-CG	5.19	1.62	1.51
1	O	299	TRP	CG-CD1	-5.18	1.29	1.36
1	O	216	THR	CB-OG1	-5.18	1.32	1.43
1	C	17	GLU	C-O	5.17	1.33	1.23
1	O	133	VAL	CB-CG1	-5.17	1.42	1.52
1	O	150	VAL	C-N	-5.17	1.22	1.34
1	C	176	GLU	N-CA	-5.16	1.36	1.46
1	O	199	VAL	N-CA	-5.16	1.36	1.46
1	O	272	ALA	CA-CB	-5.16	1.41	1.52
1	C	1	THR	CA-C	-5.15	1.39	1.52
1	C	76	SER	N-CA	-5.15	1.36	1.46
1	C	79	THR	C-O	5.14	1.33	1.23
1	O	61	SER	C-O	5.14	1.33	1.23
1	C	47(B)	TYR	CE2-CZ	5.14	1.45	1.38
1	O	35	SER	C-O	5.14	1.33	1.23
1	O	231	LEU	C-N	-5.14	1.22	1.34
1	O	54	LYS	C-O	5.13	1.33	1.23
1	O	117	PHE	CE1-CZ	5.13	1.47	1.37
1	C	228	ILE	C-O	5.13	1.33	1.23
1	C	282	CYS	CA-C	-5.13	1.39	1.52
1	O	41	PRO	C-N	5.13	1.45	1.34
1	C	11	ASP	CG-OD2	5.12	1.37	1.25
1	C	272	ALA	N-CA	-5.12	1.36	1.46
1	O	245	TYR	CZ-OH	5.12	1.46	1.37
1	O	281(A)	SER	CA-C	5.12	1.66	1.52
1	O	302	GLY	C-O	-5.11	1.15	1.23
1	C	52	TYR	CE1-CZ	5.11	1.45	1.38
1	C	3	SER	C-N	-5.10	1.22	1.34
1	C	61	SER	C-O	5.10	1.33	1.23
1	O	165	ILE	CA-CB	-5.10	1.43	1.54
1	O	278	GLU	C-N	5.10	1.45	1.34
1	C	296	GLY	N-CA	-5.09	1.38	1.46
1	O	236	GLY	CA-C	5.09	1.59	1.51
1	O	227	SER	C-N	5.09	1.45	1.34
1	O	300	ALA	CA-CB	5.09	1.63	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	154	TYR	CG-CD1	-5.08	1.32	1.39
1	C	48	THR	CB-CG2	5.08	1.69	1.52
1	C	50	CYS	C-O	-5.08	1.13	1.23
1	C	126	ILE	N-CA	5.08	1.56	1.46
1	O	300	ALA	N-CA	5.08	1.56	1.46
1	C	286	ILE	C-O	-5.07	1.13	1.23
1	C	264	GLY	C-N	5.07	1.45	1.34
1	C	50	CYS	N-CA	-5.07	1.36	1.46
1	C	202	SER	CA-CB	5.07	1.60	1.52
1	O	60	ASP	C-O	-5.07	1.13	1.23
1	O	313	PHE	C-O	-5.06	1.13	1.23
1	C	294	PRO	C-N	-5.06	1.22	1.34
1	O	250	ASN	CG-ND2	5.05	1.45	1.32
1	C	149	ASP	C-O	-5.05	1.13	1.23
1	C	52	TYR	CG-CD1	5.04	1.45	1.39
1	C	178	ASN	CA-CB	-5.04	1.40	1.53
1	C	140	ILE	CB-CG2	-5.04	1.37	1.52
1	O	296	GLY	C-N	-5.03	1.24	1.34
1	C	242	PHE	CA-C	5.03	1.66	1.52
1	C	136	ILE	CA-CB	-5.03	1.43	1.54
1	C	248	LYS	CB-CG	-5.03	1.39	1.52
1	O	51	VAL	CB-CG2	5.03	1.63	1.52
1	O	233	GLU	N-CA	-5.03	1.36	1.46
1	C	325	ALA	C-O	5.02	1.32	1.23
1	O	100	MET	CG-SD	5.01	1.94	1.81
1	O	155	TYR	CZ-OH	5.01	1.46	1.37
1	O	62	SER	CA-C	-5.00	1.40	1.52
1	C	121	VAL	CB-CG1	-5.00	1.42	1.52

All (1127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	316	ARG	NE-CZ-NH1	45.10	142.85	120.30
1	O	74	ARG	NE-CZ-NH2	42.22	141.41	120.30
1	O	157	ARG	NE-CZ-NH1	34.81	137.70	120.30
1	O	316	ARG	NE-CZ-NH2	-31.00	104.80	120.30
1	C	319	ARG	NE-CZ-NH1	28.55	134.58	120.30
1	O	157	ARG	NE-CZ-NH2	-27.09	106.75	120.30
1	O	149	ASP	CB-CG-OD2	-26.39	94.55	118.30
1	O	315	ARG	NE-CZ-NH2	26.15	133.37	120.30
1	O	154	TYR	CB-CG-CD2	25.96	136.58	121.00
1	C	158	ASP	CB-CG-OD2	-25.86	95.03	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	47(B)	TYR	CB-CG-CD1	-24.25	106.45	121.00
1	O	149	ASP	CB-CG-OD1	23.97	139.88	118.30
1	C	242	PHE	CB-CG-CD1	-23.19	104.57	120.80
1	O	87	ASP	CB-CG-OD2	-22.68	97.89	118.30
1	C	158	ASP	CB-CG-OD1	22.52	138.57	118.30
1	C	47	ARG	NE-CZ-NH2	-21.28	109.66	120.30
1	O	132	ARG	NE-CZ-NH2	20.92	130.76	120.30
1	O	74	ARG	NE-CZ-NH1	-20.92	109.84	120.30
1	C	315	ARG	NE-CZ-NH1	-19.93	110.33	120.30
1	O	307	ARG	NE-CZ-NH2	19.91	130.25	120.30
1	O	319	ARG	NE-CZ-NH2	-18.78	110.91	120.30
1	O	240	ARG	NE-CZ-NH2	18.71	129.66	120.30
1	O	276	PHE	CB-CG-CD1	-18.71	107.70	120.80
1	O	290	ASP	CB-CG-OD1	18.57	135.02	118.30
1	C	47(B)	TYR	CB-CG-CD2	18.49	132.09	121.00
1	C	74	ARG	NE-CZ-NH1	-17.87	111.36	120.30
1	O	326	ARG	CD-NE-CZ	-17.20	99.52	123.60
1	C	242	PHE	CB-CG-CD2	16.96	132.67	120.80
1	O	75	TYR	CB-CG-CD1	-16.92	110.85	121.00
1	C	83	PHE	CB-CG-CD1	16.55	132.38	120.80
1	O	276	PHE	CB-CG-CD2	16.34	132.24	120.80
1	O	325	ALA	N-CA-CB	16.00	132.50	110.10
1	O	181	TYR	CB-CG-CD2	-15.96	111.42	121.00
1	O	109	ALA	CB-CA-C	-15.83	86.36	110.10
1	C	257	ASP	CB-CG-OD1	15.52	132.27	118.30
1	O	104	VAL	CG1-CB-CG2	-15.50	86.09	110.90
1	O	244	ASP	CB-CG-OD2	-15.27	104.56	118.30
1	C	159	SER	O-C-N	15.14	146.93	122.70
1	C	9	TYR	CB-CG-CD2	14.99	129.99	121.00
1	C	289	MET	N-CA-CB	14.92	137.45	110.60
1	C	64	TYR	CB-CG-CD1	14.75	129.85	121.00
1	O	57	ASP	CB-CG-OD2	-14.67	105.10	118.30
1	C	113	MET	CG-SD-CE	14.63	123.60	100.20
1	C	132	ARG	N-CA-CB	-14.39	84.70	110.60
1	C	309	PHE	CB-CG-CD2	-14.39	110.73	120.80
1	C	118	ASP	CB-CG-OD1	14.28	131.16	118.30
1	O	87	ASP	CB-CG-OD1	14.12	131.01	118.30
1	O	285	ALA	N-CA-CB	-14.02	90.47	110.10
1	O	288	ALA	CB-CA-C	-13.90	89.25	110.10
1	C	319	ARG	NE-CZ-NH2	-13.75	113.42	120.30
1	C	289	MET	CA-CB-CG	13.74	136.66	113.30
1	C	9	TYR	CB-CG-CD1	-13.63	112.82	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	152	SER	N-CA-CB	-13.52	90.23	110.50
1	C	157	ARG	NE-CZ-NH1	13.51	127.05	120.30
1	O	120	VAL	CG1-CB-CG2	-13.44	89.39	110.90
1	C	83	PHE	CB-CG-CD2	-13.41	111.42	120.80
1	C	208	ASP	CB-CG-OD1	13.38	130.34	118.30
1	O	165	ILE	CA-CB-CG1	-13.21	85.90	111.00
1	C	150	VAL	CA-CB-CG1	-13.20	91.11	110.90
1	O	132	ARG	CD-NE-CZ	13.17	142.03	123.60
1	C	310	TYR	CG-CD1-CE1	13.10	131.78	121.30
1	O	115	ALA	CB-CA-C	-13.09	90.47	110.10
1	O	244	ASP	CB-CG-OD1	13.03	130.03	118.30
1	C	60	ASP	CB-CG-OD1	13.00	130.00	118.30
1	C	287	HIS	CB-CA-C	-13.00	84.40	110.40
1	C	64	TYR	CB-CG-CD2	-12.93	113.24	121.00
1	O	74	ARG	CD-NE-CZ	12.69	141.37	123.60
1	O	154	TYR	CG-CD2-CE2	12.67	131.44	121.30
1	O	319	ARG	NE-CZ-NH1	12.65	126.63	120.30
1	O	158	ASP	CB-CG-OD1	12.64	129.68	118.30
1	C	251	GLU	OE1-CD-OE2	-12.64	108.14	123.30
1	C	239	LYS	N-CA-CB	-12.43	88.22	110.60
1	O	91	VAL	CG1-CB-CG2	-12.41	91.04	110.90
1	O	64	TYR	CZ-CE2-CD2	-12.39	108.65	119.80
1	O	251	GLU	CB-CG-CD	12.38	147.62	114.20
1	O	13	GLN	N-CA-CB	-12.30	88.45	110.60
1	C	57	ASP	CB-CG-OD2	-12.21	107.31	118.30
1	O	181	TYR	CG-CD2-CE2	-12.14	111.58	121.30
1	C	116	GLU	CG-CD-OE2	-12.12	94.06	118.30
1	O	75	TYR	CB-CG-CD2	11.97	128.18	121.00
1	O	76	SER	CB-CA-C	-11.87	87.55	110.10
1	O	29	VAL	CA-CB-CG2	-11.81	93.18	110.90
1	C	4	VAL	CA-CB-CG2	-11.77	93.24	110.90
1	C	310	TYR	CD1-CE1-CZ	-11.76	109.22	119.80
1	C	108	PRO	N-CA-CB	11.76	117.41	103.30
1	C	56	PHE	CB-CG-CD1	11.74	129.02	120.80
1	C	274	TYR	CB-CG-CD2	-11.73	113.96	121.00
1	O	160(D)	SER	CB-CA-C	-11.73	87.81	110.10
1	O	132	ARG	NE-CZ-NH1	-11.72	114.44	120.30
1	C	294	PRO	N-CA-CB	-11.68	89.28	103.30
1	O	161	LEU	C-N-CA	-11.68	97.78	122.30
1	C	177	GLY	C-N-CA	-11.65	92.58	121.70
1	C	132	ARG	NE-CZ-NH1	-11.56	114.52	120.30
1	O	125	PHE	CD1-CE1-CZ	-11.54	106.26	120.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	290	ASP	CB-CG-OD2	-11.53	107.92	118.30
1	C	197	VAL	CG1-CB-CG2	-11.52	92.46	110.90
1	C	76	SER	N-CA-CB	-11.46	93.31	110.50
1	O	48	THR	CA-CB-CG2	-11.44	96.39	112.40
1	O	52	TYR	CA-CB-CG	-11.43	91.68	113.40
1	C	57	ASP	CB-CG-OD1	11.41	128.57	118.30
1	C	74	ARG	NH1-CZ-NH2	11.41	131.95	119.40
1	O	235	LEU	CB-CG-CD1	-11.30	91.78	111.00
1	C	17	GLU	OE1-CD-OE2	-11.29	109.75	123.30
1	O	64	TYR	CG-CD2-CE2	11.23	130.29	121.30
1	O	281(A)	SER	N-CA-CB	-11.12	93.82	110.50
1	O	262	LEU	CB-CG-CD1	-11.12	92.10	111.00
1	C	322	PHE	CB-CG-CD2	-11.08	113.04	120.80
1	O	156	ASN	N-CA-CB	11.05	130.49	110.60
1	C	175	TYR	CZ-CE2-CD2	-11.02	109.89	119.80
1	O	15	TYR	CB-CG-CD2	11.01	127.61	121.00
1	C	87	ASP	CB-CG-OD1	10.97	128.18	118.30
1	O	208	ASP	CB-CG-OD2	-10.97	108.43	118.30
1	C	293	PRO	CA-N-CD	-10.93	96.20	111.50
1	O	64	TYR	CG-CD1-CE1	-10.92	112.57	121.30
1	C	58	ALA	CB-CA-C	-10.90	93.75	110.10
1	O	270	THR	CA-CB-CG2	-10.85	97.21	112.40
1	O	176	GLU	CG-CD-OE2	-10.78	96.74	118.30
1	O	110	LEU	N-CA-CB	-10.78	88.85	110.40
1	C	153	PHE	CB-CG-CD2	-10.77	113.26	120.80
1	C	118	ASP	CB-CG-OD2	-10.77	108.61	118.30
1	O	77	THR	OG1-CB-CG2	-10.76	85.25	110.00
1	O	109	ALA	O-C-N	10.75	139.91	122.70
1	C	240	ARG	NE-CZ-NH1	10.64	125.62	120.30
1	O	15	TYR	CZ-CE2-CD2	-10.62	110.24	119.80
1	C	289	MET	CB-CA-C	-10.62	89.17	110.40
1	O	154	TYR	CB-CG-CD1	-10.61	114.63	121.00
1	O	145	VAL	CA-CB-CG1	10.61	126.81	110.90
1	C	320	ILE	C-N-CA	-10.60	100.03	122.30
1	C	183	ASN	CB-CA-C	-10.59	89.21	110.40
1	C	287	HIS	CA-CB-CG	-10.59	95.60	113.60
1	O	47	ARG	NE-CZ-NH2	10.52	125.56	120.30
1	O	118	ASP	CB-CG-OD2	-10.51	108.84	118.30
1	C	53	HIS	N-CA-CB	-10.50	91.69	110.60
1	C	244	ASP	CA-CB-CG	10.48	136.45	113.40
1	O	309	PHE	CD1-CE1-CZ	-10.47	107.53	120.10
1	C	148	GLU	OE1-CD-OE2	10.46	135.85	123.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	202	SER	CB-CA-C	10.45	129.95	110.10
1	O	62	SER	CA-C-O	-10.38	98.30	120.10
1	C	157	ARG	CB-CG-CD	10.35	138.51	111.60
1	O	230	LYS	CD-CE-NZ	10.34	135.48	111.70
1	O	178	ASN	CA-CB-CG	-10.29	90.75	113.40
1	C	47(B)	TYR	CZ-CE2-CD2	-10.21	110.61	119.80
1	O	112	PHE	CZ-CE2-CD2	-10.20	107.86	120.10
1	C	289	MET	CG-SD-CE	10.20	116.52	100.20
1	C	220	TYR	CB-CG-CD1	10.18	127.11	121.00
1	C	49	ALA	N-CA-CB	-10.13	95.91	110.10
1	O	314	ASP	CB-CG-OD1	10.12	127.41	118.30
1	C	257	ASP	CB-CG-OD2	-10.11	109.20	118.30
1	O	100	MET	CG-SD-CE	-10.10	84.04	100.20
1	C	134	THR	CA-CB-CG2	10.09	126.52	112.40
1	C	227	SER	CB-CA-C	-10.07	90.96	110.10
1	O	122	GLY	CA-C-O	10.05	138.69	120.60
1	C	225	THR	CA-CB-CG2	-10.05	98.33	112.40
1	O	246	VAL	CG1-CB-CG2	10.03	126.95	110.90
1	C	5	ILE	CA-CB-CG1	-9.99	92.01	111.00
1	O	276	PHE	CZ-CE2-CD2	-9.99	108.11	120.10
1	C	83	PHE	CD1-CE1-CZ	-9.99	108.12	120.10
1	O	311	THR	OG1-CB-CG2	-9.99	87.03	110.00
1	O	17	GLU	CG-CD-OE2	-9.96	98.37	118.30
1	O	280	TYR	OH-CZ-CE2	-9.92	93.31	120.10
1	C	313	PHE	CG-CD1-CE1	-9.91	109.89	120.80
1	O	251	GLU	CB-CA-C	9.91	130.22	110.40
1	C	208	ASP	CB-CG-OD2	-9.90	109.39	118.30
1	O	96	VAL	CB-CA-C	-9.87	92.64	111.40
1	O	74	ARG	NH1-CZ-NH2	-9.82	108.60	119.40
1	C	30	VAL	CG1-CB-CG2	-9.78	95.26	110.90
1	O	157	ARG	CD-NE-CZ	9.77	137.28	123.60
1	C	248	LYS	N-CA-CB	-9.74	93.06	110.60
1	C	79	THR	CA-CB-CG2	9.72	126.01	112.40
1	C	239	LYS	CB-CA-C	9.71	129.82	110.40
1	C	240	ARG	CA-CB-CG	9.71	134.77	113.40
1	C	96	VAL	CG1-CB-CG2	-9.66	95.45	110.90
1	O	250	ASN	C-N-CA	9.65	145.84	121.70
1	O	278	GLU	CA-C-O	-9.65	99.83	120.10
1	O	171	ASP	CB-CG-OD1	-9.64	109.62	118.30
1	C	173	GLN	CA-CB-CG	-9.63	92.21	113.40
1	C	154	TYR	CB-CG-CD1	-9.61	115.23	121.00
1	O	189	VAL	CG1-CB-CG2	-9.61	95.52	110.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	245	TYR	CB-CG-CD2	-9.58	115.25	121.00
1	O	207	GLU	N-CA-CB	9.57	127.83	110.60
1	O	150	VAL	CG1-CB-CG2	-9.56	95.60	110.90
1	C	220	TYR	CG-CD2-CE2	9.55	128.94	121.30
1	O	269	LEU	O-C-N	-9.54	107.44	122.70
1	O	114	LEU	CB-CG-CD2	-9.51	94.83	111.00
1	O	310	TYR	CZ-CE2-CD2	9.51	128.36	119.80
1	C	69	THR	OG1-CB-CG2	-9.50	88.16	110.00
1	C	182	ILE	CA-CB-CG2	9.48	129.85	110.90
1	O	118	ASP	CB-CG-OD1	9.47	126.83	118.30
1	O	315	ARG	CG-CD-NE	9.45	131.63	111.80
1	O	114	LEU	CA-CB-CG	-9.44	93.58	115.30
1	C	310	TYR	CG-CD2-CE2	-9.44	113.75	121.30
1	C	30	VAL	CA-CB-CG1	9.41	125.02	110.90
1	O	240	ARG	N-CA-CB	9.39	127.50	110.60
1	O	65	LYS	CB-CA-C	9.35	129.10	110.40
1	C	60	ASP	CB-CG-OD2	-9.34	109.90	118.30
1	O	57	ASP	CB-CG-OD1	9.34	126.70	118.30
1	C	55	LEU	CB-CG-CD2	9.32	126.85	111.00
1	O	194	MET	CA-C-O	9.30	139.63	120.10
1	C	187	THR	CA-CB-CG2	-9.27	99.42	112.40
1	C	38	VAL	CA-CB-CG2	-9.26	97.01	110.90
1	O	224	SER	CB-CA-C	-9.26	92.51	110.10
1	O	175	TYR	CB-CG-CD2	-9.25	115.45	121.00
1	C	315	ARG	CG-CD-NE	-9.24	92.41	111.80
1	O	240	ARG	NE-CZ-NH1	-9.23	115.68	120.30
1	O	276	PHE	CG-CD2-CE2	9.22	130.95	120.80
1	O	150	VAL	O-C-N	-9.20	107.97	122.70
1	O	15	TYR	CB-CG-CD1	-9.20	115.48	121.00
1	C	69	THR	CA-CB-OG1	-9.13	89.82	109.00
1	O	296	GLY	CA-C-O	-9.12	104.19	120.60
1	O	220	TYR	CB-CG-CD2	9.11	126.47	121.00
1	O	289	MET	CA-CB-CG	-9.09	97.84	113.30
1	C	70	GLU	N-CA-CB	9.07	126.92	110.60
1	C	155	TYR	CD1-CE1-CZ	9.06	127.96	119.80
1	C	239	LYS	CA-CB-CG	9.06	133.33	113.40
1	O	75	TYR	CG-CD2-CE2	-9.05	114.06	121.30
1	O	313	PHE	CZ-CE2-CD2	-9.04	109.25	120.10
1	O	324	LEU	CB-CA-C	-9.01	93.08	110.20
1	C	120	VAL	CG1-CB-CG2	-9.01	96.48	110.90
1	O	112	PHE	CB-CG-CD1	-8.98	114.51	120.80
1	C	255	LEU	N-CA-CB	-8.98	92.44	110.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	280	TYR	N-CA-CB	8.96	126.72	110.60
1	O	312	GLU	CG-CD-OE1	8.96	136.22	118.30
1	O	268	THR	CA-CB-CG2	8.94	124.91	112.40
1	C	132	ARG	CB-CG-CD	-8.93	88.39	111.60
1	C	313	PHE	CD1-CE1-CZ	8.92	130.80	120.10
1	O	143	GLN	C-N-CA	-8.92	103.57	122.30
1	C	285	ALA	CB-CA-C	8.90	123.45	110.10
1	C	154	TYR	CB-CG-CD2	8.89	126.33	121.00
1	O	80	VAL	N-CA-C	-8.89	86.99	111.00
1	O	121	VAL	CG1-CB-CG2	-8.88	96.70	110.90
1	C	6	LEU	CB-CG-CD1	-8.86	95.94	111.00
1	O	250	ASN	N-CA-CB	-8.84	94.69	110.60
1	C	267	TYR	CZ-CE2-CD2	-8.82	111.87	119.80
1	C	83	PHE	CG-CD1-CE1	8.81	130.49	120.80
1	O	46	SER	CB-CA-C	-8.80	93.38	110.10
1	O	182	ILE	CB-CA-C	-8.79	94.02	111.60
1	C	311	THR	CA-CB-CG2	8.79	124.70	112.40
1	O	145	VAL	N-CA-CB	-8.78	92.19	111.50
1	O	270	THR	OG1-CB-CG2	-8.77	89.83	110.00
1	C	99	GLN	N-CA-CB	-8.77	94.82	110.60
1	C	7	THR	OG1-CB-CG2	-8.75	89.88	110.00
1	O	315	ARG	NH1-CZ-NH2	-8.74	109.79	119.40
1	O	151	PHE	N-CA-CB	8.71	126.27	110.60
1	O	222	SER	CB-CA-C	-8.70	93.57	110.10
1	C	114	LEU	CB-CA-C	-8.69	93.69	110.20
1	C	233	GLU	CB-CA-C	-8.68	93.04	110.40
1	O	161	LEU	N-CA-CB	-8.63	93.13	110.40
1	O	28	LYS	CB-CA-C	-8.62	93.15	110.40
1	O	111	PRO	CB-CA-C	-8.62	90.46	112.00
1	O	307	ARG	NH1-CZ-NH2	-8.61	109.92	119.40
1	C	316	ARG	O-C-N	8.60	136.46	122.70
1	C	186	LYS	CB-CG-CD	8.60	133.96	111.60
1	C	49	ALA	O-C-N	-8.60	108.95	122.70
1	C	10	MET	CA-CB-CG	-8.59	98.69	113.30
1	O	66	HIS	CB-CA-C	-8.58	93.24	110.40
1	O	155	TYR	CA-CB-CG	8.58	129.70	113.40
1	O	291	ILE	CA-CB-CG2	-8.58	93.74	110.90
1	O	313	PHE	CB-CG-CD2	-8.58	114.80	120.80
1	C	293	PRO	N-CA-CB	8.57	113.58	103.30
1	O	205	LEU	CA-CB-CG	8.53	134.93	115.30
1	O	0	THR	N-CA-CB	-8.51	94.13	110.30
1	O	254	THR	N-CA-CB	-8.51	94.14	110.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	132	ARG	CA-CB-CG	8.49	132.09	113.40
1	O	164	GLN	CG-CD-OE1	-8.49	104.61	121.60
1	O	260	PHE	CB-CG-CD1	8.49	126.74	120.80
1	C	322	PHE	CB-CG-CD1	8.48	126.74	120.80
1	O	30	VAL	N-CA-CB	8.48	130.16	111.50
1	C	149	ASP	CB-CG-OD1	-8.45	110.69	118.30
1	C	326	ARG	NE-CZ-NH2	-8.45	116.07	120.30
1	O	81	SER	CA-C-N	8.45	133.09	116.20
1	O	121	VAL	CA-C-N	8.45	133.09	116.20
1	O	281(C)	LYS	CA-CB-CG	-8.44	94.84	113.40
1	C	175	TYR	CB-CG-CD2	-8.44	115.94	121.00
1	O	134	THR	CA-CB-CG2	-8.43	100.60	112.40
1	O	271	SER	N-CA-CB	8.41	123.12	110.50
1	C	326	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	C	-2	GLY	O-C-N	8.40	136.15	122.70
1	O	44	LYS	O-C-N	-8.40	109.26	122.70
1	C	178	ASN	N-CA-CB	-8.40	95.49	110.60
1	O	64	TYR	CA-CB-CG	-8.38	97.47	113.40
1	C	323	ALA	CB-CA-C	-8.37	97.55	110.10
1	O	278	GLU	CB-CA-C	-8.35	93.69	110.40
1	O	205	LEU	N-CA-CB	-8.34	93.73	110.40
1	C	266	GLU	CA-CB-CG	-8.33	95.07	113.40
1	O	94	ILE	CA-CB-CG1	-8.31	95.21	111.00
1	C	85	SER	CB-CA-C	8.30	125.88	110.10
1	O	154	TYR	CD1-CG-CD2	-8.29	108.78	117.90
1	C	322	PHE	CG-CD2-CE2	-8.28	111.69	120.80
1	O	289	MET	CG-SD-CE	-8.26	86.98	100.20
1	C	191	GLN	CA-CB-CG	8.26	131.57	113.40
1	C	54	LYS	CB-CA-C	-8.25	93.90	110.40
1	C	316	ARG	CD-NE-CZ	-8.23	112.08	123.60
1	C	310	TYR	CZ-CE2-CD2	8.22	127.20	119.80
1	O	194	MET	CG-SD-CE	8.20	113.32	100.20
1	C	86	GLN	N-CA-CB	8.19	125.34	110.60
1	C	185	ILE	O-C-N	-8.15	109.66	122.70
1	C	74	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	C	208	ASP	CA-CB-CG	-8.12	95.55	113.40
1	O	58	ALA	O-C-N	-8.11	109.72	122.70
1	C	134	THR	CA-CB-OG1	-8.10	91.99	109.00
1	C	181	TYR	CD1-CE1-CZ	-8.09	112.52	119.80
1	C	47(B)	TYR	CG-CD1-CE1	-8.08	114.84	121.30
1	O	326	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	O	281(C)	LYS	CB-CA-C	8.07	126.53	110.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	179	PHE	CB-CA-C	-8.06	94.27	110.40
1	O	154	TYR	CD1-CE1-CZ	8.06	127.05	119.80
1	O	318	ASN	CB-CG-OD1	-8.05	105.50	121.60
1	O	111	PRO	N-CD-CG	-8.04	91.14	103.20
1	O	184	LEU	CB-CG-CD2	8.03	124.66	111.00
1	O	155	TYR	CD1-CE1-CZ	8.03	127.03	119.80
1	C	14	TYR	CB-CG-CD2	8.02	125.81	121.00
1	C	146	LEU	C-N-CA	-8.01	101.67	121.70
1	O	47	ARG	NH1-CZ-NH2	-8.01	110.59	119.40
1	C	9	TYR	CD1-CE1-CZ	8.00	127.00	119.80
1	C	322	PHE	CZ-CE2-CD2	8.00	129.69	120.10
1	C	25	GLN	CA-C-O	-7.99	103.31	120.10
1	C	87	ASP	CB-CG-OD2	-7.99	111.11	118.30
1	O	307	ARG	CA-CB-CG	7.99	130.97	113.40
1	O	47	ARG	CD-NE-CZ	-7.98	112.42	123.60
1	O	274	TYR	CG-CD2-CE2	-7.98	114.92	121.30
1	O	242	PHE	N-CA-C	-7.97	89.48	111.00
1	O	252	GLY	CA-C-O	-7.96	106.27	120.60
1	O	37	ASN	CA-CB-CG	7.96	130.91	113.40
1	O	276	PHE	CG-CD1-CE1	-7.96	112.05	120.80
1	C	206	CYS	N-CA-CB	7.95	124.90	110.60
1	O	190	TRP	CB-CG-CD1	-7.94	116.67	127.00
1	O	85	SER	CB-CA-C	7.94	125.19	110.10
1	O	234	ALA	N-CA-CB	-7.93	99.00	110.10
1	C	148	GLU	N-CA-CB	-7.92	96.35	110.60
1	C	109	ALA	CB-CA-C	-7.91	98.23	110.10
1	C	127	GLU	CG-CD-OE1	7.91	134.12	118.30
1	O	157	ARG	O-C-N	-7.91	110.05	122.70
1	C	266	GLU	OE1-CD-OE2	7.91	132.79	123.30
1	C	315	ARG	NE-CZ-NH2	7.90	124.25	120.30
1	O	323	ALA	CB-CA-C	-7.89	98.26	110.10
1	C	250	ASN	C-N-CA	7.87	141.38	121.70
1	C	245	TYR	CB-CG-CD1	7.86	125.71	121.00
1	C	116	GLU	OE1-CD-OE2	7.85	132.72	123.30
1	O	269	LEU	CD1-CG-CD2	-7.84	86.97	110.50
1	O	189	VAL	CA-CB-CG1	7.84	122.66	110.90
1	C	195	LYS	CA-C-O	-7.84	103.64	120.10
1	O	201	SER	O-C-N	7.82	135.21	122.70
1	O	31	PHE	CB-CG-CD1	7.81	126.27	120.80
1	C	166	VAL	CA-CB-CG1	-7.80	99.20	110.90
1	C	320	ILE	CA-CB-CG2	-7.79	95.32	110.90
1	C	281(C)	LYS	CB-CA-C	-7.79	94.82	110.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	57	ASP	CB-CA-C	-7.74	94.92	110.40
1	O	12	THR	O-C-N	-7.74	110.31	122.70
1	O	31	PHE	CG-CD2-CE2	7.73	129.30	120.80
1	C	267	TYR	OH-CZ-CE2	-7.73	99.23	120.10
1	C	212	ALA	N-CA-CB	-7.71	99.30	110.10
1	C	33	THR	O-C-N	-7.71	110.10	123.20
1	C	316	ARG	N-CA-CB	7.70	124.47	110.60
1	C	215	ASP	CA-CB-CG	7.70	130.34	113.40
1	O	280	TYR	CE1-CZ-OH	7.68	140.83	120.10
1	C	313	PHE	CB-CG-CD1	-7.67	115.43	120.80
1	C	233	GLU	CB-CG-CD	-7.63	93.60	114.20
1	C	190	TRP	CB-CG-CD2	7.61	136.49	126.60
1	C	77	THR	C-N-CA	7.60	138.26	122.30
1	C	242	PHE	CG-CD1-CE1	-7.59	112.45	120.80
1	C	262	LEU	N-CA-CB	-7.59	95.22	110.40
1	O	52	TYR	CB-CG-CD1	-7.58	116.45	121.00
1	O	158	ASP	CB-CG-OD2	-7.57	111.48	118.30
1	O	241	LEU	CB-CG-CD1	-7.56	98.14	111.00
1	O	190	TRP	CG-CD2-CE3	7.55	140.70	133.90
1	O	52	TYR	CB-CG-CD2	7.55	125.53	121.00
1	C	44	LYS	CD-CE-NZ	7.53	129.02	111.70
1	O	309	PHE	CE1-CZ-CE2	7.52	133.53	120.00
1	C	193	GLN	CA-CB-CG	-7.51	96.87	113.40
1	C	288	ALA	N-CA-CB	7.51	120.61	110.10
1	C	290	ASP	O-C-N	-7.51	110.68	122.70
1	O	72	THR	CA-CB-CG2	-7.51	101.89	112.40
1	O	36	SER	O-C-N	-7.50	110.70	122.70
1	O	290	ASP	CA-C-O	-7.49	104.37	120.10
1	O	269	LEU	CA-CB-CG	7.49	132.52	115.30
1	O	88	ILE	CB-CG1-CD1	-7.48	92.97	113.90
1	O	113	MET	CB-CA-C	7.47	125.34	110.40
1	C	185	ILE	N-CA-CB	-7.47	93.63	110.80
1	O	220	TYR	CG-CD1-CE1	7.46	127.27	121.30
1	C	299	TRP	CE3-CZ3-CH2	7.46	129.40	121.20
1	O	39	TRP	CH2-CZ2-CE2	-7.46	109.94	117.40
1	C	322	PHE	CD1-CE1-CZ	-7.45	111.16	120.10
1	C	123	MET	CG-SD-CE	7.44	112.10	100.20
1	O	160(D)	SER	N-CA-CB	7.43	121.65	110.50
1	C	60	ASP	CA-CB-CG	7.43	129.75	113.40
1	O	14	TYR	CB-CG-CD2	-7.43	116.54	121.00
1	C	310	TYR	CA-C-O	-7.43	104.50	120.10
1	O	125	PHE	CG-CD1-CE1	7.42	128.96	120.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	9	TYR	CG-CD2-CE2	7.42	127.23	121.30
1	C	77	THR	N-CA-C	7.41	131.01	111.00
1	C	125	PHE	CG-CD1-CE1	7.40	128.94	120.80
1	O	318	ASN	CB-CA-C	-7.39	95.62	110.40
1	O	176	GLU	CB-CG-CD	-7.39	94.25	114.20
1	C	170	SER	CA-C-O	-7.38	104.60	120.10
1	C	128	GLN	CB-CA-C	7.37	125.14	110.40
1	O	137	PHE	CG-CD1-CE1	7.37	128.90	120.80
1	O	194	MET	CA-C-N	-7.37	100.99	117.20
1	C	142	SER	CA-CB-OG	-7.36	91.33	111.20
1	O	245	TYR	CB-CG-CD2	-7.35	116.59	121.00
1	C	116	GLU	CG-CD-OE1	7.35	132.99	118.30
1	C	305	PHE	CB-CG-CD1	7.33	125.94	120.80
1	O	273	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	O	193	GLN	CA-C-O	-7.31	104.75	120.10
1	C	0	THR	OG1-CB-CG2	7.30	126.79	110.00
1	C	181	TYR	CB-CA-C	-7.29	95.82	110.40
1	O	315	ARG	NE-CZ-NH1	-7.29	116.66	120.30
1	O	14	TYR	CB-CG-CD1	7.29	125.37	121.00
1	O	280	TYR	CB-CG-CD2	7.28	125.37	121.00
1	O	60	ASP	N-CA-C	-7.27	91.37	111.00
1	O	309	PHE	CB-CG-CD2	-7.27	115.71	120.80
1	C	157	ARG	C-N-CA	-7.26	103.54	121.70
1	O	178	ASN	CB-CA-C	7.26	124.93	110.40
1	O	293	PRO	N-CA-CB	7.26	112.01	103.30
1	C	47(B)	TYR	CA-CB-CG	-7.25	99.63	113.40
1	O	318	ASN	CB-CG-ND2	7.25	134.10	116.70
1	C	148	GLU	CB-CG-CD	-7.25	94.64	114.20
1	C	195	LYS	CA-CB-CG	-7.24	97.46	113.40
1	C	174	HIS	CG-CD2-NE2	-7.24	95.44	109.20
1	C	309	PHE	CG-CD2-CE2	-7.22	112.86	120.80
1	O	179	PHE	C-N-CA	7.21	139.74	121.70
1	O	232	MET	N-CA-CB	-7.21	97.62	110.60
1	O	96	VAL	CA-CB-CG2	7.21	121.72	110.90
1	C	189	VAL	CA-CB-CG2	-7.21	100.09	110.90
1	O	227	SER	O-C-N	7.20	134.23	122.70
1	O	117	PHE	CD1-CG-CD2	-7.20	108.94	118.30
1	O	227	SER	CB-CA-C	7.20	123.77	110.10
1	O	242	PHE	N-CA-CB	-7.20	97.65	110.60
1	C	184	LEU	N-CA-CB	-7.18	96.04	110.40
1	O	-1	ASN	N-CA-CB	7.18	123.52	110.60
1	O	106	GLU	OE1-CD-OE2	7.17	131.91	123.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	281(B)	LYS	CD-CE-NZ	7.17	128.19	111.70
1	C	239	LYS	N-CA-C	7.17	130.35	111.00
1	C	220	TYR	CD1-CG-CD2	-7.17	110.02	117.90
1	O	246	VAL	O-C-N	7.17	134.16	122.70
1	C	113	MET	CA-CB-CG	-7.16	101.12	113.30
1	C	105	THR	O-C-N	-7.16	111.25	122.70
1	O	208	ASP	C-N-CA	7.16	137.33	122.30
1	C	91	VAL	CG1-CB-CG2	-7.15	99.45	110.90
1	C	149	ASP	O-C-N	7.15	134.15	122.70
1	O	161	LEU	CB-CG-CD1	7.15	123.15	111.00
1	C	195	LYS	N-CA-C	7.14	130.28	111.00
1	O	207	GLU	C-N-CA	-7.14	103.85	121.70
1	O	99	GLN	CB-CA-C	-7.14	96.13	110.40
1	O	252	GLY	O-C-N	7.14	134.66	121.10
1	O	266	GLU	CG-CD-OE2	7.13	132.57	118.30
1	C	133	VAL	CB-CA-C	-7.13	97.85	111.40
1	C	281	SER	N-CA-C	7.13	130.25	111.00
1	O	94	ILE	CA-CB-CG2	-7.12	96.66	110.90
1	C	186	LYS	O-C-N	-7.11	111.32	122.70
1	C	125	PHE	N-CA-CB	-7.10	97.82	110.60
1	C	60	ASP	N-CA-CB	-7.10	97.83	110.60
1	O	96	VAL	O-C-N	-7.09	111.35	122.70
1	O	254	THR	OG1-CB-CG2	7.09	126.31	110.00
1	C	155	TYR	O-C-N	-7.08	111.36	122.70
1	C	44	LYS	CA-CB-CG	7.08	128.99	113.40
1	C	107	MET	CG-SD-CE	7.06	111.50	100.20
1	C	324	LEU	N-CA-CB	-7.06	96.28	110.40
1	C	261	HIS	O-C-N	7.06	133.99	122.70
1	C	259	SER	CB-CA-C	7.05	123.50	110.10
1	O	117	PHE	CB-CG-CD2	7.05	125.73	120.80
1	C	47(B)	TYR	CA-C-O	-7.05	105.30	120.10
1	O	76	SER	O-C-N	7.05	133.97	122.70
1	O	203	THR	N-CA-CB	7.04	123.68	110.30
1	C	308	LYS	CB-CA-C	7.03	124.45	110.40
1	C	149	ASP	CB-CG-OD2	7.03	124.62	118.30
1	O	127	GLU	CA-CB-CG	7.01	128.83	113.40
1	C	33	THR	CA-C-N	7.00	130.21	116.20
1	C	278	GLU	CB-CG-CD	7.00	133.11	114.20
1	O	80	VAL	CB-CA-C	7.00	124.71	111.40
1	O	31	PHE	CD1-CG-CD2	-6.99	109.22	118.30
1	O	197	VAL	N-CA-C	-6.99	92.14	111.00
1	C	34	GLY	O-C-N	-6.98	111.53	122.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	69	THR	CA-CB-CG2	6.96	122.15	112.40
1	O	32	ASP	CA-CB-CG	6.95	128.69	113.40
1	O	278	GLU	N-CA-CB	6.95	123.11	110.60
1	O	304	THR	CA-CB-OG1	6.95	123.59	109.00
1	O	39	TRP	CB-CG-CD1	-6.95	117.97	127.00
1	O	92	GLY	C-N-CA	-6.95	107.71	122.30
1	O	124	GLY	C-N-CA	-6.95	104.33	121.70
1	O	284	LEU	CB-CG-CD2	-6.95	99.19	111.00
1	O	-1	ASN	CA-C-O	6.94	134.68	120.10
1	O	44	LYS	CD-CE-NZ	6.94	127.66	111.70
1	O	150	VAL	N-CA-CB	-6.94	96.24	111.50
1	O	8	ASN	N-CA-CB	-6.94	98.11	110.60
1	O	142	SER	CB-CA-C	6.93	123.26	110.10
1	C	95	THR	CA-CB-CG2	-6.93	102.70	112.40
1	O	75	TYR	CD1-CE1-CZ	-6.91	113.58	119.80
1	C	17	GLU	CA-CB-CG	-6.90	98.22	113.40
1	C	46	SER	CA-CB-OG	-6.89	92.58	111.20
1	C	110	LEU	CB-CG-CD2	-6.88	99.30	111.00
1	O	164	GLN	N-CA-CB	-6.88	98.21	110.60
1	O	267	TYR	CG-CD2-CE2	6.88	126.80	121.30
1	O	267	TYR	CZ-CE2-CD2	-6.88	113.61	119.80
1	C	90	THR	CA-CB-OG1	6.87	123.43	109.00
1	O	209	GLY	O-C-N	6.87	133.69	122.70
1	O	303	ALA	N-CA-CB	-6.87	100.48	110.10
1	C	175	TYR	CE1-CZ-CE2	6.87	130.79	119.80
1	C	67	ASN	N-CA-CB	6.86	122.95	110.60
1	C	310	TYR	CB-CG-CD1	6.84	125.10	121.00
1	O	180	HIS	CA-CB-CG	-6.84	101.97	113.60
1	O	107	MET	CB-CG-SD	-6.83	91.90	112.40
1	C	22	THR	C-N-CD	-6.83	105.57	120.60
1	C	287	HIS	N-CA-CB	-6.82	98.32	110.60
1	O	185	ILE	CG1-CB-CG2	-6.82	96.39	111.40
1	O	-1	ASN	O-C-N	-6.82	111.79	122.70
1	O	112	PHE	N-CA-C	6.82	129.41	111.00
1	C	151	PHE	O-C-N	-6.81	111.80	122.70
1	C	304	THR	O-C-N	6.81	133.60	122.70
1	C	27	PHE	N-CA-CB	-6.81	98.35	110.60
1	O	17	GLU	O-C-N	6.81	133.59	122.70
1	C	235	LEU	O-C-N	-6.81	111.63	123.20
1	O	176	GLU	OE1-CD-OE2	6.80	131.46	123.30
1	O	32	ASP	N-CA-CB	-6.80	98.36	110.60
1	O	114	LEU	CB-CA-C	-6.80	97.28	110.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	179	PHE	CB-CG-CD1	6.80	125.56	120.80
1	C	56	PHE	CB-CG-CD2	-6.79	116.05	120.80
1	C	313	PHE	CG-CD2-CE2	6.78	128.26	120.80
1	O	138	ASP	CB-CG-OD1	6.78	124.41	118.30
1	O	273	ASP	CB-CG-OD1	6.78	124.40	118.30
1	O	59	SER	CA-CB-OG	-6.78	92.91	111.20
1	O	229	GLU	N-CA-CB	-6.77	98.41	110.60
1	O	130	ILE	CB-CA-C	-6.77	98.07	111.60
1	O	13	GLN	CA-C-O	-6.77	105.89	120.10
1	O	133	VAL	CG1-CB-CG2	-6.76	100.08	110.90
1	O	266	GLU	CG-CD-OE1	-6.76	104.77	118.30
1	C	319	ARG	NH1-CZ-NH2	-6.75	111.97	119.40
1	O	287	HIS	O-C-N	-6.75	111.89	122.70
1	C	222	SER	CB-CA-C	-6.75	97.27	110.10
1	C	313	PHE	CZ-CE2-CD2	-6.75	112.00	120.10
1	O	155	TYR	CG-CD1-CE1	-6.75	115.90	121.30
1	O	176	GLU	CG-CD-OE1	6.75	131.80	118.30
1	O	281(B)	LYS	CB-CG-CD	6.75	129.15	111.60
1	O	49	ALA	CB-CA-C	-6.74	99.99	110.10
1	C	26	THR	O-C-N	-6.73	111.93	122.70
1	C	65	LYS	N-CA-CB	-6.73	98.48	110.60
1	C	281(A)	SER	CB-CA-C	-6.73	97.31	110.10
1	C	251	GLU	CA-C-N	-6.73	102.74	116.20
1	C	27	PHE	CB-CG-CD2	6.73	125.51	120.80
1	C	132	ARG	CG-CD-NE	6.73	125.92	111.80
1	O	163	GLY	CA-C-O	-6.72	108.50	120.60
1	O	270	THR	CB-CA-C	-6.72	93.44	111.60
1	O	310	TYR	CA-C-O	-6.72	105.98	120.10
1	C	235	LEU	CB-CA-C	-6.72	97.43	110.20
1	O	310	TYR	N-CA-CB	-6.71	98.52	110.60
1	O	284	LEU	N-CA-CB	6.71	123.82	110.40
1	C	181	TYR	CA-C-O	-6.70	106.03	120.10
1	O	47	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	C	278	GLU	OE1-CD-OE2	-6.70	115.26	123.30
1	C	231	LEU	CB-CG-CD2	6.70	122.38	111.00
1	C	325	ALA	O-C-N	-6.69	112.00	122.70
1	O	56	PHE	CA-C-O	6.69	134.15	120.10
1	O	261	HIS	C-N-CA	-6.69	104.98	121.70
1	C	294	PRO	CA-C-O	6.68	136.23	120.20
1	C	294	PRO	O-C-N	-6.68	112.02	122.70
1	C	247	VAL	CG1-CB-CG2	6.68	121.58	110.90
1	C	326	ARG	N-CA-C	-6.67	92.98	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	181	TYR	CD1-CE1-CZ	-6.67	113.80	119.80
1	C	113	MET	O-C-N	-6.66	112.04	122.70
1	O	80	VAL	CA-CB-CG2	-6.66	100.91	110.90
1	O	47(A)	LEU	CB-CG-CD2	6.66	122.31	111.00
1	O	223	GLY	C-N-CA	-6.66	105.06	121.70
1	O	312	GLU	CG-CD-OE2	-6.66	104.99	118.30
1	C	153	PHE	CB-CG-CD1	6.65	125.46	120.80
1	C	322	PHE	CG-CD1-CE1	6.65	128.12	120.80
1	O	275	VAL	CA-CB-CG2	-6.65	100.93	110.90
1	C	157	ARG	NH1-CZ-NH2	-6.64	112.09	119.40
1	C	325	ALA	CA-C-O	6.64	134.04	120.10
1	O	204	LEU	CB-CG-CD2	6.64	122.28	111.00
1	O	97	THR	OG1-CB-CG2	-6.63	94.74	110.00
1	O	154	TYR	OH-CZ-CE2	6.62	137.96	120.10
1	O	58	ALA	N-CA-CB	6.61	119.36	110.10
1	O	183	ASN	N-CA-C	6.59	128.80	111.00
1	O	175	TYR	CB-CG-CD1	6.59	124.95	121.00
1	C	257	ASP	N-CA-CB	-6.56	98.79	110.60
1	C	4	VAL	CG1-CB-CG2	6.55	121.39	110.90
1	C	47	ARG	CB-CG-CD	-6.55	94.56	111.60
1	C	47	ARG	NH1-CZ-NH2	6.55	126.61	119.40
1	O	135	PRO	N-CA-CB	-6.54	95.40	102.60
1	O	117	PHE	CG-CD2-CE2	6.54	128.00	120.80
1	C	146	LEU	CB-CG-CD1	-6.54	99.89	111.00
1	O	67	ASN	CB-CG-OD1	-6.51	108.57	121.60
1	C	191	GLN	C-N-CA	-6.51	105.42	121.70
1	C	276	PHE	CG-CD1-CE1	6.51	127.96	120.80
1	O	9	TYR	CB-CG-CD1	6.51	124.90	121.00
1	O	35	SER	CB-CA-C	-6.51	97.74	110.10
1	C	59	SER	CA-CB-OG	-6.50	93.64	111.20
1	O	269	LEU	CB-CG-CD2	-6.50	99.95	111.00
1	O	121	VAL	CA-C-O	-6.50	106.45	120.10
1	C	116	GLU	CB-CA-C	-6.50	97.41	110.40
1	C	28	LYS	CB-CA-C	-6.49	97.41	110.40
1	C	189	VAL	CB-CA-C	-6.49	99.08	111.40
1	O	205	LEU	CB-CA-C	6.49	122.52	110.20
1	C	127	GLU	CG-CD-OE2	-6.49	105.33	118.30
1	O	110	LEU	CB-CG-CD2	-6.48	99.98	111.00
1	O	181	TYR	CA-CB-CG	-6.48	101.09	113.40
1	C	70	GLU	CG-CD-OE2	-6.48	105.35	118.30
1	O	145	VAL	N-CA-C	6.48	128.49	111.00
1	C	205	LEU	CB-CG-CD1	-6.47	100.01	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	257	ASP	CA-C-N	6.46	131.42	117.20
1	O	17	GLU	CG-CD-OE1	6.46	131.22	118.30
1	C	207	GLU	N-CA-C	6.46	128.43	111.00
1	O	299	TRP	CD1-NE1-CE2	6.45	114.81	109.00
1	C	208	ASP	CB-CA-C	-6.45	97.50	110.40
1	O	144	GLY	O-C-N	-6.45	112.38	122.70
1	O	221	ILE	N-CA-C	-6.45	93.59	111.00
1	O	181	TYR	CD1-CG-CD2	6.45	124.99	117.90
1	C	71	LEU	N-CA-CB	-6.44	97.52	110.40
1	O	15	TYR	CG-CD2-CE2	6.44	126.45	121.30
1	C	181	TYR	CA-CB-CG	-6.43	101.19	113.40
1	O	269	LEU	CB-CG-CD1	-6.43	100.07	111.00
1	O	316	ARG	NH1-CZ-NH2	-6.43	112.33	119.40
1	C	220	TYR	CG-CD1-CE1	6.43	126.44	121.30
1	O	199	VAL	N-CA-C	-6.43	93.65	111.00
1	C	173	GLN	CG-CD-OE1	-6.42	108.77	121.60
1	C	304	THR	CA-CB-OG1	6.42	122.47	109.00
1	O	59	SER	CA-C-N	-6.41	103.09	117.20
1	O	0	THR	N-CA-C	6.41	128.31	111.00
1	O	322	PHE	CA-C-N	6.41	131.30	117.20
1	O	26	THR	O-C-N	6.40	132.95	122.70
1	O	32	ASP	CB-CG-OD1	6.40	124.06	118.30
1	C	121	VAL	O-C-N	-6.40	112.33	123.20
1	C	184	LEU	C-N-CA	6.39	137.68	121.70
1	O	85	SER	O-C-N	6.39	132.93	122.70
1	O	102	GLY	O-C-N	-6.39	112.48	122.70
1	C	241	LEU	CB-CA-C	-6.38	98.07	110.20
1	O	62	SER	CA-C-N	6.38	131.24	117.20
1	C	9	TYR	CG-CD1-CE1	-6.37	116.20	121.30
1	C	228	ILE	CG1-CB-CG2	-6.36	97.40	111.40
1	O	167	LEU	CB-CG-CD1	-6.36	100.20	111.00
1	O	281(D)	LEU	N-CA-CB	-6.36	97.69	110.40
1	O	276	PHE	CD1-CE1-CZ	6.35	127.72	120.10
1	C	3	SER	CB-CA-C	-6.35	98.04	110.10
1	C	268	THR	OG1-CB-CG2	6.35	124.60	110.00
1	C	315	ARG	CD-NE-CZ	6.35	132.49	123.60
1	C	97	THR	N-CA-CB	6.35	122.36	110.30
1	O	274	TYR	N-CA-C	6.34	128.11	111.00
1	C	207	GLU	C-N-CA	-6.32	105.89	121.70
1	O	122	GLY	O-C-N	-6.32	112.59	122.70
1	C	-2	GLY	C-N-CA	-6.32	105.90	121.70
1	C	270	THR	OG1-CB-CG2	-6.31	95.48	110.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	22	THR	CA-CB-OG1	-6.31	95.74	109.00
1	O	250	ASN	CA-CB-CG	-6.31	99.51	113.40
1	C	13	GLN	CG-CD-NE2	-6.31	101.56	116.70
1	C	257	ASP	CA-C-O	-6.31	106.85	120.10
1	O	24	PRO	O-C-N	6.30	132.78	122.70
1	O	103	GLU	CA-C-O	-6.30	106.88	120.10
1	O	203	THR	OG1-CB-CG2	-6.30	95.52	110.00
1	O	310	TYR	CB-CG-CD1	6.29	124.78	121.00
1	O	304	THR	OG1-CB-CG2	-6.28	95.55	110.00
1	C	278	GLU	CG-CD-OE1	6.27	130.83	118.30
1	O	182	ILE	CA-CB-CG2	-6.26	98.37	110.90
1	O	198	SER	CA-CB-OG	-6.26	94.29	111.20
1	C	125	PHE	CD1-CE1-CZ	-6.26	112.58	120.10
1	C	251	GLU	CG-CD-OE2	6.26	130.82	118.30
1	O	62	SER	CA-CB-OG	-6.25	94.32	111.20
1	O	186	LYS	CB-CA-C	-6.25	97.90	110.40
1	C	13	GLN	CB-CG-CD	-6.25	95.36	111.60
1	C	102	GLY	O-C-N	6.24	132.69	122.70
1	O	77	THR	CA-CB-CG2	6.24	121.13	112.40
1	O	117	PHE	CB-CG-CD1	6.24	125.17	120.80
1	O	125	PHE	CB-CA-C	6.24	122.87	110.40
1	C	99	GLN	O-C-N	6.22	132.65	122.70
1	O	108	PRO	CB-CA-C	-6.21	96.47	112.00
1	C	121	VAL	CA-CB-CG2	6.19	120.19	110.90
1	O	85	SER	CA-C-O	-6.19	107.09	120.10
1	O	320	ILE	CA-C-N	6.19	128.58	116.20
1	O	33	THR	CA-C-N	-6.19	103.82	116.20
1	C	47(B)	TYR	CB-CA-C	-6.19	98.03	110.40
1	C	47(B)	TYR	CG-CD2-CE2	6.19	126.25	121.30
1	C	269	LEU	C-N-CA	6.18	137.16	121.70
1	O	145	VAL	CA-C-N	6.18	130.79	117.20
1	O	176	GLU	C-N-CA	-6.18	109.33	122.30
1	O	265	LYS	CG-CD-CE	-6.17	93.39	111.90
1	C	192	ILE	CA-CB-CG1	6.17	122.71	111.00
1	O	175	TYR	C-N-CA	-6.16	106.30	121.70
1	O	235	LEU	CA-C-O	6.16	133.03	120.10
1	O	101	PHE	CD1-CE1-CZ	-6.16	112.71	120.10
1	C	63	SER	N-CA-CB	-6.15	101.27	110.50
1	O	68	GLY	O-C-N	-6.15	112.86	122.70
1	O	143	GLN	CG-CD-OE1	6.15	133.90	121.60
1	C	81	SER	CA-CB-OG	-6.14	94.61	111.20
1	C	65	LYS	CB-CG-CD	-6.14	95.63	111.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	77	THR	CA-C-O	-6.14	107.20	120.10
1	O	50	CYS	CA-CB-SG	-6.14	102.95	114.00
1	O	313	PHE	CE1-CZ-CE2	6.14	131.05	120.00
1	C	21	GLY	N-CA-C	6.13	128.44	113.10
1	O	109	ALA	CA-C-N	-6.13	103.71	117.20
1	O	254	THR	O-C-N	-6.13	112.89	122.70
1	O	39	TRP	N-CA-CB	6.13	121.63	110.60
1	C	155	TYR	CG-CD1-CE1	-6.11	116.41	121.30
1	O	61	SER	CA-C-N	-6.11	103.76	117.20
1	C	112	PHE	CD1-CE1-CZ	6.11	127.43	120.10
1	C	67	ASN	CB-CG-OD1	-6.11	109.39	121.60
1	O	117	PHE	CB-CA-C	-6.10	98.20	110.40
1	O	186	LYS	CB-CG-CD	6.09	127.45	111.60
1	O	32	ASP	CB-CA-C	-6.09	98.21	110.40
1	O	64	TYR	CB-CG-CD1	-6.08	117.35	121.00
1	O	182	ILE	CA-CB-CG1	6.08	122.55	111.00
1	O	12	THR	CA-C-N	6.08	130.57	117.20
1	O	301	LEU	N-CA-CB	-6.08	98.25	110.40
1	C	74	ARG	O-C-N	-6.07	112.98	122.70
1	O	324	LEU	CB-CG-CD2	-6.07	100.67	111.00
1	O	326	ARG	N-CA-CB	-6.07	99.67	110.60
1	C	46	SER	CB-CA-C	-6.07	98.56	110.10
1	C	107	MET	CB-CG-SD	6.06	130.58	112.40
1	C	178	ASN	CB-CG-OD1	-6.06	109.48	121.60
1	O	100	MET	N-CA-CB	-6.06	99.69	110.60
1	O	235	LEU	N-CA-CB	-6.05	98.29	110.40
1	O	246	VAL	C-N-CA	6.05	136.83	121.70
1	C	161	LEU	CA-CB-CG	-6.05	101.39	115.30
1	O	220	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	O	240	ARG	CG-CD-NE	-6.04	99.11	111.80
1	O	272	ALA	CA-C-O	-6.04	107.41	120.10
1	C	179	PHE	CB-CG-CD1	6.03	125.02	120.80
1	C	283	THR	CA-CB-OG1	-6.03	96.33	109.00
1	O	47(B)	TYR	CB-CA-C	-6.02	98.35	110.40
1	O	83	PHE	CG-CD1-CE1	6.02	127.42	120.80
1	O	112	PHE	CE1-CZ-CE2	6.02	130.84	120.00
1	C	17	GLU	CG-CD-OE2	6.01	130.32	118.30
1	O	250	ASN	CB-CA-C	6.01	122.42	110.40
1	C	287	HIS	C-N-CA	-6.01	106.68	121.70
1	O	156	ASN	C-N-CA	6.01	136.72	121.70
1	O	208	ASP	O-C-N	6.01	133.42	123.20
1	O	292	PRO	O-C-N	6.01	132.52	121.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	SER	CA-C-N	-6.01	103.98	117.20
1	O	232	MET	CA-CB-CG	6.01	123.51	113.30
1	C	213	LEU	CD1-CG-CD2	-6.00	92.49	110.50
1	C	35	SER	N-CA-CB	6.00	119.50	110.50
1	C	174	HIS	CE1-NE2-CD2	6.00	121.60	106.60
1	O	81	SER	CA-C-O	-6.00	107.50	120.10
1	C	89	ILE	CA-CB-CG2	-6.00	98.91	110.90
1	O	35	SER	CA-C-N	-5.99	104.02	117.20
1	C	137	PHE	CZ-CE2-CD2	-5.99	112.91	120.10
1	O	106	GLU	CB-CA-C	-5.99	98.42	110.40
1	O	260	PHE	CD1-CG-CD2	-5.99	110.52	118.30
1	C	258	ILE	CA-CB-CG1	-5.99	99.63	111.00
1	O	64	TYR	CD1-CE1-CZ	5.99	125.19	119.80
1	C	244	ASP	CA-C-O	-5.98	107.54	120.10
1	O	180	HIS	N-CA-CB	5.98	121.36	110.60
1	O	230	LYS	N-CA-CB	-5.98	99.84	110.60
1	C	279	SER	N-CA-CB	-5.98	101.54	110.50
1	O	58	ALA	CA-C-O	5.97	132.64	120.10
1	O	213	LEU	N-CA-CB	-5.97	98.46	110.40
1	C	22	THR	CA-C-O	-5.96	107.58	120.10
1	C	246	VAL	N-CA-CB	-5.96	98.38	111.50
1	C	232	MET	CA-C-O	5.96	132.62	120.10
1	C	193	GLN	N-CA-CB	-5.96	99.88	110.60
1	O	100	MET	CA-C-O	5.96	132.61	120.10
1	O	38	VAL	CG1-CB-CG2	-5.95	101.37	110.90
1	C	23	PRO	O-C-N	5.95	132.41	121.10
1	C	190	TRP	CD1-CG-CD2	-5.95	101.54	106.30
1	C	70	GLU	CA-CB-CG	5.94	126.46	113.40
1	C	90	THR	CA-CB-CG2	-5.93	104.09	112.40
1	O	30	VAL	CB-CA-C	-5.93	100.13	111.40
1	C	44	LYS	CG-CD-CE	5.93	129.69	111.90
1	O	13	GLN	CB-CA-C	-5.93	98.54	110.40
1	C	315	ARG	O-C-N	5.92	132.18	122.70
1	C	122	GLY	CA-C-O	5.92	131.26	120.60
1	O	281	SER	CB-CA-C	-5.92	98.85	110.10
1	O	17	GLU	OE1-CD-OE2	5.92	130.40	123.30
1	O	112	PHE	CG-CD1-CE1	-5.92	114.29	120.80
1	O	318	ASN	N-CA-CB	-5.92	99.94	110.60
1	O	143	GLN	CB-CA-C	-5.92	98.56	110.40
1	C	299	TRP	CD2-CE3-CZ3	-5.91	111.12	118.80
1	O	304	THR	CA-CB-CG2	-5.91	104.13	112.40
1	C	183	ASN	CB-CG-ND2	-5.91	102.53	116.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	240	ARG	CB-CA-C	5.90	122.20	110.40
1	C	281(B)	LYS	CG-CD-CE	5.90	129.59	111.90
1	C	325	ALA	N-CA-CB	-5.89	101.86	110.10
1	C	73	LEU	CB-CG-CD1	5.89	121.01	111.00
1	C	194	MET	O-C-N	-5.89	113.28	122.70
1	C	18	ILE	O-C-N	5.88	133.20	123.20
1	C	110	LEU	N-CA-C	-5.88	95.12	111.00
1	O	14	TYR	CD1-CE1-CZ	5.88	125.09	119.80
1	O	238	LYS	CB-CG-CD	5.88	126.88	111.60
1	C	91	VAL	O-C-N	-5.87	113.22	123.20
1	O	189	VAL	CB-CA-C	-5.87	100.25	111.40
1	O	238	LYS	CD-CE-NZ	5.87	125.21	111.70
1	C	104	VAL	CA-CB-CG1	5.87	119.70	110.90
1	O	257	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	O	70	GLU	CA-CB-CG	-5.86	100.50	113.40
1	C	9	TYR	CZ-CE2-CD2	-5.86	114.53	119.80
1	O	117	PHE	CG-CD1-CE1	5.85	127.24	120.80
1	O	231	LEU	CB-CG-CD2	5.85	120.94	111.00
1	C	25	GLN	CA-C-N	5.82	130.01	117.20
1	O	150	VAL	CA-CB-CG1	5.82	119.64	110.90
1	O	292	PRO	N-CA-C	5.82	127.24	112.10
1	C	191	GLN	CB-CA-C	5.82	122.04	110.40
1	C	139	ASN	CB-CG-OD1	-5.82	109.96	121.60
1	C	230	LYS	CG-CD-CE	5.82	129.34	111.90
1	C	199	VAL	CG1-CB-CG2	5.81	120.20	110.90
1	O	133	VAL	CA-CB-CG2	5.81	119.62	110.90
1	C	250	ASN	N-CA-CB	-5.81	100.14	110.60
1	O	325	ALA	O-C-N	5.81	131.99	122.70
1	O	101	PHE	CB-CG-CD1	-5.80	116.74	120.80
1	C	191	GLN	N-CA-CB	-5.80	100.17	110.60
1	C	249	CYS	N-CA-CB	5.80	121.03	110.60
1	O	158	ASP	O-C-N	5.79	131.97	122.70
1	O	62	SER	CB-CA-C	-5.79	99.09	110.10
1	O	191	GLN	CA-CB-CG	5.79	126.14	113.40
1	C	231	LEU	CB-CG-CD1	5.79	120.84	111.00
1	O	72	THR	OG1-CB-CG2	5.79	123.31	110.00
1	O	284	LEU	CB-CG-CD1	-5.79	101.16	111.00
1	C	52	TYR	CZ-CE2-CD2	-5.78	114.59	119.80
1	O	45	CYS	C-N-CA	-5.78	107.24	121.70
1	C	14	TYR	CA-CB-CG	5.78	124.38	113.40
1	O	226	SER	C-N-CA	-5.78	107.25	121.70
1	O	199	VAL	CG1-CB-CG2	-5.77	101.67	110.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	77	THR	CB-CA-C	-5.77	96.03	111.60
1	C	235	LEU	C-N-CA	-5.75	110.22	122.30
1	O	100	MET	C-N-CA	-5.75	107.31	121.70
1	O	281	SER	N-CA-CB	5.75	119.13	110.50
1	C	155	TYR	CE1-CZ-CE2	-5.75	110.60	119.80
1	O	120	VAL	CA-CB-CG1	5.75	119.53	110.90
1	O	219	SER	CA-CB-OG	5.75	126.72	111.20
1	O	75	TYR	N-CA-C	-5.75	95.48	111.00
1	O	134	THR	CB-CA-C	-5.75	96.08	111.60
1	C	284	LEU	CA-C-O	5.73	132.14	120.10
1	O	258	ILE	N-CA-C	-5.73	95.52	111.00
1	C	263	GLY	O-C-N	-5.73	113.46	123.20
1	C	164	GLN	CB-CA-C	-5.73	98.95	110.40
1	C	32	ASP	CB-CG-OD2	5.72	123.45	118.30
1	O	239	LYS	C-N-CA	-5.72	107.39	121.70
1	O	90	THR	OG1-CB-CG2	-5.72	96.84	110.00
1	O	189	VAL	N-CA-CB	5.72	124.08	111.50
1	O	38	VAL	CA-CB-CG2	5.72	119.48	110.90
1	O	51	VAL	CA-C-O	5.72	132.10	120.10
1	C	165	ILE	CA-CB-CG2	5.71	122.32	110.90
1	C	323	ALA	N-CA-C	-5.71	95.58	111.00
1	O	228	ILE	N-CA-CB	5.71	123.94	110.80
1	C	284	LEU	O-C-N	-5.71	113.56	122.70
1	O	193	GLN	CA-CB-CG	5.71	125.95	113.40
1	C	285	ALA	C-N-CA	5.70	135.96	121.70
1	O	249	CYS	CB-CA-C	5.70	121.80	110.40
1	O	15	TYR	CE1-CZ-CE2	5.70	128.92	119.80
1	O	322	PHE	CG-CD2-CE2	5.70	127.07	120.80
1	C	32	ASP	CA-CB-CG	5.70	125.93	113.40
1	O	207	GLU	CB-CA-C	-5.69	99.01	110.40
1	O	183	ASN	CB-CA-C	5.69	121.78	110.40
1	C	112	PHE	CG-CD2-CE2	5.69	127.06	120.80
1	O	260	PHE	CG-CD2-CE2	5.69	127.05	120.80
1	C	86	GLN	O-C-N	5.68	131.80	122.70
1	O	18	ILE	CG1-CB-CG2	-5.68	98.89	111.40
1	C	207	GLU	CA-CB-CG	-5.68	100.90	113.40
1	O	22	THR	CA-CB-CG2	-5.68	104.45	112.40
1	C	173	GLN	CB-CG-CD	5.68	126.36	111.60
1	O	249	CYS	N-CA-CB	5.68	120.82	110.60
1	C	267	TYR	CG-CD2-CE2	5.67	125.84	121.30
1	O	165	ILE	CA-CB-CG2	5.67	122.24	110.90
1	O	231	LEU	N-CA-CB	-5.67	99.06	110.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	237	ALA	O-C-N	5.67	131.77	122.70
1	O	148	GLU	CA-CB-CG	-5.67	100.93	113.40
1	O	190	TRP	N-CA-CB	5.67	120.80	110.60
1	O	204	LEU	C-N-CA	-5.67	107.54	121.70
1	O	22	THR	CB-CA-C	-5.66	96.31	111.60
1	O	240	ARG	CA-C-N	-5.66	104.74	117.20
1	C	201	SER	O-C-N	5.66	131.76	122.70
1	C	185	ILE	CA-C-N	5.65	129.64	117.20
1	O	120	VAL	CB-CA-C	5.65	122.14	111.40
1	C	293	PRO	CA-CB-CG	-5.64	93.28	104.00
1	O	215	ASP	CB-CG-OD1	5.64	123.37	118.30
1	C	158	ASP	C-N-CA	5.63	135.77	121.70
1	C	59	SER	CA-C-O	5.63	131.92	120.10
1	C	148	GLU	CG-CD-OE2	-5.62	107.06	118.30
1	O	274	TYR	CD1-CE1-CZ	-5.62	114.74	119.80
1	C	47(A)	LEU	N-CA-C	-5.62	95.84	111.00
1	C	141	ILE	O-C-N	-5.61	113.72	122.70
1	O	94	ILE	CG1-CB-CG2	-5.61	99.05	111.40
1	C	200	GLY	CA-C-O	5.61	130.69	120.60
1	C	54	LYS	CD-CE-NZ	5.61	124.59	111.70
1	O	160(D)	SER	CA-C-N	5.61	129.53	117.20
1	C	59	SER	O-C-N	-5.60	113.74	122.70
1	O	99	GLN	O-C-N	5.60	131.66	122.70
1	O	156	ASN	O-C-N	-5.60	113.74	122.70
1	C	47	ARG	CD-NE-CZ	5.59	131.43	123.60
1	O	253	PRO	CB-CA-C	-5.59	98.02	112.00
1	C	155	TYR	CZ-CE2-CD2	5.59	124.83	119.80
1	O	190	TRP	CB-CG-CD2	5.59	133.87	126.60
1	C	239	LYS	O-C-N	-5.59	113.76	122.70
1	O	137	PHE	O-C-N	-5.59	113.76	122.70
1	O	75	TYR	CG-CD1-CE1	5.59	125.77	121.30
1	O	137	PHE	CD1-CE1-CZ	-5.59	113.40	120.10
1	O	154	TYR	CZ-CE2-CD2	-5.58	114.77	119.80
1	C	244	ASP	N-CA-CB	-5.58	100.55	110.60
1	O	133	VAL	CA-CB-CG1	-5.58	102.53	110.90
1	O	299	TRP	NE1-CE2-CD2	-5.58	101.72	107.30
1	O	226	SER	CB-CA-C	-5.58	99.50	110.10
1	O	279	SER	CA-CB-OG	5.58	126.27	111.20
1	O	311	THR	CA-CB-OG1	-5.58	97.29	109.00
1	C	125	PHE	CB-CG-CD1	5.58	124.70	120.80
1	C	128	GLN	CA-C-O	5.58	131.81	120.10
1	C	165	ILE	CB-CA-C	-5.57	100.45	111.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	84	LEU	C-N-CA	-5.57	107.76	121.70
1	O	212	ALA	CA-C-O	-5.57	108.41	120.10
1	C	120	VAL	N-CA-CB	-5.57	99.25	111.50
1	O	266	GLU	CA-CB-CG	5.57	125.65	113.40
1	C	110	LEU	N-CA-CB	-5.56	99.27	110.40
1	O	207	GLU	OE1-CD-OE2	5.56	129.97	123.30
1	C	304	THR	CA-C-N	-5.55	104.98	117.20
1	C	47	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	O	255	LEU	CD1-CG-CD2	-5.55	93.86	110.50
1	O	164	GLN	CB-CG-CD	-5.54	97.19	111.60
1	C	255	LEU	CB-CG-CD1	5.54	120.42	111.00
1	C	176	GLU	CA-C-O	5.54	131.72	120.10
1	O	205	LEU	CB-CG-CD1	-5.54	101.59	111.00
1	C	185	ILE	CG1-CB-CG2	-5.53	99.23	111.40
1	C	16	GLY	N-CA-C	-5.53	99.28	113.10
1	C	171	ASP	CB-CG-OD1	5.52	123.27	118.30
1	O	121	VAL	CA-CB-CG1	5.52	119.18	110.90
1	C	230	LYS	CB-CA-C	-5.52	99.36	110.40
1	C	80	VAL	N-CA-C	-5.51	96.11	111.00
1	C	45	CYS	CB-CA-C	-5.51	99.38	110.40
1	C	190	TRP	CE2-CD2-CE3	-5.51	112.09	118.70
1	O	213	LEU	N-CA-C	-5.51	96.13	111.00
1	C	117	PHE	N-CA-CB	-5.51	100.69	110.60
1	C	274	TYR	CB-CG-CD1	5.51	124.30	121.00
1	C	291	ILE	N-CA-C	-5.50	96.15	111.00
1	C	254	THR	N-CA-CB	-5.50	99.85	110.30
1	O	114	LEU	CA-C-N	5.50	129.30	117.20
1	O	282	CYS	O-C-N	-5.50	113.90	122.70
1	C	7	THR	CA-CB-CG2	5.50	120.10	112.40
1	C	173	GLN	O-C-N	5.49	131.49	122.70
1	O	99	GLN	CA-C-N	-5.49	105.12	117.20
1	C	99	GLN	CB-CA-C	5.49	121.37	110.40
1	O	249	CYS	CA-CB-SG	-5.48	104.13	114.00
1	C	65	LYS	O-C-N	5.48	131.47	122.70
1	O	100	MET	O-C-N	-5.48	113.93	122.70
1	O	148	GLU	CG-CD-OE1	5.48	129.26	118.30
1	C	242	PHE	CZ-CE2-CD2	-5.48	113.53	120.10
1	O	106	GLU	CG-CD-OE2	-5.47	107.35	118.30
1	C	201	SER	CB-CA-C	-5.47	99.70	110.10
1	O	94	ILE	CA-C-O	-5.46	108.62	120.10
1	O	170	SER	CA-C-N	5.46	129.22	117.20
1	O	75	TYR	CB-CA-C	5.46	121.33	110.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4	VAL	O-C-N	-5.46	113.96	122.70
1	C	240	ARG	CD-NE-CZ	5.46	131.24	123.60
1	C	319	ARG	CG-CD-NE	-5.45	100.35	111.80
1	C	48	THR	CB-CA-C	5.45	126.31	111.60
1	O	147	LYS	CD-CE-NZ	5.44	124.22	111.70
1	O	13	GLN	O-C-N	5.44	131.41	122.70
1	O	125	PHE	CB-CG-CD1	-5.44	116.99	120.80
1	O	128	GLN	CA-C-N	5.44	129.17	117.20
1	C	-1	ASN	N-CA-CB	5.44	120.39	110.60
1	C	280	TYR	CB-CG-CD1	-5.44	117.74	121.00
1	O	101	PHE	CG-CD2-CE2	-5.43	114.82	120.80
1	C	84	LEU	CD1-CG-CD2	-5.41	94.26	110.50
1	C	196	GLY	CA-C-N	5.41	129.10	117.20
1	O	303	ALA	CB-CA-C	-5.41	101.99	110.10
1	C	233	GLU	O-C-N	5.40	131.35	122.70
1	O	178	ASN	CA-C-N	5.40	129.08	117.20
1	C	267	TYR	CB-CA-C	5.40	121.19	110.40
1	C	20	ILE	CA-CB-CG1	5.39	121.25	111.00
1	C	315	ARG	NH1-CZ-NH2	5.39	125.33	119.40
1	C	25	GLN	CB-CG-CD	5.39	125.61	111.60
1	O	311	THR	CA-CB-CG2	5.39	119.94	112.40
1	C	306	ILE	CA-CB-CG1	5.38	121.23	111.00
1	O	33	THR	CA-CB-CG2	-5.38	104.86	112.40
1	O	179	PHE	CZ-CE2-CD2	5.38	126.56	120.10
1	C	245	TYR	OH-CZ-CE2	-5.38	105.59	120.10
1	O	145	VAL	C-N-CA	-5.38	108.26	121.70
1	C	110	LEU	CA-C-O	-5.37	108.82	120.10
1	O	13	GLN	CG-CD-OE1	-5.37	110.85	121.60
1	O	156	ASN	CA-C-O	5.37	131.38	120.10
1	C	201	SER	CA-C-O	-5.37	108.83	120.10
1	O	310	TYR	CE1-CZ-CE2	-5.36	111.22	119.80
1	C	13	GLN	OE1-CD-NE2	5.36	134.23	121.90
1	C	137	PHE	CG-CD2-CE2	5.36	126.70	120.80
1	C	267	TYR	CE1-CZ-CE2	5.35	128.36	119.80
1	O	29	VAL	N-CA-CB	5.35	123.28	111.50
1	O	212	ALA	N-CA-CB	-5.35	102.61	110.10
1	O	307	ARG	CB-CA-C	5.35	121.10	110.40
1	C	124	GLY	O-C-N	-5.35	114.15	122.70
1	C	130	ILE	CA-CB-CG1	-5.34	100.85	111.00
1	O	80	VAL	CA-CB-CG1	5.34	118.92	110.90
1	O	246	VAL	CA-C-N	-5.34	105.44	117.20
1	O	298	THR	CA-CB-CG2	-5.34	104.92	112.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	72	THR	OG1-CB-CG2	5.34	122.29	110.00
1	C	282	CYS	C-N-CA	-5.34	108.35	121.70
1	C	316	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	C	281(C)	LYS	N-CA-C	-5.32	96.63	111.00
1	C	324	LEU	CB-CG-CD1	5.32	120.05	111.00
1	O	314	ASP	O-C-N	5.32	131.21	122.70
1	C	112	PHE	CZ-CE2-CD2	-5.32	113.72	120.10
1	O	278	GLU	O-C-N	5.32	131.21	122.70
1	O	31	PHE	CE1-CZ-CE2	-5.31	110.44	120.00
1	O	179	PHE	CG-CD1-CE1	5.31	126.64	120.80
1	O	72	THR	CA-CB-OG1	-5.31	97.85	109.00
1	O	289	MET	N-CA-CB	5.31	120.16	110.60
1	O	232	MET	CG-SD-CE	5.31	108.69	100.20
1	C	179	PHE	CB-CG-CD2	-5.31	117.09	120.80
1	C	226	SER	CA-CB-OG	-5.30	96.88	111.20
1	O	320	ILE	N-CA-CB	-5.30	98.61	110.80
1	O	195	LYS	CA-C-N	5.30	126.79	116.20
1	O	13	GLN	C-N-CA	5.29	134.93	121.70
1	C	301	LEU	CA-C-N	5.29	126.78	116.20
1	O	19	GLY	N-CA-C	-5.29	99.87	113.10
1	O	157	ARG	CA-C-N	5.29	128.84	117.20
1	C	307	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	C	296	GLY	N-CA-C	-5.29	99.89	113.10
1	C	318	ASN	C-N-CA	-5.29	108.48	121.70
1	O	157	ARG	CB-CG-CD	5.28	125.33	111.60
1	C	117	PHE	CB-CG-CD1	5.28	124.50	120.80
1	O	278	GLU	CA-C-N	5.28	128.82	117.20
1	O	285	ALA	CB-CA-C	5.28	118.02	110.10
1	C	115	ALA	N-CA-CB	-5.27	102.72	110.10
1	C	130	ILE	N-CA-CB	-5.27	98.68	110.80
1	O	31	PHE	CD1-CE1-CZ	5.27	126.42	120.10
1	O	52	TYR	CZ-CE2-CD2	-5.26	115.06	119.80
1	O	220	TYR	CD1-CE1-CZ	-5.26	115.06	119.80
1	C	14	TYR	CD1-CG-CD2	-5.26	112.11	117.90
1	C	183	ASN	CB-CG-OD1	5.26	132.12	121.60
1	C	208	ASP	N-CA-CB	-5.26	101.13	110.60
1	O	279	SER	CB-CA-C	-5.26	100.11	110.10
1	C	295	THR	N-CA-CB	-5.26	100.31	110.30
1	O	199	VAL	CA-C-N	-5.26	105.69	116.20
1	C	75	TYR	CG-CD2-CE2	-5.25	117.10	121.30
1	C	52	TYR	CB-CG-CD1	5.25	124.15	121.00
1	C	159	SER	CA-C-O	-5.25	109.07	120.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	184	LEU	CB-CG-CD2	-5.25	102.08	111.00
1	C	115	ALA	O-C-N	-5.24	114.31	122.70
1	C	212	ALA	CB-CA-C	5.24	117.97	110.10
1	C	263	GLY	CA-C-O	5.24	130.04	120.60
1	O	92	GLY	CA-C-O	5.24	130.04	120.60
1	O	112	PHE	CG-CD2-CE2	5.24	126.56	120.80
1	O	28	LYS	N-CA-CB	5.24	120.03	110.60
1	O	279	SER	N-CA-CB	-5.24	102.64	110.50
1	C	260	PHE	CA-C-O	5.23	131.09	120.10
1	O	58	ALA	C-N-CA	-5.23	108.62	121.70
1	O	111	PRO	C-N-CA	-5.23	108.62	121.70
1	C	155	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	C	123	MET	N-CA-CB	5.23	120.01	110.60
1	C	294	PRO	N-CA-C	-5.23	98.51	112.10
1	C	199	VAL	O-C-N	-5.22	114.32	123.20
1	O	215	ASP	N-CA-CB	-5.22	101.20	110.60
1	O	323	ALA	N-CA-CB	5.21	117.40	110.10
1	C	274	TYR	CZ-CE2-CD2	5.21	124.49	119.80
1	O	207	GLU	CG-CD-OE2	-5.21	107.88	118.30
1	C	167	LEU	CD1-CG-CD2	-5.21	94.87	110.50
1	O	148	GLU	CG-CD-OE2	-5.21	107.89	118.30
1	O	292	PRO	N-CD-CG	-5.21	95.39	103.20
1	C	70	GLU	CG-CD-OE1	5.20	128.71	118.30
1	C	111	PRO	N-CA-CB	-5.20	96.88	102.60
1	C	108	PRO	CA-CB-CG	-5.20	94.13	104.00
1	O	1	THR	N-CA-CB	-5.20	100.43	110.30
1	C	166	VAL	O-C-N	5.19	131.00	122.70
1	O	47	ARG	CA-C-O	5.19	131.00	120.10
1	C	280	TYR	CZ-CE2-CD2	-5.19	115.13	119.80
1	C	281(B)	LYS	CD-CE-NZ	5.18	123.62	111.70
1	C	-2	GLY	CA-C-O	-5.18	111.28	120.60
1	C	13	GLN	CB-CA-C	-5.18	100.04	110.40
1	C	179	PHE	C-N-CA	5.18	134.65	121.70
1	C	245	TYR	O-C-N	-5.18	114.42	122.70
1	C	312	GLU	CG-CD-OE1	5.17	128.65	118.30
1	C	188	GLY	N-CA-C	-5.17	100.18	113.10
1	O	263	GLY	O-C-N	-5.17	114.42	123.20
1	C	255	LEU	CA-CB-CG	-5.16	103.42	115.30
1	O	242	PHE	CB-CG-CD1	5.16	124.41	120.80
1	O	134	THR	O-C-N	5.16	130.91	121.10
1	O	203	THR	CA-C-O	5.16	130.94	120.10
1	O	225	THR	CA-CB-CG2	-5.16	105.18	112.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	294	PRO	CA-N-CD	5.16	118.92	111.70
1	C	91	VAL	CA-CB-CG2	-5.16	103.16	110.90
1	C	106	GLU	CG-CD-OE1	5.15	128.60	118.30
1	C	192	ILE	CG1-CB-CG2	5.14	122.71	111.40
1	O	52	TYR	N-CA-CB	-5.14	101.34	110.60
1	O	26	THR	CA-C-O	-5.14	109.31	120.10
1	O	144	GLY	CA-C-N	5.14	128.50	117.20
1	O	247	VAL	N-CA-CB	-5.14	100.20	111.50
1	O	120	VAL	CA-CB-CG2	-5.13	103.20	110.90
1	C	57	ASP	C-N-CA	-5.12	108.89	121.70
1	O	155	TYR	N-CA-CB	-5.12	101.38	110.60
1	C	215	ASP	N-CA-CB	-5.12	101.38	110.60
1	O	165	ILE	CB-CA-C	-5.12	101.36	111.60
1	C	181	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	C	313	PHE	N-CA-CB	-5.12	101.39	110.60
1	O	127	GLU	CG-CD-OE1	5.12	128.53	118.30
1	O	45	CYS	CA-CB-SG	-5.11	104.80	114.00
1	C	110	LEU	CA-CB-CG	-5.11	103.55	115.30
1	O	72	THR	CA-C-N	5.10	128.43	117.20
1	O	308	LYS	CA-CB-CG	-5.10	102.17	113.40
1	C	100	MET	CG-SD-CE	-5.10	92.04	100.20
1	C	233	GLU	OE1-CD-OE2	5.10	129.42	123.30
1	C	313	PHE	CA-C-N	5.10	128.42	117.20
1	C	39	TRP	CB-CA-C	-5.09	100.21	110.40
1	C	217	GLY	C-N-CA	5.09	134.43	121.70
1	C	238	LYS	CA-CB-CG	-5.09	102.19	113.40
1	C	267	TYR	CB-CG-CD1	-5.09	117.94	121.00
1	C	309	PHE	CB-CG-CD1	5.09	124.37	120.80
1	C	205	LEU	C-N-CA	5.08	134.40	121.70
1	C	42	SER	CB-CA-C	-5.08	100.45	110.10
1	C	297	PRO	O-C-N	5.08	130.82	122.70
1	O	247	VAL	CB-CA-C	5.08	121.05	111.40
1	C	229	GLU	N-CA-CB	-5.08	101.46	110.60
1	O	75	TYR	CZ-CE2-CD2	5.07	124.36	119.80
1	C	160(D)	SER	N-CA-CB	-5.06	102.91	110.50
1	O	125	PHE	CE1-CZ-CE2	5.06	129.11	120.00
1	C	318	ASN	N-CA-C	5.06	124.66	111.00
1	C	254	THR	OG1-CB-CG2	5.06	121.63	110.00
1	O	114	LEU	N-CA-CB	5.06	120.51	110.40
1	C	23	PRO	N-CD-CG	-5.05	95.62	103.20
1	O	191	GLN	C-N-CA	-5.05	109.06	121.70
1	O	41	PRO	CA-CB-CG	5.05	114.40	104.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	280	TYR	CD1-CE1-CZ	-5.05	115.26	119.80
1	C	245	TYR	CE1-CZ-OH	5.05	133.72	120.10
1	O	48	THR	CA-CB-OG1	5.05	119.60	109.00
1	C	314	ASP	CA-C-O	5.04	130.68	120.10
1	C	67	ASN	O-C-N	-5.04	114.64	123.20
1	C	267	TYR	CD1-CE1-CZ	-5.04	115.27	119.80
1	O	87	ASP	CA-CB-CG	-5.03	102.33	113.40
1	O	314	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	O	27	PHE	C-N-CA	5.03	134.28	121.70
1	O	180	HIS	O-C-N	-5.03	114.65	122.70
1	O	210	CYS	CB-CA-C	5.03	120.46	110.40
1	C	292	PRO	CA-CB-CG	-5.03	94.45	104.00
1	O	238	LYS	CG-CD-CE	5.02	126.97	111.90
1	C	152	SER	CA-C-O	-5.02	109.56	120.10
1	C	22	THR	C-N-CA	5.02	143.08	122.00
1	O	44	LYS	N-CA-CB	5.02	119.63	110.60
1	O	110	LEU	CB-CA-C	-5.02	100.67	110.20
1	C	88	ILE	CA-CB-CG1	-5.01	101.48	111.00
1	O	175	TYR	CD1-CE1-CZ	-5.01	115.29	119.80
1	O	237	ALA	N-CA-CB	5.01	117.12	110.10
1	O	323	ALA	CA-C-O	-5.01	109.58	120.10
1	C	-1	ASN	CA-CB-CG	-5.01	102.38	113.40
1	O	136	ILE	CA-C-N	5.00	128.21	117.20
1	C	268	THR	CB-CA-C	-5.00	98.10	111.60
1	O	208	ASP	CB-CG-OD1	5.00	122.80	118.30

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	182	ILE	CB
1	C	311	THR	CB
1	O	156	ASN	CA
1	O	183	ASN	CA
1	O	202	SER	CA
1	O	208	ASP	CA
1	O	249	CYS	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	154	TYR	Sidechain
1	C	220	TYR	Sidechain

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	O	157	ARG	Mainchain
1	O	272	ALA	Mainchain
1	O	310	TYR	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	C	2567	0	2487	301	0
1	O	2557	0	2486	371	0
2	C	35	0	43	11	0
2	O	35	0	43	15	0
3	C	15	0	0	3	0
3	O	7	0	0	2	0
All	All	5216	0	5059	674	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 66.

All (674) 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:C:186:LYS:CE	1:C:186:LYS:CD	1.75	1.64
1:C:186:LYS:CG	1:C:186:LYS:CD	1.76	1.61
1:O:204:LEU:CB	1:O:204:LEU:CG	1.79	1.60
1:C:281(C):LYS:CD	1:C:281(C):LYS:CE	1.76	1.59
1:O:173:GLN:CG	1:O:173:GLN:CB	1.76	1.59
1:O:204:LEU:CG	1:O:204:LEU:CD2	1.81	1.58
1:O:238:LYS:CD	1:O:238:LYS:CG	1.75	1.57
1:C:281(B):LYS:CD	1:C:281(B):LYS:CG	1.78	1.57
1:O:186:LYS:CB	1:O:186:LYS:CG	1.82	1.57
1:C:44:LYS:CD	1:C:44:LYS:CE	1.82	1.57
1:O:239:LYS:CD	1:O:239:LYS:CE	1.76	1.56
1:C:186:LYS:CA	1:C:186:LYS:CB	1.75	1.56
1:C:265:LYS:CE	1:C:265:LYS:NZ	1.67	1.55
1:O:251:GLU:CA	1:O:251:GLU:CB	1.80	1.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:GLU:CD	1:C:278:GLU:CG	1.75	1.54
1:C:248:LYS:NZ	1:C:248:LYS:CE	1.67	1.54
1:C:44:LYS:NZ	1:C:44:LYS:CE	1.72	1.53
1:O:147:LYS:CD	1:O:147:LYS:CG	1.81	1.53
1:C:208:ASP:N	1:C:208:ASP:CA	1.68	1.52
1:O:251:GLU:CD	1:O:251:GLU:CG	1.77	1.51
1:O:230:LYS:CD	1:O:230:LYS:CE	1.80	1.51
1:O:160(D):SER:N	1:O:160(D):SER:CA	1.69	1.51
1:O:238:LYS:CE	1:O:238:LYS:NZ	1.72	1.50
1:O:178:ASN:CB	1:O:178:ASN:CG	1.76	1.50
1:O:316:ARG:NH1	1:O:316:ARG:CZ	1.72	1.50
1:O:158:ASP:CB	1:O:158:ASP:CG	1.78	1.49
1:C:281(C):LYS:CE	1:C:281(C):LYS:NZ	1.72	1.48
1:O:281(B):LYS:CE	1:O:281(B):LYS:NZ	1.73	1.47
1:O:44:LYS:NZ	1:O:44:LYS:CE	1.75	1.45
1:C:238:LYS:NZ	1:C:238:LYS:CE	1.78	1.45
1:O:173:GLN:CG	1:O:173:GLN:CD	1.84	1.44
1:C:226:SER:CB	1:C:226:SER:OG	1.64	1.44
1:O:173:GLN:NE2	1:O:173:GLN:CD	1.68	1.43
1:C:224:SER:CB	1:C:224:SER:OG	1.63	1.43
1:O:230:LYS:CE	1:O:230:LYS:NZ	1.80	1.42
1:O:158:ASP:CG	1:O:158:ASP:OD1	1.63	1.36
1:O:202:SER:OG	1:O:202:SER:CB	1.74	1.32
1:C:47:ARG:HE	1:C:47:ARG:N	1.36	1.22
1:C:47:ARG:NE	1:C:47:ARG:H	1.39	1.21
1:C:250:ASN:HD22	1:C:251:GLU:N	1.39	1.20
1:C:205:LEU:HD12	1:C:227:SER:HB3	1.30	1.11
1:O:279:SER:OG	1:O:281(C):LYS:HD3	1.48	1.09
1:C:88:ILE:HG22	1:C:97:THR:HG22	1.14	1.09
1:O:194:MET:HE2	1:O:197:VAL:HG22	1.41	1.03
1:O:-1:ASN:HA	1:O:147:LYS:HD2	1.36	1.02
1:C:49:ALA:HA	1:C:113:MET:HE3	1.38	1.01
1:O:-1:ASN:H2	1:O:147:LYS:HE3	1.25	0.98
1:O:251:GLU:HA	1:O:251:GLU:CB	1.92	0.97
1:O:-1:ASN:HA	1:O:147:LYS:CD	1.96	0.94
1:O:194:MET:CE	1:O:197:VAL:HG22	1.97	0.94
1:C:41:PRO:HB3	1:C:107:MET:HE2	1.50	0.93
1:O:64:TYR:HE1	1:O:85:SER:HG	1.03	0.93
1:C:261:HIS:HB2	1:C:266:GLU:OE2	1.68	0.92
1:O:273:ASP:OD1	1:O:308:LYS:HE2	1.69	0.92
1:O:250:ASN:HB2	1:O:281(A):SER:HA	1.52	0.92

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:185:ILE:HG22	1:O:186:LYS:HG2	1.52	0.91
1:O:-1:ASN:N	1:O:147:LYS:HE3	1.84	0.91
1:C:250:ASN:ND2	1:C:251:GLU:N	2.18	0.91
1:C:49:ALA:HA	1:C:113:MET:CE	2.01	0.91
1:C:293:PRO:HA	1:C:296:GLY:O	1.71	0.91
1:O:126:ILE:CD1	1:O:132:ARG:HG3	2.02	0.90
1:O:-1:ASN:CA	1:O:147:LYS:HE3	2.03	0.88
1:C:-1:ASN:HD22	1:C:-1:ASN:C	1.75	0.88
1:C:250:ASN:HD21	1:C:251:GLU:HG3	1.37	0.88
1:O:178:ASN:CA	1:O:178:ASN:CG	2.42	0.87
1:O:47:ARG:HB2	1:O:51:VAL:HG22	1.56	0.86
1:C:172:PRO:HA	1:C:175:TYR:CE1	2.11	0.86
1:O:240:ARG:HH12	1:O:242:PHE:HB2	1.38	0.85
1:C:147:LYS:HB3	1:C:147:LYS:NZ	1.91	0.85
1:O:178:ASN:HA	1:O:178:ASN:CG	1.97	0.85
1:O:203:THR:CG2	1:O:207:GLU:HG3	2.06	0.85
1:O:194:MET:HE2	1:O:197:VAL:CG2	2.07	0.84
1:C:147:LYS:HZ3	1:C:147:LYS:HB3	1.41	0.84
1:O:194:MET:O	1:O:209:GLY:HA2	1.78	0.83
1:C:88:ILE:HG22	1:C:97:THR:CG2	2.06	0.83
1:O:195:LYS:HD2	3:O:2006:HOH:O	1.78	0.83
1:O:198:SER:HB2	1:O:203:THR:HA	1.60	0.83
1:C:225:THR:O	1:C:229:GLU:HB2	1.79	0.82
1:O:326:ARG:HH21	1:O:326:ARG:HB3	1.41	0.82
1:O:126:ILE:HD11	1:O:132:ARG:HG3	1.60	0.82
1:C:157:ARG:HH21	1:O:161:LEU:HD13	1.45	0.82
1:O:205:LEU:CG	1:O:230:LYS:HE2	2.09	0.81
1:O:281:SER:HB2	1:O:281(C):LYS:HD2	1.62	0.81
1:O:47:ARG:HB2	1:O:51:VAL:CG2	2.10	0.81
1:C:207:GLU:C	1:C:208:ASP:CA	2.48	0.81
1:C:-1:ASN:ND2	1:C:-1:ASN:C	2.34	0.80
1:O:71:LEU:HD13	1:O:84:LEU:HD13	1.62	0.80
1:C:65:LYS:HB3	1:C:86:GLN:HG3	1.64	0.80
1:O:51:VAL:HG12	1:O:52:TYR:CD2	2.16	0.79
1:O:99:GLN:NE2	1:O:139:ASN:ND2	2.30	0.79
1:O:205:LEU:HB2	1:O:230:LYS:NZ	1.97	0.79
1:O:205:LEU:HG	1:O:230:LYS:HE2	1.63	0.79
1:C:143:GLN:HB2	1:C:145:VAL:HG11	1.65	0.79
1:O:281:SER:CB	1:O:281(C):LYS:HD2	2.12	0.78
1:C:292:PRO:HB2	1:C:294:PRO:HD2	1.65	0.78
1:O:275:VAL:HG22	1:O:284:LEU:HD22	1.63	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:157:ARG:O	1:O:159:SER:N	2.17	0.78
1:O:148:GLU:HG3	1:O:168:GLY:O	1.83	0.77
1:C:226:SER:CA	1:C:226:SER:OG	2.33	0.77
1:O:195:LYS:NZ	1:O:264:GLY:HA2	2.00	0.77
1:C:149:ASP:H	1:C:316:ARG:CD	1.98	0.77
1:C:183:ASN:HA	1:C:319:ARG:HB3	1.67	0.76
1:C:147:LYS:NZ	1:C:147:LYS:CB	2.48	0.76
1:C:274:TYR:CD1	1:C:275:VAL:HG23	2.20	0.76
1:O:286:ILE:O	1:O:287:HIS:HD2	1.68	0.75
1:O:202:SER:O	1:O:204:LEU:HD23	1.87	0.75
1:O:240:ARG:NH1	1:O:242:PHE:O	2.20	0.75
1:O:240:ARG:CG	1:O:241:LEU:H	1.98	0.75
1:O:156:ASN:OD1	1:O:162:GLY:N	2.18	0.75
1:C:149:ASP:H	1:C:316:ARG:HD2	1.52	0.75
1:O:18:ILE:HG12	1:O:29:VAL:HG11	1.67	0.74
1:O:240:ARG:HH11	1:O:242:PHE:H	1.34	0.74
1:C:146:LEU:HD22	1:C:168:GLY:HA3	1.68	0.73
1:C:238:LYS:N	1:C:238:LYS:HD3	2.04	0.73
1:O:203:THR:HG23	1:O:207:GLU:HG3	1.69	0.73
1:O:326:ARG:HH21	1:O:326:ARG:CB	2.01	0.73
1:C:221:ILE:O	1:C:286:ILE:HA	1.87	0.73
1:C:51:VAL:HG23	1:C:52:TYR:CD1	2.23	0.72
1:C:226:SER:N	1:C:226:SER:OG	2.22	0.72
1:O:99:GLN:NE2	1:O:139:ASN:HD22	1.86	0.72
1:C:326:ARG:NH1	1:O:1:THR:HG22	2.05	0.71
1:C:41:PRO:CB	1:C:107:MET:HE2	2.20	0.71
1:C:185:ILE:HG23	1:C:186:LYS:N	2.05	0.71
1:O:3:SER:HA	1:O:165:ILE:O	1.90	0.71
1:O:262:LEU:HD23	1:O:267:TYR:CD1	2.25	0.71
1:C:248:LYS:CB	1:C:251:GLU:OE1	2.38	0.71
1:O:270:THR:O	1:O:273:ASP:HB2	1.89	0.71
1:O:126:ILE:HD13	1:O:132:ARG:HD3	1.73	0.70
1:O:205:LEU:HD21	1:O:227:SER:HB2	1.72	0.70
1:C:208:ASP:N	1:C:208:ASP:CB	2.53	0.70
1:O:291:ILE:O	1:O:296:GLY:HA3	1.92	0.70
1:O:206:CYS:SG	1:O:206:CYS:O	2.50	0.69
1:C:326:ARG:HH11	1:O:1:THR:HG22	1.57	0.69
1:O:141:ILE:HD13	1:O:146:LEU:HD12	1.74	0.69
1:C:234:ALA:O	1:C:236:GLY:N	2.24	0.69
1:C:250:ASN:ND2	1:C:251:GLU:HG3	2.06	0.69
1:O:126:ILE:HD13	1:O:132:ARG:HG3	1.73	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:47(B):TYR:OH	1:O:106:GLU:HG3	1.91	0.69
1:O:39:TRP:NE1	1:O:120:VAL:HG12	2.08	0.69
1:O:182:ILE:HD12	1:O:263:GLY:HA3	1.75	0.69
1:O:29:VAL:HG23	1:O:30:VAL:N	1.96	0.68
1:O:46:SER:OG	1:O:47(A):LEU:N	2.23	0.68
1:C:52:TYR:HB2	1:C:113:MET:HE2	1.76	0.68
1:O:0:THR:O	1:O:147:LYS:N	2.26	0.68
1:O:18:ILE:HG12	1:O:29:VAL:CG1	2.23	0.68
1:O:204:LEU:HB2	1:O:230:LYS:NZ	2.09	0.68
1:O:240:ARG:NH1	1:O:242:PHE:H	1.92	0.68
1:C:144:GLY:C	1:C:145:VAL:HG12	2.14	0.68
1:O:51:VAL:O	1:O:52:TYR:CD2	2.47	0.68
1:O:222:SER:HA	1:O:287:HIS:O	1.93	0.68
1:O:155:TYR:OH	1:O:216:THR:O	2.10	0.68
1:O:203:THR:HG21	1:O:207:GLU:HG3	1.77	0.67
1:C:126:ILE:HG12	1:C:132:ARG:NH2	2.08	0.67
1:C:189:VAL:O	1:C:189:VAL:HG12	1.87	0.67
1:C:205:LEU:HD23	1:C:205:LEU:N	2.10	0.67
1:O:51:VAL:O	1:O:52:TYR:HD2	1.77	0.67
1:C:52:TYR:HB2	1:C:113:MET:CE	2.24	0.67
1:O:204:LEU:HG	1:O:204:LEU:CD2	2.15	0.66
1:O:195:LYS:HZ2	1:O:264:GLY:HA2	1.57	0.66
1:O:96:VAL:HG21	1:O:136:ILE:HD11	1.77	0.66
1:C:276:PHE:CE1	1:C:285:ALA:HB2	2.30	0.66
1:O:28:LYS:HB2	1:O:117:PHE:CA	2.26	0.66
1:C:226:SER:CB	1:C:226:SER:HG	2.07	0.66
1:O:67:ASN:HB3	1:O:84:LEU:O	1.96	0.66
1:C:293:PRO:O	1:C:294:PRO:O	2.13	0.66
1:C:291:ILE:O	1:C:296:GLY:HA3	1.96	0.66
1:C:292:PRO:O	1:C:294:PRO:N	2.29	0.66
1:O:265:LYS:HG2	1:O:267:TYR:CE1	2.30	0.66
1:C:20:ILE:HD12	1:C:89:ILE:HG12	1.77	0.66
1:O:108:PRO:HG2	1:O:112:PHE:HD2	1.60	0.65
1:O:194:MET:CE	1:O:260:PHE:HD2	2.10	0.65
1:C:195:LYS:NZ	1:C:261:HIS:NE2	2.43	0.65
1:O:204:LEU:CG	1:O:204:LEU:CA	2.73	0.65
1:O:109:ALA:O	1:O:113:MET:HB3	1.96	0.65
1:C:3:SER:HA	1:C:165:ILE:O	1.96	0.65
1:C:2:SER:O	1:C:167:LEU:N	2.25	0.65
1:O:14:TYR:O	1:O:30:VAL:HG12	1.97	0.65
1:O:28:LYS:CB	1:O:117:PHE:HA	2.26	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:ASP:OD1	1:C:158:ASP:HB2	1.96	0.65
1:C:185:ILE:HG23	1:C:186:LYS:H	1.62	0.65
1:O:141:ILE:CD1	1:O:146:LEU:HD12	2.26	0.64
1:O:-1:ASN:HA	1:O:147:LYS:CE	2.27	0.64
1:O:84:LEU:HD21	1:O:133:VAL:HG21	1.78	0.64
1:C:203:THR:CG2	1:C:207:GLU:HB3	2.28	0.64
1:O:311:THR:HG23	1:O:322:PHE:CE2	2.32	0.64
1:O:-1:ASN:CA	1:O:147:LYS:CD	2.74	0.64
1:O:240:ARG:HG3	1:O:241:LEU:H	1.61	0.64
1:O:46:SER:OG	1:O:47(A):LEU:HB2	1.98	0.64
1:C:250:ASN:HD22	1:C:250:ASN:C	2.01	0.64
1:C:182:ILE:HG21	1:C:192:ILE:HG13	1.79	0.64
1:C:293:PRO:CD	1:C:294:PRO:HD2	2.27	0.64
1:C:250:ASN:HD22	1:C:251:GLU:H	1.43	0.64
1:O:293:PRO:HA	1:O:297:PRO:HD3	1.80	0.64
1:C:27:PHE:CZ	1:C:56:PHE:HB2	2.33	0.63
1:O:126:ILE:HD13	1:O:132:ARG:CD	2.28	0.63
1:O:296:GLY:HA2	1:O:298:THR:HG22	1.79	0.63
1:O:183:ASN:HB3	1:O:319:ARG:HB3	1.81	0.63
1:O:-1:ASN:CA	1:O:147:LYS:CE	2.76	0.63
1:O:132:ARG:HH21	1:O:132:ARG:HA	1.63	0.63
1:O:170:SER:O	1:O:172:PRO:HD3	1.97	0.63
1:O:240:ARG:NH1	1:O:242:PHE:HB2	2.13	0.63
1:C:181:TYR:CD2	1:C:321:GLY:HA3	2.34	0.63
1:C:191:GLN:OE1	1:C:211:LEU:HB3	1.99	0.63
1:O:194:MET:HE1	1:O:260:PHE:HD2	1.62	0.63
1:C:248:LYS:HB3	1:C:251:GLU:OE1	1.99	0.62
1:O:132:ARG:CZ	1:O:132:ARG:HB2	2.29	0.62
1:C:0:THR:HG22	1:C:1:THR:N	2.13	0.62
1:O:204:LEU:CB	1:O:230:LYS:HZ3	2.12	0.62
1:O:84:LEU:HB3	1:O:100:MET:CE	2.29	0.62
1:O:240:ARG:CG	1:O:241:LEU:N	2.63	0.62
1:O:28:LYS:HB2	1:O:117:PHE:HA	1.80	0.62
1:O:202:SER:C	1:O:204:LEU:HD23	2.20	0.62
1:C:149:ASP:O	1:C:315:ARG:HB2	2.00	0.62
1:O:109:ALA:HB3	1:O:110:LEU:CB	2.28	0.62
1:C:248:LYS:HB3	1:C:251:GLU:CD	2.20	0.62
1:C:41:PRO:HG3	1:C:107:MET:CE	2.29	0.62
1:C:48:THR:O	1:C:113:MET:HE1	2.01	0.61
1:O:250:ASN:HB2	1:O:281(A):SER:CA	2.27	0.61
1:C:224:SER:CB	1:C:224:SER:HG	2.07	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:SER:HB2	2:C:1327:C47:H261	1.81	0.61
1:O:108:PRO:HG2	1:O:112:PHE:CD2	2.35	0.61
1:O:47(B):TYR:CE1	1:O:106:GLU:HA	2.35	0.61
1:C:250:ASN:ND2	1:C:251:GLU:H	1.96	0.61
1:C:181:TYR:HA	1:C:321:GLY:HA2	1.83	0.61
1:C:281(B):LYS:O	1:C:281(C):LYS:HG2	2.01	0.61
2:C:1327:C47:O16	2:C:1327:C47:H202	2.00	0.61
1:C:239:LYS:O	1:C:241:LEU:N	2.33	0.60
1:O:223:GLY:O	1:O:289:MET:N	2.31	0.60
1:C:293:PRO:O	1:C:294:PRO:C	2.39	0.60
1:O:292:PRO:O	1:O:294:PRO:HD2	2.01	0.60
1:C:131:GLY:O	1:C:132:ARG:HB3	1.98	0.60
1:O:173:GLN:CA	1:O:173:GLN:CG	2.75	0.60
1:C:148:GLU:HB3	1:C:150:VAL:HG23	1.82	0.60
1:O:286:ILE:O	1:O:287:HIS:CD2	2.54	0.60
1:O:109:ALA:HB3	1:O:110:LEU:HB2	1.82	0.60
1:C:76:SER:OG	1:C:289:MET:HG3	2.01	0.60
1:C:187:THR:HB	1:C:318:ASN:ND2	2.17	0.60
1:C:292:PRO:C	1:C:294:PRO:HD2	2.23	0.59
1:O:-1:ASN:C	1:O:147:LYS:HG2	2.22	0.59
1:O:186:LYS:HD3	1:O:191:GLN:HE22	1.67	0.59
1:C:2:SER:O	1:C:166:VAL:HA	2.02	0.59
1:O:202:SER:O	1:O:204:LEU:CD2	2.50	0.59
1:O:226:SER:O	1:O:229:GLU:HB2	2.03	0.59
1:C:186:LYS:CB	1:C:186:LYS:N	2.65	0.59
1:O:27:PHE:CE2	1:O:54:LYS:HG2	2.37	0.59
1:C:203:THR:HG22	1:C:207:GLU:HB3	1.85	0.59
1:O:281:SER:HB2	1:O:281(C):LYS:CD	2.31	0.59
1:O:84:LEU:HD12	1:O:101:PHE:O	2.03	0.59
1:O:28:LYS:CG	1:O:117:PHE:HA	2.32	0.59
1:O:279:SER:HG	1:O:281(C):LYS:HD3	1.65	0.59
1:O:154:TYR:HE2	1:O:161:LEU:HD23	1.66	0.59
1:O:130:ILE:HG22	1:O:130:ILE:O	1.93	0.58
1:O:184:LEU:HB2	1:O:318:ASN:O	2.02	0.58
1:C:41:PRO:HG3	1:C:107:MET:HE1	1.85	0.58
1:C:-1:ASN:HD22	1:C:0:THR:N	2.02	0.58
1:O:41:PRO:HD3	1:O:118:ASP:O	2.02	0.58
1:O:43:SER:C	1:O:45:CYS:H	2.06	0.58
1:O:249:CYS:HB3	1:O:279:SER:O	2.04	0.58
1:O:19:GLY:O	1:O:89:ILE:HA	2.04	0.58
1:C:149:ASP:H	1:C:316:ARG:HD3	1.69	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:294:PRO:HG2	1:O:295:THR:H	1.68	0.57
1:C:191:GLN:OE1	1:C:298:THR:OG1	2.22	0.57
1:O:216:THR:HG22	1:O:306:ILE:CD1	2.33	0.57
1:C:89:ILE:HG22	1:C:90:THR:N	2.18	0.57
1:O:314:ASP:HB3	1:O:319:ARG:O	2.03	0.57
1:O:183:ASN:HB3	1:O:319:ARG:CB	2.34	0.57
1:C:111:PRO:HB2	2:C:1327:C47:H10	1.86	0.57
1:C:293:PRO:HD2	1:C:294:PRO:HD2	1.85	0.57
1:O:80:VAL:HG13	1:O:112:PHE:CE2	2.39	0.57
1:C:250:ASN:HD22	1:C:251:GLU:CA	2.16	0.57
1:C:202:SER:O	1:C:204:LEU:N	2.36	0.57
1:O:204:LEU:CB	1:O:204:LEU:HG	2.18	0.57
1:C:228:ILE:HG13	1:C:287:HIS:O	2.05	0.57
1:O:76:SER:OG	2:O:1327:C47:H282	2.05	0.57
2:O:1327:C47:H24	2:O:1327:C47:O30	2.04	0.57
1:O:72:THR:HA	1:O:81:SER:HA	1.87	0.57
1:O:205:LEU:HB2	1:O:230:LYS:HZ3	1.69	0.56
1:C:195:LYS:HZ3	1:C:261:HIS:CD2	2.23	0.56
1:C:207:GLU:O	1:C:208:ASP:HA	2.04	0.56
1:C:65:LYS:CB	1:C:86:GLN:HG3	2.35	0.56
1:C:146:LEU:HD22	1:C:168:GLY:CA	2.34	0.56
1:C:39:TRP:HA	1:C:102:GLY:O	2.04	0.56
1:O:205:LEU:HD12	1:O:230:LYS:CE	2.36	0.56
1:O:0:THR:CG2	1:O:1:THR:N	2.67	0.56
1:O:126:ILE:HD13	1:O:132:ARG:CG	2.35	0.56
1:C:141:ILE:HG12	1:C:149:ASP:OD2	2.06	0.56
1:O:240:ARG:HH12	1:O:242:PHE:CB	2.14	0.56
1:O:242:PHE:O	1:O:244:ASP:O	2.22	0.56
1:C:27:PHE:HZ	1:C:56:PHE:HB2	1.70	0.56
1:C:293:PRO:HD2	1:C:294:PRO:CD	2.35	0.56
1:O:185:ILE:HG23	1:O:185:ILE:O	2.05	0.56
1:C:205:LEU:HD12	1:C:227:SER:CB	2.21	0.56
1:C:71:LEU:HD22	1:C:84:LEU:HD21	1.87	0.56
1:C:126:ILE:HG12	1:C:132:ARG:CZ	2.36	0.56
1:C:91:VAL:O	1:C:91:VAL:HG23	2.04	0.56
1:O:147:LYS:CD	1:O:147:LYS:HA	2.36	0.56
1:C:75:TYR:CG	2:C:1327:C47:H201	2.41	0.56
1:O:220:TYR:O	1:O:302:GLY:HA3	2.06	0.55
1:C:79:THR:O	1:C:108:PRO:HD2	2.06	0.55
1:C:41:PRO:HB3	1:C:107:MET:CE	2.33	0.55
1:C:-1:ASN:O	1:C:-1:ASN:ND2	2.38	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:ASP:OD2	1:C:307:ARG:NH2	2.39	0.55
1:O:83:PHE:HE1	1:O:105:THR:CG2	2.20	0.55
1:O:217:GLY:O	2:O:1327:C47:H142	2.06	0.55
1:O:94:ILE:HG22	1:O:95:THR:N	2.21	0.55
2:O:1327:C47:H11	2:O:1327:C47:O16	2.06	0.55
1:O:50:CYS:SG	1:O:107:MET:HE3	2.46	0.55
1:C:9:TYR:O	1:C:12:THR:N	2.37	0.55
1:C:181:TYR:HA	1:C:320:ILE:O	2.07	0.55
1:C:238:LYS:O	1:C:245:TYR:HA	2.07	0.55
1:C:206:CYS:O	1:C:206:CYS:SG	2.65	0.55
1:O:0:THR:N	1:O:147:LYS:HE3	2.22	0.54
1:O:219:SER:O	1:O:303:ALA:HB3	2.07	0.54
1:C:144:GLY:N	1:C:145:VAL:HG12	2.22	0.54
1:C:242:PHE:O	1:C:287:HIS:HE1	1.89	0.54
1:O:270:THR:H	1:O:273:ASP:HB2	1.72	0.54
1:C:184:LEU:HB2	1:C:318:ASN:O	2.08	0.54
1:O:191:GLN:OE1	1:O:211:LEU:HD13	2.08	0.54
1:O:108:PRO:HB2	1:O:111:PRO:CD	2.37	0.54
1:C:3:SER:CA	1:C:165:ILE:O	2.55	0.54
1:C:217:GLY:O	2:C:1327:C47:H142	2.08	0.54
1:O:10:MET:O	1:O:11:ASP:HB2	2.04	0.54
1:C:150:VAL:HG12	1:C:313:PHE:O	2.08	0.54
1:C:35:SER:HB2	3:C:2002:HOH:O	2.08	0.54
1:C:195:LYS:HZ3	1:C:261:HIS:CE1	2.23	0.53
1:C:187:THR:HB	1:C:318:ASN:HD22	1.71	0.53
1:O:108:PRO:HB2	1:O:111:PRO:HD2	1.88	0.53
1:C:181:TYR:CD2	1:C:321:GLY:CA	2.92	0.53
1:O:10:MET:C	1:O:12:THR:H	2.12	0.53
1:O:186:LYS:CB	1:O:186:LYS:NZ	2.71	0.53
1:O:48:THR:O	1:O:51:VAL:N	2.41	0.53
1:O:319:ARG:NH2	3:O:2007:HOH:O	2.33	0.53
1:O:80:VAL:HG12	1:O:108:PRO:HD2	1.88	0.53
1:C:75:TYR:CD1	2:C:1327:C47:H332	2.44	0.53
1:C:221:ILE:HG22	1:C:286:ILE:HG23	1.89	0.53
1:O:204:LEU:HB2	1:O:230:LYS:HZ3	1.71	0.53
1:O:186:LYS:HD3	1:O:191:GLN:NE2	2.24	0.53
1:O:99:GLN:HE21	1:O:139:ASN:ND2	2.06	0.53
1:C:207:GLU:O	1:C:208:ASP:CA	2.56	0.52
1:C:136:ILE:CG2	1:C:137:PHE:N	2.71	0.52
1:O:274:TYR:CD1	1:O:275:VAL:HG23	2.44	0.52
1:O:271:SER:O	1:O:272:ALA:O	2.27	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:75:TYR:CB	2:O:1327:C47:H201	2.39	0.52
1:O:36:SER:OG	1:O:128:GLN:HB2	2.08	0.52
1:C:186:LYS:CA	1:C:186:LYS:CG	2.81	0.52
1:O:46:SER:HG	1:O:47(A):LEU:H	1.55	0.52
1:C:172:PRO:CA	1:C:175:TYR:CE1	2.89	0.52
1:O:84:LEU:HD21	1:O:133:VAL:CG2	2.40	0.52
1:C:150:VAL:CG1	1:C:314:ASP:HA	2.39	0.52
1:O:193:GLN:HE21	1:O:209:GLY:HA3	1.74	0.52
1:O:181:TYR:N	1:O:181:TYR:CD1	2.71	0.52
1:C:292:PRO:CB	1:C:294:PRO:HD2	2.38	0.52
1:O:203:THR:CG2	1:O:203:THR:O	2.58	0.51
1:O:130:ILE:CD1	2:O:1327:C47:H351	2.39	0.51
1:O:203:THR:HG23	1:O:203:THR:O	2.08	0.51
1:O:108:PRO:C	1:O:110:LEU:H	2.11	0.51
1:C:291:ILE:HG22	1:C:296:GLY:HA3	1.91	0.51
1:C:189:VAL:CG1	1:C:191:GLN:HB2	2.40	0.51
1:O:247:VAL:HA	1:O:251:GLU:OE2	2.10	0.51
1:C:140:ILE:HA	1:C:143:GLN:HG3	1.93	0.51
1:C:205:LEU:CD1	1:C:227:SER:HB3	2.21	0.51
1:C:64:TYR:CG	1:C:65:LYS:N	2.73	0.51
2:O:1327:C47:H202	2:O:1327:C47:O16	2.10	0.51
1:C:2:SER:O	1:C:166:VAL:HG13	2.10	0.51
1:O:320:ILE:O	1:O:320:ILE:HG22	2.10	0.51
1:O:202:SER:O	1:O:204:LEU:N	2.43	0.51
1:O:204:LEU:CB	1:O:230:LYS:NZ	2.73	0.51
1:O:265:LYS:HG2	1:O:267:TYR:CZ	2.46	0.51
1:O:84:LEU:HB3	1:O:100:MET:HE2	1.93	0.51
1:C:10:MET:O	1:C:11:ASP:HB2	2.09	0.50
1:O:50:CYS:O	1:O:55:LEU:HD11	2.12	0.50
1:C:4:VAL:O	1:C:5:ILE:HG13	2.12	0.50
1:O:231:LEU:O	1:O:234:ALA:HB3	2.12	0.50
1:C:89:ILE:CG2	1:C:90:THR:N	2.72	0.50
1:C:237:ALA:HB1	1:C:246:VAL:H	1.74	0.50
1:O:99:GLN:HE22	1:O:139:ASN:ND2	2.07	0.50
1:O:75:TYR:HD1	2:O:1327:C47:H332	1.75	0.50
1:C:126:ILE:CG1	1:C:132:ARG:NH2	2.72	0.50
1:O:77:THR:OG1	1:O:77:THR:O	2.08	0.50
1:C:251:GLU:O	1:C:254:THR:HB	2.12	0.50
1:O:28:LYS:O	1:O:118:ASP:N	2.39	0.50
2:C:1327:C47:O16	2:C:1327:C47:H11	2.12	0.50
1:C:293:PRO:CA	1:C:296:GLY:O	2.54	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:LYS:HE3	1:C:251:GLU:OE1	2.12	0.50
1:O:160(D):SER:N	1:O:160(D):SER:HA	2.05	0.50
1:O:240:ARG:NH1	1:O:242:PHE:C	2.65	0.50
1:C:141:ILE:CG2	1:C:141:ILE:O	2.58	0.50
1:C:47:ARG:NE	1:C:47:ARG:N	2.19	0.50
1:O:195:LYS:HZ1	1:O:264:GLY:HA2	1.74	0.50
1:O:0:THR:HB	1:O:145:VAL:O	2.12	0.50
1:O:23:PRO:O	1:O:23:PRO:HG2	2.11	0.49
1:O:74:ARG:O	2:O:1327:C47:H352	2.12	0.49
1:O:317:ASN:O	1:O:318:ASN:C	2.50	0.49
1:O:233:GLU:OE1	1:O:233:GLU:HA	2.12	0.49
1:C:292:PRO:HG2	1:C:294:PRO:HG2	1.95	0.49
1:O:186:LYS:NZ	1:O:186:LYS:HB2	2.28	0.49
1:O:71:LEU:O	1:O:82:GLY:N	2.41	0.49
1:O:241:LEU:HB3	1:O:242:PHE:CD1	2.46	0.49
1:C:284:LEU:N	1:C:284:LEU:HD23	2.27	0.49
1:O:205:LEU:HB2	1:O:230:LYS:CE	2.42	0.49
1:C:150:VAL:HG12	1:C:314:ASP:HA	1.95	0.49
1:C:242:PHE:O	1:C:287:HIS:CE1	2.65	0.49
1:O:147:LYS:C	1:O:148:GLU:HG2	2.33	0.49
1:O:83:PHE:HE1	1:O:105:THR:HG23	1.77	0.49
1:O:205:LEU:HD23	1:O:206:CYS:H	1.77	0.49
1:C:41:PRO:CB	1:C:107:MET:CE	2.90	0.49
1:O:5:ILE:HG23	1:O:161:LEU:HD12	1.95	0.49
1:O:137:PHE:CE1	1:O:141:ILE:HG12	2.48	0.48
1:O:28:LYS:HG3	1:O:117:PHE:HA	1.94	0.48
1:C:281(B):LYS:O	1:C:281(B):LYS:HD3	2.13	0.48
1:C:246:VAL:HG23	1:C:283:THR:HA	1.95	0.48
1:O:185:ILE:HG22	1:O:186:LYS:CG	2.36	0.48
1:O:239:LYS:HA	1:O:245:TYR:HA	1.96	0.48
1:C:52:TYR:CD1	1:C:113:MET:HE1	2.48	0.48
1:O:269:LEU:HD22	1:O:273:ASP:HB3	1.94	0.48
1:O:48:THR:O	1:O:52:TYR:N	2.38	0.48
1:O:76:SER:HB3	1:O:291:ILE:CG2	2.43	0.48
1:C:4:VAL:HG12	1:C:5:ILE:N	2.29	0.48
1:O:197:VAL:O	1:O:205:LEU:N	2.44	0.48
1:C:248:LYS:HB2	1:C:251:GLU:OE1	2.13	0.48
1:C:164:GLN:HE21	1:C:164:GLN:HB3	1.55	0.48
1:C:198:SER:O	1:C:258:ILE:HA	2.13	0.48
1:O:53:HIS:HD2	1:O:118:ASP:OD1	1.96	0.48
1:O:204:LEU:CB	1:O:204:LEU:CD1	2.88	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:205:LEU:CD1	1:O:230:LYS:HE2	2.44	0.48
1:O:262:LEU:CD2	1:O:267:TYR:CD1	2.94	0.48
1:C:171:ASP:C	1:C:171:ASP:OD2	2.51	0.48
1:C:292:PRO:C	1:C:294:PRO:CD	2.82	0.48
1:C:0:THR:CG2	1:C:1:THR:N	2.76	0.48
1:O:202:SER:O	1:O:204:LEU:HG	2.13	0.47
1:C:175:TYR:O	1:C:326:ARG:HD2	2.14	0.47
1:C:109:ALA:O	1:C:113:MET:CB	2.62	0.47
1:C:175:TYR:HA	1:C:324:LEU:O	2.14	0.47
1:O:5:ILE:CG2	1:O:161:LEU:HD12	2.44	0.47
1:O:240:ARG:HD2	1:O:241:LEU:HB2	1.97	0.47
1:C:315:ARG:NH1	3:C:2014:HOH:O	2.43	0.47
1:C:326:ARG:NH1	1:O:1:THR:O	2.46	0.47
1:O:132:ARG:NH2	1:O:132:ARG:HB2	2.30	0.47
1:C:4:VAL:HG12	1:C:5:ILE:H	1.77	0.47
1:C:291:ILE:HA	1:C:292:PRO:HD2	1.69	0.47
1:O:186:LYS:CB	1:O:186:LYS:HZ3	2.26	0.47
1:O:0:THR:H	1:O:147:LYS:HE3	1.79	0.47
1:O:51:VAL:CG1	1:O:52:TYR:CE2	2.98	0.47
1:O:156:ASN:OD1	1:O:161:LEU:HB3	2.13	0.47
1:O:35:SER:O	1:O:124:GLY:N	2.47	0.47
1:C:21:GLY:O	1:C:24:PRO:HA	2.14	0.47
1:C:292:PRO:HB2	1:C:293:PRO:CD	2.43	0.47
1:O:232:MET:HG3	1:O:245:TYR:CE1	2.50	0.47
1:C:202:SER:O	1:C:204:LEU:HD12	2.14	0.47
1:C:241:LEU:HD13	1:C:241:LEU:HA	1.71	0.47
1:C:52:TYR:HD1	1:C:113:MET:HE1	1.79	0.47
1:C:0:THR:OG1	1:C:145:VAL:HG23	2.14	0.47
1:O:47:ARG:HA	1:O:51:VAL:HG23	1.95	0.47
1:O:51:VAL:C	1:O:52:TYR:CD2	2.88	0.47
1:C:228:ILE:HA	1:C:228:ILE:HD13	1.13	0.47
1:C:76:SER:HG	1:C:289:MET:CG	2.27	0.47
1:C:296:GLY:HA2	1:C:298:THR:HB	1.97	0.47
1:O:205:LEU:HB2	1:O:230:LYS:HE2	1.97	0.47
1:O:18:ILE:O	1:O:26:THR:HA	2.15	0.47
1:O:265:LYS:HG3	1:O:266:GLU:N	2.30	0.47
1:C:77:THR:HG23	1:C:289:MET:SD	2.55	0.47
1:C:195:LYS:HZ1	1:C:263:GLY:CA	2.28	0.47
1:C:143:GLN:HB2	1:C:145:VAL:CG1	2.40	0.47
1:O:233:GLU:CA	1:O:233:GLU:OE1	2.63	0.46
1:O:186:LYS:O	1:O:186:LYS:HG3	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:64:TYR:OH	1:O:66:HIS:HA	2.15	0.46
1:O:16:GLY:N	1:O:29:VAL:O	2.45	0.46
1:O:194:MET:HE3	1:O:197:VAL:HG22	1.89	0.46
1:C:205:LEU:HD11	1:C:227:SER:O	2.15	0.46
1:O:58:ALA:HB1	1:O:64:TYR:CG	2.51	0.46
1:C:125:PHE:CE1	1:C:315:ARG:NE	2.84	0.46
1:O:80:VAL:CG1	1:O:112:PHE:CE2	2.98	0.46
1:C:205:LEU:C	1:C:207:GLU:H	2.19	0.46
1:C:65:LYS:HB3	1:C:86:GLN:CG	2.40	0.46
1:O:240:ARG:CD	1:O:241:LEU:H	2.28	0.46
1:C:172:PRO:HA	1:C:175:TYR:CD1	2.49	0.46
1:O:51:VAL:HG12	1:O:52:TYR:CE2	2.51	0.46
1:C:130:ILE:HG23	1:C:130:ILE:HD13	1.66	0.46
1:C:104:VAL:HG13	1:C:106:GLU:O	2.16	0.46
1:C:292:PRO:CB	1:C:293:PRO:HD3	2.45	0.46
1:O:20:ILE:HG12	1:O:89:ILE:HG12	1.98	0.46
1:O:75:TYR:HD1	2:O:1327:C47:C33	2.29	0.46
1:O:253:PRO:HG2	1:O:280:TYR:CE1	2.51	0.46
1:C:185:ILE:CG2	1:C:191:GLN:O	2.63	0.46
1:O:251:GLU:CG	1:O:251:GLU:CA	2.87	0.45
1:C:228:ILE:HG23	1:C:228:ILE:HD12	1.51	0.45
1:O:174:HIS:HA	1:O:326:ARG:O	2.16	0.45
1:O:111:PRO:HB2	2:O:1327:C47:H10	1.98	0.45
1:C:281(D):LEU:HD23	1:C:281(D):LEU:HA	1.72	0.45
1:C:194:MET:HE2	1:C:194:MET:HB3	1.76	0.45
1:C:241:LEU:HD12	1:C:241:LEU:O	2.16	0.45
1:O:187:THR:HG23	1:O:187:THR:O	2.16	0.45
1:C:22:THR:HG1	1:C:63:SER:CB	2.26	0.45
1:C:195:LYS:HZ1	1:C:263:GLY:N	2.14	0.45
1:O:270:THR:N	1:O:273:ASP:HB2	2.32	0.45
1:C:136:ILE:HG23	1:C:137:PHE:N	2.30	0.45
1:O:114:LEU:HD23	1:O:114:LEU:HA	1.44	0.45
1:C:3:SER:HB3	1:C:165:ILE:O	2.17	0.45
1:C:10:MET:C	1:C:12:THR:N	2.69	0.45
1:C:84:LEU:HA	1:C:84:LEU:HD23	1.65	0.45
1:C:293:PRO:N	1:C:294:PRO:HD2	2.31	0.45
1:O:42:SER:O	1:O:55:LEU:HD22	2.16	0.45
1:C:4:VAL:H	1:C:4:VAL:HG23	1.51	0.45
1:O:213:LEU:O	1:O:300:ALA:HA	2.16	0.45
1:O:0:THR:HG23	1:O:1:THR:N	2.30	0.45
1:C:239:LYS:HG2	1:C:245:TYR:CE2	2.52	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:158:ASP:CG	1:O:158:ASP:CA	2.78	0.45
1:O:262:LEU:N	1:O:265:LYS:O	2.49	0.45
1:O:96:VAL:HG12	1:O:97:THR:N	2.30	0.45
1:C:189:VAL:HG11	1:C:191:GLN:HB2	1.99	0.45
1:O:56:PHE:CE1	1:O:58:ALA:HB2	2.52	0.45
1:C:147:LYS:HG3	1:C:148:GLU:OE1	2.17	0.45
1:O:286:ILE:C	1:O:287:HIS:HD2	2.20	0.45
1:C:170:SER:HB2	1:C:310:TYR:HE1	1.80	0.45
1:C:189:VAL:HG12	1:C:191:GLN:H	1.82	0.45
1:C:202:SER:O	1:C:204:LEU:CD1	2.65	0.45
1:C:224:SER:OG	1:C:224:SER:C	2.55	0.45
1:O:89:ILE:HG22	1:O:90:THR:N	2.26	0.45
1:C:166:VAL:HG12	1:C:167:LEU:N	2.32	0.45
1:C:268:THR:CG2	1:C:269:LEU:N	2.79	0.45
1:C:41:PRO:CG	1:C:107:MET:HE2	2.48	0.44
1:O:195:LYS:NZ	1:O:264:GLY:CA	2.78	0.44
1:C:132:ARG:HD2	1:C:132:ARG:HA	1.73	0.44
2:C:1327:C47:H172	2:C:1327:C47:H142	1.76	0.44
1:O:20:ILE:HG22	1:O:56:PHE:CE2	2.51	0.44
1:O:57:ASP:O	1:O:60:ASP:HB2	2.17	0.44
1:O:209:GLY:O	1:O:210:CYS:HB3	2.16	0.44
1:C:248:LYS:HD2	1:C:281(A):SER:O	2.17	0.44
1:O:51:VAL:HG12	1:O:52:TYR:CG	2.52	0.44
1:O:326:ARG:CG	1:O:326:ARG:NH2	2.70	0.44
1:C:292:PRO:CB	1:C:293:PRO:CD	2.96	0.44
1:O:186:LYS:HB2	1:O:186:LYS:HZ2	1.83	0.44
1:O:66:HIS:CG	1:O:67:ASN:N	2.85	0.44
2:C:1327:C47:H171	3:C:2015:HOH:O	2.17	0.44
1:O:199:VAL:HG22	1:O:231:LEU:HD12	2.00	0.44
1:O:185:ILE:HD12	1:O:211:LEU:HD22	1.99	0.44
1:C:41:PRO:HG3	1:C:107:MET:HE2	1.99	0.44
1:O:63:SER:O	1:O:64:TYR:C	2.53	0.44
1:C:152:SER:OG	1:C:169:GLY:O	2.26	0.44
1:O:240:ARG:HG3	1:O:241:LEU:N	2.30	0.44
1:C:147:LYS:HG2	1:C:148:GLU:N	2.31	0.44
1:C:65:LYS:HE2	1:C:65:LYS:HB2	1.86	0.44
1:O:286:ILE:C	1:O:287:HIS:CD2	2.90	0.44
1:O:86:GLN:O	1:O:87:ASP:HB2	2.18	0.44
1:C:291:ILE:HG22	1:C:296:GLY:CA	2.48	0.44
1:C:195:LYS:NZ	1:C:264:GLY:H	2.16	0.44
1:O:326:ARG:HH21	1:O:326:ARG:HD2	1.27	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:176:GLU:HG2	1:O:324:LEU:HB2	2.00	0.44
1:O:152:SER:HA	1:O:311:THR:O	2.18	0.43
1:O:65:LYS:O	1:O:86:GLN:HB2	2.18	0.43
1:C:180:HIS:O	1:C:322:PHE:N	2.44	0.43
1:C:291:ILE:HD13	1:C:298:THR:CG2	2.48	0.43
1:O:20:ILE:CG1	1:O:89:ILE:HG12	2.49	0.43
1:C:99:GLN:OE1	1:C:139:ASN:ND2	2.36	0.43
1:C:186:LYS:CB	1:C:186:LYS:C	2.74	0.43
1:C:291:ILE:HD13	1:C:298:THR:HG22	2.01	0.43
1:O:39:TRP:CE2	1:O:120:VAL:HG12	2.53	0.43
1:C:13:GLN:CG	2:C:1327:C47:H6C1	2.48	0.43
1:O:10:MET:C	1:O:12:THR:N	2.72	0.43
1:O:36:SER:HG	1:O:128:GLN:HB2	1.83	0.43
1:O:208:ASP:O	1:O:208:ASP:OD2	2.35	0.43
1:C:293:PRO:CD	1:C:294:PRO:CD	2.95	0.43
1:O:291:ILE:H	1:O:291:ILE:HG12	1.69	0.43
1:O:130:ILE:HD11	2:O:1327:C47:H351	2.01	0.43
1:C:303:ALA:O	1:C:307:ARG:HB3	2.18	0.43
1:O:281(C):LYS:HB3	1:O:281(C):LYS:HE3	1.45	0.43
1:O:28:LYS:CB	1:O:117:PHE:CA	2.91	0.43
1:C:270:THR:HG21	1:O:17:GLU:CD	2.39	0.43
1:C:151:PHE:CE2	1:C:313:PHE:CD1	3.07	0.43
1:O:107:MET:HA	1:O:108:PRO:HD2	1.22	0.43
1:O:75:TYR:HB2	2:O:1327:C47:H201	2.00	0.43
1:O:199:VAL:CG2	1:O:231:LEU:HD12	2.48	0.43
1:O:221:ILE:HG13	1:O:304:THR:HB	2.00	0.43
1:C:185:ILE:CG2	1:C:186:LYS:N	2.78	0.43
1:O:245:TYR:C	1:O:246:VAL:HG13	2.39	0.43
1:O:326:ARG:CB	1:O:326:ARG:NH2	2.76	0.43
1:O:109:ALA:HB3	1:O:110:LEU:HB3	2.00	0.43
1:O:141:ILE:HD11	1:O:146:LEU:HD12	2.01	0.43
1:C:161:LEU:HD12	1:C:161:LEU:HA	1.39	0.43
1:C:28:LYS:C	1:C:29:VAL:HG13	2.38	0.43
1:C:149:ASP:N	1:C:316:ARG:HD3	2.34	0.43
1:C:189:VAL:HG12	1:C:191:GLN:N	2.34	0.42
1:O:270:THR:HB	1:O:272:ALA:H	1.84	0.42
1:C:21:GLY:O	1:C:23:PRO:C	2.57	0.42
1:C:228:ILE:O	1:C:232:MET:HG2	2.20	0.42
1:O:326:ARG:HB3	1:O:326:ARG:NH2	2.22	0.42
1:C:221:ILE:O	1:C:286:ILE:HG23	2.19	0.42
1:C:185:ILE:HG21	1:C:191:GLN:HB3	2.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:245:TYR:O	1:O:246:VAL:CG1	2.68	0.42
1:O:84:LEU:HG	1:O:100:MET:CE	2.49	0.42
1:O:107:MET:HE2	1:O:107:MET:HB2	1.13	0.42
1:O:184:LEU:HA	1:O:184:LEU:HD12	1.47	0.42
1:O:232:MET:HA	1:O:235:LEU:HB2	2.00	0.42
1:C:237:ALA:HB1	1:C:246:VAL:N	2.34	0.42
1:C:171:ASP:OD2	1:C:173:GLN:HB2	2.19	0.42
1:O:185:ILE:HG21	1:O:185:ILE:HD13	1.78	0.42
1:O:232:MET:HG3	1:O:245:TYR:CD1	2.55	0.42
1:O:272:ALA:HB3	1:O:273:ASP:H	1.61	0.42
1:O:49:ALA:HB1	1:O:107:MET:HG2	2.01	0.42
1:O:317:ASN:HB3	1:O:319:ARG:HD3	2.01	0.42
1:O:205:LEU:CB	1:O:230:LYS:HE2	2.50	0.42
1:O:160(D):SER:N	1:O:160(D):SER:C	2.65	0.42
1:O:207:GLU:OE2	1:O:207:GLU:N	2.51	0.42
1:O:43:SER:C	1:O:45:CYS:N	2.63	0.42
1:C:205:LEU:CD2	1:C:205:LEU:N	2.82	0.42
1:C:140:ILE:HD13	1:C:140:ILE:HG21	1.75	0.42
1:C:8:ASN:HD21	1:C:158:ASP:HB2	1.85	0.42
1:O:261:HIS:C	1:O:261:HIS:CD2	2.93	0.42
1:C:292:PRO:HB2	1:C:293:PRO:HD3	2.02	0.42
1:O:194:MET:HE1	1:O:260:PHE:CD2	2.49	0.42
1:C:237:ALA:HB1	1:C:246:VAL:O	2.20	0.42
1:O:23:PRO:O	1:O:23:PRO:CG	2.68	0.42
1:O:178:ASN:HD22	1:O:179:PHE:N	2.16	0.42
1:C:46:SER:OG	1:C:47:ARG:N	2.44	0.42
1:C:88:ILE:HD13	1:C:88:ILE:HG21	1.80	0.42
1:O:235:LEU:HD12	1:O:284:LEU:HD11	2.01	0.41
1:O:292:PRO:C	1:O:294:PRO:HD2	2.41	0.41
1:O:88:ILE:HA	1:O:96:VAL:O	2.19	0.41
1:C:314:ASP:O	1:C:318:ASN:HA	2.20	0.41
1:C:36:SER:OG	1:C:124:GLY:C	2.58	0.41
1:C:35:SER:HB3	2:C:1327:C47:H331	2.03	0.41
1:O:5:ILE:HG23	1:O:161:LEU:CD1	2.50	0.41
1:C:126:ILE:HG13	1:C:126:ILE:O	2.20	0.41
1:C:38:VAL:HG23	1:C:38:VAL:H	1.59	0.41
1:O:194:MET:HE3	1:O:260:PHE:HD2	1.84	0.41
1:O:137:PHE:CE1	1:O:141:ILE:CG1	3.03	0.41
1:C:13:GLN:HE21	1:C:13:GLN:HB3	0.89	0.41
1:C:76:SER:OG	1:C:289:MET:CG	2.69	0.41
1:C:215:ASP:OD1	1:C:218:ALA:HB2	2.21	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:PRO:CG	1:C:107:MET:CE	2.96	0.41
1:O:51:VAL:CG1	1:O:52:TYR:CD2	2.96	0.41
1:C:65:LYS:HD3	1:C:65:LYS:HA	1.76	0.41
1:C:125:PHE:HE1	1:C:315:ARG:CD	2.33	0.41
1:C:205:LEU:HA	1:C:207:GLU:OE1	2.21	0.41
1:C:149:ASP:HB3	1:C:315:ARG:CB	2.50	0.41
1:C:198:SER:HB2	1:C:259:SER:HB2	2.02	0.41
1:C:52:TYR:CD1	1:C:113:MET:CE	3.03	0.41
1:O:126:ILE:CD1	1:O:132:ARG:CG	2.87	0.41
1:O:75:TYR:HA	2:O:1327:C47:H332	2.03	0.41
1:O:0:THR:N	1:O:147:LYS:CE	2.83	0.41
1:C:204:LEU:O	1:C:230:LYS:NZ	2.40	0.41
1:O:84:LEU:HG	1:O:100:MET:HG3	2.02	0.41
1:O:132:ARG:CG	1:O:132:ARG:O	2.68	0.41
1:C:147:LYS:NZ	1:C:147:LYS:HB2	2.32	0.41
1:C:255:LEU:HB3	1:C:274:TYR:OH	2.20	0.41
1:O:76:SER:HB3	1:O:291:ILE:HG21	2.03	0.41
1:O:4:VAL:O	1:O:164:GLN:HA	2.21	0.41
1:C:186:LYS:CD	1:C:186:LYS:HG3	2.20	0.41
1:O:186:LYS:CG	1:O:186:LYS:O	2.68	0.41
1:O:292:PRO:HA	1:O:293:PRO:HD3	1.80	0.41
1:C:147:LYS:CG	1:C:148:GLU:HB2	2.51	0.40
1:O:5:ILE:HD13	1:O:5:ILE:HG21	1.69	0.40
1:O:291:ILE:HA	1:O:292:PRO:HD3	1.62	0.40
1:O:184:LEU:HB3	1:O:318:ASN:ND2	2.37	0.40
1:O:240:ARG:NH2	1:O:244:ASP:HB2	2.36	0.40
1:C:228:ILE:O	1:C:229:GLU:C	2.59	0.40
1:O:130:ILE:HD13	2:O:1327:C47:H351	2.03	0.40
1:O:233:GLU:O	1:O:233:GLU:OE1	2.38	0.40
1:C:147:LYS:HG2	1:C:148:GLU:HB2	2.03	0.40
1:O:294:PRO:HG2	1:O:295:THR:N	2.36	0.40
1:C:267:TYR:OH	1:C:322:PHE:HB2	2.21	0.40
1:C:253:PRO:HG3	1:C:280:TYR:CE2	2.56	0.40
1:C:292:PRO:O	1:C:294:PRO:CD	2.70	0.40
1:C:147:LYS:HB2	1:C:147:LYS:HZ2	1.85	0.40
1:O:262:LEU:HD23	1:O:267:TYR:HD1	1.78	0.40
1:O:88:ILE:HG21	1:O:88:ILE:HD13	1.40	0.40
1:C:23:PRO:HA	1:C:24:PRO:HD3	1.71	0.40
1:C:294:PRO:HB2	1:C:295:THR:HG23	2.04	0.40
1:C:197:VAL:O	1:C:203:THR:HA	2.21	0.40
1:C:204:LEU:HB3	1:C:205:LEU:HD22	2.03	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:126:ILE:HG22	1:O:127:GLU:OE1	2.22	0.40
1:O:83:PHE:CE1	1:O:105:THR:HG23	2.56	0.40
1:O:192:ILE:HG21	1:O:192:ILE:HD13	1.83	0.40
1:O:134:THR:HG22	1:O:135:PRO:N	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	330/340 (97%)	283 (86%)	34 (10%)	13 (4%)	4	12
1	O	328/340 (96%)	274 (84%)	34 (10%)	20 (6%)	2	5
All	All	658/680 (97%)	557 (85%)	68 (10%)	33 (5%)	3	8

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	185	ILE
1	C	207	GLU
1	C	234	ALA
1	C	235	LEU
1	C	240	ARG
1	O	58	ALA
1	O	77	THR
1	O	186	LYS
1	O	244	ASP
1	O	293	PRO
1	C	145	VAL
1	C	203	THR
1	C	241	LEU
1	C	252	GLY

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	293	PRO
1	O	149	ASP
1	O	209	GLY
1	C	144	GLY
1	O	60	ASP
1	O	87	ASP
1	O	203	THR
1	O	272	ALA
1	O	273	ASP
1	O	277	GLN
1	O	278	GLU
1	O	53	HIS
1	O	145	VAL
1	C	281(C)	LYS
1	O	271	SER
1	C	281(A)	SER
1	O	252	GLY
1	O	294	PRO
1	O	256	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	C	283/290 (98%)	214 (76%)	69 (24%)	1	2
1	O	282/290 (97%)	193 (68%)	89 (32%)	0	1
All	All	565/580 (97%)	407 (72%)	158 (28%)	0	1

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	-1	ASN
1	C	3	SER
1	C	5	ILE
1	C	22	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	26	THR
1	C	42	SER
1	C	44	LYS
1	C	47	ARG
1	C	54	LYS
1	C	60	ASP
1	C	69	THR
1	C	81	SER
1	C	90	THR
1	C	95	THR
1	C	106	GLU
1	C	107	MET
1	C	110	LEU
1	C	113	MET
1	C	120	VAL
1	C	123	MET
1	C	130	ILE
1	C	134	THR
1	C	136	ILE
1	C	138	ASP
1	C	143	GLN
1	C	145	VAL
1	C	147	LYS
1	C	150	VAL
1	C	157	ARG
1	C	164	GLN
1	C	182	ILE
1	C	187	THR
1	C	192	ILE
1	C	193	GLN
1	C	195	LYS
1	C	199	VAL
1	C	202	SER
1	C	205	LEU
1	C	208	ASP
1	C	213	LEU
1	C	219	SER
1	C	226	SER
1	C	228	ILE
1	C	229	GLU
1	C	230	LYS
1	C	231	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	233	GLU
1	C	239	LYS
1	C	240	ARG
1	C	241	LEU
1	C	247	VAL
1	C	249	CYS
1	C	250	ASN
1	C	274	TYR
1	C	278	GLU
1	C	279	SER
1	C	281	SER
1	C	281(C)	LYS
1	C	284	LEU
1	C	294	PRO
1	C	301	LEU
1	C	304	THR
1	C	307	ARG
1	C	311	THR
1	C	312	GLU
1	C	315	ARG
1	C	316	ARG
1	C	319	ARG
1	C	324	LEU
1	O	-1	ASN
1	O	0	THR
1	O	1	THR
1	O	2	SER
1	O	3	SER
1	O	13	GLN
1	O	14	TYR
1	O	17	GLU
1	O	22	THR
1	O	23	PRO
1	O	25	GLN
1	O	26	THR
1	O	32	ASP
1	O	35	SER
1	O	36	SER
1	O	37	ASN
1	O	44	LYS
1	O	47	ARG
1	O	48	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	O	62	SER
1	O	63	SER
1	O	65	LYS
1	O	69	THR
1	O	71	LEU
1	O	76	SER
1	O	80	VAL
1	O	83	PHE
1	O	84	LEU
1	O	85	SER
1	O	87	ASP
1	O	90	THR
1	O	91	VAL
1	O	106	GLU
1	O	118	ASP
1	O	126	ILE
1	O	132	ARG
1	O	138	ASP
1	O	141	ILE
1	O	143	GLN
1	O	147	LYS
1	O	149	ASP
1	O	152	SER
1	O	157	ARG
1	O	158	ASP
1	O	164	GLN
1	O	171	ASP
1	O	178	ASN
1	O	184	LEU
1	O	185	ILE
1	O	186	LYS
1	O	189	VAL
1	O	195	LYS
1	O	198	SER
1	O	201	SER
1	O	202	SER
1	O	205	LEU
1	O	206	CYS
1	O	207	GLU
1	O	208	ASP
1	O	213	LEU
1	O	219	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	O	227	SER
1	O	230	LYS
1	O	232	MET
1	O	233	GLU
1	O	235	LEU
1	O	238	LYS
1	O	241	LEU
1	O	247	VAL
1	O	248	LYS
1	O	251	GLU
1	O	253	PRO
1	O	262	LEU
1	O	265	LYS
1	O	270	THR
1	O	271	SER
1	O	278	GLU
1	O	279	SER
1	O	281	SER
1	O	281(C)	LYS
1	O	281(D)	LEU
1	O	283	THR
1	O	284	LEU
1	O	291	ILE
1	O	295	THR
1	O	308	LYS
1	O	315	ARG
1	O	324	LEU
1	O	326	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	-1	ASN
1	C	13	GLN
1	C	164	GLN
1	C	250	ASN
1	C	277	GLN
1	C	287	HIS
1	C	318	ASN
1	O	99	GLN
1	O	139	ASN
1	O	164	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	O	174	HIS
1	O	178	ASN
1	O	183	ASN
1	O	191	GLN
1	O	193	GLN
1	O	287	HIS
1	O	318	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands 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	C47	C	1327	-	36,36,36	3.12	20 (55%)	35,50,50	3.35	18 (51%)
2	C47	O	1327	-	36,36,36	3.92	20 (55%)	35,50,50	3.94	20 (57%)

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	C47	C	1327	-	-	0/37/49/49	0/2/2/2
2	C47	O	1327	-	-	0/37/49/49	0/2/2/2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	1327	C47	C12-C7	-8.26	1.28	1.40
2	C	1327	C47	C17-C18	-5.91	1.45	1.54
2	O	1327	C47	C6-C7	-4.86	1.43	1.51
2	C	1327	C47	C21-C18	-4.70	1.44	1.55
2	O	1327	C47	C26-C27	-4.24	1.42	1.54
2	C	1327	C47	C14-C5	-4.23	1.46	1.53
2	C	1327	C47	C14-N13	-4.05	1.41	1.47
2	O	1327	C47	C26-C24	-3.19	1.44	1.52
2	C	1327	C47	C29-N31	-2.82	1.27	1.33
2	O	1327	C47	C14-N13	-2.82	1.43	1.47
2	C	1327	C47	O30-C29	-2.71	1.18	1.23
2	C	1327	C47	C19-C18	-2.65	1.48	1.53
2	C	1327	C47	C33-C32	-2.42	1.41	1.51
2	O	1327	C47	C17-C15	-2.38	1.48	1.51
2	O	1327	C47	C32-N31	-2.10	1.41	1.46
2	O	1327	C47	C10-C9	2.17	1.43	1.38
2	O	1327	C47	C11-C12	2.25	1.43	1.39
2	C	1327	C47	C27-C29	2.30	1.55	1.51
2	O	1327	C47	C24-C22	2.31	1.55	1.53
2	C	1327	C47	O25-C24	2.52	1.49	1.43
2	C	1327	C47	C8-C7	2.80	1.44	1.39
2	C	1327	C47	C15-N13	3.01	1.41	1.36
2	C	1327	C47	O2-C1	3.02	1.52	1.45
2	C	1327	C47	C22-N23	3.10	1.58	1.47
2	C	1327	C47	C12-C7	3.13	1.44	1.40
2	C	1327	C47	C26-C24	3.25	1.61	1.52
2	O	1327	C47	C9-C8	3.36	1.45	1.38
2	O	1327	C47	C21-C22	3.58	1.57	1.53
2	O	1327	C47	C10-C11	3.59	1.46	1.38
2	O	1327	C47	C29-N31	3.86	1.41	1.33
2	O	1327	C47	C6-C5	4.15	1.64	1.52
2	C	1327	C47	O2-C3	4.18	1.43	1.33
2	O	1327	C47	O16-C15	5.37	1.35	1.23
2	C	1327	C47	C12-N13	5.66	1.51	1.41
2	C	1327	C47	C9-C8	6.50	1.52	1.38
2	O	1327	C47	C19-C18	6.86	1.67	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	1327	C47	O2-C3	6.95	1.51	1.33
2	O	1327	C47	C12-N13	7.08	1.54	1.41
2	C	1327	C47	C11-C12	7.11	1.52	1.39
2	O	1327	C47	O4-C3	11.88	1.51	1.21

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1327	C47	O25-C24-C22	-8.91	96.28	109.49
2	C	1327	C47	C27-C26-C24	-6.87	105.71	114.24
2	O	1327	C47	C27-C26-C24	-6.09	106.67	114.24
2	O	1327	C47	C6-C7-C12	-6.05	111.98	120.07
2	O	1327	C47	C19-C18-C17	-5.29	98.98	109.30
2	O	1327	C47	C10-C9-C8	-5.19	112.58	120.19
2	O	1327	C47	O4-C3-C5	-4.84	103.33	123.10
2	C	1327	C47	C7-C12-N13	-3.41	114.26	117.30
2	C	1327	C47	O2-C3-O4	-3.40	116.77	123.79
2	C	1327	C47	O30-C29-N31	-3.17	116.73	123.08
2	C	1327	C47	C20-C18-C19	-2.93	105.35	109.49
2	O	1327	C47	C14-C5-C6	-2.92	103.18	109.19
2	O	1327	C47	C28-C27-C26	-2.89	105.63	111.42
2	O	1327	C47	O16-C15-C17	-2.58	116.20	121.64
2	C	1327	C47	C1-O2-C3	-2.41	110.34	115.99
2	C	1327	C47	C14-C5-C6	-2.29	104.47	109.19
2	C	1327	C47	C9-C8-C7	-2.29	117.35	120.90
2	C	1327	C47	C33-C32-N31	-2.25	105.61	112.19
2	C	1327	C47	C21-C22-N23	-2.03	103.20	109.13
2	O	1327	C47	C11-C12-C7	-2.01	117.06	120.00
2	O	1327	C47	C28-C27-C29	2.07	112.26	109.34
2	C	1327	C47	C19-C18-C17	2.09	113.39	109.30
2	O	1327	C47	C11-C12-N13	2.25	124.54	121.35
2	C	1327	C47	C11-C12-N13	2.36	124.69	121.35
2	C	1327	C47	C10-C9-C8	2.36	123.65	120.19
2	O	1327	C47	O16-C15-N13	2.39	125.29	121.93
2	O	1327	C47	C27-C29-N31	2.59	120.50	116.84
2	C	1327	C47	C20-C18-C17	2.66	114.48	109.30
2	O	1327	C47	C20-C18-C17	3.41	115.96	109.30
2	C	1327	C47	C27-C29-N31	3.61	121.95	116.84
2	O	1327	C47	O2-C3-C5	5.06	120.41	111.87
2	O	1327	C47	C8-C7-C12	5.23	124.62	118.10
2	O	1327	C47	O25-C24-C26	5.38	119.64	109.22
2	O	1327	C47	O2-C3-O4	6.02	136.22	123.79

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	O	1327	C47	O25-C24-C22	7.00	119.86	109.49
2	C	1327	C47	O2-C3-C5	7.93	125.25	111.87
2	C	1327	C47	C28-C27-C29	8.48	121.30	109.34
2	O	1327	C47	C20-C18-C19	12.02	126.47	109.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1327	C47	11	0
2	O	1327	C47	15	0

## 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 ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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