



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:21 AM UTC

PDB ID : 4RUB / pdb_00004rub
Title : A CRYSTAL FORM OF RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE FROM NICOTIANA TABACUM IN THE ACTIVATED STATE
Authors : Schreuder, H.; Cascio, D.; Curmi, P.M.G.; Eisenberg, D.
Deposited on : 1990-05-25
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

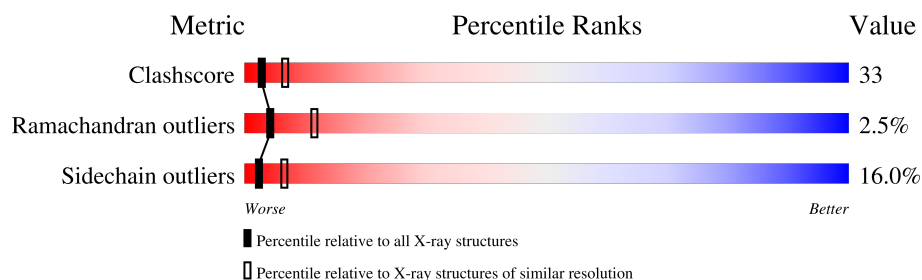
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	477	17% 45% 29% 7% .
1	B	477	17% 45% 29% 7% .
1	C	477	18% 42% 31% 7% .
1	D	477	19% 43% 28% 8% .
2	S	123	12% 45% 34% 9%
2	T	123	17% 47% 26% 10%
2	U	123	7% 37% 47% 8%
2	V	123	11% 44% 32% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CAP	A	490	-	X	-	-
4	CAP	B	490	-	X	-	-
4	CAP	C	490	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18708 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 RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	1
			3628	2307	641	664	16			
1	B	465	Total	C	N	O	S	0	0	1
			3628	2307	641	664	16			
1	C	465	Total	C	N	O	S	0	0	1
			3628	2307	641	664	16			
1	D	465	Total	C	N	O	S	0	0	1
			3628	2307	641	664	16			

- Molecule 2 is a protein called RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	123	Total	C	N	O	S	0	0	0
			1024	669	163	186	6			
2	T	123	Total	C	N	O	S	0	0	0
			1024	669	163	186	6			
2	U	123	Total	C	N	O	S	0	0	0
			1024	669	163	186	6			
2	V	123	Total	C	N	O	S	0	0	0
			1024	669	163	186	6			

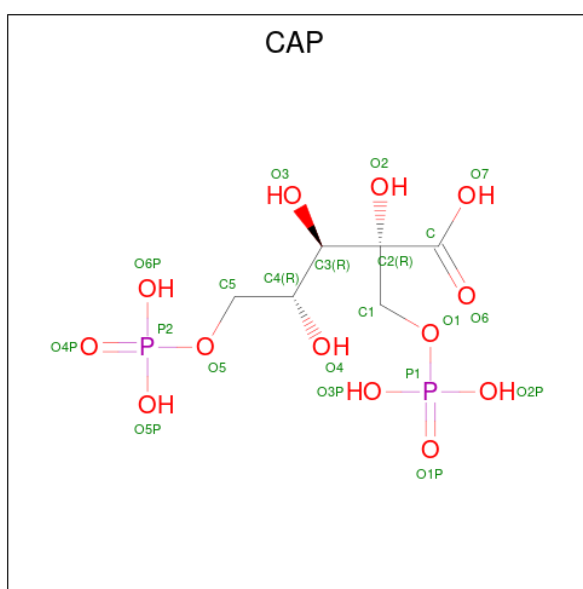
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	88	GLY	GLU	conflict	UNP P69249
T	88	GLY	GLU	conflict	UNP P69249
U	88	GLY	GLU	conflict	UNP P69249
V	88	GLY	GLU	conflict	UNP P69249

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (CCD ID: CAP) (formula: $C_6H_{14}O_{13}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O P 21 6 13 2	0	0
4	B	1	Total C O P 21 6 13 2	0	0
4	C	1	Total C O P 21 6 13 2	0	0
4	D	1	Total C O P 21 6 13 2	0	0

- Molecule 5 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



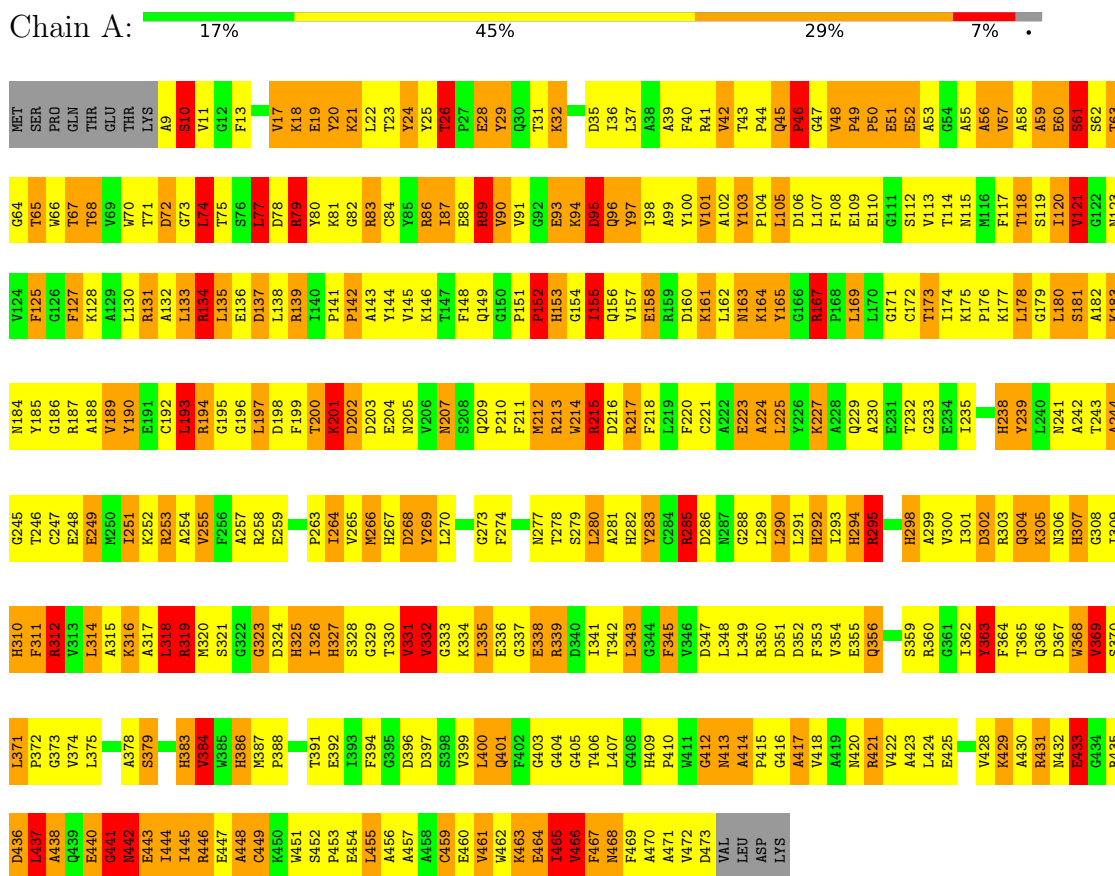
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		
5	C	1	Total	C	O	0	0
			3	1	2		
5	D	1	Total	C	O	0	0
			3	1	2		

3 Residue-property plots

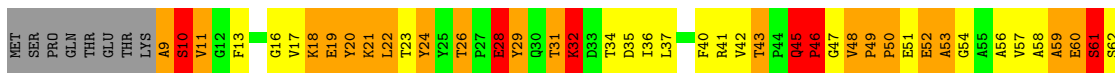
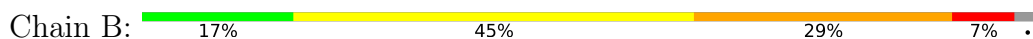
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)



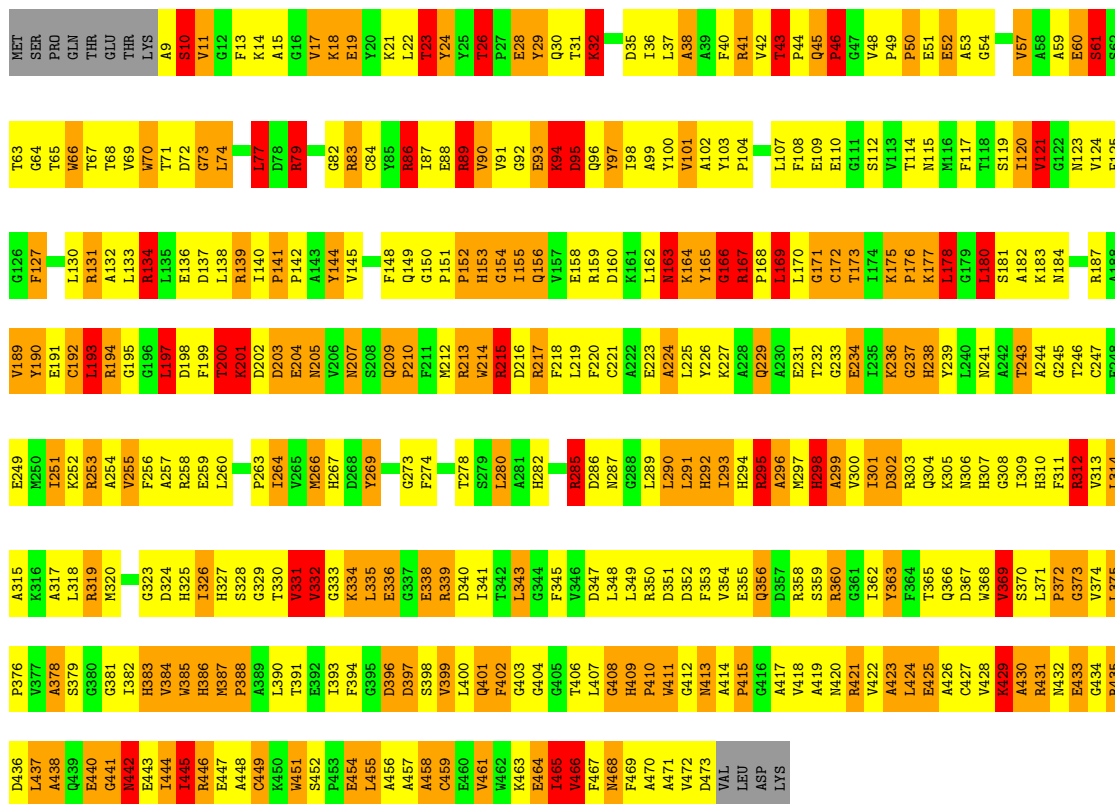
- Molecule 1: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)





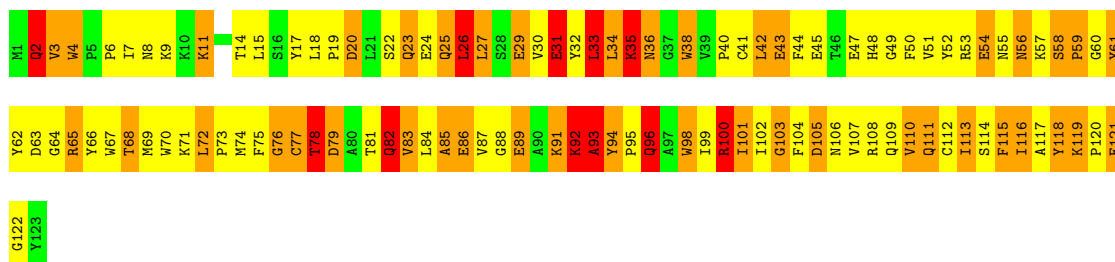
• Molecule 1: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)

Chain D: 

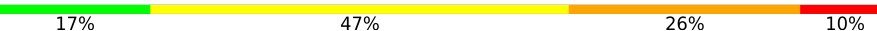


• Molecule 2: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)

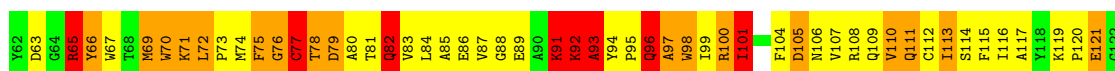
Chain S: 



• Molecule 2: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)

Chain T: 

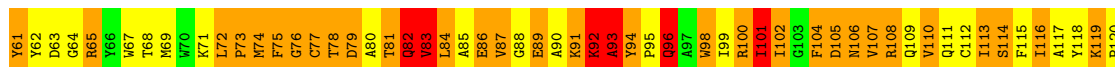




Y123

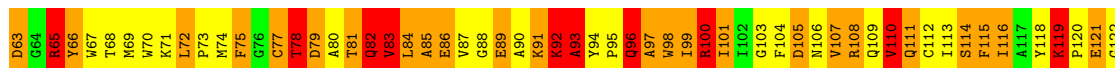
- Molecule 2: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)

Chain U: 7% 37% 47% 8%

E121
G122
Y123

- Molecule 2: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE (FORM IV)

Chain V: 11% 44% 32% 13%



Y123

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	204.60Å 204.60Å 117.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.202 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18708	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: FMT, CAP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.21	120/3716 (3.2%)	3.12	541/5038 (10.7%)
1	B	2.18	113/3716 (3.0%)	3.13	542/5038 (10.8%)
1	C	2.28	150/3716 (4.0%)	3.09	526/5038 (10.4%)
1	D	2.19	110/3716 (3.0%)	3.08	535/5038 (10.6%)
2	S	1.97	31/1057 (2.9%)	3.09	148/1435 (10.3%)
2	T	1.96	26/1057 (2.5%)	2.88	122/1435 (8.5%)
2	U	2.26	48/1057 (4.5%)	3.10	140/1435 (9.8%)
2	V	2.13	28/1057 (2.6%)	3.13	141/1435 (9.8%)
All	All	2.19	626/19092 (3.3%)	3.09	2695/25892 (10.4%)

All (626) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	7	ILE	C-O	13.43	1.37	1.23
1	B	175	LYS	N-CA	11.56	1.55	1.45
1	C	266	MET	C-O	11.43	1.38	1.23
2	V	82	GLN	C-O	10.95	1.36	1.24
2	V	7	ILE	C-O	10.76	1.38	1.24
1	A	238	HIS	CE1-NE2	-10.75	1.21	1.32
1	C	201	LYS	CA-CB	10.33	1.71	1.53
1	D	290	LEU	C-O	10.24	1.35	1.23
1	C	238	HIS	CE1-NE2	-10.22	1.22	1.32
1	B	141	PRO	C-O	9.96	1.33	1.24
1	D	201	LYS	CA-CB	9.89	1.70	1.53
1	C	310	HIS	C-O	9.64	1.35	1.23
1	C	323	GLY	N-CA	9.64	1.59	1.45
1	A	201	LYS	CA-CB	9.32	1.69	1.53
1	A	72	ASP	C-O	9.25	1.35	1.24
1	C	298	HIS	CD2-NE2	9.24	1.48	1.37
1	C	127	PHE	C-O	9.22	1.34	1.23
1	D	290	LEU	N-CA	9.20	1.56	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	319	ARG	CD-NE	-9.20	1.33	1.46
2	S	7	ILE	C-O	9.03	1.35	1.24
1	B	201	LYS	CA-CB	9.02	1.68	1.53
1	C	405	GLY	C-O	8.97	1.36	1.23
2	U	102	ILE	C-O	8.96	1.33	1.23
1	C	243	THR	CB-OG1	8.90	1.57	1.43
1	A	238	HIS	CG-CD2	-8.84	1.26	1.35
1	B	201	LYS	N-CA	-8.81	1.35	1.46
1	C	238	HIS	C-O	8.80	1.33	1.23
1	C	201	LYS	N-CA	-8.78	1.35	1.46
2	V	8	ASN	N-CA	8.75	1.57	1.46
1	A	175	LYS	N-CA	8.72	1.53	1.45
1	B	140	ILE	N-CA	8.71	1.52	1.46
1	C	256	PHE	C-O	8.67	1.34	1.24
1	C	445	ILE	N-CA	8.66	1.57	1.46
1	A	267	HIS	CD2-NE2	8.63	1.47	1.37
1	C	293	ILE	C-N	-8.60	1.22	1.33
2	U	54	GLU	C-O	8.45	1.33	1.24
1	B	367	ASP	N-CA	8.37	1.56	1.46
1	D	329	GLY	N-CA	8.35	1.53	1.45
2	V	62	TYR	N-CA	8.34	1.56	1.46
2	T	92	LYS	C-O	8.32	1.33	1.23
1	A	319	ARG	NE-CZ	-8.30	1.24	1.33
2	V	93	ALA	N-CA	8.30	1.56	1.46
1	D	258	ARG	NE-CZ	8.24	1.42	1.33
1	A	368	TRP	C-N	-8.23	1.22	1.33
2	U	59	PRO	C-O	8.22	1.33	1.23
1	A	135	LEU	N-CA	8.18	1.56	1.46
1	B	175	LYS	CA-CB	-8.16	1.44	1.54
1	C	435	ARG	N-CA	8.16	1.56	1.45
1	D	237	GLY	C-O	8.16	1.32	1.24
1	D	403	GLY	N-CA	8.14	1.57	1.45
1	A	119	SER	C-O	8.13	1.34	1.24
1	B	365	THR	C-O	8.12	1.33	1.23
1	D	306	ASN	C-O	8.12	1.34	1.23
1	B	189	VAL	C-N	-8.10	1.23	1.33
1	D	123	ASN	C-N	-8.10	1.23	1.34
1	A	319	ARG	CD-NE	-8.08	1.34	1.46
2	U	94	TYR	N-CA	8.07	1.55	1.46
1	B	120	ILE	C-N	-8.04	1.26	1.33
1	D	291	LEU	C-O	8.03	1.33	1.24
1	A	252	LYS	C-N	-7.98	1.23	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	421	ARG	C-O	7.96	1.33	1.24
1	D	385	TRP	CA-CB	7.96	1.65	1.53
1	B	292	HIS	ND1-CE1	-7.92	1.24	1.32
1	C	429	LYS	N-CA	7.92	1.56	1.46
1	C	306	ASN	C-O	7.90	1.33	1.23
1	D	421	ARG	C-O	7.87	1.33	1.24
1	B	282	HIS	CE1-NE2	-7.87	1.24	1.32
1	D	153	HIS	CE1-NE2	7.86	1.40	1.32
1	D	26	THR	CA-CB	7.82	1.62	1.53
1	A	103	TYR	C-O	7.82	1.33	1.24
2	T	7	ILE	C-O	7.80	1.32	1.23
2	S	8	ASN	N-CA	7.79	1.58	1.46
2	U	98	TRP	C-O	7.78	1.33	1.23
2	T	39	VAL	N-CA	7.77	1.52	1.46
1	C	177	LYS	C-O	7.77	1.33	1.24
2	U	7	ILE	CA-CB	7.77	1.64	1.54
1	D	264	ILE	N-CA	7.76	1.55	1.46
1	A	24	TYR	C-O	7.74	1.34	1.23
1	A	465	ILE	CA-CB	7.71	1.63	1.54
1	C	153	HIS	C-O	7.69	1.35	1.23
1	D	132	ALA	N-CA	7.67	1.55	1.45
1	A	134	ARG	CZ-NH1	7.66	1.43	1.32
1	C	156	GLN	CD-NE2	7.66	1.49	1.33
1	D	332	VAL	C-O	7.65	1.33	1.24
2	U	65	ARG	NE-CZ	7.63	1.41	1.33
1	A	386	HIS	CE1-NE2	7.59	1.40	1.32
1	C	367	ASP	N-CA	7.56	1.55	1.46
2	U	8	ASN	N-CA	7.54	1.57	1.46
1	C	175	LYS	N-CA	7.54	1.52	1.45
1	C	69	VAL	N-CA	7.52	1.55	1.46
1	A	121	VAL	N-CA	7.44	1.54	1.46
1	D	197	LEU	C-O	7.42	1.32	1.23
1	C	267	HIS	CE1-NE2	-7.42	1.25	1.32
1	C	332	VAL	C-O	7.34	1.32	1.24
1	B	64	GLY	N-CA	7.33	1.51	1.44
1	C	141	PRO	CA-C	-7.31	1.47	1.52
1	D	201	LYS	N-CA	-7.29	1.37	1.46
2	U	116	ILE	N-CA	7.28	1.55	1.46
2	T	8	ASN	N-CA	7.27	1.55	1.46
1	B	248	GLU	C-O	7.25	1.32	1.24
2	S	92	LYS	C-O	7.25	1.32	1.24
1	C	205	ASN	N-CA	7.25	1.54	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	267	HIS	ND1-CE1	7.22	1.39	1.32
2	U	104	PHE	CA-CB	7.20	1.63	1.53
1	D	115	ASN	C-O	-7.18	1.15	1.24
1	B	69	VAL	N-CA	7.17	1.54	1.46
2	T	92	LYS	N-CA	7.17	1.54	1.46
1	D	411	TRP	C-O	7.17	1.33	1.24
1	A	201	LYS	N-CA	-7.16	1.37	1.46
1	D	140	ILE	N-CA	7.16	1.51	1.46
1	C	161	LYS	C-O	7.12	1.32	1.24
2	V	65	ARG	NE-CZ	7.11	1.40	1.33
1	C	365	THR	N-CA	7.10	1.55	1.46
1	B	206	VAL	C-O	-7.09	1.13	1.23
1	C	267	HIS	CG-ND1	-7.08	1.30	1.38
2	U	98	TRP	CA-C	7.06	1.61	1.52
2	U	100	ARG	N-CA	7.05	1.55	1.45
1	C	36	ILE	C-O	7.04	1.33	1.24
2	V	92	LYS	C-O	7.03	1.32	1.24
2	V	50	PHE	N-CA	7.03	1.54	1.45
1	C	267	HIS	ND1-CE1	7.02	1.39	1.32
1	A	148	PHE	C-O	-7.00	1.15	1.23
2	V	114	SER	N-CA	7.00	1.53	1.46
1	C	206	VAL	CA-C	6.98	1.60	1.53
2	S	59	PRO	C-O	6.97	1.31	1.23
1	A	350	ARG	CD-NE	-6.96	1.36	1.46
1	B	294	HIS	ND1-CE1	-6.95	1.25	1.32
1	C	285	ARG	CZ-NH1	6.95	1.42	1.32
1	A	244	ALA	C-O	6.95	1.32	1.23
2	V	67	TRP	N-CA	6.94	1.54	1.45
1	D	301	ILE	CA-CB	6.94	1.63	1.54
1	C	401	GLN	CA-CB	6.92	1.64	1.53
1	A	267	HIS	CE1-NE2	-6.91	1.25	1.32
1	C	292	HIS	CE1-NE2	6.91	1.39	1.32
1	C	153	HIS	ND1-CE1	-6.90	1.25	1.32
1	A	200	THR	C-N	-6.89	1.25	1.33
2	T	106	ASN	C-O	6.89	1.32	1.24
1	A	39	ALA	C-O	6.87	1.32	1.23
1	D	319	ARG	NE-CZ	-6.87	1.25	1.33
2	V	88	GLY	N-CA	6.86	1.54	1.45
1	D	312	ARG	N-CA	6.85	1.54	1.46
1	A	374	VAL	C-O	-6.81	1.16	1.24
1	A	214	TRP	N-CA	-6.81	1.38	1.46
1	C	109	GLU	C-N	-6.80	1.24	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	148	PHE	N-CA	6.79	1.54	1.45
1	C	395	GLY	N-CA	6.78	1.52	1.45
1	C	431	ARG	NE-CZ	6.78	1.40	1.33
1	A	154	GLY	CA-C	-6.78	1.45	1.52
1	A	362	ILE	C-O	6.77	1.33	1.23
1	A	217	ARG	CD-NE	-6.76	1.36	1.46
2	T	57	LYS	N-CA	6.76	1.53	1.46
1	D	296	ALA	N-CA	6.72	1.54	1.46
1	A	26	THR	CA-CB	6.71	1.61	1.53
2	U	71	LYS	C-O	6.71	1.31	1.24
1	A	169	LEU	CA-CB	-6.69	1.43	1.53
1	D	285	ARG	NE-CZ	6.64	1.40	1.33
1	C	111	GLY	C-O	6.64	1.32	1.23
1	C	425	GLU	N-CA	6.64	1.54	1.46
1	A	223	GLU	C-O	-6.61	1.16	1.24
1	B	128	LYS	N-CA	6.61	1.54	1.46
1	B	350	ARG	CD-NE	-6.61	1.36	1.46
2	U	59	PRO	N-CA	6.60	1.55	1.47
1	C	220	PHE	C-O	6.59	1.31	1.24
1	D	399	VAL	N-CA	6.59	1.53	1.46
1	A	370	SER	C-O	6.58	1.34	1.24
2	V	106	ASN	C-O	6.57	1.32	1.24
1	D	237	GLY	N-CA	6.57	1.51	1.45
1	A	311	PHE	C-O	6.56	1.31	1.24
1	D	278	THR	C-N	-6.55	1.25	1.33
1	C	128	LYS	CA-CB	-6.54	1.43	1.53
1	A	367	ASP	CA-CB	-6.52	1.44	1.53
2	S	53	ARG	C-N	-6.50	1.25	1.33
1	D	440	GLU	C-O	6.50	1.32	1.24
2	T	7	ILE	CA-CB	6.50	1.62	1.55
2	U	98	TRP	CA-CB	-6.49	1.43	1.53
2	U	38	TRP	C-O	6.49	1.31	1.23
1	B	173	THR	C-N	-6.47	1.26	1.33
1	B	306	ASN	C-O	6.47	1.32	1.23
2	U	101	ILE	C-O	6.47	1.31	1.24
1	D	429	LYS	N-CA	6.47	1.54	1.46
2	S	7	ILE	CA-C	-6.46	1.46	1.52
1	C	329	GLY	CA-C	6.45	1.59	1.52
1	A	279	SER	CA-CB	-6.45	1.43	1.53
2	U	110	VAL	N-CA	6.44	1.53	1.46
2	U	49	GLY	C-O	6.44	1.32	1.23
1	D	280	LEU	C-O	6.43	1.31	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	388	PRO	N-CD	6.43	1.56	1.47
1	B	153	HIS	CE1-NE2	-6.42	1.26	1.32
1	D	325	HIS	ND1-CE1	6.42	1.39	1.32
2	T	99	ILE	N-CA	6.42	1.53	1.46
2	V	83	VAL	N-CA	6.41	1.54	1.46
2	V	90	ALA	C-O	6.41	1.32	1.24
2	S	93	ALA	C-O	6.41	1.32	1.24
1	A	224	ALA	N-CA	-6.39	1.38	1.46
1	B	144	TYR	C-N	6.38	1.41	1.33
1	C	312	ARG	N-CA	6.38	1.54	1.46
1	C	416	GLY	C-O	6.38	1.31	1.23
1	C	409	HIS	CE1-NE2	6.37	1.39	1.32
2	T	55	ASN	C-O	6.37	1.32	1.24
1	C	158	GLU	C-N	6.36	1.42	1.33
1	D	112	SER	C-N	6.35	1.42	1.33
1	B	248	GLU	CA-CB	-6.34	1.43	1.53
1	A	285	ARG	CD-NE	6.33	1.55	1.46
2	U	116	ILE	C-O	6.33	1.31	1.24
1	B	125	PHE	C-N	-6.33	1.26	1.33
2	T	66	TYR	C-O	-6.33	1.16	1.23
1	C	253	ARG	CZ-NH1	6.33	1.41	1.32
2	V	42	LEU	C-O	6.33	1.31	1.23
1	C	404	GLY	N-CA	6.32	1.53	1.45
2	U	58	SER	N-CA	6.31	1.55	1.46
1	D	455	LEU	C-O	6.31	1.31	1.24
1	A	332	VAL	CA-CB	6.30	1.63	1.54
1	D	335	LEU	N-CA	6.30	1.53	1.45
2	S	92	LYS	C-N	-6.30	1.24	1.33
1	B	133	LEU	N-CA	6.30	1.53	1.46
1	A	202	ASP	C-N	-6.29	1.24	1.33
1	C	133	LEU	N-CA	6.29	1.53	1.45
1	D	175	LYS	N-CA	6.29	1.50	1.45
2	S	105	ASP	C-N	-6.29	1.25	1.33
1	B	24	TYR	C-O	6.28	1.32	1.23
1	D	295	ARG	C-O	6.28	1.33	1.23
1	C	406	THR	CB-OG1	6.28	1.53	1.43
1	A	282	HIS	CE1-NE2	-6.28	1.26	1.32
1	B	292	HIS	CD2-NE2	-6.28	1.30	1.37
2	S	99	ILE	C-N	-6.28	1.24	1.33
1	B	285	ARG	C-O	-6.27	1.16	1.24
1	D	91	VAL	CA-C	6.26	1.60	1.52
1	C	133	LEU	C-N	-6.26	1.25	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	141	PRO	C-O	6.25	1.30	1.24
2	V	118	TYR	C-O	6.25	1.31	1.24
2	U	76	GLY	C-O	6.24	1.32	1.23
1	D	169	LEU	C-O	6.24	1.31	1.23
1	C	170	LEU	C-O	6.24	1.31	1.23
1	B	366	GLN	N-CA	6.23	1.53	1.46
1	A	383	HIS	C-O	-6.23	1.16	1.23
1	C	278	THR	C-O	6.23	1.31	1.24
1	B	311	PHE	C-N	-6.23	1.25	1.34
1	B	169	LEU	C-O	6.21	1.31	1.23
1	B	222	ALA	CA-CB	-6.20	1.43	1.53
1	C	114	THR	CB-OG1	6.20	1.53	1.43
1	A	70	TRP	C-O	6.20	1.31	1.24
2	T	7	ILE	CA-C	-6.20	1.45	1.52
2	V	69	MET	CG-SD	6.18	1.96	1.80
1	B	240	LEU	N-CA	6.18	1.54	1.46
1	C	87	ILE	C-N	-6.17	1.25	1.33
1	A	154	GLY	C-O	6.17	1.31	1.23
1	D	289	LEU	C-O	6.17	1.31	1.23
1	B	205	ASN	N-CA	6.15	1.53	1.46
1	B	296	ALA	C-O	6.15	1.31	1.23
1	D	141	PRO	CA-CB	6.15	1.60	1.54
2	U	114	SER	N-CA	6.14	1.54	1.46
1	C	345	PHE	N-CA	6.14	1.54	1.46
1	D	408	GLY	C-O	6.14	1.32	1.23
1	C	238	HIS	CG-ND1	-6.13	1.31	1.38
1	A	345	PHE	N-CA	6.13	1.54	1.46
1	B	253	ARG	C-O	6.13	1.31	1.24
1	C	199	PHE	N-CA	-6.13	1.38	1.46
1	C	180	LEU	C-O	6.12	1.31	1.23
2	U	82	GLN	N-CA	6.12	1.53	1.46
1	A	119	SER	C-N	-6.12	1.26	1.34
1	A	238	HIS	CD2-NE2	6.12	1.44	1.37
1	D	422	VAL	C-O	6.12	1.30	1.24
1	D	409	HIS	CE1-NE2	6.11	1.38	1.32
1	B	210	PRO	C-N	-6.10	1.25	1.33
1	D	428	VAL	N-CA	6.10	1.53	1.46
1	B	31	THR	C-O	6.09	1.31	1.23
1	B	316	LYS	C-O	6.09	1.31	1.24
1	C	24	TYR	C-O	6.09	1.32	1.24
1	C	386	HIS	CA-CB	-6.09	1.45	1.54
1	D	232	THR	CB-OG1	6.08	1.53	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	150	GLY	N-CA	6.08	1.53	1.44
1	D	191	GLU	N-CA	6.07	1.53	1.46
2	U	100	ARG	C-O	6.07	1.31	1.23
1	C	233	GLY	C-O	6.05	1.32	1.23
1	C	258	ARG	N-CA	6.03	1.53	1.46
1	B	390	LEU	C-O	6.03	1.31	1.24
2	V	110	VAL	CA-C	6.03	1.59	1.52
1	C	53	ALA	C-N	-6.02	1.26	1.33
1	C	238	HIS	CD2-NE2	6.02	1.44	1.37
1	C	210	PRO	CA-CB	-6.02	1.44	1.53
1	C	386	HIS	CG-ND1	6.02	1.44	1.38
1	C	173	THR	CB-OG1	6.00	1.53	1.43
1	B	192	CYS	C-O	-6.00	1.17	1.24
1	A	342	THR	CB-OG1	5.99	1.53	1.43
1	B	244	ALA	C-N	-5.97	1.26	1.34
2	V	98	TRP	CA-C	5.96	1.60	1.52
2	S	34	LEU	N-CA	5.95	1.53	1.46
1	A	187	ARG	C-O	-5.94	1.17	1.24
1	D	212	MET	C-O	5.94	1.30	1.23
1	D	386	HIS	N-CA	5.93	1.54	1.45
1	B	350	ARG	CA-CB	-5.92	1.44	1.53
1	B	415	PRO	CA-CB	-5.91	1.44	1.53
1	C	215	ARG	N-CA	5.91	1.53	1.46
1	A	355	GLU	C-O	5.90	1.31	1.23
1	B	34	THR	C-O	5.90	1.32	1.24
1	C	181	SER	CB-OG	5.90	1.53	1.42
1	D	299	ALA	N-CA	5.90	1.54	1.46
2	S	58	SER	CB-OG	-5.89	1.30	1.42
1	C	324	ASP	C-N	-5.88	1.25	1.33
1	A	277	ASN	C-O	-5.87	1.17	1.24
1	B	63	THR	CA-CB	5.87	1.62	1.54
1	B	152	PRO	C-O	-5.87	1.16	1.24
1	D	247	CYS	C-N	-5.87	1.26	1.33
1	D	424	LEU	C-O	5.86	1.30	1.24
2	U	90	ALA	C-O	5.86	1.31	1.24
1	A	225	LEU	CB-CG	-5.85	1.41	1.53
1	C	99	ALA	N-CA	5.85	1.53	1.46
1	B	367	ASP	CA-CB	-5.85	1.45	1.53
1	B	186	GLY	CA-C	-5.83	1.45	1.52
2	U	39	VAL	CA-C	-5.83	1.48	1.53
1	D	217	ARG	CZ-NH2	5.83	1.41	1.33
1	C	302	ASP	C-O	5.83	1.31	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	ALA	C-N	-5.83	1.26	1.33
1	B	230	ALA	C-N	-5.82	1.26	1.33
1	D	374	VAL	N-CA	-5.82	1.39	1.46
1	B	80	TYR	CA-CB	5.81	1.62	1.53
1	A	465	ILE	C-N	-5.81	1.26	1.33
1	B	175	LYS	C-O	5.81	1.29	1.24
1	C	66	TRP	C-N	-5.81	1.25	1.33
1	D	266	MET	C-O	5.81	1.31	1.23
1	D	378	ALA	C-O	5.79	1.30	1.24
1	A	46	PRO	CA-CB	5.79	1.61	1.53
1	A	248	GLU	CA-CB	-5.78	1.44	1.53
2	V	105	ASP	CA-C	5.78	1.59	1.52
1	C	413	ASN	C-O	5.78	1.31	1.24
1	A	319	ARG	N-CA	5.77	1.53	1.46
1	C	424	LEU	C-O	5.77	1.30	1.24
1	A	32	LYS	CA-C	5.77	1.60	1.52
2	T	65	ARG	CD-NE	-5.77	1.38	1.46
1	B	32	LYS	CA-CB	-5.76	1.44	1.53
1	B	285	ARG	CD-NE	-5.76	1.38	1.46
1	D	171	GLY	N-CA	5.76	1.51	1.45
1	A	249	GLU	C-N	-5.76	1.26	1.33
1	A	25	TYR	N-CA	5.75	1.53	1.46
1	B	76	SER	C-O	5.75	1.30	1.24
2	T	98	TRP	C-N	-5.74	1.25	1.33
1	D	210	PRO	CA-CB	-5.73	1.45	1.53
1	B	238	HIS	C-N	-5.73	1.25	1.33
1	C	191	GLU	N-CA	5.73	1.52	1.46
2	U	73	PRO	C-O	5.73	1.30	1.23
2	S	53	ARG	CZ-NH2	-5.72	1.26	1.33
2	T	101	ILE	C-N	-5.72	1.26	1.33
1	D	159	ARG	NE-CZ	5.72	1.39	1.33
1	A	63	THR	C-O	5.71	1.31	1.24
1	C	356	GLN	C-O	5.71	1.30	1.23
1	C	215	ARG	CZ-NH1	5.71	1.40	1.32
1	D	52	GLU	CA-CB	-5.71	1.44	1.53
1	D	150	GLY	N-CA	5.71	1.52	1.44
1	C	261	GLY	C-O	5.71	1.32	1.24
1	B	428	VAL	N-CA	5.70	1.53	1.46
1	C	217	ARG	NE-CZ	-5.70	1.26	1.33
1	C	319	ARG	NE-CZ	-5.70	1.26	1.33
1	A	270	LEU	C-O	5.70	1.31	1.24
1	B	83	ARG	C-O	-5.69	1.16	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	212	MET	N-CA	5.69	1.53	1.46
1	C	119	SER	C-O	5.69	1.29	1.23
2	V	7	ILE	CA-CB	5.69	1.63	1.55
1	C	465	ILE	CA-CB	5.69	1.61	1.54
1	C	240	LEU	N-CA	5.68	1.53	1.46
1	A	229	GLN	CA-CB	-5.68	1.44	1.53
1	A	332	VAL	C-O	5.67	1.30	1.24
1	B	139	ARG	C-O	5.67	1.30	1.24
2	S	98	TRP	CA-C	5.66	1.59	1.52
1	C	322	GLY	CA-C	-5.66	1.44	1.51
1	C	80	TYR	CA-CB	5.66	1.62	1.53
1	D	223	GLU	C-N	-5.66	1.26	1.33
1	A	238	HIS	ND1-CE1	-5.65	1.26	1.32
1	B	252	LYS	N-CA	-5.65	1.39	1.46
2	S	59	PRO	C-N	-5.65	1.25	1.33
1	D	469	PHE	CA-C	5.64	1.59	1.52
1	C	298	HIS	CE1-NE2	-5.64	1.26	1.32
1	B	131	ARG	N-CA	5.64	1.53	1.45
1	A	423	ALA	C-N	-5.64	1.26	1.33
1	C	343	LEU	N-CA	5.63	1.53	1.46
1	C	432	ASN	C-O	5.63	1.31	1.24
1	C	120	ILE	C-N	-5.62	1.25	1.33
2	S	94	TYR	CA-CB	-5.62	1.47	1.53
1	D	17	VAL	C-N	-5.62	1.26	1.33
1	B	245	GLY	C-O	5.62	1.30	1.24
1	B	237	GLY	CA-C	5.62	1.57	1.51
1	A	18	LYS	C-O	5.61	1.30	1.23
1	B	319	ARG	CD-NE	-5.61	1.38	1.46
1	B	192	CYS	C-N	-5.61	1.26	1.33
1	B	325	HIS	C-N	-5.61	1.25	1.33
1	A	464	GLU	C-O	5.61	1.32	1.24
2	V	12	TYR	CA-CB	5.61	1.61	1.53
2	U	50	PHE	N-CA	5.59	1.53	1.45
1	A	360	ARG	NE-CZ	5.59	1.39	1.33
1	B	58	ALA	C-O	5.59	1.31	1.24
1	B	247	CYS	CA-CB	-5.58	1.44	1.53
1	D	234	GLU	C-O	5.58	1.30	1.23
1	A	298	HIS	CE1-NE2	-5.58	1.26	1.32
1	C	63	THR	C-O	5.57	1.31	1.24
1	C	193	LEU	C-O	5.56	1.30	1.24
1	D	18	LYS	C-O	5.55	1.30	1.23
1	D	233	GLY	N-CA	5.55	1.53	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	237	GLY	C-N	-5.55	1.26	1.33
1	A	306	ASN	C-O	5.54	1.30	1.23
1	C	44	PRO	C-O	-5.54	1.16	1.24
1	A	215	ARG	CD-NE	5.54	1.54	1.46
1	C	234	GLU	C-O	5.54	1.30	1.24
1	C	319	ARG	C-N	-5.53	1.26	1.33
1	A	58	ALA	C-O	5.53	1.31	1.24
1	A	278	THR	CA-C	-5.53	1.45	1.52
1	B	245	GLY	N-CA	-5.52	1.38	1.45
1	D	319	ARG	C-N	-5.52	1.26	1.33
1	D	355	GLU	C-N	-5.51	1.26	1.33
1	A	193	LEU	N-CA	5.51	1.53	1.46
1	A	218	PHE	C-N	-5.50	1.26	1.33
2	U	74	MET	CG-SD	5.50	1.94	1.80
1	B	252	LYS	C-O	5.49	1.30	1.24
1	A	347	ASP	C-N	-5.49	1.26	1.34
1	B	287	ASN	C-N	-5.49	1.27	1.33
1	B	282	HIS	C-O	5.48	1.30	1.24
1	D	139	ARG	C-O	5.48	1.30	1.24
1	D	229	GLN	N-CA	5.48	1.53	1.46
1	B	26	THR	CA-CB	5.47	1.60	1.53
2	U	41	CYS	C-O	5.47	1.30	1.23
2	V	53	ARG	CZ-NH1	5.47	1.40	1.32
2	S	51	VAL	C-N	-5.47	1.26	1.33
2	T	107	VAL	C-N	-5.47	1.25	1.33
1	C	319	ARG	CZ-NH1	5.47	1.40	1.32
1	A	242	ALA	CA-CB	-5.46	1.44	1.53
1	A	359	SER	CA-CB	-5.46	1.44	1.53
1	B	83	ARG	CZ-NH2	5.46	1.40	1.33
1	A	440	GLU	C-O	5.45	1.32	1.24
1	C	140	ILE	N-CA	5.44	1.50	1.46
2	U	50	PHE	C-O	5.44	1.30	1.23
1	A	374	VAL	N-CA	-5.44	1.39	1.46
2	S	73	PRO	N-CD	-5.43	1.40	1.47
1	C	310	HIS	ND1-CE1	5.43	1.38	1.32
1	A	144	TYR	N-CA	5.43	1.53	1.46
1	C	89	ARG	CA-CB	-5.43	1.45	1.53
1	C	299	ALA	N-CA	5.43	1.53	1.46
1	D	166	GLY	C-O	5.43	1.31	1.23
1	C	123	ASN	CA-CB	5.43	1.61	1.54
2	T	111	GLN	CA-CB	-5.43	1.46	1.53
1	B	283	TYR	CA-CB	-5.42	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	408	GLY	C-O	5.42	1.31	1.23
1	A	141	PRO	C-O	5.42	1.29	1.24
1	B	241	ASN	N-CA	5.42	1.52	1.46
2	U	111	GLN	CA-CB	-5.41	1.45	1.53
1	D	201	LYS	CE-NZ	-5.41	1.33	1.49
1	D	245	GLY	CA-C	-5.41	1.44	1.51
1	B	116	MET	C-N	-5.41	1.26	1.33
1	B	327	HIS	N-CA	5.41	1.52	1.46
2	T	59	PRO	CA-CB	-5.40	1.46	1.53
1	D	352	ASP	C-N	-5.40	1.26	1.33
1	B	203	ASP	CA-C	5.40	1.59	1.52
2	S	55	ASN	C-N	-5.39	1.26	1.33
1	C	294	HIS	C-O	5.39	1.30	1.24
1	C	121	VAL	CA-C	-5.39	1.46	1.52
1	C	99	ALA	CA-CB	-5.39	1.45	1.53
1	A	416	GLY	C-N	-5.39	1.26	1.33
1	B	114	THR	CB-OG1	5.39	1.52	1.43
2	U	67	TRP	N-CA	5.38	1.53	1.45
1	C	52	GLU	CA-CB	-5.38	1.45	1.53
1	C	26	THR	CA-CB	5.38	1.60	1.53
1	A	153	HIS	CG-ND1	-5.38	1.32	1.38
2	T	7	ILE	C-N	-5.37	1.26	1.33
1	B	288	GLY	CA-C	-5.36	1.46	1.51
2	S	54	GLU	CA-C	-5.36	1.46	1.53
1	D	14	LYS	C-O	5.36	1.30	1.24
2	U	98	TRP	C-N	-5.36	1.25	1.33
1	A	257	ALA	CA-CB	-5.35	1.45	1.53
1	B	127	PHE	C-O	5.35	1.30	1.23
1	A	79	ARG	NE-CZ	5.35	1.39	1.33
1	C	451	TRP	C-O	5.35	1.31	1.24
1	C	301	ILE	CA-CB	5.35	1.61	1.54
1	A	345	PHE	CA-CB	-5.34	1.44	1.53
2	S	7	ILE	CA-CB	5.34	1.62	1.55
1	A	36	ILE	C-O	5.34	1.31	1.24
1	A	155	ILE	C-N	-5.34	1.27	1.33
2	T	53	ARG	CA-CB	-5.34	1.48	1.53
1	B	61	SER	C-N	-5.33	1.26	1.33
1	D	312	ARG	C-O	5.33	1.30	1.24
1	A	47	GLY	N-CA	5.33	1.52	1.45
1	A	189	VAL	C-N	-5.32	1.27	1.33
1	D	53	ALA	C-N	-5.32	1.27	1.33
2	U	29	GLU	C-O	5.31	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	63	ASP	CA-CB	-5.31	1.44	1.53
2	T	51	VAL	C-O	-5.31	1.17	1.24
1	C	18	LYS	C-O	5.31	1.30	1.23
1	B	53	ALA	C-N	-5.31	1.27	1.33
1	B	291	LEU	CB-CG	-5.30	1.42	1.53
2	U	62	TYR	C-O	5.30	1.29	1.23
1	A	301	ILE	N-CA	-5.30	1.39	1.46
1	A	72	ASP	CG-OD2	5.29	1.35	1.25
1	B	80	TYR	C-O	5.29	1.30	1.24
1	D	345	PHE	CA-CB	-5.29	1.44	1.53
1	D	345	PHE	C-O	5.29	1.30	1.24
1	B	184	ASN	C-O	5.29	1.30	1.24
1	A	333	GLY	CA-C	-5.29	1.44	1.51
1	A	46	PRO	C-O	5.28	1.30	1.24
1	C	185	TYR	N-CA	5.28	1.52	1.46
1	C	321	SER	CA-CB	-5.28	1.45	1.53
2	S	76	GLY	C-O	5.28	1.31	1.23
1	D	363	TYR	C-O	5.28	1.30	1.24
1	C	139	ARG	CA-CB	5.28	1.60	1.53
1	A	205	ASN	C-N	-5.27	1.27	1.33
1	C	323	GLY	CA-C	5.27	1.59	1.51
1	D	176	PRO	C-O	5.27	1.33	1.23
2	U	46	THR	C-O	5.26	1.31	1.24
1	C	358	ARG	NE-CZ	5.25	1.38	1.33
2	S	4	TRP	C-N	-5.25	1.27	1.33
1	C	33	ASP	N-CA	5.25	1.52	1.46
1	C	121	VAL	C-O	5.25	1.30	1.24
2	U	17	TYR	C-O	5.25	1.30	1.24
1	D	238	HIS	CD2-NE2	5.25	1.43	1.37
1	A	196	GLY	CA-C	-5.25	1.44	1.51
1	A	200	THR	N-CA	5.25	1.52	1.45
1	B	223	GLU	C-O	5.25	1.30	1.24
1	C	342	THR	N-CA	-5.25	1.40	1.46
1	C	140	ILE	C-N	-5.24	1.27	1.33
1	B	276	ALA	C-N	-5.24	1.27	1.33
2	T	93	ALA	N-CA	5.24	1.52	1.46
2	V	101	ILE	C-O	5.24	1.29	1.24
1	C	435	ARG	NE-CZ	5.24	1.38	1.33
2	S	11	LYS	C-O	-5.23	1.16	1.23
2	S	62	TYR	C-N	-5.23	1.25	1.33
1	D	152	PRO	C-O	-5.23	1.17	1.24
1	D	435	ARG	N-CA	5.23	1.52	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	65	ARG	CD-NE	-5.23	1.39	1.46
1	C	322	GLY	C-N	-5.22	1.25	1.33
1	D	251	ILE	C-N	-5.22	1.27	1.33
2	V	13	GLU	CA-C	-5.22	1.47	1.53
1	A	120	ILE	CA-C	-5.22	1.46	1.52
1	A	353	PHE	C-N	-5.22	1.27	1.33
1	C	468	ASN	CA-C	5.22	1.59	1.52
1	A	61	SER	CA-CB	5.21	1.62	1.53
1	C	40	PHE	N-CA	5.21	1.52	1.46
2	V	116	ILE	N-CA	5.21	1.52	1.46
1	A	65	THR	N-CA	5.20	1.53	1.46
1	B	282	HIS	CG-CD2	-5.20	1.30	1.35
1	C	234	GLU	N-CA	5.20	1.52	1.46
1	A	61	SER	N-CA	-5.20	1.39	1.46
1	D	201	LYS	CA-C	-5.19	1.46	1.52
2	T	43	GLU	C-N	-5.19	1.26	1.33
1	D	57	VAL	CA-CB	-5.19	1.48	1.54
2	U	63	ASP	CA-C	5.18	1.60	1.53
1	C	215	ARG	CD-NE	5.18	1.53	1.46
1	A	288	GLY	C-N	-5.18	1.25	1.33
1	A	264	ILE	CA-C	-5.18	1.46	1.52
1	B	254	ALA	CA-CB	-5.18	1.45	1.53
1	C	19	GLU	C-N	-5.18	1.27	1.33
1	C	266	MET	CA-CB	5.18	1.63	1.54
2	U	31	GLU	C-O	5.17	1.30	1.24
1	A	363	TYR	C-O	5.17	1.30	1.24
1	D	24	TYR	C-O	5.17	1.30	1.24
1	C	213	ARG	CA-CB	-5.16	1.45	1.53
1	D	70	TRP	C-N	-5.16	1.26	1.33
1	B	207	ASN	C-N	-5.16	1.26	1.33
1	B	127	PHE	N-CA	5.16	1.52	1.46
1	B	229	GLN	CD-NE2	-5.15	1.22	1.33
2	S	58	SER	CA-CB	-5.15	1.46	1.53
1	D	339	ARG	CZ-NH1	5.14	1.40	1.32
2	U	7	ILE	CA-C	-5.14	1.47	1.52
1	C	325	HIS	C-N	-5.14	1.27	1.33
1	D	347	ASP	N-CA	5.14	1.52	1.46
1	B	127	PHE	CA-C	-5.13	1.46	1.52
1	B	302	ASP	C-O	5.13	1.30	1.24
1	B	339	ARG	N-CA	-5.13	1.40	1.46
1	B	227	LYS	CA-CB	-5.12	1.45	1.53
1	D	156	GLN	CD-NE2	5.12	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	ASN	C-N	-5.12	1.27	1.33
1	A	230	ALA	C-N	-5.12	1.27	1.33
2	V	91	LYS	N-CA	5.12	1.52	1.46
2	T	54	GLU	CA-C	-5.11	1.47	1.53
1	D	332	VAL	CA-CB	5.11	1.61	1.54
1	D	36	ILE	C-O	5.11	1.30	1.24
1	A	291	LEU	N-CA	5.11	1.52	1.46
1	D	315	ALA	N-CA	5.11	1.52	1.46
1	A	201	LYS	CE-NZ	-5.10	1.34	1.49
2	U	3	VAL	N-CA	-5.10	1.40	1.46
1	C	327	HIS	CD2-NE2	5.10	1.43	1.37
1	C	383	HIS	ND1-CE1	5.09	1.37	1.32
1	B	420	ASN	C-O	5.09	1.30	1.24
1	C	409	HIS	CD2-NE2	-5.09	1.32	1.37
2	U	87	VAL	C-N	5.09	1.40	1.33
1	A	52	GLU	N-CA	5.08	1.52	1.46
2	T	70	TRP	C-O	5.08	1.30	1.24
1	B	177	LYS	C-O	5.08	1.30	1.24
1	D	428	VAL	C-O	5.08	1.30	1.24
1	A	180	LEU	CA-C	-5.08	1.46	1.52
1	B	70	TRP	C-O	5.08	1.30	1.24
1	D	68	THR	CA-CB	5.07	1.60	1.53
2	S	73	PRO	CA-CB	-5.07	1.47	1.53
1	D	375	LEU	CA-CB	5.07	1.61	1.53
1	D	264	ILE	CA-C	-5.07	1.46	1.52
1	B	421	ARG	N-CA	5.06	1.52	1.46
1	D	319	ARG	N-CA	5.06	1.52	1.46
1	D	330	THR	C-N	-5.06	1.26	1.33
1	C	216	ASP	N-CA	-5.05	1.40	1.46
1	D	260	LEU	C-O	5.05	1.30	1.24
2	S	66	TYR	C-O	-5.05	1.17	1.23
1	B	263	PRO	CA-C	-5.04	1.45	1.52
1	C	326	ILE	C-N	-5.04	1.26	1.33
1	C	416	GLY	N-CA	5.04	1.52	1.45
2	U	113	ILE	CA-CB	5.04	1.60	1.55
1	A	156	GLN	C-O	5.04	1.29	1.24
2	S	110	VAL	C-N	-5.03	1.26	1.33
1	C	348	LEU	C-O	5.03	1.30	1.24
1	A	263	PRO	C-N	-5.03	1.27	1.33
1	C	307	HIS	CD2-NE2	5.03	1.43	1.37
1	A	175	LYS	CA-CB	-5.03	1.47	1.54
1	C	110	GLU	CB-CG	-5.03	1.37	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	50	PHE	C-N	5.03	1.40	1.33
2	T	100	ARG	N-CA	5.03	1.52	1.45
1	D	249	GLU	N-CA	5.03	1.52	1.46
1	A	48	VAL	N-CA	-5.02	1.42	1.46
1	C	209	GLN	C-O	5.02	1.30	1.24
1	D	170	LEU	N-CA	5.02	1.52	1.46
1	B	303	ARG	C-O	5.02	1.29	1.24
1	B	413	ASN	C-O	5.02	1.29	1.24
1	C	30	GLN	N-CA	-5.02	1.40	1.46
1	C	325	HIS	CE1-NE2	-5.01	1.27	1.32
1	D	125	PHE	C-N	-5.01	1.28	1.33
1	B	90	VAL	N-CA	5.01	1.52	1.46
1	D	83	ARG	CD-NE	-5.01	1.39	1.46
1	B	153	HIS	CG-CD2	-5.01	1.30	1.35
1	B	197	LEU	C-O	5.01	1.30	1.23
1	A	225	LEU	C-N	-5.01	1.27	1.33
2	U	113	ILE	C-O	5.01	1.30	1.23
1	A	310	HIS	C-O	5.01	1.30	1.23
1	B	16	GLY	N-CA	5.01	1.49	1.45
2	V	53	ARG	C-N	-5.00	1.26	1.33

All (2695) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	ARG	CD-NE-CZ	24.79	159.11	124.40
1	A	72	ASP	CA-CB-CG	23.76	136.36	112.60
2	S	7	ILE	CA-C-O	-23.61	99.79	120.80
1	C	319	ARG	CD-NE-CZ	23.38	157.13	124.40
2	U	7	ILE	N-CA-C	22.31	129.97	111.90
2	V	7	ILE	N-CA-C	22.16	129.13	111.62
1	D	72	ASP	CA-CB-CG	21.75	134.35	112.60
1	B	72	ASP	CA-CB-CG	21.53	134.13	112.60
1	C	72	ASP	CA-CB-CG	20.93	133.53	112.60
2	V	7	ILE	CA-C-O	-19.95	103.05	120.80
2	T	7	ILE	CA-C-O	-19.90	101.63	120.73
1	C	350	ARG	NE-CZ-NH2	-18.66	102.40	119.20
1	B	127	PHE	CA-CB-CG	-17.75	96.05	113.80
2	S	7	ILE	N-CA-C	17.75	125.64	111.62
2	T	7	ILE	N-CA-C	17.48	126.59	111.56
1	D	319	ARG	CD-NE-CZ	17.43	148.80	124.40
1	B	319	ARG	CD-NE-CZ	17.11	148.35	124.40
2	S	63	ASP	CA-CB-CG	16.99	129.59	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	ARG	CD-NE-CZ	16.09	146.93	124.40
1	A	350	ARG	CD-NE-CZ	15.89	146.65	124.40
1	B	201	LYS	CA-CB-CG	15.73	145.55	114.10
1	B	217	ARG	CD-NE-CZ	15.41	145.97	124.40
1	A	89	ARG	CD-NE-CZ	15.34	145.87	124.40
1	D	386	HIS	CA-CB-CG	15.21	129.01	113.80
1	B	347	ASP	CA-CB-CG	14.90	127.50	112.60
2	U	75	PHE	CA-C-O	-14.85	105.54	121.87
1	A	207	ASN	OD1-CG-ND2	14.80	137.40	122.60
1	A	121	VAL	N-CA-CB	-14.76	93.17	112.36
2	V	63	ASP	CA-CB-CG	14.68	127.28	112.60
2	U	36	ASN	OD1-CG-ND2	14.65	137.25	122.60
1	C	413	ASN	CA-CB-CG	14.35	126.94	112.60
1	C	207	ASN	CA-CB-CG	14.21	126.81	112.60
1	D	294	HIS	CA-C-O	-14.20	104.91	120.38
2	U	7	ILE	CA-C-O	-14.19	106.96	120.30
1	A	139	ARG	NE-CZ-NH2	14.11	131.90	119.20
2	S	82	GLN	CB-CG-CD	13.95	136.31	112.60
1	A	292	HIS	CA-C-O	-13.56	105.85	120.36
2	T	39	VAL	CA-C-O	-13.27	111.69	119.12
1	C	200	THR	CA-C-O	-13.18	106.13	121.68
1	C	386	HIS	CA-CB-CG	13.17	126.97	113.80
1	D	121	VAL	N-CA-CB	-13.14	95.07	112.16
2	U	55	ASN	CA-CB-CG	-12.98	99.62	112.60
1	B	226	TYR	CA-C-O	-12.94	106.71	120.42
1	D	139	ARG	NE-CZ-NH1	-12.82	108.68	121.50
1	D	139	ARG	NE-CZ-NH2	12.79	130.71	119.20
1	B	377	VAL	CA-C-O	12.66	134.08	120.53
1	D	217	ARG	CD-NE-CZ	12.66	142.12	124.40
1	B	89	ARG	CD-NE-CZ	12.64	142.09	124.40
1	D	127	PHE	CA-CB-CG	-12.60	101.20	113.80
1	D	397	ASP	O-C-N	12.57	139.03	122.56
1	A	127	PHE	CA-CB-CG	-12.55	101.25	113.80
1	C	89	ARG	CD-NE-CZ	12.49	141.89	124.40
1	D	89	ARG	CD-NE-CZ	12.43	141.79	124.40
2	U	39	VAL	CA-C-O	-12.22	111.94	119.15
1	D	215	ARG	NE-CZ-NH2	12.21	130.19	119.20
1	C	46	PRO	N-CA-CB	-12.15	90.49	103.25
2	S	18	LEU	O-C-N	12.08	132.07	121.20
1	C	140	ILE	CA-C-O	-11.94	112.10	119.15
1	A	40	PHE	CA-CB-CG	11.93	125.73	113.80
1	A	341	ILE	O-C-N	11.93	133.60	121.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	GLU	CA-CB-CG	11.92	137.95	114.10
1	A	156	GLN	CB-CG-CD	11.91	132.85	112.60
2	V	59	PRO	CA-C-O	-11.90	107.77	121.34
1	B	270	LEU	CA-C-O	-11.86	105.54	120.00
1	B	26	THR	N-CA-CB	-11.83	95.41	110.79
1	C	220	PHE	CA-C-O	-11.82	107.90	120.42
1	A	359	SER	N-CA-C	-11.74	98.18	110.97
1	B	193	LEU	CA-C-O	-11.74	108.34	120.90
1	B	141	PRO	O-C-N	-11.67	115.67	121.15
1	C	153	HIS	CA-CB-CG	-11.66	102.14	113.80
2	S	7	ILE	CA-C-N	-11.65	107.13	123.20
2	S	7	ILE	C-N-CA	-11.65	107.13	123.20
1	D	201	LYS	CG-CD-CE	-11.64	84.52	111.30
1	B	139	ARG	NE-CZ-NH2	11.62	129.65	119.20
2	T	105	ASP	CA-C-O	-11.58	109.05	122.13
1	C	243	THR	O-C-N	11.50	137.07	122.93
1	B	91	VAL	O-C-N	11.49	134.39	122.67
1	B	207	ASN	OD1-CG-ND2	-11.47	111.12	122.60
2	V	57	LYS	CA-C-O	-11.43	106.52	119.78
1	B	153	HIS	CA-CB-CG	-11.42	102.38	113.80
1	B	469	PHE	CA-CB-CG	11.35	125.15	113.80
1	B	259	GLU	CB-CG-CD	11.30	131.81	112.60
1	B	218	PHE	CA-CB-CG	11.22	125.02	113.80
2	S	53	ARG	NE-CZ-NH2	11.21	129.29	119.20
2	V	32	TYR	CA-C-O	11.21	132.43	120.55
1	B	141	PRO	CA-C-O	11.19	129.57	120.73
2	T	7	ILE	CB-CA-C	-11.18	100.81	111.44
2	S	2	GLN	OE1-CD-NE2	11.17	133.77	122.60
1	B	277	ASN	CA-CB-CG	-11.16	101.44	112.60
1	C	215	ARG	NE-CZ-NH1	-11.14	110.36	121.50
2	U	106	ASN	CA-CB-CG	-11.13	101.47	112.60
1	B	156	GLN	CB-CG-CD	11.10	131.47	112.60
1	A	442	ASN	CA-CB-CG	-11.09	101.51	112.60
2	S	56	ASN	CA-CB-CG	11.09	123.69	112.60
1	D	328	SER	CA-C-O	-11.06	106.88	119.05
1	A	338	GLU	CA-C-O	11.02	132.39	120.71
1	D	433	GLU	CA-CB-CG	11.01	136.12	114.10
2	S	98	TRP	N-CA-C	-10.98	91.91	109.59
1	B	396	ASP	CA-CB-CG	10.98	123.58	112.60
2	V	55	ASN	CA-CB-CG	-10.96	101.64	112.60
1	D	140	ILE	CA-C-O	-10.95	112.99	119.12
1	D	95	ASP	CA-CB-CG	-10.95	101.65	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	ASP	CA-CB-CG	10.93	123.53	112.60
1	C	217	ARG	CD-NE-CZ	10.89	139.65	124.40
1	C	217	ARG	NE-CZ-NH2	-10.88	109.41	119.20
2	V	48	HIS	CA-CB-CG	-10.88	102.92	113.80
1	A	433	GLU	CB-CG-CD	10.86	131.06	112.60
1	B	46	PRO	N-CA-CB	-10.83	91.88	103.25
1	C	52	GLU	N-CA-C	-10.82	95.00	111.56
2	V	55	ASN	OD1-CG-ND2	10.82	133.42	122.60
1	B	238	HIS	CA-C-O	-10.81	108.66	120.33
1	B	215	ARG	NE-CZ-NH1	-10.80	110.70	121.50
1	C	191	GLU	CA-C-O	-10.78	109.21	121.07
1	B	433	GLU	CA-CB-CG	10.75	135.60	114.10
1	C	90	VAL	O-C-N	10.73	135.18	122.62
1	B	156	GLN	CG-CD-OE1	10.71	142.23	120.80
2	U	8	ASN	CA-CB-CG	10.71	123.31	112.60
1	C	127	PHE	CA-CB-CG	-10.70	103.10	113.80
1	A	149	GLN	O-C-N	10.70	136.13	122.23
2	S	92	LYS	CA-C-O	-10.68	108.10	120.49
2	V	79	ASP	CA-CB-CG	-10.66	101.94	112.60
1	B	215	ARG	NE-CZ-NH2	10.65	128.78	119.20
1	A	134	ARG	NE-CZ-NH1	-10.60	110.90	121.50
1	C	95	ASP	CA-CB-CG	-10.59	102.01	112.60
2	V	99	ILE	O-C-N	10.58	134.32	123.00
1	A	207	ASN	CA-CB-CG	10.56	123.16	112.60
1	A	156	GLN	OE1-CD-NE2	-10.54	112.06	122.60
2	U	101	ILE	CA-C-O	-10.52	109.34	120.39
1	D	401	GLN	CA-C-O	10.52	131.85	120.38
1	D	205	ASN	OD1-CG-ND2	10.52	133.12	122.60
1	D	218	PHE	CA-CB-CG	10.52	124.32	113.80
1	D	371	LEU	N-CA-C	-10.49	96.92	109.93
1	A	289	LEU	CA-C-O	-10.48	109.17	120.80
1	B	442	ASN	CA-CB-CG	-10.47	102.13	112.60
1	C	123	ASN	OD1-CG-ND2	10.47	133.07	122.60
2	U	72	LEU	O-C-N	10.45	130.21	121.32
2	V	59	PRO	O-C-N	10.45	135.68	123.03
1	A	216	ASP	CA-C-O	-10.43	108.66	120.24
1	D	203	ASP	N-CA-C	-10.41	95.07	110.48
1	D	360	ARG	CD-NE-CZ	-10.41	109.83	124.40
2	U	65	ARG	NE-CZ-NH2	-10.41	109.83	119.20
1	D	291	LEU	CA-C-O	-10.40	109.13	120.36
1	A	245	GLY	CA-C-O	-10.39	107.19	119.45
1	D	156	GLN	CB-CG-CD	10.38	130.24	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	55	ASN	CA-CB-CG	-10.38	102.22	112.60
1	A	196	GLY	CA-C-N	10.35	137.18	120.94
1	A	196	GLY	C-N-CA	10.35	137.18	120.94
1	B	200	THR	CA-C-O	-10.33	109.59	121.58
1	A	465	ILE	N-CA-C	10.33	123.46	108.58
1	A	409	HIS	CA-CB-CG	10.32	124.12	113.80
1	B	288	GLY	CA-C-N	10.31	138.01	122.65
1	B	288	GLY	C-N-CA	10.31	138.01	122.65
1	B	48	VAL	O-C-N	10.31	129.50	121.46
1	A	149	GLN	OE1-CD-NE2	10.30	132.90	122.60
1	D	298	HIS	CA-CB-CG	10.27	124.07	113.80
2	S	72	LEU	O-C-N	10.26	129.56	121.55
1	D	359	SER	N-CA-C	-10.26	99.79	110.97
1	C	401	GLN	N-CA-C	10.24	125.56	109.07
1	D	64	GLY	N-CA-C	10.24	130.02	112.51
1	B	13	PHE	CA-CB-CG	10.24	124.04	113.80
2	T	60	GLY	CA-C-O	10.23	130.38	119.02
1	A	110	GLU	CA-C-O	-10.23	110.71	121.55
2	U	63	ASP	CA-CB-CG	10.22	122.82	112.60
1	B	350	ARG	NE-CZ-NH2	-10.20	110.02	119.20
1	B	88	GLU	CA-CB-CG	10.19	134.48	114.10
1	A	213	ARG	NE-CZ-NH2	10.18	128.36	119.20
2	S	100	ARG	N-CA-CB	-10.17	93.86	111.55
1	C	270	LEU	CA-C-O	-10.16	108.96	120.24
1	B	155	ILE	CA-C-O	-10.16	108.08	120.78
2	U	105	ASP	CA-C-O	-10.15	110.21	121.58
1	D	350	ARG	NE-CZ-NH2	-10.13	110.08	119.20
2	V	98	TRP	N-CA-C	-10.12	93.15	109.76
1	A	223	GLU	CA-C-N	10.08	133.55	120.44
1	A	223	GLU	C-N-CA	10.08	133.55	120.44
1	B	413	ASN	CA-CB-CG	10.07	122.67	112.60
1	C	160	ASP	O-C-N	10.07	132.80	122.12
1	B	91	VAL	N-CA-CB	10.06	123.61	110.13
1	C	259	GLU	CB-CG-CD	10.03	129.66	112.60
2	U	111	GLN	N-CA-C	-10.01	93.93	109.25
1	A	442	ASN	OD1-CG-ND2	10.00	132.60	122.60
1	B	139	ARG	CD-NE-CZ	-10.00	110.40	124.40
1	B	43	THR	O-C-N	9.99	129.74	121.44
1	C	241	ASN	OD1-CG-ND2	9.99	132.59	122.60
1	D	52	GLU	N-CA-C	-9.98	99.41	112.68
2	V	109	GLN	CA-C-O	-9.96	109.99	121.65
1	B	139	ARG	NE-CZ-NH1	-9.94	111.56	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	GLN	O-C-N	9.93	135.14	122.23
2	V	6	PRO	CA-C-N	-9.93	112.64	123.16
2	V	6	PRO	C-N-CA	-9.93	112.64	123.16
1	A	48	VAL	O-C-N	9.91	128.58	121.55
1	B	345	PHE	CA-CB-CG	9.89	123.69	113.80
1	B	409	HIS	CA-CB-CG	9.87	123.67	113.80
1	B	201	LYS	CG-CD-CE	-9.87	88.60	111.30
1	A	216	ASP	O-C-N	9.87	135.06	122.23
1	C	266	MET	N-CA-CB	-9.85	94.55	111.69
1	C	433	GLU	CA-CB-CG	9.84	133.79	114.10
1	A	211	PHE	CA-C-O	-9.83	108.99	120.10
2	S	7	ILE	CB-CA-C	-9.81	102.32	111.05
2	U	109	GLN	CB-CG-CD	9.80	129.25	112.60
2	U	75	PHE	O-C-N	9.78	134.19	122.75
1	A	46	PRO	N-CA-CB	-9.77	93.00	103.25
1	D	46	PRO	N-CA-CB	-9.76	93.01	103.25
1	D	338	GLU	CA-C-O	9.76	131.63	120.80
1	C	79	ARG	O-C-N	9.75	134.90	122.23
1	B	139	ARG	CA-C-O	-9.72	110.17	120.58
2	V	72	LEU	O-C-N	9.70	127.92	121.71
1	A	39	ALA	CA-C-O	-9.69	110.84	120.92
1	B	40	PHE	CA-CB-CG	9.69	123.49	113.80
1	C	79	ARG	NE-CZ-NH1	-9.69	111.81	121.50
1	D	48	VAL	N-CA-C	9.69	117.14	107.55
1	D	266	MET	N-CA-CB	-9.68	94.84	111.69
1	C	203	ASP	N-CA-C	-9.67	94.92	110.20
2	T	57	LYS	CA-C-O	-9.66	108.57	119.78
1	C	301	ILE	N-CA-C	9.65	120.11	111.81
2	V	7	ILE	CB-CA-C	-9.63	102.48	111.05
1	D	402	PHE	CA-C-O	9.63	132.95	121.11
1	B	246	THR	CA-C-O	-9.62	110.18	121.44
1	A	278	THR	CA-CB-OG1	-9.62	95.17	109.60
1	D	53	ALA	CA-C-N	9.62	130.85	119.99
1	D	53	ALA	C-N-CA	9.62	130.85	119.99
1	A	95	ASP	CA-CB-CG	-9.60	103.00	112.60
1	A	125	PHE	CA-CB-CG	9.60	123.39	113.80
2	S	79	ASP	CA-CB-CG	-9.55	103.05	112.60
1	D	244	ALA	CA-C-O	9.55	132.59	121.32
1	C	293	ILE	CA-C-N	9.54	136.46	123.00
1	C	293	ILE	C-N-CA	9.54	136.46	123.00
1	D	48	VAL	O-C-N	9.53	127.38	121.37
1	D	89	ARG	CA-CB-CG	9.47	133.04	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	82	GLY	N-CA-C	-9.46	99.12	112.37
1	A	328	SER	CA-C-O	-9.45	108.65	119.05
1	C	157	VAL	CA-C-O	-9.45	111.13	120.95
1	C	220	PHE	O-C-N	9.45	132.92	122.15
1	D	86	ARG	NE-CZ-NH2	9.45	127.70	119.20
1	D	201	LYS	CA-CB-CG	9.44	132.98	114.10
1	C	110	GLU	CB-CG-CD	9.44	128.65	112.60
2	T	50	PHE	O-C-N	-9.43	112.33	123.27
1	D	79	ARG	NE-CZ-NH1	-9.42	112.08	121.50
1	A	117	PHE	CA-C-O	-9.41	110.94	120.82
1	A	466	VAL	CA-C-O	-9.41	111.98	121.49
1	B	180	LEU	N-CA-CB	-9.41	95.29	110.63
2	V	115	PHE	O-C-N	9.41	134.21	123.48
2	V	8	ASN	CA-CB-CG	9.41	122.01	112.60
2	T	49	GLY	CA-C-O	-9.39	110.87	120.45
2	U	92	LYS	CA-C-O	-9.39	109.60	120.49
1	C	360	ARG	NE-CZ-NH1	-9.39	112.11	121.50
1	D	19	GLU	CA-CB-CG	9.38	132.87	114.10
2	U	93	ALA	CA-C-N	-9.38	111.80	123.15
2	U	93	ALA	C-N-CA	-9.38	111.80	123.15
1	A	63	THR	CA-C-O	-9.37	107.91	118.69
1	A	36	ILE	CA-C-O	-9.37	109.12	121.02
2	S	105	ASP	CA-C-O	-9.35	111.11	121.58
2	U	48	HIS	CA-CB-CG	-9.35	104.45	113.80
2	T	75	PHE	CA-C-O	-9.34	111.59	121.87
1	D	345	PHE	CA-CB-CG	9.34	123.14	113.80
2	U	65	ARG	CD-NE-CZ	-9.33	111.34	124.40
1	C	201	LYS	N-CA-CB	-9.33	97.09	111.46
1	A	190	TYR	CA-C-O	9.32	130.70	120.63
1	B	338	GLU	CA-C-O	9.32	131.15	120.80
1	C	41	ARG	NE-CZ-NH2	9.31	127.58	119.20
2	U	79	ASP	CA-CB-CG	-9.31	103.29	112.60
1	D	350	ARG	CD-NE-CZ	9.29	137.41	124.40
1	A	249	GLU	N-CA-CB	9.29	123.45	109.98
1	C	338	GLU	CA-C-O	9.29	131.11	120.80
1	D	220	PHE	CA-C-O	-9.28	109.94	120.24
1	D	421	ARG	NE-CZ-NH1	-9.28	112.22	121.50
1	C	231	GLU	CA-C-O	-9.27	110.88	121.07
1	A	156	GLN	CG-CD-OE1	9.26	139.33	120.80
1	B	202	ASP	CA-CB-CG	9.26	121.86	112.60
2	V	4	TRP	O-C-N	9.25	129.36	121.31
1	B	149	GLN	CA-C-O	-9.24	109.98	120.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	LYS	CB-CA-C	-9.24	93.44	110.62
1	B	121	VAL	N-CA-CB	-9.22	98.56	112.67
1	C	156	GLN	CB-CG-CD	9.21	128.26	112.60
1	A	266	MET	CA-C-O	-9.21	111.39	121.33
1	A	88	GLU	CA-C-O	-9.21	109.57	120.43
1	A	17	VAL	CA-C-O	-9.20	110.85	121.98
1	B	366	GLN	CA-C-O	-9.20	110.45	120.30
1	D	13	PHE	CA-CB-CG	9.20	123.00	113.80
1	D	125	PHE	CA-CB-CG	9.20	123.00	113.80
1	A	304	GLN	OE1-CD-NE2	-9.19	113.41	122.60
1	C	471	ALA	N-CA-C	9.18	122.45	110.43
2	V	82	GLN	OE1-CD-NE2	-9.17	113.43	122.60
1	D	82	GLY	N-CA-C	-9.16	99.54	112.37
1	D	404	GLY	O-C-N	9.16	131.20	122.13
1	A	257	ALA	N-CA-C	-9.15	101.30	111.28
2	S	111	GLN	N-CA-C	-9.14	94.43	108.96
1	C	91	VAL	O-C-N	9.12	132.42	122.66
1	A	19	GLU	N-CA-CB	9.12	123.30	110.17
1	C	156	GLN	CG-CD-OE1	9.12	139.03	120.80
2	U	82	GLN	CB-CG-CD	9.10	128.08	112.60
1	D	156	GLN	CG-CD-OE1	9.09	138.97	120.80
2	S	65	ARG	NE-CZ-NH2	-9.08	111.03	119.20
1	C	91	VAL	N-CA-CB	9.07	120.92	110.49
1	A	139	ARG	NE-CZ-NH1	-9.06	112.44	121.50
2	S	101	ILE	CA-C-O	-9.06	110.87	120.39
2	T	79	ASP	CA-CB-CG	-9.06	103.54	112.60
1	D	156	GLN	OE1-CD-NE2	-9.05	113.55	122.60
1	B	53	ALA	CA-C-N	9.04	129.97	119.94
1	B	53	ALA	C-N-CA	9.04	129.97	119.94
1	C	29	TYR	CA-C-N	9.04	135.94	123.11
1	C	29	TYR	C-N-CA	9.04	135.94	123.11
1	A	332	VAL	N-CA-CB	-9.01	96.36	111.23
2	V	114	SER	CB-CA-C	9.00	124.21	109.72
1	C	233	GLY	N-CA-C	-8.97	101.27	115.08
1	A	246	THR	CA-C-O	-8.97	111.27	121.40
1	C	265	VAL	O-C-N	8.96	132.33	122.92
1	C	88	GLU	CA-C-O	-8.95	110.97	120.99
2	V	61	TYR	O-C-N	8.94	133.41	123.22
2	U	100	ARG	N-CA-CB	-8.93	96.14	111.69
1	D	123	ASN	OD1-CG-ND2	8.93	131.53	122.60
1	D	108	PHE	O-C-N	8.93	134.55	123.21
2	V	37	GLY	CA-C-N	-8.92	108.66	121.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	37	GLY	C-N-CA	-8.92	108.66	121.42
2	S	75	PHE	CA-C-O	-8.91	112.10	121.55
2	U	98	TRP	N-CA-C	-8.91	95.14	109.76
1	D	243	THR	CA-C-O	-8.89	110.78	120.92
2	U	110	VAL	O-C-N	8.88	132.50	123.00
2	V	82	GLN	CB-CA-C	8.87	124.81	110.88
1	C	49	PRO	N-CA-C	-8.87	99.88	110.70
1	C	390	LEU	O-C-N	8.86	131.25	122.03
1	D	183	LYS	N-CA-C	8.86	120.94	111.28
1	A	215	ARG	CD-NE-CZ	-8.85	112.01	124.40
1	C	121	VAL	N-CA-CB	-8.85	96.63	111.23
2	S	107	VAL	O-C-N	8.84	133.51	121.84
1	D	213	ARG	CB-CA-C	8.84	124.11	109.53
1	C	442	ASN	CA-CB-CG	-8.83	103.77	112.60
1	B	123	ASN	CA-CB-CG	-8.82	103.78	112.60
1	C	89	ARG	O-C-N	8.80	132.92	123.06
1	A	174	ILE	CA-C-O	-8.80	111.68	121.36
2	T	82	GLN	OE1-CD-NE2	-8.80	113.80	122.60
1	C	341	ILE	O-C-N	8.80	130.53	121.91
1	C	445	ILE	CB-CA-C	8.79	124.03	112.24
1	C	40	PHE	CA-CB-CG	8.79	122.59	113.80
1	D	30	GLN	OE1-CD-NE2	8.79	131.39	122.60
1	B	340	ASP	O-C-N	8.79	132.16	122.15
1	B	156	GLN	OE1-CD-NE2	-8.78	113.82	122.60
1	A	364	PHE	CA-CB-CG	8.78	122.58	113.80
1	C	79	ARG	NH1-CZ-NH2	8.77	130.71	119.30
2	T	36	ASN	OD1-CG-ND2	8.75	131.35	122.60
1	D	258	ARG	CB-CG-CD	8.75	131.42	111.30
1	B	370	SER	CA-C-O	-8.74	110.00	120.32
2	T	63	ASP	CA-CB-CG	8.74	121.34	112.60
1	A	201	LYS	CA-CB-CG	8.74	131.57	114.10
1	B	212	MET	O-C-N	8.72	134.19	122.59
1	A	198	ASP	CA-C-O	8.71	129.79	119.60
1	B	82	GLY	N-CA-C	-8.71	100.80	112.82
1	A	446	ARG	CA-C-O	8.71	129.95	120.20
1	A	286	ASP	CA-C-O	-8.70	108.68	119.38
2	V	96	GLN	OE1-CD-NE2	8.69	131.29	122.60
2	T	67	TRP	CA-C-O	-8.69	111.09	121.60
2	T	110	VAL	CA-CB-CG1	8.68	125.15	110.40
2	S	4	TRP	O-C-N	8.67	128.85	121.31
1	D	442	ASN	CA-CB-CG	-8.66	103.94	112.60
1	D	338	GLU	CB-CG-CD	8.65	127.31	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	98	TRP	N-CA-CB	8.65	124.80	110.52
1	A	103	TYR	CA-C-O	8.65	127.85	119.55
1	A	360	ARG	CD-NE-CZ	-8.65	112.30	124.40
1	A	309	ILE	CA-C-O	-8.64	109.91	121.32
2	U	33	LEU	CB-CA-C	8.64	124.66	110.92
1	B	362	ILE	CA-C-O	-8.62	112.57	121.70
1	A	401	GLN	N-CA-C	8.62	123.28	109.24
2	V	85	ALA	CA-C-O	8.62	130.12	120.90
1	B	13	PHE	O-C-N	8.60	133.10	123.04
1	D	249	GLU	O-C-N	8.59	131.37	122.09
1	D	326	ILE	N-CA-CB	8.58	125.44	111.36
1	A	220	PHE	CA-C-O	-8.58	111.33	120.42
1	B	331	VAL	CA-C-N	8.58	137.41	121.97
1	B	331	VAL	C-N-CA	8.58	137.41	121.97
1	D	17	VAL	CA-C-O	-8.58	112.61	122.13
1	D	153	HIS	CA-CB-CG	-8.58	105.22	113.80
1	D	91	VAL	O-C-N	8.58	131.42	122.67
1	C	230	ALA	O-C-N	8.57	130.94	122.03
1	B	274	PHE	CA-CB-CG	8.56	122.36	113.80
1	B	300	VAL	CA-C-O	-8.56	111.22	120.47
1	A	153	HIS	CA-CB-CG	-8.56	105.24	113.80
1	A	325	HIS	CA-CB-CG	8.55	122.35	113.80
1	B	54	GLY	CA-C-O	-8.55	111.77	121.00
1	A	200	THR	CA-C-O	-8.54	111.67	121.58
1	C	306	ASN	CA-CB-CG	-8.54	104.06	112.60
1	C	160	ASP	CA-C-O	-8.54	111.40	120.63
1	D	290	LEU	CA-C-O	-8.54	111.20	121.28
1	A	91	VAL	N-CA-CB	8.54	120.31	110.49
1	D	24	TYR	CB-CA-C	8.53	124.97	110.56
1	D	257	ALA	N-CA-C	-8.53	100.62	111.02
1	B	461	VAL	O-C-N	8.52	130.26	121.91
1	C	447	GLU	CA-C-O	8.51	129.76	120.82
1	C	321	SER	O-C-N	-8.50	112.91	122.09
1	C	351	ASP	N-CA-C	8.50	121.75	110.53
1	C	170	LEU	CA-C-O	-8.50	111.56	121.16
1	B	133	LEU	CA-C-O	-8.49	110.09	120.54
1	B	49	PRO	N-CA-C	-8.49	100.34	110.70
1	B	376	PRO	CA-C-N	8.49	134.16	123.12
1	B	376	PRO	C-N-CA	8.49	134.16	123.12
1	C	93	GLU	CA-C-O	8.49	129.90	120.31
1	B	72	ASP	CA-C-O	8.48	129.79	120.63
1	C	295	ARG	CD-NE-CZ	-8.48	112.52	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	36	ASN	CA-CB-CG	-8.48	104.12	112.60
2	S	82	GLN	OE1-CD-NE2	-8.47	114.13	122.60
1	B	167	ARG	O-C-N	8.46	131.06	121.32
2	V	39	VAL	N-CA-C	-8.46	101.35	108.63
1	A	292	HIS	O-C-N	8.46	132.86	123.22
2	S	109	GLN	CB-CG-CD	8.46	126.98	112.60
1	C	42	VAL	CA-C-N	8.46	132.82	122.42
1	C	42	VAL	C-N-CA	8.46	132.82	122.42
1	D	83	ARG	CD-NE-CZ	8.46	136.24	124.40
1	D	213	ARG	CA-CB-CG	-8.44	97.22	114.10
1	A	61	SER	CB-CA-C	-8.43	95.93	110.17
1	A	314	LEU	N-CA-C	-8.43	102.05	111.07
1	D	24	TYR	N-CA-CB	-8.43	98.25	110.56
1	A	321	SER	CA-C-O	-8.42	111.98	120.82
1	D	327	HIS	CA-CB-CG	8.41	122.21	113.80
1	B	217	ARG	NH1-CZ-NH2	-8.40	108.38	119.30
1	D	332	VAL	N-CA-CB	-8.38	97.40	111.23
1	A	203	ASP	N-CA-C	-8.38	96.96	110.20
1	B	383	HIS	O-C-N	8.38	132.74	123.10
1	C	469	PHE	CA-CB-CG	8.38	122.18	113.80
2	V	56	ASN	O-C-N	8.38	132.39	123.42
1	D	200	THR	CA-C-O	-8.38	111.80	121.68
1	B	466	VAL	CA-C-O	-8.37	113.03	121.49
1	B	156	GLN	CG-CD-NE2	-8.35	103.87	116.40
2	T	109	GLN	CA-C-O	-8.34	111.60	122.03
1	D	79	ARG	NH1-CZ-NH2	8.33	130.13	119.30
1	D	123	ASN	CA-C-N	8.33	132.27	120.53
1	D	123	ASN	C-N-CA	8.33	132.27	120.53
1	B	88	GLU	O-C-N	8.32	132.73	123.33
1	D	328	SER	O-C-N	8.32	132.58	122.35
1	A	321	SER	O-C-N	8.32	130.63	122.07
1	C	61	SER	CA-CB-OG	-8.31	94.48	111.10
1	B	461	VAL	CA-C-O	-8.31	112.36	121.17
1	A	213	ARG	CB-CG-CD	8.30	130.40	111.30
1	D	131	ARG	N-CA-C	-8.30	103.75	114.04
1	B	67	THR	CA-C-O	-8.30	112.19	121.40
1	C	287	ASN	OD1-CG-ND2	8.30	130.90	122.60
2	V	105	ASP	CA-C-O	-8.29	112.29	121.58
1	A	82	GLY	CA-C-O	-8.29	113.89	121.18
1	C	140	ILE	CA-C-N	8.29	125.63	119.66
1	C	140	ILE	C-N-CA	8.29	125.63	119.66
1	D	292	HIS	CA-C-O	-8.28	111.50	120.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	ALA	N-CA-C	8.28	121.27	110.43
2	T	110	VAL	CA-C-O	-8.27	111.69	121.28
2	V	48	HIS	O-C-N	8.26	135.45	122.81
1	A	26	THR	N-CA-CB	-8.26	100.06	110.79
2	U	92	LYS	N-CA-C	-8.25	96.63	109.25
1	A	180	LEU	CB-CA-C	8.24	123.43	109.50
2	T	36	ASN	CA-CB-CG	-8.24	104.36	112.60
1	C	354	VAL	CA-C-O	8.24	128.38	120.31
2	V	26	LEU	CB-CA-C	8.24	124.47	110.79
2	S	53	ARG	NE-CZ-NH1	-8.22	113.28	121.50
2	T	98	TRP	N-CA-C	-8.21	95.85	109.07
2	S	34	LEU	CB-CA-C	8.21	123.60	110.96
1	C	115	ASN	CA-C-O	-8.21	112.38	121.00
2	U	18	LEU	N-CA-C	-8.21	100.46	110.31
2	T	82	GLN	CB-CG-CD	8.21	126.55	112.60
1	B	377	VAL	O-C-N	-8.20	113.50	123.10
1	D	302	ASP	N-CA-C	8.20	122.07	112.72
1	C	92	GLY	O-C-N	8.20	133.36	122.70
2	S	92	LYS	N-CA-C	-8.20	96.71	109.25
1	B	287	ASN	OD1-CG-ND2	8.19	130.79	122.60
1	C	99	ALA	CA-C-O	-8.19	111.50	120.92
2	S	55	ASN	OD1-CG-ND2	8.18	130.78	122.60
1	C	326	ILE	N-CA-CB	8.18	124.77	111.36
1	D	163	ASN	CA-C-O	-8.18	111.55	121.28
1	B	350	ARG	CD-NE-CZ	8.17	135.84	124.40
2	U	7	ILE	CB-CA-C	-8.17	103.46	111.30
1	C	130	LEU	O-C-N	8.16	134.05	123.11
1	D	338	GLU	CA-C-N	8.16	133.07	120.82
1	D	338	GLU	C-N-CA	8.16	133.07	120.82
2	V	75	PHE	CA-C-O	-8.16	112.40	121.87
2	V	120	PRO	N-CA-C	-8.14	97.29	110.40
1	A	67	THR	CA-C-O	-8.13	112.74	121.36
1	B	466	VAL	O-C-N	8.13	132.34	122.58
1	A	469	PHE	CA-CB-CG	8.13	121.93	113.80
1	B	211	PHE	CA-C-O	-8.12	109.66	119.49
2	V	98	TRP	CA-C-O	-8.12	111.79	120.80
1	C	64	GLY	N-CA-C	8.11	126.87	112.10
2	S	55	ASN	CA-CB-CG	-8.11	104.49	112.60
1	C	201	LYS	CA-CB-CG	8.11	130.33	114.10
1	B	269	TYR	CA-CB-CG	8.10	128.49	113.90
1	A	24	TYR	CB-CA-C	8.10	123.62	110.09
1	C	173	THR	CA-CB-CG2	8.10	124.27	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	386	HIS	CA-CB-CG	8.10	121.89	113.80
1	B	178	LEU	CA-C-N	8.09	134.48	122.10
1	B	178	LEU	C-N-CA	8.09	134.48	122.10
1	D	13	PHE	CA-C-O	-8.09	111.50	120.81
2	S	100	ARG	CB-CG-CD	8.08	129.89	111.30
1	B	45	GLN	CA-CB-CG	8.07	130.23	114.10
1	D	115	ASN	OD1-CG-ND2	-8.07	114.53	122.60
1	B	200	THR	N-CA-C	-8.06	97.16	109.41
1	D	91	VAL	N-CA-CB	8.05	120.92	110.13
1	B	37	LEU	CA-C-O	-8.05	112.02	121.11
2	S	18	LEU	CA-C-O	-8.04	111.95	120.87
2	S	33	LEU	O-C-N	8.04	130.68	122.08
1	C	110	GLU	CG-CD-OE2	8.04	136.89	118.40
2	V	82	GLN	CB-CG-CD	8.04	126.26	112.60
1	B	24	TYR	CB-CA-C	8.04	123.51	110.09
1	A	165	TYR	CA-C-N	8.03	137.16	121.41
1	A	165	TYR	C-N-CA	8.03	137.16	121.41
1	A	203	ASP	N-CA-CB	8.03	122.19	110.06
2	T	60	GLY	O-C-N	-8.03	112.19	122.39
1	A	180	LEU	N-CA-CB	-8.02	97.55	110.63
1	D	465	ILE	N-CA-C	8.02	120.13	108.58
1	A	13	PHE	CA-CB-CG	8.02	121.82	113.80
2	S	25	GLN	O-C-N	8.02	130.43	122.09
1	D	201	LYS	CB-CA-C	-8.01	95.47	111.17
1	B	88	GLU	CA-C-O	-8.01	112.02	120.99
1	D	291	LEU	O-C-N	8.01	132.83	123.30
1	B	45	GLN	N-CA-C	-8.00	99.99	110.07
1	C	360	ARG	CD-NE-CZ	-8.00	113.20	124.40
1	D	336	GLU	N-CA-C	8.00	120.64	110.24
2	V	23	GLN	OE1-CD-NE2	7.99	130.59	122.60
1	B	79	ARG	CB-CA-C	-7.98	96.09	110.70
2	U	73	PRO	CB-CA-C	7.98	121.70	111.64
1	B	360	ARG	NE-CZ-NH1	-7.98	113.52	121.50
1	D	469	PHE	CA-CB-CG	7.98	121.78	113.80
1	B	303	ARG	CA-C-N	7.98	132.07	120.82
1	B	303	ARG	C-N-CA	7.98	132.07	120.82
1	D	396	ASP	CA-CB-CG	7.97	120.57	112.60
1	B	201	LYS	N-CA-CB	-7.97	99.21	111.56
2	V	92	LYS	N-CA-C	-7.97	97.09	109.76
1	A	96	GLN	CA-CB-CG	7.96	130.03	114.10
1	B	112	SER	N-CA-C	7.95	122.99	107.57
1	B	334	LYS	CA-C-O	-7.94	109.89	119.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	92	LYS	CA-C-O	-7.93	111.69	120.81
1	C	41	ARG	NE-CZ-NH1	-7.93	113.57	121.50
2	V	37	GLY	O-C-N	7.93	130.75	122.51
2	S	63	ASP	N-CA-C	-7.92	98.80	110.52
1	D	312	ARG	CA-C-O	-7.92	112.43	120.90
2	S	93	ALA	CA-C-N	-7.92	113.57	123.15
2	S	93	ALA	C-N-CA	-7.92	113.57	123.15
1	B	324	ASP	CA-CB-CG	7.91	120.51	112.60
1	D	369	VAL	CA-C-O	7.91	130.67	120.78
1	A	141	PRO	CB-CA-C	-7.91	103.74	111.17
1	A	137	ASP	CA-CB-CG	-7.90	104.70	112.60
1	C	52	GLU	N-CA-CB	7.90	122.46	110.14
1	C	466	VAL	CA-C-O	-7.90	113.51	121.49
1	B	401	GLN	N-CA-C	7.90	122.71	109.76
1	C	130	LEU	CA-C-O	-7.90	112.22	121.46
1	B	90	VAL	O-C-N	7.90	131.86	122.62
1	B	445	ILE	CB-CA-C	7.89	122.82	112.24
2	T	47	GLU	N-CA-C	7.89	123.83	114.04
1	D	43	THR	O-C-N	7.89	127.98	121.44
1	D	294	HIS	O-C-N	7.89	132.60	123.29
1	A	110	GLU	CA-CB-CG	7.88	129.87	114.10
1	B	52	GLU	N-CA-CB	7.88	122.43	110.14
1	A	436	ASP	O-C-N	7.88	134.94	122.96
1	B	465	ILE	N-CA-C	7.88	119.92	108.58
1	A	217	ARG	N-CA-CB	7.87	121.48	110.07
1	C	217	ARG	NE-CZ-NH1	7.85	129.35	121.50
1	C	319	ARG	CA-CB-CG	7.85	129.80	114.10
1	A	212	MET	O-C-N	7.85	133.03	122.59
1	A	63	THR	CA-C-N	-7.84	115.49	122.47
1	A	63	THR	C-N-CA	-7.84	115.49	122.47
1	C	215	ARG	CA-C-N	7.84	131.10	120.44
1	C	215	ARG	C-N-CA	7.84	131.10	120.44
1	A	343	LEU	O-C-N	7.83	131.38	122.22
1	D	112	SER	N-CA-C	7.83	123.42	107.69
1	C	350	ARG	NH1-CZ-NH2	7.82	129.47	119.30
1	C	290	LEU	N-CA-C	-7.82	96.94	109.76
1	A	312	ARG	NH1-CZ-NH2	7.82	129.46	119.30
2	V	92	LYS	CA-C-O	-7.81	111.78	120.69
1	B	167	ARG	NE-CZ-NH2	7.81	126.23	119.20
1	B	413	ASN	N-CA-C	7.81	120.55	111.02
1	B	36	ILE	CA-C-O	-7.80	111.89	120.71
2	V	25	GLN	O-C-N	7.80	130.21	122.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	121	GLU	CA-CB-CG	7.79	129.68	114.10
1	C	424	LEU	CA-C-O	-7.78	112.69	120.70
1	D	207	ASN	CA-CB-CG	7.78	120.38	112.60
2	U	73	PRO	N-CA-C	-7.78	99.06	111.03
1	D	92	GLY	O-C-N	7.78	132.81	122.70
2	U	71	LYS	CB-CA-C	-7.77	107.61	116.63
1	D	169	LEU	CA-C-O	-7.77	112.54	121.47
1	B	217	ARG	N-CA-CB	7.76	121.26	110.01
1	B	215	ARG	CD-NE-CZ	-7.76	113.53	124.40
2	U	53	ARG	CD-NE-CZ	-7.75	113.55	124.40
1	D	83	ARG	NE-CZ-NH1	-7.75	113.75	121.50
1	D	391	THR	N-CA-CB	7.75	121.49	109.94
1	B	191	GLU	O-C-N	-7.75	113.97	122.03
1	D	172	CYS	N-CA-CB	-7.74	97.80	110.81
1	A	13	PHE	N-CA-C	-7.74	98.35	109.96
1	A	113	VAL	O-C-N	-7.74	114.06	121.87
2	T	119	LYS	N-CA-C	-7.74	100.33	110.39
1	B	89	ARG	O-C-N	7.73	131.72	123.06
2	V	111	GLN	N-CA-C	-7.73	96.69	108.67
1	C	57	VAL	N-CA-CB	7.72	120.13	110.47
2	U	2	GLN	N-CA-CB	7.72	124.95	111.13
1	D	401	GLN	N-CA-C	7.72	121.50	109.07
1	C	135	LEU	CB-CA-C	7.72	122.45	109.80
1	A	91	VAL	O-C-N	7.70	130.90	122.66
1	C	134	ARG	NE-CZ-NH1	-7.70	113.80	121.50
2	U	119	LYS	N-CA-C	-7.70	100.31	110.40
2	V	34	LEU	CB-CA-C	7.70	122.82	110.96
1	A	63	THR	O-C-N	7.70	130.12	122.19
1	C	387	MET	CA-CB-CG	-7.70	98.71	114.10
2	U	40	PRO	O-C-N	7.69	132.75	123.06
2	T	100	ARG	N-CA-CB	-7.69	98.31	111.69
1	C	206	VAL	N-CA-CB	7.69	120.42	111.66
1	A	399	VAL	CA-C-O	-7.68	112.40	120.39
1	A	312	ARG	NE-CZ-NH1	-7.68	113.82	121.50
1	C	433	GLU	CB-CG-CD	7.68	125.66	112.60
1	D	438	ALA	CA-C-O	-7.68	112.99	120.90
2	T	92	LYS	N-CA-C	-7.68	98.44	109.96
1	C	49	PRO	CB-CA-C	7.66	120.27	110.92
1	D	269	TYR	N-CA-C	7.66	120.52	111.71
1	B	45	GLN	OE1-CD-NE2	-7.66	114.94	122.60
2	T	36	ASN	N-CA-C	7.65	121.87	112.23
1	C	69	VAL	CA-C-O	-7.65	112.37	120.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	ILE	CA-C-O	7.65	123.66	119.15
1	B	174	ILE	CA-C-O	-7.65	112.95	121.36
1	B	418	VAL	CA-C-O	7.64	130.34	120.78
1	A	324	ASP	N-CA-C	-7.64	104.09	113.41
1	A	201	LYS	N-CA-CB	-7.64	99.72	111.56
1	D	201	LYS	N-CA-CB	-7.64	99.70	111.46
1	D	386	HIS	N-CA-C	-7.64	103.51	114.12
1	D	471	ALA	N-CA-C	7.63	120.73	110.35
1	B	133	LEU	O-C-N	7.62	132.33	123.41
1	C	110	GLU	N-CA-CB	-7.62	99.46	110.36
1	A	215	ARG	NE-CZ-NH1	-7.62	113.88	121.50
1	D	119	SER	O-C-N	7.61	131.09	122.11
2	U	63	ASP	N-CA-C	-7.61	99.26	110.52
1	C	364	PHE	CA-CB-CG	7.61	121.41	113.80
1	D	194	ARG	NE-CZ-NH1	7.60	129.10	121.50
1	A	24	TYR	N-CA-CB	-7.60	99.25	110.49
1	D	104	PRO	CA-C-O	-7.59	112.75	121.56
1	C	345	PHE	CA-CB-CG	7.59	121.39	113.80
1	A	351	ASP	N-CA-C	7.59	120.55	110.53
1	A	356	GLN	CA-C-O	-7.59	112.80	121.15
1	D	254	ALA	N-CA-C	-7.59	103.01	111.28
1	D	30	GLN	O-C-N	7.58	132.69	123.13
2	T	82	GLN	CB-CA-C	7.58	123.38	110.79
1	C	465	ILE	CA-C-O	-7.58	112.46	120.57
2	T	106	ASN	CA-CB-CG	-7.58	105.02	112.60
1	D	36	ILE	N-CA-C	-7.57	97.68	108.58
1	D	408	GLY	CA-C-N	7.57	130.81	120.67
1	D	408	GLY	C-N-CA	7.57	130.81	120.67
1	A	259	GLU	CB-CG-CD	7.57	125.46	112.60
1	B	445	ILE	N-CA-C	-7.56	102.76	111.00
1	C	332	VAL	N-CA-CB	-7.56	98.75	111.23
1	D	410	PRO	O-C-N	7.56	131.32	122.17
1	C	156	GLN	OE1-CD-NE2	-7.56	115.04	122.60
2	T	40	PRO	CB-CA-C	-7.55	101.17	111.21
1	A	258	ARG	NH1-CZ-NH2	-7.55	109.49	119.30
1	B	465	ILE	CB-CA-C	-7.55	101.55	110.91
1	A	167	ARG	O-C-N	7.54	129.99	121.32
1	B	141	PRO	N-CA-CB	-7.53	99.30	103.22
1	B	217	ARG	NE-CZ-NH1	7.53	129.03	121.50
1	B	50	PRO	O-C-N	7.52	131.26	122.23
2	U	29	GLU	CB-CG-CD	7.52	125.38	112.60
2	U	58	SER	CB-CA-C	7.52	124.98	110.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	84	LEU	O-C-N	7.52	130.09	122.12
1	C	174	ILE	CA-C-O	-7.51	112.49	121.28
1	C	285	ARG	NE-CZ-NH2	7.51	125.96	119.20
1	C	465	ILE	N-CA-C	7.51	119.10	108.36
1	D	347	ASP	CA-CB-CG	7.51	120.11	112.60
1	C	19	GLU	N-CA-CB	7.50	121.69	110.29
1	C	82	GLY	CA-C-O	-7.50	113.02	121.94
1	C	295	ARG	O-C-N	7.50	132.11	122.06
1	A	112	SER	N-CA-C	7.49	122.10	107.57
1	D	41	ARG	NH1-CZ-NH2	7.49	129.04	119.30
1	D	324	ASP	CB-CA-C	7.49	124.40	110.70
1	D	183	LYS	O-C-N	-7.48	114.19	122.12
1	B	61	SER	CB-CA-C	-7.48	96.81	109.38
2	V	53	ARG	CA-C-O	-7.48	108.64	122.62
1	A	178	LEU	CA-C-O	-7.47	112.66	121.11
1	A	167	ARG	NE-CZ-NH1	-7.47	114.03	121.50
1	D	428	VAL	O-C-N	7.47	129.12	121.87
1	A	89	ARG	CA-CB-CG	7.47	129.04	114.10
2	S	8	ASN	CA-CB-CG	7.47	120.07	112.60
1	B	298	HIS	N-CA-C	7.47	119.42	111.28
1	B	310	HIS	CA-C-O	-7.47	112.54	121.05
1	C	183	LYS	CA-CB-CG	-7.47	99.17	114.10
2	V	18	LEU	N-CA-C	-7.47	100.62	110.40
1	D	88	GLU	CA-C-O	-7.46	111.36	120.54
2	V	2	GLN	N-CA-CB	7.46	124.64	111.13
1	D	354	VAL	O-C-N	7.46	130.94	123.18
1	A	203	ASP	CA-CB-CG	7.46	120.06	112.60
1	D	461	VAL	N-CA-C	7.46	117.58	110.42
1	B	330	THR	O-C-N	7.45	130.53	122.34
1	C	133	LEU	CA-C-O	-7.45	112.42	121.06
1	C	110	GLU	CA-C-O	-7.44	113.24	121.87
1	B	244	ALA	CA-C-N	7.44	129.71	120.34
1	B	244	ALA	C-N-CA	7.44	129.71	120.34
2	T	97	ALA	CA-C-O	-7.43	113.04	121.81
1	D	101	VAL	O-C-N	7.43	130.84	123.03
1	A	60	GLU	CA-C-N	7.43	134.01	122.49
1	A	60	GLU	C-N-CA	7.43	134.01	122.49
1	A	309	ILE	O-C-N	7.43	130.83	123.03
1	C	201	LYS	N-CA-C	7.43	119.45	108.60
1	A	75	THR	CA-C-O	-7.42	112.90	120.77
1	A	373	GLY	CA-C-N	7.42	132.39	123.19
1	A	373	GLY	C-N-CA	7.42	132.39	123.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	386	HIS	ND1-CE1-NE2	-7.42	100.98	108.40
2	V	119	LYS	N-CA-C	-7.42	100.69	110.40
2	S	104	PHE	N-CA-C	7.41	121.55	109.76
2	S	40	PRO	CA-C-O	-7.41	112.42	121.31
1	C	175	LYS	O-C-N	-7.41	115.77	121.55
1	C	246	THR	CA-C-O	-7.41	112.46	121.06
1	A	82	GLY	N-CA-C	-7.41	98.51	111.62
1	D	187	ARG	O-C-N	7.40	129.99	122.08
1	A	326	ILE	N-CA-CB	7.39	123.49	111.36
1	B	236	LYS	CA-C-O	-7.39	112.81	121.46
2	U	98	TRP	N-CA-CB	7.39	122.72	110.52
2	S	55	ASN	CA-C-O	-7.38	110.30	119.38
1	A	135	LEU	CB-CA-C	7.37	121.92	109.75
1	C	163	ASN	CA-CB-CG	-7.37	105.23	112.60
1	A	215	ARG	CB-CG-CD	7.37	128.25	111.30
1	B	371	LEU	N-CA-C	-7.36	100.48	109.83
1	D	466	VAL	CA-C-N	-7.35	112.28	122.87
1	D	466	VAL	C-N-CA	-7.35	112.28	122.87
1	B	417	ALA	N-CA-C	-7.35	102.87	111.03
1	C	223	GLU	CA-C-O	7.35	128.76	120.90
1	D	287	ASN	CA-CB-CG	-7.35	105.25	112.60
1	C	292	HIS	CA-C-O	-7.34	112.24	120.32
1	D	287	ASN	CB-CG-ND2	-7.34	105.39	116.40
2	S	65	ARG	CG-CD-NE	7.34	128.15	112.00
2	V	43	GLU	CB-CG-CD	7.34	125.08	112.60
1	C	352	ASP	O-C-N	7.34	131.77	122.23
1	A	448	ALA	O-C-N	7.33	130.51	122.15
1	D	203	ASP	O-C-N	7.33	131.24	122.96
2	U	25	GLN	O-C-N	7.33	129.89	122.12
1	D	290	LEU	N-CA-C	-7.33	98.37	110.17
2	V	5	PRO	CA-C-O	7.33	126.18	120.90
1	A	270	LEU	CA-C-O	-7.32	112.11	120.24
1	C	112	SER	N-CA-C	7.32	122.19	107.41
1	C	389	ALA	O-C-N	7.32	129.99	122.09
2	U	55	ASN	N-CA-C	7.31	121.46	112.54
1	A	218	PHE	CA-CB-CG	7.31	121.11	113.80
1	D	331	VAL	CA-C-N	7.31	135.13	121.97
1	D	331	VAL	C-N-CA	7.31	135.13	121.97
1	B	351	ASP	CA-CB-CG	-7.31	105.29	112.60
1	B	324	ASP	N-CA-C	-7.30	103.99	113.12
1	C	157	VAL	O-C-N	7.30	128.95	121.87
1	A	193	LEU	CA-C-O	-7.30	112.75	120.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	111	GLN	N-CA-CB	7.29	121.76	109.87
2	T	113	ILE	CA-C-O	-7.29	115.11	121.09
1	C	144	TYR	N-CA-C	-7.29	104.92	113.88
1	C	468	ASN	N-CA-CB	7.29	122.19	110.16
1	B	29	TYR	N-CA-C	7.28	121.05	110.42
2	U	88	GLY	CA-C-O	7.28	128.86	121.00
1	D	89	ARG	N-CA-CB	7.28	121.35	110.29
1	A	278	THR	CA-C-O	-7.28	112.83	120.55
2	S	4	TRP	CA-C-O	-7.27	112.38	119.51
1	D	390	LEU	O-C-N	7.27	129.86	122.08
1	D	123	ASN	N-CA-C	7.27	123.06	114.04
1	B	230	ALA	O-C-N	7.27	129.94	122.09
1	B	420	ASN	OD1-CG-ND2	7.27	129.87	122.60
1	A	414	ALA	CA-C-N	7.26	126.80	119.24
1	A	414	ALA	C-N-CA	7.26	126.80	119.24
1	B	393	ILE	O-C-N	7.26	128.92	121.87
1	B	442	ASN	OD1-CG-ND2	7.26	129.87	122.60
2	V	57	LYS	N-CA-CB	7.26	123.55	111.49
1	A	238	HIS	CA-C-O	-7.26	112.54	120.24
1	A	232	THR	CA-CB-OG1	-7.26	98.71	109.60
1	A	456	ALA	O-C-N	7.25	129.84	122.08
1	B	224	ALA	CA-C-O	-7.25	112.74	120.42
1	A	193	LEU	N-CA-CB	-7.25	99.19	110.06
2	S	26	LEU	CB-CA-C	7.24	122.81	110.79
2	S	109	GLN	CA-C-O	-7.24	113.18	121.65
1	C	43	THR	O-C-N	7.24	127.06	121.27
1	D	432	ASN	CA-C-O	-7.24	112.88	120.55
1	B	433	GLU	CB-CG-CD	7.24	124.90	112.60
1	C	371	LEU	CA-C-N	7.24	127.66	119.92
1	C	371	LEU	C-N-CA	7.24	127.66	119.92
1	B	246	THR	O-C-N	7.24	132.56	123.15
1	B	336	GLU	CA-C-O	-7.23	113.63	121.44
2	S	31	GLU	CA-C-N	7.23	129.97	120.28
2	S	31	GLU	C-N-CA	7.23	129.97	120.28
1	B	326	ILE	N-CA-CB	7.23	123.31	111.45
1	B	18	LYS	CA-C-O	-7.23	112.94	120.89
1	B	223	GLU	CB-CG-CD	7.22	124.88	112.60
1	C	103	TYR	N-CA-CB	-7.22	97.67	109.94
1	D	420	ASN	O-C-N	7.22	129.77	122.12
1	D	334	LYS	N-CA-C	7.20	121.17	112.38
1	B	144	TYR	CA-C-N	-7.20	111.49	120.56
1	B	144	TYR	C-N-CA	-7.20	111.49	120.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	440	GLU	N-CA-C	7.20	121.75	113.19
1	A	80	TYR	CA-C-O	-7.19	111.28	119.41
1	C	201	LYS	CG-CD-CE	-7.19	94.76	111.30
1	A	79	ARG	CB-CA-C	-7.19	98.62	110.85
1	B	434	GLY	CA-C-O	-7.19	111.19	118.96
1	B	346	VAL	N-CA-C	-7.18	103.53	110.42
1	B	351	ASP	N-CA-C	7.18	119.24	110.41
2	S	119	LYS	N-CA-C	-7.18	101.06	110.39
1	A	445	ILE	CB-CA-C	7.18	122.12	112.22
1	C	36	ILE	N-CA-C	-7.18	97.96	108.87
2	U	7	ILE	CA-C-N	-7.18	112.54	122.87
2	U	7	ILE	C-N-CA	-7.18	112.54	122.87
1	B	127	PHE	CA-C-O	-7.17	113.30	121.19
1	A	432	ASN	CA-CB-CG	7.17	119.77	112.60
1	A	366	GLN	CA-C-O	-7.17	112.63	120.30
1	B	432	ASN	CA-C-O	-7.17	112.95	120.55
1	D	329	GLY	CA-C-O	-7.17	116.86	122.52
2	S	100	ARG	CG-CD-NE	7.16	127.75	112.00
1	B	52	GLU	N-CA-C	-7.16	100.61	111.56
1	D	40	PHE	CA-CB-CG	7.16	120.96	113.80
1	C	265	VAL	CA-C-O	-7.15	113.29	121.44
2	U	61	TYR	O-C-N	7.15	131.35	123.27
1	D	119	SER	CA-C-O	-7.15	113.39	120.89
2	T	98	TRP	N-CA-CB	7.15	121.79	110.57
1	A	401	GLN	OE1-CD-NE2	-7.14	115.46	122.60
1	A	465	ILE	CA-C-O	-7.14	112.64	120.71
1	B	290	LEU	O-C-N	7.14	131.44	123.16
1	B	89	ARG	CA-CB-CG	7.14	128.38	114.10
1	C	266	MET	CA-C-O	-7.14	113.33	121.40
1	A	444	ILE	CA-C-N	-7.14	110.28	120.42
1	A	444	ILE	C-N-CA	-7.14	110.28	120.42
1	C	60	GLU	CG-CD-OE2	7.14	134.82	118.40
1	D	232	THR	CA-C-O	-7.14	111.37	119.79
1	D	345	PHE	CA-C-O	-7.13	110.61	119.38
1	A	330	THR	O-C-N	7.13	129.53	122.19
1	D	86	ARG	O-C-N	7.13	132.07	122.59
1	D	183	LYS	CA-C-O	7.12	128.10	120.55
1	C	258	ARG	NH1-CZ-NH2	-7.12	110.04	119.30
1	A	86	ARG	N-CA-CB	7.12	122.52	110.49
1	C	431	ARG	O-C-N	7.11	129.40	122.07
1	D	137	ASP	N-CA-CB	-7.11	100.75	111.56
1	B	452	SER	CA-C-N	7.11	126.63	119.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	452	SER	C-N-CA	7.11	126.63	119.24
1	D	30	GLN	CA-C-O	-7.11	112.85	120.46
1	B	259	GLU	CA-C-N	7.11	132.59	120.72
1	B	259	GLU	C-N-CA	7.11	132.59	120.72
1	B	374	VAL	N-CA-CB	-7.11	99.49	110.86
1	C	324	ASP	N-CA-C	-7.10	104.24	113.12
1	C	48	VAL	O-C-N	7.09	125.84	121.37
1	C	10	SER	N-CA-CB	7.09	122.47	110.49
1	B	13	PHE	N-CA-C	-7.08	98.50	109.76
1	B	360	ARG	CD-NE-CZ	-7.08	114.49	124.40
2	V	93	ALA	CA-C-N	-7.08	114.59	123.15
2	V	93	ALA	C-N-CA	-7.08	114.59	123.15
1	A	295	ARG	NE-CZ-NH1	7.08	128.58	121.50
1	C	132	ALA	CA-C-O	-7.08	112.08	120.43
1	D	165	TYR	CA-C-N	7.08	135.28	121.41
1	D	165	TYR	C-N-CA	7.08	135.28	121.41
1	D	431	ARG	CD-NE-CZ	-7.08	114.49	124.40
1	A	430	ALA	N-CA-C	-7.07	103.50	111.07
1	A	144	TYR	N-CA-C	-7.07	104.78	113.41
1	C	432	ASN	CA-CB-CG	7.07	119.67	112.60
1	C	343	LEU	O-C-N	7.07	130.49	122.22
1	C	197	LEU	N-CA-C	-7.06	100.03	110.48
2	U	82	GLN	CB-CA-C	7.06	122.51	110.79
1	B	41	ARG	NE-CZ-NH2	7.06	125.55	119.20
1	B	354	VAL	O-C-N	7.05	130.51	123.18
1	B	175	LYS	CB-CA-C	7.05	119.93	109.22
1	B	448	ALA	O-C-N	7.05	130.19	122.15
1	A	125	PHE	CA-C-O	-7.03	110.24	119.10
1	D	223	GLU	CB-CG-CD	7.03	124.56	112.60
1	D	432	ASN	OD1-CG-ND2	-7.03	115.57	122.60
1	A	194	ARG	O-C-N	7.03	131.53	122.39
1	D	79	ARG	O-C-N	7.03	130.16	122.15
1	A	51	GLU	CB-CG-CD	7.03	124.55	112.60
1	A	279	SER	N-CA-C	-7.02	103.63	111.28
1	B	302	ASP	N-CA-C	7.02	121.55	112.92
1	C	314	LEU	CA-C-N	7.02	129.56	120.44
1	C	314	LEU	C-N-CA	7.02	129.56	120.44
1	D	139	ARG	CD-NE-CZ	-7.02	114.58	124.40
1	D	350	ARG	CB-CG-CD	-7.01	95.17	111.30
2	T	104	PHE	CA-CB-CG	-7.01	106.79	113.80
1	D	391	THR	CA-C-O	-7.00	113.41	120.90
1	C	156	GLN	CG-CD-NE2	-7.00	105.90	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	LEU	CA-C-O	-7.00	113.49	120.70
1	B	279	SER	CA-C-N	7.00	130.23	120.29
1	B	279	SER	C-N-CA	7.00	130.23	120.29
1	D	366	GLN	CA-C-O	-7.00	112.62	120.32
2	T	14	THR	CA-CB-OG1	-7.00	99.11	109.60
1	C	428	VAL	O-C-N	6.99	128.65	121.87
2	V	98	TRP	O-C-N	6.99	131.37	123.19
1	A	417	ALA	N-CA-C	-6.98	103.28	111.03
1	D	189	VAL	CA-C-N	6.98	129.97	120.54
1	D	189	VAL	C-N-CA	6.98	129.97	120.54
2	V	96	GLN	O-C-N	6.98	130.72	122.34
2	V	36	ASN	N-CA-C	6.97	122.03	112.90
1	D	446	ARG	NE-CZ-NH2	6.96	125.47	119.20
1	C	89	ARG	CA-CB-CG	6.96	128.03	114.10
1	C	131	ARG	N-CA-C	-6.96	105.33	114.31
1	B	130	LEU	CA-C-N	-6.96	110.70	122.11
1	B	130	LEU	C-N-CA	-6.96	110.70	122.11
1	C	355	GLU	N-CA-CB	-6.96	99.74	109.97
1	D	41	ARG	NE-CZ-NH1	-6.96	114.54	121.50
2	S	89	GLU	CA-CB-CG	6.96	128.01	114.10
1	C	253	ARG	NH1-CZ-NH2	6.95	128.33	119.30
1	A	99	ALA	CA-C-O	-6.94	112.93	120.92
1	C	115	ASN	O-C-N	6.94	129.25	122.03
1	B	96	GLN	CA-CB-CG	6.94	127.98	114.10
1	C	356	GLN	OE1-CD-NE2	6.94	129.54	122.60
1	A	455	LEU	O-C-N	6.93	129.47	122.12
1	B	75	THR	O-C-N	6.93	131.81	122.59
1	B	13	PHE	N-CA-CB	6.92	120.68	109.95
1	C	286	ASP	O-C-N	6.92	131.71	122.43
1	D	214	TRP	CA-C-O	-6.92	113.15	120.63
1	C	68	THR	CA-C-N	-6.92	114.61	123.19
1	C	68	THR	C-N-CA	-6.92	114.61	123.19
2	S	51	VAL	O-C-N	6.92	129.75	122.62
1	B	62	SER	CA-C-N	-6.92	111.38	122.24
1	B	62	SER	C-N-CA	-6.92	111.38	122.24
1	B	191	GLU	CB-CG-CD	6.92	124.36	112.60
2	S	50	PHE	CA-CB-CG	6.91	120.71	113.80
1	D	330	THR	CA-CB-OG1	-6.91	99.23	109.60
2	T	48	HIS	CA-CB-CG	-6.91	106.89	113.80
1	A	49	PRO	O-C-N	6.91	129.61	121.46
2	S	82	GLN	CB-CA-C	6.90	121.71	110.88
2	S	115	PHE	CA-C-N	-6.90	112.14	121.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	115	PHE	C-N-CA	-6.90	112.14	121.66
1	B	34	THR	CA-C-O	-6.90	111.45	119.59
1	C	180	LEU	N-CA-CB	-6.90	99.17	110.41
1	D	280	LEU	CB-CA-C	6.90	122.58	110.85
1	B	438	ALA	CA-C-O	-6.89	113.80	120.90
1	C	258	ARG	NE-CZ-NH1	6.89	128.39	121.50
1	A	229	GLN	CA-C-O	-6.89	113.59	120.82
1	A	461	VAL	CA-C-N	-6.89	111.85	122.60
1	A	461	VAL	C-N-CA	-6.89	111.85	122.60
1	D	367	ASP	CA-C-O	-6.89	112.74	120.32
1	C	26	THR	N-CA-CB	-6.89	101.84	110.79
1	B	71	THR	O-C-N	6.89	131.75	122.59
1	B	144	TYR	N-CA-C	-6.89	105.41	113.88
1	A	304	GLN	CB-CA-C	6.88	120.64	109.90
1	D	41	ARG	CD-NE-CZ	-6.88	114.77	124.40
2	S	73	PRO	CB-CA-C	6.88	119.78	111.46
1	A	247	CYS	O-C-N	6.88	129.41	122.12
2	T	96	GLN	CB-CG-CD	6.88	124.29	112.60
1	C	89	ARG	N-CA-CB	6.87	121.61	110.41
1	D	159	ARG	CD-NE-CZ	-6.87	114.78	124.40
1	D	465	ILE	CB-CA-C	-6.87	102.39	110.91
1	B	298	HIS	CA-CB-CG	6.87	120.67	113.80
1	B	360	ARG	N-CA-C	6.87	121.10	113.21
1	D	61	SER	CA-CB-OG	-6.87	97.37	111.10
1	B	37	LEU	O-C-N	6.86	132.11	123.19
1	C	338	GLU	CB-CG-CD	6.86	124.27	112.60
2	U	8	ASN	O-C-N	6.86	131.20	122.28
2	U	96	GLN	CB-CG-CD	6.86	124.27	112.60
1	A	258	ARG	NE-CZ-NH1	6.86	128.36	121.50
2	V	58	SER	CB-CA-C	6.86	123.68	110.17
1	C	114	THR	CA-CB-OG1	-6.85	99.32	109.60
2	U	44	PHE	CA-C-O	-6.85	113.42	121.44
1	D	190	TYR	CA-C-N	-6.85	111.53	120.44
1	D	190	TYR	C-N-CA	-6.85	111.53	120.44
2	U	98	TRP	CA-C-N	-6.83	113.44	122.94
2	U	98	TRP	C-N-CA	-6.83	113.44	122.94
2	U	98	TRP	CA-C-O	-6.83	113.22	120.80
1	D	306	ASN	CA-CB-CG	-6.83	105.77	112.60
1	D	184	ASN	OD1-CG-ND2	6.83	129.43	122.60
1	C	87	ILE	CA-C-O	-6.83	113.70	121.75
1	D	36	ILE	CA-C-O	-6.82	113.00	120.71
1	D	232	THR	CA-CB-OG1	-6.82	99.37	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	167	ARG	NE-CZ-NH2	6.82	125.34	119.20
2	S	66	TYR	CB-CG-CD2	6.82	131.03	120.80
1	A	465	ILE	N-CA-CB	-6.82	103.29	110.72
1	B	290	LEU	CA-C-O	-6.82	113.08	120.92
1	C	199	PHE	N-CA-C	6.82	120.65	109.06
1	A	194	ARG	N-CA-CB	6.81	121.90	110.32
1	A	127	PHE	CA-C-O	-6.81	113.70	121.19
1	D	45	GLN	CA-C-N	6.81	128.35	119.84
1	D	45	GLN	C-N-CA	6.81	128.35	119.84
1	A	117	PHE	O-C-N	6.81	129.08	122.07
2	V	80	ALA	CA-C-O	6.81	127.98	120.63
1	B	432	ASN	OD1-CG-ND2	-6.80	115.80	122.60
1	A	158	GLU	N-CA-CB	6.80	119.87	110.01
1	C	400	LEU	O-C-N	6.80	131.39	123.30
1	B	431	ARG	O-C-N	6.80	129.35	122.08
1	D	269	TYR	CA-C-O	-6.79	112.42	120.10
1	D	466	VAL	O-C-N	6.79	130.22	122.82
1	B	428	VAL	CB-CA-C	6.79	120.66	111.97
1	A	52	GLU	N-CA-C	-6.79	102.27	112.04
2	U	86	GLU	O-C-N	6.79	129.91	122.11
2	S	85	ALA	CA-C-N	6.78	129.70	120.54
2	S	85	ALA	C-N-CA	6.78	129.70	120.54
1	B	98	ILE	CA-C-O	-6.78	111.84	120.86
1	B	131	ARG	N-CA-C	-6.78	105.29	113.97
1	B	248	GLU	CB-CG-CD	6.78	124.13	112.60
1	C	139	ARG	CA-C-N	-6.78	117.71	122.59
1	C	139	ARG	C-N-CA	-6.78	117.71	122.59
1	C	352	ASP	N-CA-CB	6.78	120.30	110.20
1	A	83	ARG	NE-CZ-NH2	6.78	125.30	119.20
1	B	170	LEU	N-CA-CB	-6.78	99.78	110.69
1	A	264	ILE	CA-CB-CG2	6.78	122.02	110.50
1	C	208	SER	CB-CA-C	6.78	120.13	110.24
1	D	49	PRO	N-CA-C	-6.77	102.44	110.70
1	D	303	ARG	O-C-N	-6.77	115.07	122.38
2	T	45	GLU	CA-CB-CG	6.76	127.63	114.10
2	T	100	ARG	CA-C-O	-6.76	113.76	121.40
1	C	110	GLU	CA-CB-CG	6.76	127.62	114.10
1	B	259	GLU	N-CA-CB	6.76	120.01	109.94
2	U	110	VAL	CA-C-O	-6.76	113.44	121.28
1	B	286	ASP	O-C-N	6.76	131.78	122.46
1	C	324	ASP	CB-CA-C	6.76	120.71	109.56
2	S	48	HIS	O-C-N	6.75	133.14	122.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	TYR	N-CA-CB	6.75	121.17	110.57
1	C	165	TYR	CA-C-N	6.75	134.64	121.41
1	C	165	TYR	C-N-CA	6.75	134.64	121.41
1	D	431	ARG	NE-CZ-NH2	-6.75	113.12	119.20
1	A	394	PHE	N-CA-C	6.75	121.74	112.90
2	V	66	TYR	O-C-N	6.75	131.12	122.89
1	A	413	ASN	N-CA-C	6.75	119.25	111.02
1	A	459	CYS	O-C-N	6.75	129.10	122.09
1	B	201	LYS	N-CA-C	6.75	119.11	108.79
1	C	394	PHE	CA-C-O	-6.75	111.71	119.60
1	B	341	ILE	N-CA-C	-6.74	104.19	110.53
1	B	466	VAL	N-CA-C	-6.74	98.59	108.23
1	B	449	CYS	N-CA-C	-6.74	103.17	111.33
1	B	367	ASP	CA-CB-CG	6.74	119.34	112.60
2	T	65	ARG	CG-CD-NE	6.74	126.83	112.00
2	T	111	GLN	N-CA-C	-6.74	98.22	108.67
1	A	121	VAL	CB-CA-C	6.74	118.34	110.93
1	A	201	LYS	CG-CD-CE	-6.74	95.80	111.30
1	B	301	ILE	CB-CG1-CD1	-6.74	99.65	113.80
1	C	325	HIS	CA-C-N	6.74	132.83	122.25
1	C	325	HIS	C-N-CA	6.74	132.83	122.25
1	D	23	THR	CA-C-N	-6.74	111.87	122.65
1	D	23	THR	C-N-CA	-6.74	111.87	122.65
1	B	264	ILE	CB-CG1-CD1	-6.73	99.66	113.80
1	B	303	ARG	N-CA-C	6.73	119.92	111.24
1	B	95	ASP	CA-CB-CG	-6.73	105.87	112.60
1	C	268	ASP	CA-C-O	-6.73	113.78	121.66
2	S	98	TRP	N-CA-CB	6.73	121.52	110.69
1	B	118	THR	N-CA-C	-6.73	103.95	111.28
2	U	59	PRO	O-C-N	6.73	131.17	123.03
1	D	207	ASN	OD1-CG-ND2	-6.73	115.87	122.60
2	V	2	GLN	O-C-N	6.73	131.28	123.41
1	C	113	VAL	N-CA-C	-6.72	103.76	110.62
1	D	163	ASN	CB-CA-C	-6.72	102.18	111.73
1	A	201	LYS	CB-CA-C	-6.72	98.12	110.62
1	B	286	ASP	CA-C-O	-6.72	110.32	119.05
1	A	406	THR	CA-C-O	-6.72	111.85	119.98
1	A	391	THR	CA-CB-OG1	-6.72	99.53	109.60
2	T	38	TRP	CB-CA-C	6.72	120.88	109.53
1	B	338	GLU	O-C-N	-6.71	115.33	123.19
2	S	40	PRO	CB-CA-C	-6.71	102.28	111.21
1	B	158	GLU	N-CA-CB	6.71	119.74	110.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	ASN	OD1-CG-ND2	6.70	129.30	122.60
1	B	359	SER	N-CA-C	-6.70	103.66	110.97
1	D	445	ILE	N-CA-C	-6.70	103.95	110.72
1	D	124	VAL	CA-C-O	-6.70	114.08	121.05
2	T	91	LYS	N-CA-C	-6.70	104.05	111.82
1	D	351	ASP	N-CA-C	6.70	119.17	110.53
1	D	360	ARG	NE-CZ-NH1	-6.70	114.80	121.50
1	B	188	ALA	CA-C-N	6.70	129.07	120.70
1	B	188	ALA	C-N-CA	6.70	129.07	120.70
1	D	193	LEU	CA-C-O	-6.70	113.79	120.82
1	C	359	SER	CA-CB-OG	6.69	124.49	111.10
1	A	422	VAL	CA-C-O	-6.69	114.08	121.17
1	A	45	GLN	CA-C-N	6.69	128.20	119.84
1	A	45	GLN	C-N-CA	6.69	128.20	119.84
1	B	377	VAL	CA-C-N	6.69	131.53	122.84
1	B	377	VAL	C-N-CA	6.69	131.53	122.84
2	S	45	GLU	O-C-N	6.69	131.52	123.36
1	A	345	PHE	CA-CB-CG	6.68	120.48	113.80
1	C	435	ARG	CD-NE-CZ	-6.68	115.05	124.40
1	C	444	ILE	CA-C-N	-6.68	109.87	120.55
1	C	444	ILE	C-N-CA	-6.68	109.87	120.55
1	A	164	LYS	CA-C-O	6.67	127.31	120.24
1	A	365	THR	CA-C-O	-6.67	113.14	120.81
2	T	40	PRO	CA-C-O	-6.67	113.31	121.31
1	B	92	GLY	O-C-N	6.67	131.37	122.70
1	B	404	GLY	O-C-N	6.67	128.59	122.19
1	C	19	GLU	CA-CB-CG	6.67	127.43	114.10
2	S	52	TYR	CA-CB-CG	6.66	125.89	113.90
1	C	170	LEU	O-C-N	6.66	131.56	123.16
1	D	327	HIS	N-CA-C	-6.66	99.16	109.76
1	A	132	ALA	CA-C-O	-6.66	112.35	120.54
1	A	365	THR	O-C-N	6.66	131.12	122.93
1	B	109	GLU	CB-CG-CD	6.65	123.91	112.60
1	C	130	LEU	CA-C-N	-6.65	111.79	122.24
1	C	130	LEU	C-N-CA	-6.65	111.79	122.24
1	C	332	VAL	N-CA-C	6.65	123.18	109.34
1	D	282	HIS	CB-CG-CD2	-6.65	122.55	131.20
1	B	393	ILE	CA-C-O	-6.65	114.03	120.95
1	C	468	ASN	O-C-N	6.65	130.80	123.22
1	B	319	ARG	NE-CZ-NH1	6.65	128.15	121.50
1	C	321	SER	CB-CA-C	6.65	121.40	110.90
1	A	120	ILE	N-CA-C	6.64	118.19	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	39	VAL	O-C-N	6.64	127.35	121.57
1	B	94	LYS	CA-C-O	-6.64	111.01	120.51
1	B	266	MET	N-CA-CB	-6.64	100.57	111.66
2	U	109	GLN	CA-C-O	-6.64	113.88	121.65
1	B	288	GLY	N-CA-C	6.64	125.71	113.76
1	A	148	PHE	CA-CB-CG	-6.64	107.16	113.80
1	A	235	ILE	CA-C-O	-6.64	113.43	121.13
1	B	456	ALA	O-C-N	6.64	129.18	122.08
1	D	149	GLN	O-C-N	6.63	132.03	122.28
1	B	23	THR	O-C-N	6.63	130.20	122.25
1	C	61	SER	CB-CA-C	-6.62	98.46	109.99
1	D	79	ARG	CG-CD-NE	6.62	126.58	112.00
1	A	57	VAL	CA-C-O	-6.62	114.15	121.17
1	C	138	LEU	O-C-N	6.62	131.34	123.33
1	C	350	ARG	NE-CZ-NH1	6.62	128.12	121.50
1	B	207	ASN	CA-CB-CG	6.62	119.22	112.60
1	B	324	ASP	CA-C-O	-6.62	111.77	119.78
2	T	6	PRO	CA-C-N	-6.62	116.39	123.08
2	T	6	PRO	C-N-CA	-6.62	116.39	123.08
1	A	200	THR	N-CA-C	-6.62	99.35	109.41
1	A	255	VAL	O-C-N	-6.62	115.45	121.87
1	B	304	GLN	O-C-N	-6.62	114.75	122.95
1	A	469	PHE	N-CA-CB	6.61	121.75	110.57
1	D	163	ASN	O-C-N	6.61	131.27	122.41
1	C	434	GLY	CA-C-O	-6.61	111.33	118.86
1	B	34	THR	CA-CB-OG1	-6.61	99.69	109.60
1	B	290	LEU	N-CA-C	-6.60	98.86	109.96
1	A	97	TYR	CB-CA-C	-6.60	97.23	110.30
1	A	173	THR	CA-CB-CG2	6.60	121.72	110.50
1	A	298	HIS	CA-C-O	-6.60	113.84	120.90
1	A	306	ASN	OD1-CG-ND2	-6.60	116.00	122.60
1	C	139	ARG	CD-NE-CZ	-6.60	115.16	124.40
1	D	412	GLY	CA-C-O	6.60	128.64	122.57
1	C	75	THR	CA-C-O	-6.59	113.79	120.77
1	C	141	PRO	O-C-N	-6.58	118.06	121.15
2	S	18	LEU	N-CA-C	-6.58	100.49	110.50
1	D	32	LYS	N-CA-CB	6.58	121.36	110.63
2	V	100	ARG	CA-CB-CG	6.58	127.27	114.10
1	C	99	ALA	CB-CA-C	6.58	120.39	109.53
1	C	26	THR	CA-CB-CG2	6.58	121.68	110.50
1	A	249	GLU	O-C-N	6.57	129.13	122.03
1	A	169	LEU	CA-CB-CG	6.57	139.30	116.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	201	LYS	CB-CA-C	-6.57	98.29	111.17
1	D	285	ARG	CD-NE-CZ	-6.57	115.20	124.40
1	A	294	HIS	N-CA-C	-6.57	98.19	108.90
1	A	10	SER	N-CA-CB	6.57	121.59	110.49
1	A	436	ASP	CA-C-O	-6.57	112.29	120.57
1	D	467	PHE	CA-C-N	-6.57	112.11	121.50
1	D	467	PHE	C-N-CA	-6.57	112.11	121.50
2	V	67	TRP	CA-C-O	-6.57	113.93	121.68
1	A	179	GLY	N-CA-C	6.56	124.45	115.00
1	B	123	ASN	N-CA-C	6.56	121.95	113.88
1	A	339	ARG	NH1-CZ-NH2	6.56	127.82	119.30
1	D	28	GLU	CG-CD-OE2	-6.56	103.32	118.40
1	D	194	ARG	CD-NE-CZ	6.56	133.58	124.40
2	U	43	GLU	CA-CB-CG	6.56	127.21	114.10
2	T	8	ASN	CA-C-O	-6.55	111.14	120.51
1	C	216	ASP	CA-C-O	-6.55	113.95	120.70
1	A	259	GLU	CA-C-O	-6.55	113.61	120.55
1	B	149	GLN	N-CA-C	-6.55	103.63	111.69
1	A	88	GLU	O-C-N	6.55	130.95	123.48
1	B	173	THR	O-C-N	-6.55	115.75	123.22
1	C	123	ASN	N-CA-C	6.55	122.76	114.31
1	A	56	ALA	N-CA-C	-6.55	104.22	111.36
1	C	350	ARG	CB-CG-CD	-6.54	96.25	111.30
1	B	235	ILE	CB-CG1-CD1	6.54	127.54	113.80
1	C	153	HIS	CB-CA-C	-6.54	98.72	110.23
1	B	221	CYS	CA-C-O	-6.54	111.58	119.49
1	C	153	HIS	N-CA-C	6.54	121.88	113.18
1	C	441	GLY	CA-C-N	6.53	134.02	121.54
1	C	441	GLY	C-N-CA	6.53	134.02	121.54
1	D	340	ASP	O-C-N	6.53	129.15	122.09
1	A	359	SER	CB-CA-C	6.53	121.02	110.96
1	B	50	PRO	CA-C-O	-6.53	109.67	119.86
1	D	345	PHE	O-C-N	6.53	131.17	122.43
1	A	169	LEU	CB-CA-C	6.52	120.66	109.51
1	D	300	VAL	N-CA-C	-6.52	102.94	111.09
1	A	468	ASN	O-C-N	6.52	130.65	123.22
1	A	83	ARG	CA-C-O	6.52	129.01	120.21
1	A	139	ARG	CA-C-N	-6.52	117.90	122.59
1	A	139	ARG	C-N-CA	-6.52	117.90	122.59
2	S	43	GLU	CB-CG-CD	6.52	123.68	112.60
1	D	221	CYS	CA-C-O	-6.52	111.61	119.49
1	A	89	ARG	N-CA-CB	6.51	120.19	110.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	40	PRO	O-C-N	6.51	130.91	123.10
1	B	203	ASP	N-CA-C	-6.51	100.84	110.48
1	B	404	GLY	N-CA-C	-6.51	104.92	112.73
1	C	68	THR	O-C-N	6.51	130.62	123.27
1	C	198	ASP	CA-C-O	6.51	127.46	120.24
1	B	145	VAL	N-CA-CB	6.51	118.16	110.55
1	C	45	GLN	N-CA-C	-6.51	100.19	109.62
1	C	279	SER	CA-C-N	6.51	128.90	120.44
1	C	279	SER	C-N-CA	6.51	128.90	120.44
1	D	41	ARG	CA-C-O	-6.51	113.81	120.84
1	D	461	VAL	O-C-N	6.51	128.29	121.91
1	A	350	ARG	N-CA-C	6.50	121.25	113.12
1	C	260	LEU	O-C-N	-6.50	113.48	122.46
1	D	397	ASP	CA-C-O	-6.50	114.51	122.64
2	V	81	THR	O-C-N	6.50	129.01	122.12
1	C	44	PRO	N-CA-CB	6.50	110.07	103.25
1	B	264	ILE	CA-CB-CG2	6.49	121.54	110.50
1	B	330	THR	CA-C-O	-6.49	111.56	118.77
1	C	17	VAL	CA-C-O	-6.49	114.90	121.59
2	U	40	PRO	CA-C-O	-6.49	113.69	121.48
2	T	8	ASN	O-C-N	6.49	131.22	122.59
1	B	370	SER	CA-CB-OG	-6.48	98.13	111.10
2	S	106	ASN	N-CA-C	6.48	120.65	112.87
1	D	319	ARG	NE-CZ-NH1	-6.48	115.02	121.50
1	C	13	PHE	N-CA-C	-6.48	100.07	109.59
2	T	25	GLN	O-C-N	6.47	128.82	122.09
1	D	341	ILE	O-C-N	6.47	128.25	121.91
1	C	57	VAL	CA-C-O	-6.46	114.33	121.05
1	D	335	LEU	CA-C-O	-6.46	113.90	121.46
1	B	107	LEU	N-CA-C	6.46	120.90	112.89
1	C	132	ALA	O-C-N	6.46	130.84	123.48
2	U	93	ALA	CA-C-O	-6.46	111.27	120.51
1	D	469	PHE	N-CA-CB	6.46	121.49	110.57
1	D	72	ASP	CA-C-O	6.46	127.40	120.10
1	D	334	LYS	CA-CB-CG	6.46	127.02	114.10
1	A	202	ASP	N-CA-C	-6.45	100.93	110.48
1	A	444	ILE	O-C-N	6.45	128.93	121.96
1	D	458	ALA	O-C-N	6.45	128.74	122.03
1	C	110	GLU	CA-C-N	6.45	134.05	121.41
1	C	110	GLU	C-N-CA	6.45	134.05	121.41
2	T	34	LEU	CB-CA-C	6.45	121.00	110.88
1	B	234	GLU	CB-CG-CD	6.45	123.56	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	ARG	CB-CG-CD	6.45	126.12	111.30
1	A	248	GLU	CA-CB-CG	6.44	126.99	114.10
2	U	28	SER	CA-CB-OG	-6.44	98.21	111.10
1	B	191	GLU	CB-CA-C	6.44	120.87	110.96
2	T	56	ASN	O-C-N	6.43	129.83	123.46
1	D	120	ILE	N-CA-C	6.43	117.95	110.62
1	D	149	GLN	OE1-CD-NE2	6.43	129.03	122.60
2	S	68	THR	CA-C-O	-6.43	113.27	120.54
2	T	82	GLN	CA-CB-CG	6.43	126.96	114.10
1	A	49	PRO	N-CA-C	-6.43	102.86	110.70
2	S	113	ILE	O-C-N	6.42	129.35	122.67
1	A	428	VAL	CB-CA-C	6.42	120.19	111.97
1	A	319	ARG	CB-CG-CD	6.42	126.07	111.30
2	S	36	ASN	N-CA-C	6.42	121.31	112.90
1	B	204	GLU	CA-C-O	-6.42	112.03	119.61
1	C	353	PHE	O-C-N	6.42	131.10	123.27
1	A	48	VAL	N-CA-C	6.42	113.40	107.56
2	V	53	ARG	CD-NE-CZ	-6.42	115.42	124.40
1	A	93	GLU	CA-C-O	6.42	129.68	120.51
1	A	161	LYS	CA-C-O	-6.41	114.10	120.70
2	S	64	GLY	CA-C-O	6.41	126.43	119.06
1	D	201	LYS	N-CA-C	6.41	117.96	108.60
1	A	130	LEU	CA-C-O	-6.41	113.81	121.56
1	B	270	LEU	O-C-N	6.41	131.70	122.28
1	B	460	GLU	CA-C-N	6.41	128.63	120.56
1	B	460	GLU	C-N-CA	6.41	128.63	120.56
1	C	256	PHE	CA-C-O	-6.41	114.09	120.82
2	U	36	ASN	N-CA-C	6.41	121.29	112.90
1	D	169	LEU	CA-C-N	-6.41	113.64	122.93
1	D	169	LEU	C-N-CA	-6.41	113.64	122.93
1	D	409	HIS	CA-CB-CG	6.40	120.20	113.80
1	A	134	ARG	NH1-CZ-NH2	6.40	127.62	119.30
1	B	327	HIS	CA-CB-CG	6.40	120.20	113.80
2	T	73	PRO	N-CA-C	-6.40	101.18	111.03
2	T	97	ALA	O-C-N	6.39	130.14	122.85
1	B	47	GLY	CA-C-N	-6.39	116.38	123.02
1	B	47	GLY	C-N-CA	-6.39	116.38	123.02
1	B	421	ARG	NE-CZ-NH1	-6.38	115.11	121.50
2	U	107	VAL	CB-CA-C	-6.38	102.65	111.65
2	T	33	LEU	CB-CA-C	6.38	121.07	110.92
1	A	114	THR	CA-CB-OG1	-6.38	100.03	109.60
1	A	314	LEU	CB-CA-C	6.38	120.90	110.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	GLU	O-C-N	6.38	129.42	122.15
2	S	78	THR	CA-C-O	6.38	126.00	118.79
1	C	243	THR	CA-C-O	-6.38	113.47	120.81
1	D	114	THR	CA-C-O	6.38	127.72	120.90
1	D	291	LEU	N-CA-CB	-6.38	99.96	110.68
1	C	109	GLU	CA-C-O	-6.38	113.48	120.81
1	D	173	THR	CA-C-O	-6.38	113.29	120.43
2	V	57	LYS	N-CA-C	-6.37	103.63	112.30
1	A	163	ASN	CA-C-N	-6.37	113.79	122.77
1	A	163	ASN	C-N-CA	-6.37	113.79	122.77
1	C	193	LEU	CA-C-O	-6.37	114.08	120.90
1	D	153	HIS	CA-C-O	-6.37	110.94	119.47
1	D	445	ILE	CB-CA-C	6.37	121.01	112.22
1	B	60	GLU	CG-CD-OE2	6.37	133.04	118.40
1	D	330	THR	CB-CA-C	-6.37	98.69	109.38
1	C	310	HIS	CA-C-O	-6.36	113.80	121.05
1	C	215	ARG	CD-NE-CZ	-6.36	115.49	124.40
1	B	217	ARG	N-CA-C	-6.36	104.27	111.07
2	U	45	GLU	O-C-N	6.36	131.26	123.44
1	A	365	THR	CA-CB-OG1	-6.36	100.06	109.60
2	V	1	MET	CA-C-N	-6.36	110.75	121.94
2	V	1	MET	C-N-CA	-6.36	110.75	121.94
1	B	97	TYR	N-CA-C	6.36	118.61	109.14
2	S	33	LEU	N-CA-C	-6.34	103.28	111.02
1	A	354	VAL	O-C-N	6.34	129.56	123.03
1	A	186	GLY	CA-C-N	6.34	129.60	120.79
1	A	186	GLY	C-N-CA	6.34	129.60	120.79
1	B	226	TYR	N-CA-C	-6.34	104.45	111.36
1	B	198	ASP	CA-CB-CG	-6.33	106.27	112.60
1	C	183	LYS	N-CA-C	6.33	118.18	111.28
2	V	97	ALA	CA-C-O	-6.33	114.25	121.72
1	C	406	THR	N-CA-C	-6.33	101.91	111.34
1	A	144	TYR	CA-C-N	-6.33	112.58	120.56
1	A	144	TYR	C-N-CA	-6.33	112.58	120.56
1	B	62	SER	O-C-N	6.33	131.01	122.59
1	D	231	GLU	O-C-N	6.33	128.61	122.03
2	U	38	TRP	CA-C-N	-6.33	118.04	122.59
2	U	38	TRP	C-N-CA	-6.33	118.04	122.59
1	C	322	GLY	O-C-N	6.32	130.92	122.70
1	A	127	PHE	O-C-N	6.32	130.65	122.87
1	C	254	ALA	O-C-N	6.32	128.66	122.09
2	U	24	GLU	O-C-N	6.32	128.60	122.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	56	ASN	CA-C-O	-6.31	114.47	121.23
1	B	63	THR	N-CA-C	6.31	122.45	114.31
1	B	179	GLY	N-CA-C	6.31	124.85	115.64
2	S	94	TYR	CB-CA-C	6.31	120.98	111.14
1	C	53	ALA	CA-C-N	6.30	127.11	119.99
1	C	53	ALA	C-N-CA	6.30	127.11	119.99
1	B	19	GLU	CA-CB-CG	6.30	126.70	114.10
1	C	425	GLU	CA-C-O	6.30	127.22	120.10
1	A	351	ASP	CA-CB-CG	-6.30	106.30	112.60
1	C	414	ALA	O-C-N	6.30	128.56	121.32
1	D	121	VAL	O-C-N	-6.30	115.23	122.09
1	D	422	VAL	O-C-N	6.29	128.44	121.90
1	C	460	GLU	CA-C-N	6.29	128.48	120.56
1	C	460	GLU	C-N-CA	6.29	128.48	120.56
1	D	114	THR	CA-CB-OG1	-6.29	100.17	109.60
2	U	57	LYS	CA-C-O	-6.28	112.98	119.51
1	B	223	GLU	CB-CA-C	-6.28	100.76	110.81
1	A	392	GLU	CA-C-N	6.28	128.70	120.60
1	A	392	GLU	C-N-CA	6.28	128.70	120.60
2	S	47	GLU	N-CA-C	6.28	124.17	110.80
1	A	53	ALA	CA-C-N	6.28	127.06	120.03
1	A	53	ALA	C-N-CA	6.28	127.06	120.03
1	C	386	HIS	N-CA-C	-6.28	105.39	114.12
1	C	448	ALA	O-C-N	6.28	129.31	122.15
1	C	26	THR	O-C-N	6.28	126.31	121.23
1	A	332	VAL	N-CA-C	6.27	122.39	109.34
2	S	98	TRP	CA-C-N	-6.27	114.22	122.94
2	S	98	TRP	C-N-CA	-6.27	114.22	122.94
2	S	120	PRO	N-CA-C	-6.27	101.78	111.13
2	T	2	GLN	CA-C-O	6.27	128.12	120.60
1	C	298	HIS	O-C-N	6.27	128.61	122.09
1	A	394	PHE	CA-C-O	-6.27	112.27	119.60
1	C	115	ASN	CA-CB-CG	-6.27	106.33	112.60
1	C	169	LEU	N-CA-C	-6.27	101.20	110.48
1	B	374	VAL	CA-C-N	6.27	129.97	121.20
1	B	374	VAL	C-N-CA	6.27	129.97	121.20
1	C	469	PHE	O-C-N	6.27	130.62	123.48
1	A	360	ARG	N-CA-C	6.26	120.41	113.21
1	A	366	GLN	O-C-N	6.26	130.54	123.27
1	D	158	GLU	N-CA-CB	6.26	119.09	110.01
1	D	183	LYS	CA-CB-CG	-6.26	101.58	114.10
1	A	26	THR	CA-CB-OG1	-6.26	100.21	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	GLU	CG-CD-OE2	6.26	132.79	118.40
1	B	170	LEU	CA-C-O	-6.26	114.08	120.71
1	D	446	ARG	CA-C-N	6.26	128.95	120.44
1	D	446	ARG	C-N-CA	6.26	128.95	120.44
1	A	90	VAL	N-CA-C	-6.25	97.98	107.73
1	D	159	ARG	O-C-N	6.25	128.51	122.07
1	D	343	LEU	CA-C-O	6.25	127.38	120.63
1	C	36	ILE	CA-C-O	-6.25	113.09	121.02
1	D	367	ASP	CA-CB-CG	6.25	118.85	112.60
1	C	89	ARG	NE-CZ-NH1	6.25	127.75	121.50
1	D	86	ARG	N-CA-CB	6.24	121.03	110.49
1	B	32	LYS	O-C-N	6.24	130.05	123.06
1	A	204	GLU	CG-CD-OE1	6.24	132.74	118.40
1	B	350	ARG	CA-CB-CG	6.23	126.57	114.10
2	T	61	TYR	O-C-N	6.23	130.30	123.13
1	D	398	SER	O-C-N	6.23	130.09	123.42
2	T	100	ARG	CA-CB-CG	6.23	126.56	114.10
2	T	119	LYS	CA-C-O	-6.23	114.21	120.63
1	C	394	PHE	CA-CB-CG	-6.23	107.57	113.80
1	A	17	VAL	CA-C-N	6.23	133.02	121.62
1	A	17	VAL	C-N-CA	6.23	133.02	121.62
1	C	29	TYR	N-CA-C	6.23	119.51	110.42
1	C	397	ASP	O-C-N	6.23	130.60	122.38
1	D	149	GLN	N-CA-C	-6.23	103.79	112.45
1	D	10	SER	O-C-N	6.23	130.87	122.59
1	B	203	ASP	CA-C-O	-6.22	114.31	121.47
1	B	312	ARG	CD-NE-CZ	-6.22	115.69	124.40
1	D	269	TYR	O-C-N	6.22	129.49	122.22
1	B	416	GLY	CA-C-O	6.21	126.79	120.45
1	C	66	TRP	N-CA-C	6.21	120.72	113.20
1	C	140	ILE	CA-CB-CG1	6.21	120.96	110.40
1	D	213	ARG	NE-CZ-NH2	6.21	124.79	119.20
2	V	45	GLU	CA-C-O	-6.21	112.64	120.28
2	V	111	GLN	N-CA-CB	6.21	119.88	109.94
2	S	48	HIS	CA-CB-CG	-6.21	107.59	113.80
2	U	120	PRO	N-CA-C	-6.21	100.40	110.40
1	A	441	GLY	CA-C-N	6.20	133.39	121.54
1	A	441	GLY	C-N-CA	6.20	133.39	121.54
1	B	259	GLU	CA-C-O	-6.20	114.26	120.90
1	A	83	ARG	NE-CZ-NH1	-6.20	115.30	121.50
1	D	19	GLU	N-CA-CB	6.20	119.10	110.17
1	B	75	THR	CA-C-O	-6.20	111.65	120.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	THR	CA-C-O	-6.20	113.85	120.42
1	C	63	THR	CA-C-O	-6.20	112.08	118.90
1	C	288	GLY	N-CA-C	6.20	123.46	114.10
1	C	366	GLN	CA-C-N	-6.20	114.53	122.77
1	C	366	GLN	C-N-CA	-6.20	114.53	122.77
1	A	64	GLY	N-CA-C	6.20	122.35	111.57
1	D	409	HIS	CA-C-N	6.20	126.66	119.47
1	D	409	HIS	C-N-CA	6.20	126.66	119.47
1	C	366	GLN	CA-C-O	-6.20	113.89	120.40
1	C	86	ARG	NE-CZ-NH2	6.19	124.77	119.20
1	D	54	GLY	CA-C-N	6.19	129.08	120.29
1	D	54	GLY	C-N-CA	6.19	129.08	120.29
1	C	325	HIS	O-C-N	-6.19	115.15	123.19
2	U	115	PHE	CA-C-N	-6.19	112.57	120.98
2	U	115	PHE	C-N-CA	-6.19	112.57	120.98
1	A	280	LEU	CA-C-O	6.18	127.11	120.55
2	S	9	LYS	CA-CB-CG	6.18	126.47	114.10
2	U	48	HIS	O-C-N	6.18	132.27	122.81
1	A	153	HIS	CA-C-O	-6.18	111.67	120.51
1	B	26	THR	CA-CB-CG2	6.18	121.01	110.50
1	C	200	THR	N-CA-C	-6.18	100.36	109.81
1	C	323	GLY	N-CA-C	-6.18	98.53	113.18
1	B	20	TYR	N-CA-C	-6.18	104.46	111.07
1	A	52	GLU	N-CA-CB	6.18	119.76	110.19
1	B	131	ARG	CB-CA-C	6.18	119.44	109.07
1	D	84	CYS	N-CA-CB	6.18	119.20	110.24
2	V	2	GLN	CA-CB-CG	6.18	126.45	114.10
1	A	372	PRO	O-C-N	6.17	130.38	122.91
1	B	390	LEU	O-C-N	6.17	128.45	122.03
2	T	96	GLN	OE1-CD-NE2	6.17	128.77	122.60
1	C	334	LYS	CA-CB-CG	6.17	126.44	114.10
1	D	238	HIS	CA-C-O	-6.17	113.67	120.33
1	B	414	ALA	CA-C-N	6.16	125.65	119.24
1	B	414	ALA	C-N-CA	6.16	125.65	119.24
1	D	338	GLU	O-C-N	-6.16	115.98	123.19
1	D	13	PHE	N-CA-C	-6.16	100.72	109.96
1	B	232	THR	CA-CB-OG1	-6.16	100.36	109.60
1	C	324	ASP	CA-CB-CG	6.16	118.76	112.60
2	U	104	PHE	N-CA-C	6.16	118.68	109.25
1	D	243	THR	O-C-N	6.16	130.59	122.95
1	A	331	VAL	CA-C-N	6.16	133.05	121.97
1	A	331	VAL	C-N-CA	6.16	133.05	121.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	ALA	CA-C-O	-6.16	113.84	120.92
1	C	416	GLY	CA-C-O	6.16	126.84	120.80
1	B	332	VAL	N-CA-CB	-6.16	101.07	111.23
1	B	365	THR	CA-CB-OG1	-6.16	100.37	109.60
2	V	82	GLN	CG-CD-NE2	6.16	125.63	116.40
1	B	36	ILE	N-CA-C	-6.15	99.72	108.58
1	B	314	LEU	CB-CA-C	6.15	120.65	110.81
1	A	371	LEU	N-CA-C	-6.15	101.83	109.64
2	U	34	LEU	CB-CA-C	6.15	120.53	110.88
1	B	10	SER	N-CA-CB	6.14	120.87	110.49
1	A	20	TYR	O-C-N	6.14	128.48	122.09
1	B	26	THR	CA-CB-OG1	-6.14	100.39	109.60
1	C	24	TYR	CB-CA-C	6.14	120.94	110.56
1	C	431	ARG	CG-CD-NE	6.14	125.51	112.00
2	U	26	LEU	N-CA-CB	-6.14	101.08	110.16
1	D	220	PHE	N-CA-CB	6.14	119.35	110.20
1	D	257	ALA	CB-CA-C	6.14	120.68	110.92
1	C	129	ALA	CA-C-O	-6.14	111.74	120.51
2	U	49	GLY	CA-C-N	-6.14	112.27	122.21
2	U	49	GLY	C-N-CA	-6.14	112.27	122.21
1	C	360	ARG	NH1-CZ-NH2	6.13	127.28	119.30
2	T	106	ASN	N-CA-C	6.13	120.31	112.34
1	B	174	ILE	O-C-N	6.13	129.13	122.63
1	C	465	ILE	CB-CA-C	-6.13	102.50	110.84
1	D	167	ARG	O-C-N	6.13	128.37	121.32
1	D	197	LEU	N-CA-C	-6.13	100.58	110.32
2	S	107	VAL	CB-CA-C	-6.13	104.03	112.24
2	S	43	GLU	CG-CD-OE2	6.12	132.49	118.40
1	C	180	LEU	CA-C-O	-6.12	114.01	121.36
1	C	117	PHE	N-CA-CB	6.12	119.65	110.22
1	C	421	ARG	CA-C-O	6.12	127.25	120.82
1	D	406	THR	CA-CB-CG2	6.12	120.91	110.50
1	B	314	LEU	CA-C-N	6.12	128.48	120.28
1	B	314	LEU	C-N-CA	6.12	128.48	120.28
1	D	204	GLU	CG-CD-OE2	-6.12	104.33	118.40
1	D	350	ARG	NE-CZ-NH1	6.12	127.62	121.50
1	A	421	ARG	NE-CZ-NH1	-6.12	115.39	121.50
1	B	233	GLY	N-CA-C	-6.12	106.27	115.32
1	C	428	VAL	CB-CA-C	6.12	120.40	112.14
1	A	396	ASP	CA-CB-CG	6.11	118.71	112.60
1	B	216	ASP	N-CA-C	-6.11	104.70	111.36
1	C	17	VAL	CA-C-N	6.11	132.33	121.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	17	VAL	C-N-CA	6.11	132.33	121.75
2	S	73	PRO	N-CA-C	-6.11	101.58	110.80
2	U	51	VAL	CA-C-O	6.11	128.41	120.78
1	A	443	GLU	N-CA-CB	6.11	119.17	110.13
1	C	177	LYS	CA-C-O	-6.10	111.78	120.51
2	S	49	GLY	CA-C-O	-6.10	109.95	120.57
1	A	264	ILE	N-CA-CB	-6.10	100.03	111.62
1	A	338	GLU	CB-CG-CD	6.09	122.95	112.60
2	T	74	MET	CB-CA-C	6.09	121.58	111.83
1	C	243	THR	CB-CA-C	-6.09	100.15	109.89
1	D	224	ALA	O-C-N	6.09	128.34	122.07
2	V	115	PHE	CA-C-O	-6.09	113.25	120.43
1	D	104	PRO	O-C-N	6.09	130.56	123.01
1	D	244	ALA	O-C-N	-6.09	113.06	122.61
1	C	278	THR	OG1-CB-CG2	6.08	121.47	109.30
2	S	93	ALA	CA-C-O	-6.08	111.81	120.51
1	B	363	TYR	N-CA-C	6.08	119.96	112.54
1	A	412	GLY	CA-C-N	6.08	129.24	120.79
1	A	412	GLY	C-N-CA	6.08	129.24	120.79
2	S	51	VAL	CA-C-O	-6.08	115.50	121.58
1	C	48	VAL	CA-C-O	6.08	123.87	119.25
1	D	347	ASP	O-C-N	6.08	130.47	122.33
1	A	97	TYR	N-CA-C	6.08	118.65	109.41
1	C	148	PHE	CA-C-O	-6.08	114.35	121.46
2	T	8	ASN	CA-CB-CG	6.08	118.68	112.60
1	C	253	ARG	NE-CZ-NH2	-6.08	113.73	119.20
1	D	289	LEU	N-CA-CB	-6.07	100.74	110.46
2	U	3	VAL	O-C-N	6.07	130.16	122.57
1	D	259	GLU	CB-CG-CD	6.07	122.92	112.60
2	V	63	ASP	N-CA-C	-6.07	101.53	110.52
1	B	394	PHE	N-CA-C	6.07	120.96	113.50
1	D	430	ALA	CA-C-O	6.07	127.19	120.82
1	B	109	GLU	N-CA-C	-6.06	100.86	109.96
1	C	281	ALA	N-CA-CB	6.06	119.03	110.12
1	D	13	PHE	O-C-N	6.06	130.39	122.93
1	D	358	ARG	NE-CZ-NH1	-6.06	115.44	121.50
1	C	23	THR	CA-C-N	-6.06	112.95	122.65
1	C	23	THR	C-N-CA	-6.06	112.95	122.65
1	D	115	ASN	CA-CB-CG	-6.06	106.54	112.60
2	S	38	TRP	CB-CG-CD2	-6.05	118.33	126.80
1	A	204	GLU	CG-CD-OE2	-6.05	104.49	118.40
2	S	88	GLY	CA-C-O	6.05	127.53	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	204	GLU	CA-C-N	-6.05	113.06	122.67
1	C	204	GLU	C-N-CA	-6.05	113.06	122.67
1	C	270	LEU	O-C-N	6.04	130.09	122.23
1	A	101	VAL	O-C-N	6.04	129.37	123.03
1	C	127	PHE	CA-C-O	-6.04	114.55	121.19
2	S	82	GLN	CA-CB-CG	6.04	126.18	114.10
1	C	249	GLU	N-CA-CB	6.04	118.77	110.01
1	D	68	THR	CA-CB-OG1	-6.04	100.54	109.60
1	A	404	GLY	N-CA-C	-6.04	105.46	112.83
1	A	405	GLY	CA-C-N	6.04	129.62	122.44
1	A	405	GLY	C-N-CA	6.04	129.62	122.44
1	C	401	GLN	N-CA-CB	-6.04	101.09	110.57
1	B	194	ARG	CA-C-O	6.04	126.79	119.49
1	B	413	ASN	CA-C-O	-6.04	114.43	121.07
1	C	461	VAL	N-CA-C	6.04	116.21	110.42
1	D	44	PRO	CA-C-O	6.03	131.58	120.60
1	B	401	GLN	CB-CG-CD	6.03	122.86	112.60
2	S	65	ARG	CD-NE-CZ	-6.03	115.96	124.40
1	C	187	ARG	O-C-N	6.03	128.30	122.03
1	C	134	ARG	CA-C-O	6.03	127.49	120.14
2	T	100	ARG	CB-CG-CD	6.02	125.16	111.30
1	C	32	LYS	N-CA-CB	6.02	120.45	110.63
1	D	387	MET	CA-CB-CG	-6.02	102.06	114.10
1	B	29	TYR	CA-C-O	6.02	126.97	120.95
1	A	152	PRO	N-CA-C	-6.02	104.78	113.75
1	A	307	HIS	CB-CA-C	-6.02	99.57	109.80
1	D	90	VAL	O-C-N	6.02	129.24	122.68
1	C	334	LYS	N-CA-C	6.02	118.63	111.71
1	C	319	ARG	N-CA-C	-6.01	105.65	112.87
1	D	121	VAL	CA-C-O	6.01	125.44	119.97
1	D	52	GLU	N-CA-CB	6.01	120.43	110.33
1	A	145	VAL	CA-C-O	-6.01	114.80	121.17
2	T	104	PHE	N-CA-C	6.01	119.43	109.46
1	B	261	GLY	O-C-N	-6.00	114.81	122.43
2	T	38	TRP	O-C-N	6.00	130.09	123.01
1	D	325	HIS	CA-CB-CG	6.00	119.80	113.80
1	D	446	ARG	NE-CZ-NH1	-6.00	115.50	121.50
1	A	227	LYS	CA-C-N	6.00	128.81	120.29
1	A	227	LYS	C-N-CA	6.00	128.81	120.29
1	C	68	THR	CB-CA-C	6.00	119.65	109.75
1	D	134	ARG	NE-CZ-NH1	-6.00	115.50	121.50
1	A	26	THR	CA-CB-CG2	5.99	120.69	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	348	LEU	N-CA-C	-5.99	104.87	111.82
2	V	98	TRP	CA-C-N	-5.99	113.16	122.69
2	V	98	TRP	C-N-CA	-5.99	113.16	122.69
2	S	104	PHE	CB-CA-C	-5.99	100.08	109.84
1	C	244	ALA	CA-C-O	-5.99	115.01	121.36
1	A	316	LYS	CA-C-N	5.99	128.58	120.38
1	A	316	LYS	C-N-CA	5.99	128.58	120.38
1	C	391	THR	N-CA-CB	5.99	118.86	109.94
1	A	218	PHE	CA-C-N	5.99	128.58	120.44
1	A	218	PHE	C-N-CA	5.99	128.58	120.44
2	V	114	SER	N-CA-C	-5.99	99.42	108.46
1	D	263	PRO	CA-C-N	-5.98	113.61	122.23
1	D	263	PRO	C-N-CA	-5.98	113.61	122.23
1	C	283	TYR	CA-CB-CG	-5.98	103.13	113.90
1	A	269	TYR	CA-C-O	-5.98	113.34	120.10
1	C	79	ARG	CG-CD-NE	5.98	125.16	112.00
1	A	224	ALA	CA-C-O	-5.98	114.55	120.82
1	A	45	GLN	N-CA-C	-5.97	102.25	109.72
1	A	469	PHE	O-C-N	5.97	130.23	123.42
1	C	300	VAL	O-C-N	5.97	128.55	121.80
1	A	356	GLN	OE1-CD-NE2	5.97	128.57	122.60
1	B	89	ARG	N-CA-CB	5.97	120.14	110.41
1	B	204	GLU	CG-CD-OE2	-5.97	104.66	118.40
1	D	312	ARG	N-CA-C	-5.97	103.95	111.11
1	A	298	HIS	CA-CB-CG	5.97	119.77	113.80
1	B	213	ARG	CD-NE-CZ	-5.97	116.05	124.40
2	U	26	LEU	CB-CA-C	5.97	120.99	110.85
1	A	133	LEU	CA-C-O	-5.96	113.44	120.60
1	C	86	ARG	N-CA-CB	5.96	120.57	110.49
1	A	315	ALA	CA-C-N	5.96	128.19	120.44
1	A	315	ALA	C-N-CA	5.96	128.19	120.44
1	B	63	THR	CA-C-N	-5.96	116.25	122.69
1	B	63	THR	C-N-CA	-5.96	116.25	122.69
1	B	264	ILE	CA-C-O	-5.96	115.05	121.19
2	V	119	LYS	O-C-N	5.96	128.42	121.21
1	B	430	ALA	N-CA-C	-5.96	104.69	111.07
1	D	189	VAL	CA-CB-CG1	5.96	120.53	110.40
1	A	99	ALA	N-CA-C	-5.96	99.96	109.96
1	C	281	ALA	CB-CA-C	-5.96	100.90	110.79
1	B	459	CYS	CB-CA-C	-5.95	101.29	110.81
2	U	65	ARG	CB-CG-CD	-5.95	97.61	111.30
1	D	156	GLN	CG-CD-NE2	-5.95	107.47	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	15	ALA	N-CA-C	5.95	117.97	110.24
1	B	405	GLY	CA-C-N	5.95	131.32	122.17
1	B	405	GLY	C-N-CA	5.95	131.32	122.17
2	T	32	TYR	CA-C-O	5.95	127.06	120.82
1	B	238	HIS	CA-CB-CG	-5.94	107.86	113.80
1	B	86	ARG	NE-CZ-NH1	-5.94	115.56	121.50
1	C	51	GLU	CB-CG-CD	5.94	122.70	112.60
1	D	393	ILE	CB-CA-C	-5.94	104.37	111.97
2	V	96	GLN	CB-CG-CD	5.94	122.70	112.60
1	B	158	GLU	N-CA-C	-5.94	104.72	111.07
1	C	302	ASP	CA-C-O	-5.94	112.61	119.56
1	A	252	LYS	CG-CD-CE	5.94	124.95	111.30
1	B	283	TYR	CB-CG-CD1	5.93	129.70	120.80
1	D	278	THR	O-C-N	5.93	128.41	122.12
1	D	370	SER	CA-C-O	-5.93	113.46	120.81
2	S	87	VAL	CA-C-N	5.93	126.52	119.94
2	S	87	VAL	C-N-CA	5.93	126.52	119.94
1	D	18	LYS	CA-C-O	-5.93	114.37	120.89
1	D	424	LEU	CA-C-O	-5.93	114.59	120.70
1	D	427	CYS	O-C-N	5.93	128.40	122.12
1	A	163	ASN	CB-CA-C	-5.92	103.92	111.86
1	B	251	ILE	O-C-N	5.92	127.93	121.83
1	A	81	LYS	O-C-N	5.92	130.19	122.97
1	D	332	VAL	N-CA-C	5.92	121.65	109.34
1	D	193	LEU	N-CA-C	5.92	117.40	111.07
1	D	391	THR	O-C-N	5.92	128.25	122.09
1	A	143	ALA	O-C-N	5.92	130.36	122.43
1	B	338	GLU	CA-C-N	5.92	130.60	121.19
1	B	338	GLU	C-N-CA	5.92	130.60	121.19
1	D	249	GLU	CA-C-O	-5.92	114.61	120.70
1	B	63	THR	CA-CB-OG1	-5.92	100.73	109.60
1	B	113	VAL	N-CA-C	-5.92	103.88	110.62
1	B	464	GLU	N-CA-C	5.92	120.23	113.19
1	A	391	THR	N-CA-CB	5.91	118.75	109.94
1	D	293	ILE	CA-C-O	-5.91	113.98	120.84
1	D	79	ARG	CB-CA-C	-5.91	100.80	110.85
1	A	303	ARG	CA-C-N	5.91	129.15	120.82
1	A	303	ARG	C-N-CA	5.91	129.15	120.82
1	D	154	GLY	CA-C-O	5.90	127.88	122.39
1	D	468	ASN	N-CA-CB	5.90	119.09	109.95
2	V	89	GLU	CB-CG-CD	5.90	122.63	112.60
1	A	413	ASN	OD1-CG-ND2	-5.90	116.70	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	75	PHE	CA-CB-CG	5.90	119.70	113.80
1	C	293	ILE	CA-C-O	-5.90	114.00	120.84
1	C	149	GLN	CB-CG-CD	5.90	122.62	112.60
1	A	183	LYS	N-CA-C	5.89	117.70	111.28
1	A	29	TYR	N-CA-C	5.89	119.02	110.42
1	B	467	PHE	CA-C-N	-5.89	113.89	122.19
1	B	467	PHE	C-N-CA	-5.89	113.89	122.19
1	A	221	CYS	O-C-N	-5.89	115.88	122.12
1	C	316	LYS	CA-C-N	5.89	128.45	120.38
1	C	316	LYS	C-N-CA	5.89	128.45	120.38
1	A	333	GLY	CA-C-N	5.89	128.76	120.28
1	A	333	GLY	C-N-CA	5.89	128.76	120.28
1	A	338	GLU	CA-C-N	5.89	129.65	120.82
1	A	338	GLU	C-N-CA	5.89	129.65	120.82
1	A	57	VAL	N-CA-CB	5.88	117.44	110.55
1	C	229	GLN	OE1-CD-NE2	5.88	128.48	122.60
1	D	274	PHE	CA-C-O	-5.88	114.31	120.55
1	C	306	ASN	CA-C-O	-5.88	112.68	118.97
1	A	149	GLN	CA-C-O	-5.88	113.72	120.24
1	A	189	VAL	CA-C-N	5.88	128.43	120.38
1	A	189	VAL	C-N-CA	5.88	128.43	120.38
1	C	461	VAL	CB-CA-C	-5.88	104.45	111.97
1	D	153	HIS	N-CA-C	5.88	121.00	113.18
1	B	28	GLU	O-C-N	5.88	128.44	122.09
1	B	43	THR	CA-C-O	-5.88	113.64	120.34
1	D	310	HIS	CA-C-O	-5.88	115.16	121.56
1	D	431	ARG	O-C-N	5.88	128.37	122.08
1	C	45	GLN	CA-C-N	5.87	127.18	119.84
1	C	45	GLN	C-N-CA	5.87	127.18	119.84
1	D	207	ASN	CB-CG-ND2	5.87	125.21	116.40
1	B	303	ARG	CG-CD-NE	-5.87	99.08	112.00
1	C	335	LEU	CA-C-N	5.87	129.45	120.82
1	C	335	LEU	C-N-CA	5.87	129.45	120.82
1	D	162	LEU	N-CA-C	-5.87	106.08	113.18
1	D	253	ARG	O-C-N	5.87	129.27	122.17
1	C	364	PHE	CA-C-O	5.87	127.87	121.06
1	C	60	GLU	CG-CD-OE1	-5.87	104.91	118.40
1	D	256	PHE	CA-CB-CG	-5.87	107.93	113.80
1	C	413	ASN	CA-C-O	-5.86	114.16	121.02
2	U	122	GLY	CA-C-N	5.86	132.26	121.70
2	U	122	GLY	C-N-CA	5.86	132.26	121.70
1	D	139	ARG	CA-C-N	-5.86	118.61	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	139	ARG	C-N-CA	-5.86	118.61	122.60
1	A	207	ASN	CA-C-O	-5.86	112.13	120.51
1	B	93	GLU	CB-CG-CD	5.86	122.56	112.60
1	D	232	THR	OG1-CB-CG2	5.86	121.02	109.30
1	C	371	LEU	N-CA-CB	-5.86	100.78	109.98
1	C	258	ARG	CB-CG-CD	5.86	124.77	111.30
1	A	181	SER	O-C-N	-5.85	116.39	122.94
1	A	468	ASN	N-CA-CB	5.85	119.81	110.16
2	T	51	VAL	O-C-N	5.85	129.88	122.57
1	D	470	ALA	CA-C-N	5.85	129.59	120.75
1	D	470	ALA	C-N-CA	5.85	129.59	120.75
1	B	183	LYS	CA-CB-CG	-5.85	102.40	114.10
1	B	186	GLY	CA-C-N	5.85	128.92	120.79
1	B	186	GLY	C-N-CA	5.85	128.92	120.79
1	D	285	ARG	NE-CZ-NH1	-5.85	115.65	121.50
1	D	330	THR	N-CA-CB	5.85	118.95	110.88
1	D	10	SER	N-CA-CB	5.85	120.37	110.49
1	D	387	MET	CA-C-N	5.84	125.71	119.28
1	D	387	MET	C-N-CA	5.84	125.71	119.28
1	B	359	SER	CA-CB-OG	5.84	122.78	111.10
1	C	128	LYS	O-C-N	-5.84	116.06	122.07
1	C	362	ILE	N-CA-CB	-5.84	105.01	111.66
1	C	365	THR	N-CA-C	-5.84	100.98	110.20
1	A	266	MET	N-CA-CB	-5.83	101.92	111.66
1	B	173	THR	CA-CB-CG2	5.83	120.42	110.50
1	C	209	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	D	137	ASP	O-C-N	-5.83	117.69	123.46
1	D	120	ILE	CA-CB-CG1	-5.83	100.49	110.40
2	V	13	GLU	CG-CD-OE2	-5.83	104.99	118.40
2	T	53	ARG	NE-CZ-NH1	-5.83	115.67	121.50
1	D	170	LEU	CA-C-O	-5.83	114.53	120.71
1	A	36	ILE	N-CA-C	-5.83	100.02	108.87
1	A	355	GLU	N-CA-CB	-5.83	101.41	109.97
1	B	366	GLN	O-C-N	5.83	130.03	123.27
1	C	303	ARG	CG-CD-NE	-5.83	99.18	112.00
1	D	296	ALA	O-C-N	-5.83	114.84	122.59
1	D	371	LEU	CA-C-N	5.83	126.15	119.92
1	D	371	LEU	C-N-CA	5.83	126.15	119.92
1	D	433	GLU	CB-CG-CD	5.83	122.50	112.60
2	U	32	TYR	O-C-N	5.82	128.29	122.12
1	D	249	GLU	N-CA-CB	5.82	118.52	110.07
1	D	341	ILE	CA-C-O	-5.82	115.00	121.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	LEU	N-CA-CB	-5.82	101.60	110.33
1	A	201	LYS	N-CA-C	5.82	117.70	108.79
1	A	310	HIS	CA-C-O	-5.82	114.38	121.36
2	T	63	ASP	N-CA-C	-5.82	101.91	110.52
2	T	110	VAL	N-CA-C	-5.82	99.37	108.86
1	D	117	PHE	CA-CB-CG	5.82	119.62	113.80
2	S	7	ILE	O-C-N	5.82	126.46	121.98
1	B	78	ASP	N-CA-C	-5.82	105.07	111.82
1	B	223	GLU	N-CA-CB	5.82	118.60	109.94
1	C	78	ASP	CA-CB-CG	5.82	118.42	112.60
1	B	192	CYS	N-CA-CB	5.81	118.44	110.01
1	D	99	ALA	N-CA-C	-5.81	100.19	109.96
1	C	79	ARG	CB-CA-C	-5.81	100.06	110.70
1	A	87	ILE	CA-C-O	-5.81	114.89	121.75
1	A	204	GLU	CA-C-O	-5.81	113.69	120.20
2	S	121	GLU	CB-CA-C	-5.81	101.98	110.06
2	T	92	LYS	CG-CD-CE	5.81	124.66	111.30
1	C	339	ARG	NH1-CZ-NH2	5.81	126.85	119.30
1	B	183	LYS	N-CA-C	5.81	117.61	111.28
1	B	291	LEU	N-CA-CB	-5.81	101.59	110.65
1	A	88	GLU	CA-CB-CG	5.80	125.70	114.10
1	A	383	HIS	CA-C-N	5.80	132.41	121.97
1	A	383	HIS	C-N-CA	5.80	132.41	121.97
1	D	51	GLU	CA-CB-CG	5.80	125.70	114.10
1	A	268	ASP	CA-CB-CG	5.79	118.39	112.60
1	C	28	GLU	CB-CA-C	-5.79	101.00	110.85
1	C	106	ASP	CA-C-O	-5.79	112.23	120.51
1	D	110	GLU	CG-CD-OE2	5.79	131.72	118.40
1	C	442	ASN	N-CA-C	5.79	123.13	110.80
1	A	374	VAL	N-CA-CB	-5.79	103.38	111.25
1	B	49	PRO	O-C-N	5.79	128.29	121.46
2	S	116	ILE	CB-CA-C	5.79	118.67	111.15
1	D	112	SER	CA-CB-OG	5.78	122.67	111.10
2	T	45	GLU	O-C-N	5.78	130.17	123.41
1	C	131	ARG	CB-CA-C	5.78	118.73	109.02
2	U	113	ILE	O-C-N	5.78	128.68	122.67
2	V	33	LEU	CB-CA-C	5.78	120.06	110.81
1	C	72	ASP	OD1-CG-OD2	-5.78	109.03	122.90
1	C	198	ASP	CA-C-N	5.78	132.31	122.37
1	C	198	ASP	C-N-CA	5.78	132.31	122.37
1	A	334	LYS	CA-CB-CG	5.78	125.66	114.10
1	C	205	ASN	CB-CA-C	5.78	120.32	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	108	ARG	NE-CZ-NH1	-5.78	115.72	121.50
1	D	79	ARG	CA-CB-CG	5.78	125.65	114.10
1	A	444	ILE	CA-C-O	-5.77	115.41	121.41
1	A	333	GLY	CA-C-O	-5.77	110.52	120.57
1	B	118	THR	N-CA-CB	5.77	118.61	110.12
1	C	241	ASN	CA-C-O	5.77	127.28	120.58
1	C	249	GLU	O-C-N	5.77	128.02	122.07
2	U	119	LYS	O-C-N	5.77	128.19	121.21
1	D	428	VAL	CA-C-O	-5.77	114.95	120.95
1	A	134	ARG	CD-NE-CZ	-5.77	116.32	124.40
1	A	79	ARG	NE-CZ-NH1	-5.76	115.73	121.50
2	U	8	ASN	OD1-CG-ND2	-5.76	116.84	122.60
1	B	301	ILE	O-C-N	5.76	129.77	122.57
1	C	469	PHE	N-CA-CB	5.76	121.19	110.99
2	U	108	ARG	O-C-N	5.76	129.44	122.35
2	T	48	HIS	O-C-N	5.76	131.62	122.81
1	C	435	ARG	CA-C-O	-5.76	115.97	122.01
1	A	193	LEU	CA-C-N	5.76	129.81	120.60
1	A	193	LEU	C-N-CA	5.76	129.81	120.60
1	C	253	ARG	N-CA-C	-5.76	104.61	111.69
1	C	42	VAL	N-CA-C	5.75	118.21	109.12
1	D	190	TYR	O-C-N	5.75	128.07	122.09
1	A	285	ARG	CG-CD-NE	-5.75	99.36	112.00
1	A	290	LEU	CA-C-O	-5.75	114.46	121.36
1	D	356	GLN	CA-C-O	-5.75	114.70	120.96
1	C	13	PHE	O-C-N	5.75	130.20	122.96
1	C	141	PRO	CB-CA-C	-5.75	105.77	111.17
1	D	214	TRP	O-C-N	5.75	128.21	122.12
1	C	328	SER	CA-C-O	-5.74	112.73	119.05
1	C	410	PRO	CA-C-N	-5.74	113.54	122.67
1	C	410	PRO	C-N-CA	-5.74	113.54	122.67
1	B	152	PRO	O-C-N	5.74	128.38	122.18
1	B	362	ILE	O-C-N	5.74	128.73	122.36
1	D	109	GLU	CB-CG-CD	5.74	122.36	112.60
2	V	30	VAL	CA-C-O	5.74	126.90	120.64
2	S	24	GLU	N-CA-C	-5.74	104.66	111.03
2	T	120	PRO	N-CA-C	-5.74	101.16	110.40
2	T	73	PRO	CB-CA-C	5.74	118.87	111.64
1	C	168	PRO	N-CD-CG	-5.74	94.60	103.20
1	D	86	ARG	NE-CZ-NH1	-5.74	115.76	121.50
1	D	115	ASN	CB-CG-OD1	5.73	132.27	120.80
1	D	419	ALA	CA-C-N	5.73	127.96	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	419	ALA	C-N-CA	5.73	127.96	120.28
1	A	67	THR	O-C-N	5.73	129.63	122.92
1	A	74	LEU	O-C-N	5.73	129.68	122.23
2	S	110	VAL	CA-CB-CG1	5.73	120.14	110.40
1	B	50	PRO	N-CA-C	-5.73	105.56	113.53
1	D	77	LEU	CA-C-O	-5.73	112.33	119.38
2	T	87	VAL	O-C-N	5.73	127.43	121.87
1	B	204	GLU	CG-CD-OE1	5.73	131.57	118.40
2	T	93	ALA	CA-C-O	-5.73	112.32	120.51
1	C	178	LEU	O-C-N	-5.73	115.44	123.11
1	D	224	ALA	CA-C-O	-5.73	114.81	120.82
1	B	198	ASP	CA-C-N	5.73	131.74	122.29
1	B	198	ASP	C-N-CA	5.73	131.74	122.29
2	S	20	ASP	CA-CB-CG	-5.72	106.88	112.60
2	T	120	PRO	O-C-N	5.72	130.04	122.89
1	D	273	GLY	CA-C-O	5.72	125.94	122.22
1	A	286	ASP	O-C-N	5.72	130.09	122.43
1	A	432	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	B	197	LEU	CA-C-N	5.72	130.35	120.58
1	B	197	LEU	C-N-CA	5.72	130.35	120.58
2	V	99	ILE	CA-C-N	-5.71	112.95	122.21
2	V	99	ILE	C-N-CA	-5.71	112.95	122.21
2	V	101	ILE	CA-C-O	-5.71	114.30	120.36
1	B	356	GLN	CA-C-O	-5.71	114.74	120.96
1	B	245	GLY	CA-C-O	-5.71	113.98	120.09
1	B	271	THR	CA-C-N	5.71	126.16	119.94
1	B	271	THR	C-N-CA	5.71	126.16	119.94
1	C	356	GLN	CA-C-O	-5.71	114.42	120.92
1	C	410	PRO	O-C-N	5.71	129.07	122.17
2	U	84	LEU	O-C-N	5.70	128.16	122.12
1	D	89	ARG	O-C-N	5.70	129.41	122.96
2	U	111	GLN	O-C-N	5.70	130.03	123.02
2	T	49	GLY	O-C-N	5.70	128.06	122.19
2	T	69	MET	CA-C-O	-5.70	114.25	120.81
1	C	192	CYS	CA-CB-SG	-5.70	101.30	114.40
1	B	28	GLU	CB-CA-C	-5.70	101.90	110.90
1	A	283	TYR	CA-CB-CG	-5.70	103.65	113.90
2	U	64	GLY	CA-C-O	-5.70	112.69	119.01
1	D	213	ARG	NH1-CZ-NH2	-5.70	111.90	119.30
1	C	48	VAL	N-CA-C	5.69	113.19	107.55
2	V	31	GLU	CA-C-N	5.69	127.91	120.28
2	V	31	GLU	C-N-CA	5.69	127.91	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	ALA	CA-C-N	5.69	127.82	120.70
1	A	188	ALA	C-N-CA	5.69	127.82	120.70
1	C	415	PRO	O-C-N	5.69	128.33	122.18
1	D	358	ARG	CA-CB-CG	-5.69	102.72	114.10
1	A	300	VAL	N-CA-C	-5.69	103.98	111.09
2	U	30	VAL	CA-C-O	5.69	126.84	120.64
1	A	32	LYS	N-CA-CB	5.69	119.68	110.41
2	T	50	PHE	CA-CB-CG	5.69	119.49	113.80
1	A	193	LEU	CA-CB-CG	5.69	136.21	116.30
1	A	465	ILE	CB-CA-C	-5.69	103.86	110.91
2	S	43	GLU	CA-CB-CG	5.69	125.48	114.10
1	C	367	ASP	O-C-N	-5.69	116.74	123.22
1	B	68	THR	CA-C-N	-5.69	116.14	123.19
1	B	68	THR	C-N-CA	-5.69	116.14	123.19
1	A	83	ARG	CD-NE-CZ	5.68	132.35	124.40
1	A	123	ASN	N-CA-C	5.68	120.87	113.88
1	D	29	TYR	O-C-N	5.68	129.47	123.11
1	D	226	TYR	O-C-N	5.68	128.63	122.15
1	A	394	PHE	CA-CB-CG	-5.68	108.12	113.80
1	B	255	VAL	O-C-N	-5.68	116.36	121.87
2	U	57	LYS	O-C-N	5.68	129.87	122.15
2	U	60	GLY	O-C-N	-5.68	115.13	122.34
1	C	134	ARG	CD-NE-CZ	-5.67	116.46	124.40
1	C	93	GLU	CB-CG-CD	5.67	122.23	112.60
1	D	412	GLY	O-C-N	-5.67	116.16	122.68
2	V	45	GLU	O-C-N	5.67	130.27	123.36
1	A	184	ASN	N-CA-C	-5.67	105.25	111.82
1	B	86	ARG	CA-C-O	5.67	128.61	120.51
1	B	22	LEU	N-CA-C	5.66	118.22	111.71
1	D	366	GLN	CA-C-N	-5.66	115.12	123.05
1	D	366	GLN	C-N-CA	-5.66	115.12	123.05
1	B	241	ASN	O-C-N	-5.66	116.06	123.02
1	D	326	ILE	O-C-N	5.66	129.66	123.09
1	D	93	GLU	CA-C-O	5.66	126.70	120.31
1	B	412	GLY	CA-C-N	5.66	128.65	120.79
1	B	412	GLY	C-N-CA	5.66	128.65	120.79
1	A	50	PRO	O-C-N	5.66	128.56	122.17
1	A	163	ASN	O-C-N	5.66	129.37	122.58
1	C	338	GLU	O-C-N	-5.66	116.57	123.19
1	D	158	GLU	CG-CD-OE2	5.66	131.41	118.40
2	S	33	LEU	CB-CA-C	5.65	119.91	110.92
2	V	87	VAL	O-C-N	5.65	127.59	121.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	64	GLY	O-C-N	-5.65	115.84	122.45
1	C	80	TYR	CA-C-O	-5.65	112.94	119.78
2	S	93	ALA	O-C-N	5.65	130.10	122.59
1	D	115	ASN	N-CA-CB	5.65	118.16	109.91
1	D	119	SER	N-CA-CB	5.65	118.12	110.10
1	D	456	ALA	O-C-N	5.65	128.12	122.08
1	A	35	ASP	CB-CA-C	-5.64	99.08	109.46
1	A	251	ILE	CA-C-O	5.64	126.82	120.95
1	B	209	GLN	CA-CB-CG	5.64	125.39	114.10
2	U	121	GLU	CB-CA-C	-5.64	102.03	110.16
1	B	297	MET	CA-C-O	-5.64	112.44	120.51
1	D	69	VAL	N-CA-CB	-5.64	103.58	111.25
1	D	231	GLU	CA-C-O	-5.64	115.07	121.00
2	S	58	SER	CA-C-O	5.64	127.67	121.01
1	D	191	GLU	CB-CA-C	5.64	119.74	110.88
2	V	108	ARG	NE-CZ-NH2	5.64	124.28	119.20
2	U	105	ASP	CB-CG-OD1	5.64	131.37	118.40
2	S	86	GLU	O-C-N	5.63	127.95	122.09
1	B	273	GLY	O-C-N	-5.63	117.91	122.64
2	V	101	ILE	O-C-N	5.63	129.28	123.20
1	A	213	ARG	CD-NE-CZ	5.63	132.28	124.40
1	D	184	ASN	N-CA-C	-5.63	105.22	111.36
2	T	29	GLU	CA-C-O	-5.63	115.10	120.90
1	D	209	GLN	O-C-N	5.63	126.11	121.32
1	D	449	CYS	N-CA-C	-5.63	105.14	111.28
2	V	92	LYS	CB-CG-CD	5.63	124.25	111.30
1	D	312	ARG	CD-NE-CZ	-5.63	116.52	124.40
1	B	19	GLU	N-CA-CB	5.62	118.27	110.17
1	A	347	ASP	N-CA-C	-5.62	105.23	111.36
1	B	155	ILE	O-C-N	5.62	129.60	122.57
1	C	172	CYS	N-CA-CB	-5.62	101.06	111.13
2	V	2	GLN	OE1-CD-NE2	5.62	128.22	122.60
1	A	308	GLY	CA-C-N	-5.62	113.22	122.67
1	A	308	GLY	C-N-CA	-5.62	113.22	122.67
2	T	39	VAL	O-C-N	5.62	125.54	121.55
2	T	109	GLN	CB-CG-CD	5.62	122.15	112.60
1	A	196	GLY	O-C-N	-5.62	115.40	122.70
1	D	26	THR	N-CA-CB	-5.62	102.12	110.99
1	A	109	GLU	CB-CG-CD	5.61	122.14	112.60
1	C	18	LYS	CA-C-O	-5.61	115.27	121.33
1	C	233	GLY	O-C-N	5.61	129.28	122.32
1	C	296	ALA	CA-C-N	5.61	132.26	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	296	ALA	C-N-CA	5.61	132.26	121.54
2	V	49	GLY	CA-C-N	-5.61	113.12	122.21
2	V	49	GLY	C-N-CA	-5.61	113.12	122.21
1	A	97	TYR	CA-C-O	5.61	128.09	121.58
1	B	145	VAL	CA-C-O	-5.61	115.22	121.17
2	V	121	GLU	CA-CB-CG	5.61	125.32	114.10
1	C	338	GLU	CA-C-N	5.61	129.23	120.82
1	C	338	GLU	C-N-CA	5.61	129.23	120.82
1	C	360	ARG	N-CA-C	5.61	119.66	113.21
1	B	311	PHE	CA-C-O	-5.61	114.58	120.63
1	D	461	VAL	CA-C-N	-5.61	113.68	122.65
1	D	461	VAL	C-N-CA	-5.61	113.68	122.65
1	C	424	LEU	O-C-N	5.60	128.14	122.09
1	D	36	ILE	N-CA-CB	5.60	116.83	110.72
1	C	330	THR	CB-CA-C	-5.60	100.39	109.13
1	D	173	THR	CA-CB-CG2	5.60	120.02	110.50
1	C	466	VAL	O-C-N	5.59	129.29	122.58
1	B	236	LYS	CG-CD-CE	5.59	124.17	111.30
2	U	8	ASN	N-CA-C	-5.59	101.88	109.54
1	D	286	ASP	O-C-N	5.59	129.92	122.43
1	A	118	THR	N-CA-CB	5.59	118.44	110.06
1	A	302	ASP	CA-C-O	-5.59	113.02	119.56
1	B	365	THR	CA-C-O	-5.59	114.90	121.16
1	A	431	ARG	CD-NE-CZ	-5.59	116.58	124.40
1	B	392	GLU	CA-CB-CG	5.59	125.27	114.10
2	U	89	GLU	CB-CG-CD	5.59	122.10	112.60
2	V	14	THR	CA-CB-OG1	-5.59	101.22	109.60
1	B	342	THR	CA-CB-OG1	-5.58	101.22	109.60
2	U	116	ILE	CB-CA-C	5.58	119.65	111.33
1	B	328	SER	CA-C-O	-5.58	112.68	119.32
2	T	2	GLN	N-CA-CB	5.58	121.12	111.13
1	C	108	PHE	O-C-N	5.58	130.49	123.23
1	C	443	GLU	O-C-N	5.58	128.93	122.17
2	U	47	GLU	N-CA-C	5.58	122.69	110.80
1	A	110	GLU	CG-CD-OE2	5.58	131.23	118.40
1	A	267	HIS	O-C-N	-5.58	117.12	123.48
1	A	278	THR	CA-C-N	5.58	127.76	120.28
1	A	278	THR	C-N-CA	5.58	127.76	120.28
1	A	68	THR	CB-CA-C	5.58	118.95	109.75
1	B	68	THR	CB-CA-C	5.58	118.95	109.75
1	D	200	THR	N-CA-C	-5.58	101.28	109.81
1	A	197	LEU	N-CA-C	-5.57	102.64	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	7	ILE	N-CA-CB	5.57	116.21	111.64
1	C	83	ARG	NE-CZ-NH1	-5.57	115.93	121.50
1	C	123	ASN	CA-C-N	5.57	129.28	120.47
1	C	123	ASN	C-N-CA	5.57	129.28	120.47
1	C	187	ARG	CD-NE-CZ	5.57	132.20	124.40
1	A	223	GLU	CB-CG-CD	5.57	122.07	112.60
1	C	68	THR	CA-CB-OG1	-5.57	101.25	109.60
1	C	377	VAL	CA-C-O	5.57	126.24	120.39
1	A	384	VAL	CB-CA-C	5.57	120.42	111.29
1	C	407	LEU	CA-C-N	5.57	132.32	121.41
1	C	407	LEU	C-N-CA	5.57	132.32	121.41
1	A	80	TYR	CA-C-N	5.57	128.75	120.90
1	A	80	TYR	C-N-CA	5.57	128.75	120.90
1	A	112	SER	O-C-N	-5.57	115.84	122.63
1	B	366	GLN	CA-C-N	-5.57	115.26	123.05
1	B	366	GLN	C-N-CA	-5.57	115.26	123.05
1	C	430	ALA	O-C-N	5.57	128.02	122.12
2	T	38	TRP	CA-C-O	-5.56	114.71	121.05
1	B	424	LEU	O-C-N	5.56	128.49	122.15
1	C	231	GLU	O-C-N	5.56	128.03	122.08
1	C	234	GLU	CA-CB-CG	5.56	125.22	114.10
1	D	319	ARG	CA-CB-CG	5.56	125.22	114.10
1	D	365	THR	N-CA-C	-5.56	101.62	109.96
2	S	118	TYR	N-CA-CB	-5.55	101.10	110.49
2	T	59	PRO	CA-C-O	-5.55	115.29	121.23
1	D	82	GLY	CA-C-O	-5.55	115.33	121.94
1	A	442	ASN	N-CA-C	5.55	122.63	110.80
1	B	108	PHE	CA-C-O	5.55	126.60	120.71
1	C	356	GLN	O-C-N	-5.55	116.06	122.95
1	B	268	ASP	CA-C-O	-5.55	115.15	120.92
1	C	219	LEU	CA-C-N	-5.55	112.41	120.29
1	C	219	LEU	C-N-CA	-5.55	112.41	120.29
1	A	42	VAL	N-CA-C	5.55	116.98	108.71
1	A	199	PHE	N-CA-C	5.55	117.62	109.24
1	D	149	GLN	CB-CG-CD	5.55	122.03	112.60
1	D	466	VAL	CA-C-O	-5.54	115.91	121.45
1	C	404	GLY	O-C-N	5.54	127.50	122.18
1	A	169	LEU	N-CA-C	-5.54	101.51	110.32
1	C	26	THR	CA-CB-OG1	-5.54	101.29	109.60
1	B	172	CYS	CA-C-N	5.54	130.14	122.77
1	B	172	CYS	C-N-CA	5.54	130.14	122.77
2	T	109	GLN	OE1-CD-NE2	5.54	128.14	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	300	VAL	CA-C-O	-5.54	114.49	120.47
2	S	2	GLN	N-CA-CB	5.54	121.02	111.00
1	C	384	VAL	CB-CA-C	5.54	120.37	111.29
1	D	164	LYS	N-CA-C	5.54	117.42	108.34
1	B	319	ARG	CA-CB-CG	5.53	125.17	114.10
1	C	80	TYR	N-CA-C	5.53	120.04	113.12
1	C	90	VAL	N-CA-CB	5.53	117.97	111.66
1	C	367	ASP	CA-CB-CG	5.53	118.13	112.60
1	D	464	GLU	N-CA-C	5.53	119.77	113.19
2	V	7	ILE	CA-C-N	-5.53	110.97	121.54
2	V	7	ILE	C-N-CA	-5.53	110.97	121.54
2	V	97	ALA	O-C-N	5.53	129.13	122.94
1	B	306	ASN	CA-C-O	-5.53	113.05	118.97
1	D	360	ARG	CA-CB-CG	-5.53	103.04	114.10
2	S	112	CYS	CA-C-N	-5.53	115.92	122.11
2	S	112	CYS	C-N-CA	-5.53	115.92	122.11
1	A	84	CYS	CA-CB-SG	-5.53	101.69	114.40
2	U	110	VAL	N-CA-C	-5.53	99.85	108.86
1	D	454	GLU	CA-C-N	-5.53	112.81	120.38
1	D	454	GLU	C-N-CA	-5.53	112.81	120.38
1	C	420	ASN	CA-C-N	-5.53	113.26	120.44
1	C	420	ASN	C-N-CA	-5.53	113.26	120.44
1	D	155	ILE	N-CA-C	5.53	120.83	109.34
1	C	139	ARG	CA-CB-CG	-5.52	103.05	114.10
1	A	453	PRO	O-C-N	5.52	128.59	122.24
1	B	281	ALA	CA-C-O	5.52	126.40	120.55
1	C	269	TYR	CB-CG-CD1	5.52	129.08	120.80
1	C	339	ARG	NE-CZ-NH2	-5.52	114.23	119.20
1	B	184	ASN	OD1-CG-ND2	5.52	128.12	122.60
1	C	142	PRO	N-CD-CG	-5.52	94.92	103.20
1	A	400	LEU	CA-C-O	-5.52	114.25	120.32
2	U	65	ARG	CG-CD-NE	5.52	124.14	112.00
1	D	428	VAL	CB-CA-C	5.52	119.59	112.14
2	S	71	LYS	CA-C-O	-5.52	112.62	120.51
1	B	111	GLY	CA-C-O	-5.51	110.97	120.57
1	B	137	ASP	CA-C-O	-5.51	115.33	121.23
1	B	164	LYS	CG-CD-CE	5.51	123.98	111.30
1	D	372	PRO	O-C-N	5.51	129.58	122.91
1	B	199	PHE	N-CA-C	5.51	117.77	109.23
1	B	406	THR	CA-C-O	-5.51	112.78	119.61
2	T	89	GLU	CA-C-O	-5.51	114.71	120.55
1	D	374	VAL	N-CA-CB	-5.51	101.02	111.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	GLU	CA-C-O	5.51	128.39	120.51
1	A	242	ALA	O-C-N	-5.51	114.77	122.37
1	C	374	VAL	O-C-N	-5.51	116.41	122.69
1	D	90	VAL	N-CA-C	-5.51	99.66	107.98
1	B	70	TRP	N-CA-C	5.50	118.04	111.71
1	C	123	ASN	CA-C-O	-5.50	112.66	118.77
1	D	394	PHE	N-CA-C	5.50	120.11	112.90
1	B	153	HIS	N-CA-C	5.50	122.52	110.80
1	B	209	GLN	OE1-CD-NE2	-5.50	117.10	122.60
1	B	215	ARG	CA-C-N	5.50	128.10	120.29
1	B	215	ARG	C-N-CA	5.50	128.10	120.29
1	A	371	LEU	CA-C-N	5.50	125.80	119.92
1	A	371	LEU	C-N-CA	5.50	125.80	119.92
1	B	259	GLU	CA-CB-CG	5.49	125.09	114.10
1	C	277	ASN	CA-CB-CG	-5.49	107.11	112.60
1	D	362	ILE	N-CA-CB	-5.49	105.40	111.66
1	B	215	ARG	CB-CG-CD	5.49	123.92	111.30
1	B	197	LEU	O-C-N	-5.49	116.76	122.96
1	C	237	GLY	O-C-N	-5.49	118.46	123.56
1	A	302	ASP	N-CA-C	5.49	119.67	112.92
1	B	296	ALA	CB-CA-C	5.49	118.28	109.61
1	C	315	ALA	CA-C-O	-5.48	115.06	120.82
1	A	113	VAL	CA-C-O	5.48	126.44	120.57
2	S	89	GLU	CG-CD-OE1	-5.48	105.79	118.40
1	B	203	ASP	N-CA-CB	5.48	118.62	110.29
1	C	88	GLU	CA-CB-CG	5.48	125.07	114.10
1	C	327	HIS	N-CA-C	-5.48	101.54	110.20
1	B	262	VAL	CA-C-N	5.48	126.69	119.84
1	B	262	VAL	C-N-CA	5.48	126.69	119.84
1	D	296	ALA	N-CA-CB	-5.48	101.23	110.49
2	T	34	LEU	CA-C-O	-5.48	115.07	120.82
1	D	60	GLU	CG-CD-OE2	5.48	131.00	118.40
1	A	413	ASN	CA-CB-CG	5.47	118.07	112.60
1	D	373	GLY	N-CA-C	-5.47	102.11	112.51
1	A	136	GLU	CA-CB-CG	5.47	125.04	114.10
1	A	306	ASN	CB-CG-ND2	5.47	124.60	116.40
1	B	97	TYR	CB-CA-C	-5.47	98.47	110.67
1	B	334	LYS	CA-CB-CG	5.47	125.04	114.10
2	S	30	VAL	CA-C-O	5.47	126.42	120.57
2	S	100	ARG	CA-CB-CG	5.47	125.04	114.10
2	S	72	LEU	CA-C-O	-5.47	115.23	120.64
1	D	53	ALA	CA-C-O	-5.47	115.06	121.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	219	LEU	O-C-N	5.47	128.38	122.15
2	T	53	ARG	NE-CZ-NH2	5.46	124.12	119.20
2	U	34	LEU	N-CA-CB	-5.46	102.09	110.01
1	D	383	HIS	CA-C-N	5.46	131.80	121.97
1	D	383	HIS	C-N-CA	5.46	131.80	121.97
1	C	158	GLU	CA-C-O	5.46	126.55	120.82
1	C	209	GLN	CB-CG-CD	5.46	121.87	112.60
1	B	393	ILE	CB-CA-C	-5.45	104.78	112.14
1	C	292	HIS	N-CA-CB	-5.45	101.99	110.55
1	C	447	GLU	CG-CD-OE1	-5.45	105.86	118.40
2	T	101	ILE	CA-C-O	-5.45	114.67	120.39
1	C	130	LEU	N-CA-CB	5.45	120.03	111.20
1	A	149	GLN	N-CA-C	-5.45	104.98	111.69
2	S	96	GLN	OE1-CD-NE2	5.45	128.05	122.60
1	B	230	ALA	CA-C-O	-5.45	115.09	120.70
1	B	254	ALA	CA-C-O	5.45	126.33	120.55
1	B	418	VAL	O-C-N	-5.45	115.76	122.57
1	A	93	GLU	CB-CG-CD	5.45	121.86	112.60
1	B	120	ILE	N-CA-C	5.45	118.69	111.17
1	B	246	THR	CA-CB-OG1	-5.45	101.43	109.60
1	D	180	LEU	N-CA-CB	-5.45	101.53	110.41
1	A	88	GLU	CG-CD-OE1	-5.44	105.88	118.40
1	C	324	ASP	CA-C-N	5.44	131.35	122.81
1	C	324	ASP	C-N-CA	5.44	131.35	122.81
1	A	13	PHE	N-CA-CB	5.44	117.95	109.85
1	A	449	CYS	N-CA-C	-5.44	104.75	111.33
1	D	399	VAL	CA-C-O	-5.44	114.68	120.39
2	S	38	TRP	CA-C-O	-5.44	115.07	121.16
2	U	54	GLU	CG-CD-OE1	-5.44	105.89	118.40
1	D	29	TYR	N-CA-C	5.44	118.36	110.42
1	D	415	PRO	O-C-N	5.44	128.31	122.17
1	A	354	VAL	CA-C-O	5.43	125.63	120.25
1	B	376	PRO	O-C-N	-5.43	116.58	123.10
1	B	435	ARG	CD-NE-CZ	-5.43	116.80	124.40
1	D	335	LEU	N-CA-CB	-5.43	102.40	111.20
1	A	187	ARG	NE-CZ-NH1	-5.43	116.07	121.50
1	D	296	ALA	CA-C-N	5.43	131.91	121.54
1	D	296	ALA	C-N-CA	5.43	131.91	121.54
1	D	372	PRO	CA-C-O	-5.43	115.16	121.95
1	A	155	ILE	CA-C-O	-5.43	114.00	120.78
2	U	14	THR	CA-CB-OG1	-5.43	101.46	109.60
2	S	119	LYS	CA-C-O	-5.42	115.04	120.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	258	ARG	CD-NE-CZ	-5.42	116.81	124.40
1	D	260	LEU	O-C-N	-5.42	114.51	122.43
1	D	444	ILE	CA-C-N	-5.42	112.72	120.42
1	D	444	ILE	C-N-CA	-5.42	112.72	120.42
1	B	165	TYR	CA-C-N	5.42	132.04	121.41
1	B	165	TYR	C-N-CA	5.42	132.04	121.41
1	B	319	ARG	NH1-CZ-NH2	-5.42	112.25	119.30
1	B	217	ARG	CA-CB-CG	5.42	124.94	114.10
1	B	254	ALA	O-C-N	-5.42	116.37	122.12
1	C	341	ILE	N-CA-C	-5.42	105.22	110.42
1	D	103	TYR	CA-C-O	-5.42	114.35	119.55
1	B	109	GLU	N-CA-CB	5.42	117.92	109.85
1	B	112	SER	O-C-N	-5.42	116.02	122.63
1	B	251	ILE	CA-C-O	-5.42	115.11	120.85
2	T	7	ILE	CA-C-N	-5.42	111.19	121.54
2	T	7	ILE	C-N-CA	-5.42	111.19	121.54
2	V	43	GLU	CA-C-N	5.42	131.07	122.62
2	V	43	GLU	C-N-CA	5.42	131.07	122.62
2	S	4	TRP	N-CA-C	-5.41	100.11	109.58
1	B	226	TYR	O-C-N	5.41	128.32	122.15
1	B	465	ILE	CA-C-O	-5.41	114.59	120.71
1	D	160	ASP	CA-C-O	-5.41	113.98	120.10
1	C	147	THR	N-CA-C	-5.41	106.53	113.02
2	T	4	TRP	O-C-N	5.41	126.02	121.31
1	C	269	TYR	N-CA-C	5.41	118.67	111.75
1	A	239	TYR	CA-CB-CG	5.40	123.63	113.90
1	C	90	VAL	N-CA-C	-5.40	98.88	107.15
2	V	4	TRP	N-CA-C	-5.40	100.12	109.58
2	V	55	ASN	N-CA-C	5.40	118.08	111.82
1	A	107	LEU	N-CA-C	5.40	119.58	112.89
1	D	223	GLU	CB-CA-C	-5.40	102.17	110.81
1	D	238	HIS	CA-CB-CG	-5.40	108.40	113.80
2	U	104	PHE	CB-CA-C	-5.40	101.44	110.29
1	D	171	GLY	CA-C-O	5.39	128.03	121.61
1	D	423	ALA	CA-C-O	5.39	126.67	120.90
1	C	255	VAL	N-CA-C	5.39	116.12	110.62
1	D	216	ASP	N-CA-C	-5.39	105.32	111.14
1	D	427	CYS	CA-C-N	-5.39	113.07	120.46
1	D	427	CYS	C-N-CA	-5.39	113.07	120.46
1	B	302	ASP	CA-C-O	-5.39	113.25	119.56
1	C	311	PHE	O-C-N	-5.39	116.06	122.20
1	B	307	HIS	CB-CA-C	-5.39	98.44	109.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	274	PHE	CA-CB-CG	5.39	119.19	113.80
2	U	32	TYR	CA-C-O	5.39	126.26	120.55
2	U	107	VAL	O-C-N	5.39	130.12	122.04
1	D	234	GLU	N-CA-CB	5.39	119.86	110.81
1	A	233	GLY	N-CA-C	-5.39	107.83	115.43
1	C	99	ALA	N-CA-C	-5.39	100.91	109.96
1	C	172	CYS	CA-C-O	-5.39	114.14	120.60
1	A	214	TRP	CA-C-O	-5.38	115.14	120.90
1	A	194	ARG	CD-NE-CZ	5.38	131.93	124.40
1	A	461	VAL	N-CA-C	5.38	116.15	110.72
1	C	56	ALA	N-CA-C	-5.38	105.33	111.14
1	C	182	ALA	CA-C-N	-5.38	113.07	120.28
1	C	182	ALA	C-N-CA	-5.38	113.07	120.28
1	D	255	VAL	N-CA-C	5.38	116.11	110.62
2	V	33	LEU	N-CA-CB	-5.38	101.92	109.94
1	A	145	VAL	O-C-N	5.37	127.18	121.91
1	A	291	LEU	N-CA-CB	-5.37	101.66	110.68
1	C	118	THR	N-CA-C	-5.37	105.59	111.82
2	U	114	SER	CB-CA-C	5.37	121.11	110.42
1	D	446	ARG	CB-CA-C	-5.37	101.55	110.68
2	U	110	VAL	N-CA-CB	5.37	121.86	111.93
1	A	26	THR	O-C-N	5.37	125.58	121.23
2	V	91	LYS	N-CA-C	-5.37	105.59	111.82
1	A	192	CYS	N-CA-CB	5.37	117.75	109.91
1	B	194	ARG	CA-C-N	5.37	127.04	120.22
1	B	194	ARG	C-N-CA	5.37	127.04	120.22
1	A	78	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	131	ARG	CB-CA-C	5.37	118.70	109.15
1	B	83	ARG	NE-CZ-NH1	-5.37	116.13	121.50
1	D	136	GLU	CG-CD-OE2	-5.36	106.06	118.40
1	D	216	ASP	CB-CA-C	5.36	119.37	110.90
2	T	50	PHE	CA-C-O	5.36	127.28	121.06
2	U	38	TRP	CA-C-O	-5.36	114.94	121.05
1	D	246	THR	CA-C-O	-5.36	114.84	121.06
1	C	238	HIS	CA-C-O	-5.36	113.07	120.52
2	V	120	PRO	O-C-N	5.36	129.59	122.89
2	V	57	LYS	O-C-N	5.36	129.60	122.26
1	D	434	GLY	CA-C-O	-5.36	113.17	118.96
1	C	215	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	D	209	GLN	CA-C-N	5.36	125.42	119.32
1	D	209	GLN	C-N-CA	5.36	125.42	119.32
1	C	282	HIS	CA-C-O	5.35	126.44	120.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	448	ALA	CA-C-O	-5.35	114.74	120.42
2	U	55	ASN	OD1-CG-ND2	5.35	127.95	122.60
1	C	358	ARG	CA-CB-CG	-5.35	103.40	114.10
1	A	19	GLU	O-C-N	5.35	129.17	122.86
1	A	350	ARG	CG-CD-NE	5.35	123.77	112.00
2	S	102	ILE	CA-C-O	-5.35	116.05	121.67
1	D	386	HIS	CE1-NE2-CD2	5.35	114.35	109.00
1	C	265	VAL	N-CA-C	-5.35	102.30	108.82
1	C	458	ALA	O-C-N	5.35	129.70	122.59
1	A	372	PRO	CA-C-O	-5.35	115.27	121.95
1	C	264	ILE	CB-CG1-CD1	-5.34	102.58	113.80
1	A	199	PHE	O-C-N	5.34	129.63	123.17
1	B	263	PRO	N-CA-C	5.34	123.47	112.47
1	C	365	THR	CA-CB-OG1	-5.34	101.59	109.60
2	U	83	VAL	O-C-N	5.34	127.05	121.87
1	D	253	ARG	NH1-CZ-NH2	5.34	126.25	119.30
1	B	365	THR	CA-C-N	-5.34	115.47	123.00
1	B	365	THR	C-N-CA	-5.34	115.47	123.00
1	D	367	ASP	CB-CG-OD1	5.34	130.68	118.40
1	A	18	LYS	CA-C-O	-5.33	115.52	121.23
1	A	470	ALA	CA-C-N	5.33	129.88	120.87
1	A	470	ALA	C-N-CA	5.33	129.88	120.87
1	B	222	ALA	N-CA-C	-5.33	105.38	111.14
1	A	265	VAL	N-CA-CB	5.33	120.02	111.23
1	B	293	ILE	CA-C-N	5.33	130.51	123.05
1	B	293	ILE	C-N-CA	5.33	130.51	123.05
2	T	4	TRP	N-CA-C	-5.33	100.25	109.58
1	A	379	SER	N-CA-C	5.33	117.36	108.99
1	C	109	GLU	CB-CG-CD	5.33	121.66	112.60
1	B	350	ARG	CB-CG-CD	-5.33	99.05	111.30
1	A	328	SER	O-C-N	5.33	128.90	122.35
1	B	219	LEU	CA-C-O	-5.32	115.23	120.82
1	D	26	THR	CA-CB-CG2	5.32	119.55	110.50
1	D	178	LEU	CA-C-N	5.32	130.87	122.51
1	D	178	LEU	C-N-CA	5.32	130.87	122.51
1	D	120	ILE	O-C-N	5.32	127.11	121.89
2	S	45	GLU	CA-C-O	-5.32	113.74	120.28
1	B	59	ALA	O-C-N	5.32	128.61	122.17
2	U	106	ASN	N-CA-C	5.32	119.25	112.87
1	C	130	LEU	N-CA-C	-5.32	101.45	109.85
1	D	319	ARG	NH1-CZ-NH2	5.32	126.21	119.30
1	B	269	TYR	N-CA-C	5.32	117.83	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	2	GLN	CA-C-O	5.32	126.98	120.60
1	D	406	THR	N-CA-C	-5.32	103.42	111.34
2	T	38	TRP	N-CA-CB	-5.32	102.03	110.06
2	V	43	GLU	CG-CD-OE1	5.32	130.63	118.40
1	C	91	VAL	CA-CB-CG1	5.31	119.43	110.40
1	D	94	LYS	CA-C-O	-5.31	112.91	120.51
1	A	108	PHE	N-CA-CB	-5.31	102.14	110.69
1	A	199	PHE	CA-CB-CG	5.31	119.11	113.80
1	A	294	HIS	CB-CA-C	5.31	119.43	109.71
1	A	319	ARG	CA-CB-CG	5.31	124.72	114.10
1	B	89	ARG	CA-C-N	-5.31	115.85	122.48
1	B	89	ARG	C-N-CA	-5.31	115.85	122.48
1	B	236	LYS	CA-C-N	5.31	127.85	121.38
1	B	236	LYS	C-N-CA	5.31	127.85	121.38
2	V	47	GLU	CG-CD-OE2	-5.31	106.19	118.40
1	A	352	ASP	CA-C-N	5.30	131.24	122.33
1	A	352	ASP	C-N-CA	5.30	131.24	122.33
1	A	369	VAL	CA-C-O	5.30	127.41	120.78
1	B	227	LYS	CA-C-O	5.30	126.16	120.70
1	D	252	LYS	N-CA-C	5.30	117.75	111.33
1	D	140	ILE	CA-C-N	5.30	123.48	119.66
1	D	140	ILE	C-N-CA	5.30	123.48	119.66
1	A	360	ARG	NH1-CZ-NH2	5.30	126.19	119.30
1	C	264	ILE	CA-C-O	5.30	126.65	121.19
2	V	61	TYR	CA-C-N	-5.30	113.26	122.37
2	V	61	TYR	C-N-CA	-5.30	113.26	122.37
1	A	86	ARG	O-C-N	5.29	129.63	122.59
2	U	73	PRO	CA-C-O	-5.29	115.57	121.23
1	D	172	CYS	CA-C-O	-5.29	113.77	120.28
1	D	134	ARG	CA-C-O	-5.29	113.07	120.21
2	S	59	PRO	CB-CA-C	5.29	118.28	111.46
1	B	266	MET	CA-C-O	-5.29	115.62	121.33
1	D	177	LYS	CB-CG-CD	-5.29	99.14	111.30
1	A	79	ARG	N-CA-C	5.29	117.12	111.36
2	T	111	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	A	264	ILE	CA-C-O	-5.28	115.75	121.19
1	B	319	ARG	N-CA-C	-5.28	105.47	112.34
1	C	334	LYS	CA-C-N	-5.28	113.93	122.81
1	C	334	LYS	C-N-CA	-5.28	113.93	122.81
2	T	110	VAL	N-CA-CB	5.28	121.70	111.93
1	D	459	CYS	O-C-N	5.28	128.18	122.11
1	C	372	PRO	CA-C-N	-5.28	115.98	122.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	372	PRO	C-N-CA	-5.28	115.98	122.15
2	U	17	TYR	CB-CA-C	5.27	118.24	109.38
1	D	294	HIS	CA-C-N	-5.27	114.19	122.95
1	D	294	HIS	C-N-CA	-5.27	114.19	122.95
1	A	263	PRO	CA-C-O	-5.27	111.00	120.60
1	B	155	ILE	CB-CG1-CD1	-5.27	102.73	113.80
1	D	236	LYS	N-CA-CB	-5.27	103.14	111.05
1	B	10	SER	O-C-N	5.27	129.60	122.59
1	A	187	ARG	CD-NE-CZ	5.27	131.78	124.40
1	A	327	HIS	N-CA-C	-5.27	101.38	109.76
2	S	74	MET	CA-C-N	5.27	128.71	120.75
2	S	74	MET	C-N-CA	5.27	128.71	120.75
1	B	303	ARG	CA-C-O	-5.27	115.27	120.80
1	C	97	TYR	N-CA-C	5.27	117.42	109.41
1	B	264	ILE	N-CA-CB	-5.27	101.61	111.62
1	A	146	LYS	CA-C-N	-5.26	112.85	122.38
1	A	146	LYS	C-N-CA	-5.26	112.85	122.38
1	B	142	PRO	CA-C-N	-5.26	111.93	120.72
1	B	142	PRO	C-N-CA	-5.26	111.93	120.72
1	A	337	GLY	CA-C-N	-5.26	115.30	122.93
1	A	337	GLY	C-N-CA	-5.26	115.30	122.93
1	C	241	ASN	O-C-N	-5.26	116.33	122.96
1	C	402	PHE	N-CA-C	5.26	118.86	107.49
1	B	400	LEU	CA-C-O	-5.26	114.53	120.32
1	C	312	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	D	83	ARG	O-C-N	5.26	129.57	123.41
1	A	77	LEU	CA-C-N	-5.26	112.32	120.31
1	A	77	LEU	C-N-CA	-5.26	112.32	120.31
1	A	83	ARG	CA-C-N	5.26	130.69	122.17
1	A	83	ARG	C-N-CA	5.26	130.69	122.17
1	A	156	GLN	CG-CD-NE2	-5.26	108.52	116.40
1	A	334	LYS	N-CA-C	5.26	117.75	111.71
1	A	353	PHE	O-C-N	5.25	129.77	123.36
1	B	139	ARG	CA-CB-CG	-5.25	103.59	114.10
1	B	371	LEU	CA-C-N	5.25	125.19	119.78
1	B	371	LEU	C-N-CA	5.25	125.19	119.78
1	B	469	PHE	N-CA-CB	5.25	119.45	110.57
2	V	56	ASN	CA-C-N	-5.25	113.36	122.14
2	V	56	ASN	C-N-CA	-5.25	113.36	122.14
1	C	41	ARG	CD-NE-CZ	-5.25	117.05	124.40
2	U	18	LEU	CA-C-N	5.25	125.19	119.78
2	U	18	LEU	C-N-CA	5.25	125.19	119.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	TYR	N-CA-CB	5.25	118.84	110.65
2	T	18	LEU	N-CA-C	-5.25	103.52	110.40
1	D	253	ARG	NE-CZ-NH2	-5.25	114.47	119.20
1	A	104	PRO	CB-CA-C	5.25	118.23	111.46
1	C	366	GLN	O-C-N	5.25	130.05	123.12
1	A	121	VAL	CA-C-O	5.25	123.94	119.38
1	A	404	GLY	O-C-N	5.25	127.26	122.17
1	C	395	GLY	O-C-N	5.25	128.71	122.68
2	V	106	ASN	OD1-CG-ND2	-5.25	117.35	122.60
1	C	285	ARG	CA-CB-CG	-5.24	103.61	114.10
1	D	413	ASN	N-CA-C	5.24	117.42	111.02
2	V	122	GLY	CA-C-N	5.24	131.14	121.70
2	V	122	GLY	C-N-CA	5.24	131.14	121.70
1	A	78	ASP	N-CA-C	-5.24	105.74	111.82
1	B	261	GLY	CA-C-N	5.24	131.82	122.13
1	B	261	GLY	C-N-CA	5.24	131.82	122.13
1	B	460	GLU	CG-CD-OE2	5.24	130.45	118.40
1	D	267	HIS	O-C-N	-5.24	117.45	123.42
1	A	45	GLN	CA-CB-CG	5.24	124.57	114.10
1	B	277	ASN	CA-C-O	5.24	126.50	121.00
1	B	337	GLY	CA-C-N	-5.24	114.85	122.65
1	B	337	GLY	C-N-CA	-5.24	114.85	122.65
2	V	78	THR	CA-C-N	-5.24	115.57	122.85
2	V	78	THR	C-N-CA	-5.24	115.57	122.85
1	D	319	ARG	CB-CA-C	5.23	121.36	110.32
1	A	334	LYS	CA-C-O	-5.23	114.19	120.10
1	B	180	LEU	CB-CA-C	5.23	118.34	109.50
1	D	82	GLY	CA-C-N	-5.23	112.73	121.94
1	D	82	GLY	C-N-CA	-5.23	112.73	121.94
1	D	97	TYR	N-CA-C	5.23	116.61	109.18
1	A	110	GLU	O-C-N	5.23	129.24	122.81
1	C	178	LEU	CA-C-N	5.23	130.83	122.25
1	C	178	LEU	C-N-CA	5.23	130.83	122.25
1	C	408	GLY	CA-C-N	5.23	127.68	120.67
1	C	408	GLY	C-N-CA	5.23	127.68	120.67
1	A	355	GLU	CG-CD-OE2	-5.23	106.37	118.40
1	A	420	ASN	OD1-CG-ND2	-5.23	117.37	122.60
2	S	26	LEU	N-CA-CB	-5.23	102.44	110.12
2	V	65	ARG	CB-CG-CD	-5.23	99.28	111.30
2	S	57	LYS	CA-C-N	-5.23	113.10	121.57
2	S	57	LYS	C-N-CA	-5.23	113.10	121.57
1	B	209	GLN	O-C-N	5.23	125.98	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	GLU	N-CA-C	-5.22	105.23	111.03
1	A	413	ASN	CB-CG-OD1	5.22	131.25	120.80
1	B	194	ARG	NH1-CZ-NH2	-5.22	112.51	119.30
1	B	301	ILE	CA-C-O	-5.22	114.25	120.78
1	B	116	MET	CA-C-O	-5.22	114.91	121.02
1	D	36	ILE	CA-CB-CG2	5.22	119.38	110.50
2	U	4	TRP	N-CA-C	-5.22	100.44	109.58
2	V	34	LEU	N-CA-CB	-5.22	102.29	109.91
1	A	78	ASP	CB-CA-C	5.22	120.69	110.67
1	A	323	GLY	CA-C-O	-5.22	111.49	120.57
2	S	103	GLY	CA-C-O	-5.22	111.49	120.57
2	T	38	TRP	CA-C-N	-5.22	119.05	122.60
2	T	38	TRP	C-N-CA	-5.22	119.05	122.60
2	T	88	GLY	CA-C-O	5.22	126.63	121.00
1	B	213	ARG	CB-CG-CD	5.21	123.29	111.30
1	A	115	ASN	O-C-N	-5.21	116.61	122.03
1	A	130	LEU	O-C-N	5.21	129.82	123.10
1	C	74	LEU	CB-CA-C	5.21	121.01	110.38
1	D	114	THR	O-C-N	-5.21	116.67	122.09
1	D	233	GLY	N-CA-C	-5.21	107.05	115.08
1	C	362	ILE	CA-C-O	-5.21	114.94	121.04
1	D	144	TYR	CB-CA-C	5.21	118.15	109.56
1	D	184	ASN	CA-CB-CG	-5.21	107.39	112.60
1	D	223	GLU	CA-C-N	5.21	127.21	120.44
1	D	223	GLU	C-N-CA	5.21	127.21	120.44
1	A	105	LEU	CB-CA-C	-5.20	102.49	110.81
1	C	250	MET	CA-C-O	-5.20	115.36	120.82
1	D	352	ASP	CA-CB-CG	-5.20	107.40	112.60
1	D	263	PRO	N-CA-C	5.20	123.19	112.47
1	A	131	ARG	N-CA-C	-5.20	107.59	114.04
1	C	406	THR	CA-C-O	-5.20	113.68	119.40
1	C	35	ASP	O-C-N	-5.20	117.09	122.96
1	A	183	LYS	CA-CB-CG	-5.20	103.71	114.10
1	B	41	ARG	NE-CZ-NH1	-5.20	116.30	121.50
1	B	322	GLY	O-C-N	5.20	129.45	122.70
1	D	421	ARG	NH1-CZ-NH2	5.20	126.05	119.30
2	V	38	TRP	CB-CA-C	5.19	118.31	109.53
1	A	355	GLU	CA-C-O	-5.19	115.34	121.16
1	B	115	ASN	CA-CB-CG	-5.19	107.41	112.60
1	D	326	ILE	N-CA-C	-5.19	101.50	108.35
2	V	55	ASN	CB-CG-OD1	-5.19	110.41	120.80
1	A	342	THR	O-C-N	5.19	127.42	122.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	392	GLU	CA-CB-CG	5.19	124.48	114.10
2	T	33	LEU	N-CA-C	-5.19	104.69	111.02
1	C	428	VAL	CA-C-O	-5.19	115.55	120.95
2	V	38	TRP	CA-C-O	-5.19	115.13	121.05
1	A	290	LEU	N-CA-C	-5.19	102.07	110.32
1	B	409	HIS	CA-C-N	5.19	125.49	119.47
1	B	409	HIS	C-N-CA	5.19	125.49	119.47
1	B	416	GLY	O-C-N	-5.19	116.85	122.19
2	U	90	ALA	CA-C-O	-5.19	114.00	119.97
1	B	213	ARG	CB-CA-C	5.19	118.09	109.53
1	B	61	SER	CA-CB-OG	-5.18	100.73	111.10
1	B	394	PHE	CA-CB-CG	-5.18	108.61	113.80
1	D	306	ASN	CB-CG-ND2	5.18	124.18	116.40
1	A	139	ARG	CA-C-O	-5.18	115.15	120.54
2	T	34	LEU	N-CA-CB	-5.18	102.50	110.01
1	D	45	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	D	292	HIS	CB-CG-CD2	-5.18	124.47	131.20
2	T	77	CYS	CA-C-O	-5.18	116.06	121.55
1	B	72	ASP	O-C-N	-5.18	116.63	122.12
1	B	440	GLU	N-CA-C	5.18	121.82	110.80
1	C	350	ARG	N-CA-C	5.18	119.68	112.90
1	C	426	ALA	N-CA-C	-5.18	105.33	110.97
1	A	29	TYR	CA-C-O	5.17	126.12	120.95
1	B	338	GLU	CB-CG-CD	5.17	121.39	112.60
1	B	468	ASN	N-CA-CB	5.17	118.70	110.16
1	B	129	ALA	CA-C-O	-5.17	112.58	119.10
1	B	454	GLU	CG-CD-OE2	-5.17	106.51	118.40
2	U	62	TYR	O-C-N	5.17	129.67	123.36
1	A	121	VAL	N-CA-C	5.17	118.11	113.10
1	A	428	VAL	CA-C-N	5.17	127.63	120.29
1	A	428	VAL	C-N-CA	5.17	127.63	120.29
2	T	107	VAL	CB-CA-C	-5.17	105.31	112.24
1	C	149	GLN	O-C-N	5.17	129.88	122.28
1	A	10	SER	O-C-N	5.17	129.46	122.59
1	B	81	LYS	CG-CD-CE	5.16	123.17	111.30
1	D	350	ARG	N-CA-C	5.16	119.71	113.41
1	C	374	VAL	N-CA-CB	-5.16	100.43	111.37
1	D	446	ARG	N-CA-C	5.16	117.58	111.33
1	B	178	LEU	CA-C-O	-5.16	115.32	121.56
1	C	190	TYR	CA-C-O	5.16	126.24	120.82
2	V	104	PHE	CB-CA-C	-5.16	101.43	109.84
2	S	102	ILE	O-C-N	5.16	128.77	123.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	402	PHE	N-CA-C	5.16	117.83	107.41
1	A	200	THR	CA-C-N	5.16	131.06	121.62
1	A	200	THR	C-N-CA	5.16	131.06	121.62
2	T	112	CYS	CA-CB-SG	-5.16	102.54	114.40
1	C	286	ASP	CA-C-N	-5.16	114.43	122.37
1	C	286	ASP	C-N-CA	-5.16	114.43	122.37
1	A	220	PHE	CA-CB-CG	5.15	118.95	113.80
1	D	298	HIS	N-CA-C	5.15	117.29	111.11
2	S	57	LYS	CA-C-O	-5.15	114.15	119.51
1	D	327	HIS	N-CA-CB	5.15	117.94	109.95
1	B	253	ARG	N-CA-C	-5.15	105.29	112.45
1	C	120	ILE	N-CA-C	5.15	118.28	111.17
1	C	249	GLU	CB-CA-C	-5.15	102.80	110.88
1	C	461	VAL	CA-C-N	-5.15	114.41	122.65
1	C	461	VAL	C-N-CA	-5.15	114.41	122.65
1	C	328	SER	O-C-N	5.15	128.68	122.35
1	C	395	GLY	N-CA-C	-5.15	105.19	112.81
1	D	224	ALA	CA-C-N	-5.15	112.87	120.28
1	D	224	ALA	C-N-CA	-5.15	112.87	120.28
1	B	140	ILE	O-C-N	-5.15	117.09	121.57
2	T	121	GLU	CB-CA-C	-5.14	102.91	110.06
1	C	357	ASP	CA-CB-CG	5.14	117.75	112.60
1	D	192	CYS	CA-C-O	-5.14	115.42	120.82
1	D	117	PHE	N-CA-CB	5.14	117.77	110.16
1	D	175	LYS	CB-CA-C	5.14	117.04	109.22
1	A	193	LEU	CB-CA-C	5.14	119.42	110.68
2	S	35	LYS	CB-CG-CD	5.14	123.12	111.30
1	B	358	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	A	225	LEU	CA-C-N	-5.14	113.39	120.28
1	A	225	LEU	C-N-CA	-5.14	113.39	120.28
1	C	24	TYR	N-CA-C	5.14	119.24	112.92
1	C	32	LYS	CB-CA-C	-5.14	100.81	109.50
1	D	107	LEU	N-CA-C	5.14	119.40	113.18
1	C	349	LEU	N-CA-CB	-5.14	102.53	110.13
2	S	32	TYR	CA-C-O	5.14	126.00	120.55
1	B	221	CYS	O-C-N	5.14	129.07	122.39
1	D	73	GLY	O-C-N	5.14	129.36	122.48
2	S	106	ASN	CA-CB-CG	-5.13	107.47	112.60
1	B	452	SER	N-CA-C	5.13	118.90	109.10
2	U	28	SER	N-CA-CB	-5.13	102.57	110.12
1	A	149	GLN	N-CA-CB	5.13	117.85	110.20
1	B	60	GLU	CA-C-N	5.13	130.29	122.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	GLU	C-N-CA	5.13	130.29	122.23
1	B	327	HIS	N-CA-C	-5.13	101.60	109.76
1	C	19	GLU	O-C-N	5.13	128.76	122.96
1	D	38	ALA	CA-C-O	5.13	126.76	120.60
1	B	83	ARG	CG-CD-NE	-5.13	100.71	112.00
1	B	110	GLU	CG-CD-OE1	-5.13	106.61	118.40
1	B	238	HIS	ND1-CE1-NE2	-5.13	103.27	108.40
1	D	191	GLU	CA-C-O	-5.13	115.44	120.82
1	D	141	PRO	N-CA-C	5.13	116.07	110.58
1	A	164	LYS	CA-C-N	5.12	130.62	122.62
1	A	164	LYS	C-N-CA	5.12	130.62	122.62
1	C	412	GLY	CA-C-N	5.12	129.34	121.19
1	C	412	GLY	C-N-CA	5.12	129.34	121.19
2	U	75	PHE	N-CA-C	-5.12	103.72	110.43
2	U	99	ILE	O-C-N	5.12	128.58	123.10
2	T	92	LYS	CB-CG-CD	5.12	123.08	111.30
1	D	131	ARG	CB-CA-C	5.12	118.27	109.15
1	A	28	GLU	CB-CA-C	-5.12	102.84	110.88
1	B	104	PRO	CA-C-O	-5.12	115.17	121.31
2	T	89	GLU	CA-CB-CG	5.12	124.34	114.10
2	U	62	TYR	CA-C-O	-5.12	113.98	120.28
2	V	100	ARG	N-CA-CB	-5.12	102.78	111.69
2	T	2	GLN	CA-CB-CG	5.12	124.33	114.10
2	T	76	GLY	O-C-N	-5.12	116.05	122.70
2	V	119	LYS	N-CA-CB	5.12	117.14	109.88
1	B	461	VAL	CB-CA-C	-5.11	105.42	111.97
2	T	52	TYR	CA-CB-CG	5.11	123.10	113.90
2	S	111	GLN	N-CA-CB	5.11	118.76	110.17
1	C	233	GLY	CA-C-N	-5.11	114.87	122.74
1	C	233	GLY	C-N-CA	-5.11	114.87	122.74
1	D	303	ARG	CA-C-N	5.11	129.39	121.26
1	D	303	ARG	C-N-CA	5.11	129.39	121.26
1	A	274	PHE	CA-CB-CG	5.11	118.91	113.80
1	C	269	TYR	CA-C-O	-5.11	114.48	120.20
1	C	435	ARG	CA-CB-CG	-5.11	103.88	114.10
2	S	122	GLY	CA-C-N	5.11	130.90	121.70
2	S	122	GLY	C-N-CA	5.11	130.90	121.70
1	B	124	VAL	CA-C-N	-5.11	111.49	120.99
1	B	124	VAL	C-N-CA	-5.11	111.49	120.99
1	B	332	VAL	N-CA-C	5.11	119.96	109.34
1	B	432	ASN	CA-CB-CG	5.11	117.71	112.60
1	C	263	PRO	N-CA-C	5.11	123.43	114.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	28	GLU	CA-C-N	5.11	129.52	121.56
1	D	28	GLU	C-N-CA	5.11	129.52	121.56
2	V	111	GLN	CA-CB-CG	-5.11	103.89	114.10
1	A	405	GLY	N-CA-C	5.10	120.52	113.99
1	C	144	TYR	CA-C-N	-5.10	114.13	120.56
1	C	144	TYR	C-N-CA	-5.10	114.13	120.56
1	D	330	THR	OG1-CB-CG2	5.10	119.51	109.30
1	B	74	LEU	N-CA-C	-5.10	106.22	112.90
1	C	207	ASN	CB-CA-C	5.10	120.57	110.42
2	V	26	LEU	N-CA-C	-5.10	105.72	111.28
2	V	104	PHE	CA-CB-CG	-5.10	108.70	113.80
2	U	56	ASN	CB-CG-ND2	5.10	124.05	116.40
1	D	77	LEU	O-C-N	5.10	129.26	122.43
1	D	246	THR	O-C-N	5.10	129.18	123.27
1	A	305	LYS	O-C-N	-5.10	115.43	122.46
1	B	136	GLU	CA-CB-CG	5.09	124.29	114.10
1	B	223	GLU	O-C-N	5.09	127.39	122.09
1	B	401	GLN	O-C-N	-5.09	117.23	123.19
1	C	138	LEU	CA-CB-CG	5.09	134.13	116.30
2	U	49	GLY	CA-C-O	-5.09	111.70	120.57
1	C	360	ARG	CA-CB-CG	-5.09	103.92	114.10
1	B	328	SER	CB-CA-C	-5.09	101.57	110.17
2	T	71	LYS	CB-CA-C	-5.09	110.31	117.23
1	C	80	TYR	CA-C-N	5.09	128.07	120.90
1	C	80	TYR	C-N-CA	5.09	128.07	120.90
1	B	9	ALA	CA-C-N	5.08	131.25	121.54
1	B	9	ALA	C-N-CA	5.08	131.25	121.54
1	A	93	GLU	CG-CD-OE2	5.08	130.09	118.40
1	A	285	ARG	NE-CZ-NH2	-5.08	114.63	119.20
1	B	178	LEU	CB-CA-C	5.08	118.86	109.71
2	S	58	SER	CA-C-N	-5.08	114.53	119.76
2	S	58	SER	C-N-CA	-5.08	114.53	119.76
1	B	447	GLU	CA-C-O	5.08	125.81	120.42
1	A	217	ARG	NH1-CZ-NH2	-5.08	112.70	119.30
1	C	452	SER	CA-C-O	5.08	125.94	119.54
1	A	294	HIS	O-C-N	5.08	129.34	123.30
1	A	253	ARG	NE-CZ-NH1	-5.08	116.42	121.50
1	A	294	HIS	CA-C-O	-5.08	114.88	120.36
2	S	2	GLN	CA-CB-CG	5.08	124.25	114.10
1	C	444	ILE	O-C-N	5.08	128.91	122.57
1	A	109	GLU	N-CA-C	-5.07	102.18	110.20
1	A	437	LEU	CA-C-O	-5.07	115.15	120.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	264	ILE	CB-CA-C	5.07	120.31	111.18
2	S	67	TRP	CA-C-O	-5.07	115.69	121.68
1	A	362	ILE	N-CA-CB	-5.07	105.88	111.66
2	S	38	TRP	N-CA-CB	-5.07	102.52	109.97
1	C	271	THR	CA-C-N	5.07	131.35	121.41
1	C	271	THR	C-N-CA	5.07	131.35	121.41
1	D	66	TRP	CA-C-O	-5.07	112.62	119.11
1	D	160	ASP	O-C-N	5.07	128.15	122.22
1	A	153	HIS	N-CA-C	5.07	121.60	110.80
1	B	310	HIS	CA-CB-CG	-5.07	108.73	113.80
1	A	46	PRO	CA-N-CD	-5.07	104.91	112.00
1	A	359	SER	O-C-N	5.07	127.30	122.03
1	A	367	ASP	CB-CG-OD1	5.07	130.05	118.40
1	C	394	PHE	N-CA-C	5.07	119.54	112.90
1	D	148	PHE	CA-CB-CG	-5.07	108.73	113.80
1	D	204	GLU	CG-CD-OE1	5.07	130.06	118.40
1	B	45	GLN	CB-CA-C	5.07	116.01	108.87
1	C	271	THR	O-C-N	-5.07	115.64	122.43
1	B	29	TYR	O-C-N	5.06	128.78	123.11
1	A	437	LEU	CA-C-N	-5.06	113.56	120.44
1	A	437	LEU	C-N-CA	-5.06	113.56	120.44
1	B	401	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	C	421	ARG	O-C-N	-5.06	116.86	122.07
1	D	220	PHE	CA-C-N	-5.06	112.50	120.60
1	D	220	PHE	C-N-CA	-5.06	112.50	120.60
2	V	14	THR	CB-CA-C	5.06	117.43	109.84
1	B	197	LEU	N-CA-C	-5.06	102.99	110.48
1	B	360	ARG	CA-C-N	5.06	131.50	121.53
1	B	360	ARG	C-N-CA	5.06	131.50	121.53
1	C	243	THR	CA-C-N	-5.06	114.07	122.11
1	C	243	THR	C-N-CA	-5.06	114.07	122.11
2	U	74	MET	CA-C-N	5.06	129.42	120.87
2	U	74	MET	C-N-CA	5.06	129.42	120.87
1	D	245	GLY	O-C-N	5.06	129.28	122.70
1	D	358	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	D	394	PHE	CA-CB-CG	-5.06	108.74	113.80
1	D	353	PHE	CA-CB-CG	5.06	118.86	113.80
1	B	371	LEU	N-CA-CB	-5.05	102.03	110.02
1	B	405	GLY	N-CA-C	5.05	120.01	114.40
1	B	417	ALA	CA-C-O	-5.05	115.69	120.90
1	C	254	ALA	N-CA-CB	5.05	117.47	109.94
1	D	178	LEU	O-C-N	-5.05	116.58	123.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	ASP	CB-CG-OD1	-5.05	106.78	118.40
1	A	59	ALA	O-C-N	5.05	128.28	122.17
1	D	385	TRP	CA-C-N	-5.05	114.30	122.23
1	D	385	TRP	C-N-CA	-5.05	114.30	122.23
1	A	257	ALA	CB-CA-C	5.05	119.17	110.79
1	C	210	PRO	N-CA-CB	5.05	108.89	103.33
1	A	44	PRO	CA-C-O	5.05	128.81	122.15
1	A	281	ALA	N-CA-CB	-5.05	102.70	110.12
1	A	329	GLY	CA-C-O	-5.05	118.53	122.52
2	T	112	CYS	CA-C-N	-5.05	116.46	122.11
2	T	112	CYS	C-N-CA	-5.05	116.46	122.11
1	D	246	THR	CA-CB-OG1	-5.05	102.03	109.60
2	V	86	GLU	O-C-N	5.05	127.34	122.09
2	U	1	MET	CA-C-O	-5.04	112.22	120.80
1	A	467	PHE	CA-C-N	-5.04	115.08	122.19
1	A	467	PHE	C-N-CA	-5.04	115.08	122.19
2	S	35	LYS	CA-CB-CG	5.04	124.19	114.10
1	D	254	ALA	N-CA-CB	5.04	117.53	110.12
2	S	61	TYR	CA-C-N	5.04	130.66	121.89
2	S	61	TYR	C-N-CA	5.04	130.66	121.89
1	C	391	THR	N-CA-C	-5.04	105.06	111.11
1	B	80	TYR	CA-C-O	-5.04	113.72	119.41
1	C	330	THR	O-C-N	5.04	127.44	122.10
1	C	252	LYS	CG-CD-CE	5.04	122.89	111.30
1	C	277	ASN	O-C-N	5.04	127.27	122.03
2	U	82	GLN	CA-CB-CG	5.04	124.17	114.10
1	D	425	GLU	CA-C-O	5.03	126.07	120.63
1	D	454	GLU	O-C-N	5.03	127.53	122.09
1	B	203	ASP	O-C-N	5.03	128.65	122.96
1	B	217	ARG	CA-C-O	-5.03	115.54	120.82
2	U	101	ILE	O-C-N	5.03	128.69	123.26
1	D	256	PHE	O-C-N	5.03	127.89	122.15
1	A	165	TYR	N-CA-C	5.03	117.44	109.50
1	A	335	LEU	CB-CA-C	5.03	119.41	109.66
2	V	107	VAL	O-C-N	5.03	128.70	121.82
1	B	98	ILE	O-C-N	5.02	129.65	122.62
1	D	226	TYR	CA-C-O	-5.02	115.09	120.42
1	C	44	PRO	O-C-N	5.02	129.42	122.64
2	U	22	SER	N-CA-C	-5.02	103.90	110.53
1	D	50	PRO	O-C-N	5.02	128.26	122.23
1	D	319	ARG	CG-CD-NE	-5.02	100.95	112.00
1	D	399	VAL	CA-CB-CG1	5.02	118.94	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	SER	O-C-N	5.02	128.32	122.24
1	C	376	PRO	N-CD-CG	-5.02	95.67	103.20
1	B	325	HIS	CA-CB-CG	5.02	118.82	113.80
2	T	26	LEU	CB-CA-C	5.02	119.38	110.85
1	D	264	ILE	CA-C-N	5.02	130.15	122.92
1	D	264	ILE	C-N-CA	5.02	130.15	122.92
1	D	410	PRO	CA-C-O	-5.02	111.71	119.64
1	C	105	LEU	O-C-N	5.02	127.45	122.08
1	B	45	GLN	CB-CG-CD	5.01	121.12	112.60
1	C	67	THR	OG1-CB-CG2	-5.01	99.27	109.30
1	A	460	GLU	CA-C-N	5.01	127.54	120.42
1	A	460	GLU	C-N-CA	5.01	127.54	120.42
1	A	217	ARG	O-C-N	5.01	127.50	122.09
1	C	198	ASP	O-C-N	-5.01	115.72	122.23
1	D	319	ARG	N-CA-C	-5.01	106.27	112.38
1	B	292	HIS	CA-C-O	-5.01	115.00	120.36
2	V	73	PRO	CB-CA-C	5.01	117.95	111.64
1	A	56	ALA	CA-C-O	5.01	125.73	120.42
1	A	141	PRO	O-C-N	-5.01	118.80	121.15
1	A	184	ASN	O-C-N	5.01	128.43	122.27
1	A	438	ALA	CA-C-O	-5.01	115.54	120.70
1	A	459	CYS	CB-CA-C	-5.01	102.80	110.81
1	C	376	PRO	O-C-N	-5.01	116.90	123.06
2	V	43	GLU	CA-CB-CG	5.01	124.11	114.10
1	D	393	ILE	CA-C-O	-5.00	115.86	121.17
1	D	451	TRP	CB-CG-CD2	-5.00	119.79	126.80
2	S	3	VAL	O-C-N	5.00	128.24	122.64
2	V	88	GLY	O-C-N	5.00	126.98	122.18
1	A	273	GLY	O-C-N	-5.00	116.20	122.70
2	S	38	TRP	CB-CA-C	5.00	118.20	109.65
1	B	384	VAL	CB-CA-C	5.00	119.49	111.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3628	0	3560	207	0
1	B	3628	0	3558	231	1
1	C	3628	0	3557	264	1
1	D	3628	0	3558	251	0
2	S	1024	0	991	70	0
2	T	1024	0	991	90	0
2	U	1024	0	991	101	0
2	V	1024	0	991	98	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	21	0	6	2	0
4	B	21	0	5	0	0
4	C	21	0	6	1	0
4	D	21	0	6	3	0
5	A	3	0	0	1	0
5	B	3	0	0	0	0
5	C	3	0	0	1	0
5	D	3	0	0	1	0
All	All	18708	0	18220	1203	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (1203) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:79:ASP:HB3	2:U:82:GLN:HE21	1.13	1.10
1:A:79:ARG:HH11	1:A:79:ARG:HG2	1.18	1.09
2:V:79:ASP:HB3	2:V:82:GLN:HE21	1.14	1.09
1:D:79:ARG:HG2	1:D:79:ARG:HH11	1.15	1.06
1:C:26:THR:HG22	1:C:29:TYR:HB2	1.37	1.05
1:C:79:ARG:HH11	1:C:79:ARG:HG2	1.18	1.04
1:C:90:VAL:HG21	1:C:96:GLN:HG2	1.37	1.02
2:T:79:ASP:HB3	2:T:82:GLN:HE21	1.18	1.02
1:D:176:PRO:HD2	1:D:180:LEU:HD22	1.43	1.01
1:A:26:THR:HG22	1:A:29:TYR:HB2	1.43	0.98
1:C:452:SER:HB3	1:C:455:LEU:HB3	1.48	0.96
2:S:27:LEU:HD23	2:S:31:GLU:OE2	1.65	0.96
2:S:79:ASP:HB3	2:S:82:GLN:HE21	1.32	0.94
1:B:304:GLN:HA	1:B:304:GLN:HE21	1.34	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ARG:HH11	1:A:89:ARG:HB2	1.35	0.92
2:V:79:ASP:CB	2:V:82:GLN:HE21	1.82	0.92
2:S:56:ASN:ND2	2:S:58:SER:H	1.68	0.92
1:B:29:TYR:OH	1:B:32:LYS:NZ	2.01	0.92
1:B:155:ILE:HG12	1:B:375:LEU:HD13	1.51	0.92
1:C:89:ARG:HB2	1:C:89:ARG:HH11	1.35	0.91
1:D:26:THR:HG22	1:D:29:TYR:HB2	1.53	0.91
1:D:293:ILE:HG21	1:D:318:LEU:CD1	2.00	0.91
1:D:383:HIS:H	1:D:386:HIS:CD2	1.88	0.91
1:D:452:SER:HB3	1:D:455:LEU:HB3	1.53	0.91
1:C:414:ALA:HB3	1:C:415:PRO:HD3	1.53	0.90
2:V:22:SER:H	2:V:25:GLN:HE21	1.18	0.90
1:D:89:ARG:HH11	1:D:89:ARG:HB2	1.37	0.90
1:D:383:HIS:H	1:D:386:HIS:HD2	1.13	0.88
1:D:414:ALA:HB3	1:D:415:PRO:HD3	1.54	0.88
2:U:11:LYS:HG3	2:U:17:TYR:CE1	2.09	0.88
2:U:79:ASP:CB	2:U:82:GLN:HE21	1.87	0.87
2:T:75:PHE:HD1	1:D:9:ALA:HB1	1.39	0.87
1:C:431:ARG:HB2	1:C:437:LEU:HD21	1.57	0.86
2:V:33:LEU:HD13	2:V:38:TRP:HB2	1.54	0.86
1:D:457:ALA:O	1:D:461:VAL:HG23	1.74	0.86
2:V:82:GLN:O	2:V:85:ALA:HB3	1.76	0.86
1:C:26:THR:CG2	1:C:29:TYR:HB2	2.06	0.86
2:T:60:GLY:O	2:T:65:ARG:NH2	2.09	0.85
1:B:304:GLN:HA	1:B:304:GLN:NE2	1.89	0.85
2:U:56:ASN:ND2	2:U:58:SER:H	1.73	0.85
1:A:26:THR:HG22	1:A:26:THR:O	1.77	0.85
1:C:455:LEU:HD12	1:C:455:LEU:O	1.77	0.85
1:A:293:ILE:HG21	1:A:318:LEU:CD1	2.06	0.84
2:S:22:SER:H	2:S:25:GLN:HE21	1.25	0.84
2:S:82:GLN:O	2:S:85:ALA:HB3	1.76	0.84
1:B:383:HIS:H	1:B:386:HIS:HD2	1.20	0.84
2:U:33:LEU:HD13	2:U:38:TRP:HB2	1.58	0.84
1:C:176:PRO:HD2	1:C:180:LEU:HD22	1.58	0.84
1:C:293:ILE:HG21	1:C:318:LEU:CD1	2.08	0.84
2:U:79:ASP:HB3	2:U:82:GLN:NE2	1.93	0.83
2:T:92:LYS:O	2:T:93:ALA:HB3	1.78	0.83
1:C:448:ALA:HA	1:C:451:TRP:CD1	2.12	0.83
1:D:26:THR:CG2	1:D:29:TYR:HB2	2.08	0.83
1:A:29:TYR:CD1	1:A:83:ARG:HD2	2.13	0.83
1:D:448:ALA:HA	1:D:451:TRP:CD1	2.12	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:THR:CG2	1:A:29:TYR:HB2	2.09	0.83
1:C:155:ILE:HG12	1:C:375:LEU:HD13	1.58	0.83
1:C:332:VAL:HG13	1:C:386:HIS:ND1	1.94	0.82
2:V:56:ASN:HB3	2:V:61:TYR:CD2	2.13	0.82
1:D:295:ARG:HG3	1:D:298:HIS:CD2	2.15	0.82
2:T:79:ASP:CB	2:T:82:GLN:HE21	1.93	0.82
1:D:79:ARG:HG2	1:D:79:ARG:NH1	1.92	0.82
1:A:155:ILE:HG12	1:A:375:LEU:HD13	1.63	0.81
2:T:77:CYS:HB2	2:T:82:GLN:OE1	1.81	0.80
1:D:414:ALA:O	1:D:418:VAL:HG23	1.81	0.80
2:U:33:LEU:HD12	2:U:33:LEU:C	2.07	0.80
1:B:293:ILE:HG21	1:B:318:LEU:CD1	2.11	0.80
1:C:387:MET:HE3	1:C:424:LEU:HB2	1.63	0.80
1:B:178:LEU:HD21	1:B:205:ASN:ND2	1.97	0.80
1:D:201:LYS:HE2	1:D:202:ASP:O	1.81	0.80
1:B:89:ARG:HH11	1:B:89:ARG:HB2	1.47	0.79
1:C:79:ARG:HG2	1:C:79:ARG:NH1	1.96	0.79
1:B:9:ALA:HB1	2:V:75:PHE:HD1	1.47	0.79
1:C:195:GLY:HA3	1:C:417:ALA:HB3	1.65	0.79
2:T:56:ASN:ND2	2:T:58:SER:H	1.81	0.78
2:V:56:ASN:ND2	2:V:58:SER:H	1.81	0.78
2:S:27:LEU:CD2	2:S:31:GLU:OE2	2.32	0.78
2:T:39:VAL:HG21	1:D:9:ALA:CB	2.13	0.78
2:U:93:ALA:C	2:U:95:PRO:HD3	2.09	0.78
1:A:79:ARG:HG2	1:A:79:ARG:NH1	1.95	0.78
1:A:90:VAL:HG21	1:A:96:GLN:HG2	1.65	0.78
1:B:383:HIS:H	1:B:386:HIS:CD2	2.02	0.78
1:B:26:THR:HG21	1:B:83:ARG:HD3	1.63	0.78
1:B:26:THR:HG22	1:B:29:TYR:HB2	1.64	0.78
1:B:79:ARG:HG2	1:B:79:ARG:HH11	1.47	0.77
2:V:93:ALA:C	2:V:95:PRO:HD3	2.09	0.77
1:A:293:ILE:HG21	1:A:318:LEU:HD13	1.65	0.77
2:S:93:ALA:C	2:S:95:PRO:HD3	2.10	0.77
2:T:92:LYS:O	2:T:93:ALA:CB	2.32	0.77
2:T:11:LYS:HG3	2:T:17:TYR:CE1	2.19	0.77
2:T:93:ALA:C	2:T:95:PRO:HD3	2.09	0.77
1:B:452:SER:HB3	1:B:455:LEU:HB3	1.67	0.77
1:D:317:ALA:HA	1:D:320:MET:HE3	1.66	0.76
1:D:293:ILE:HG13	1:D:318:LEU:HD11	1.67	0.76
1:B:9:ALA:CB	2:V:39:VAL:HG21	2.15	0.76
2:S:77:CYS:HB2	2:S:82:GLN:OE1	1.84	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:SER:HB2	1:D:156:GLN:HE22	1.49	0.76
1:D:202:ASP:OD1	1:D:238:HIS:HE1	1.67	0.76
1:B:293:ILE:HG21	1:B:318:LEU:HD13	1.67	0.76
1:B:317:ALA:HA	1:B:320:MET:HE3	1.68	0.76
1:B:202:ASP:OD1	1:B:238:HIS:HE1	1.69	0.75
1:D:171:GLY:O	1:D:402:PHE:N	2.18	0.75
1:C:387:MET:HB3	1:C:388:PRO:HD3	1.68	0.75
1:D:57:VAL:O	1:D:61:SER:HB2	1.85	0.75
1:B:71:THR:O	1:B:74:LEU:HB2	1.85	0.75
1:B:332:VAL:HG13	1:B:386:HIS:ND1	2.01	0.75
1:C:435:ARG:HD2	1:C:440:GLU:OE1	1.87	0.75
2:U:98:TRP:HD1	2:U:116:ILE:HD11	1.51	0.75
1:A:448:ALA:HA	1:A:451:TRP:CD1	2.22	0.74
1:A:71:THR:O	1:A:74:LEU:HB2	1.87	0.74
2:U:22:SER:H	2:U:25:GLN:HE21	1.33	0.74
1:A:43:THR:HG22	1:A:131:ARG:HG3	1.68	0.74
1:D:332:VAL:O	1:D:332:VAL:HG13	1.86	0.74
1:A:251:ILE:O	1:A:255:VAL:HG23	1.87	0.74
1:A:414:ALA:HB3	1:A:415:PRO:HD3	1.70	0.73
2:S:92:LYS:O	2:S:93:ALA:HB3	1.88	0.73
1:D:26:THR:HG21	1:D:83:ARG:HD3	1.67	0.73
1:C:43:THR:HG22	1:C:131:ARG:HG3	1.70	0.73
1:B:77:LEU:O	1:B:81:LYS:HG2	1.89	0.73
1:C:29:TYR:CD1	1:C:83:ARG:HD2	2.23	0.73
1:B:155:ILE:HG12	1:B:375:LEU:CD1	2.18	0.73
1:B:193:LEU:HD13	1:B:200:THR:HG23	1.70	0.73
1:C:26:THR:HG22	1:C:26:THR:O	1.89	0.73
2:S:33:LEU:HD13	2:S:38:TRP:HB2	1.70	0.73
1:A:383:HIS:H	1:A:386:HIS:HD2	1.36	0.73
2:U:82:GLN:O	2:U:85:ALA:HB3	1.89	0.73
1:D:29:TYR:OH	1:D:32:LYS:NZ	2.13	0.73
1:A:455:LEU:O	1:A:455:LEU:HD12	1.89	0.72
2:T:75:PHE:HD1	1:D:9:ALA:CB	2.01	0.72
2:V:94:TYR:HB3	2:V:97:ALA:HB2	1.71	0.72
1:A:26:THR:HG21	1:A:83:ARG:HD3	1.70	0.72
1:D:387:MET:HE3	1:D:424:LEU:HB2	1.69	0.71
1:C:304:GLN:HA	1:C:304:GLN:NE2	2.05	0.71
1:D:171:GLY:O	1:D:401:GLN:HA	1.90	0.71
1:B:414:ALA:HB3	1:B:415:PRO:HD3	1.72	0.71
1:A:19:GLU:HB3	1:A:52:GLU:OE1	1.90	0.71
1:B:332:VAL:HG13	1:B:332:VAL:O	1.91	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:ALA:HA	1:B:451:TRP:CD1	2.25	0.71
2:T:69:MET:HE3	2:T:72:LEU:HD12	1.72	0.71
1:C:181:SER:CB	1:D:156:GLN:HE22	2.03	0.71
2:U:86:GLU:HA	2:U:86:GLU:OE1	1.90	0.71
2:S:79:ASP:CB	2:S:82:GLN:HE21	2.03	0.70
1:A:29:TYR:CE2	1:A:31:THR:HA	2.25	0.70
2:U:3:VAL:HG21	2:V:70:TRP:CE3	2.27	0.70
1:C:120:ILE:HG22	1:C:121:VAL:HG23	1.73	0.70
1:C:383:HIS:H	1:C:386:HIS:CD2	2.10	0.70
1:A:293:ILE:HG13	1:A:318:LEU:HD11	1.73	0.70
2:T:75:PHE:CD1	1:D:9:ALA:CB	2.74	0.70
1:C:173:THR:HA	1:C:201:LYS:HG2	1.73	0.70
1:C:414:ALA:O	1:C:418:VAL:HG23	1.91	0.70
1:D:29:TYR:CD1	1:D:83:ARG:HD2	2.27	0.70
1:C:79:ARG:HH11	1:C:79:ARG:CG	1.91	0.70
2:V:77:CYS:HB2	2:V:82:GLN:OE1	1.92	0.70
1:C:171:GLY:O	1:C:401:GLN:HA	1.91	0.69
1:C:26:THR:HG21	1:C:83:ARG:HD3	1.74	0.69
2:V:79:ASP:HB3	2:V:82:GLN:NE2	1.98	0.69
1:D:26:THR:HG22	1:D:26:THR:O	1.92	0.69
1:B:200:THR:OG1	1:B:238:HIS:HD2	1.74	0.69
2:U:77:CYS:HB2	2:U:82:GLN:OE1	1.93	0.69
1:B:332:VAL:O	1:B:332:VAL:CG1	2.40	0.69
1:D:431:ARG:HB2	1:D:437:LEU:HD21	1.75	0.69
1:C:293:ILE:HG21	1:C:318:LEU:HD13	1.73	0.69
2:S:84:LEU:O	2:S:84:LEU:HD23	1.93	0.68
1:C:412:GLY:HA3	2:V:72:LEU:HD11	1.75	0.68
1:D:305:LYS:O	1:D:305:LYS:HG2	1.91	0.68
1:B:29:TYR:CD1	1:B:83:ARG:HD2	2.29	0.68
1:B:387:MET:HB3	1:B:388:PRO:HD3	1.74	0.68
1:B:431:ARG:HB2	1:B:437:LEU:HD21	1.75	0.68
1:C:383:HIS:H	1:C:386:HIS:HD2	1.39	0.68
1:B:19:GLU:HB3	1:B:52:GLU:OE1	1.94	0.68
1:C:52:GLU:O	1:C:53:ALA:C	2.36	0.68
2:V:79:ASP:H	2:V:82:GLN:NE2	1.91	0.68
1:B:178:LEU:CD2	1:B:205:ASN:ND2	2.57	0.68
2:S:11:LYS:HG3	2:S:17:TYR:CE1	2.28	0.68
1:D:293:ILE:HG21	1:D:318:LEU:HD13	1.72	0.68
1:A:332:VAL:HG13	1:A:386:HIS:ND1	2.08	0.67
1:A:443:GLU:O	1:A:447:GLU:HG3	1.94	0.67
1:B:194:ARG:NH2	2:T:4:TRP:O	2.26	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:94:TYR:N	2:T:95:PRO:HD3	2.09	0.67
1:A:26:THR:O	1:A:26:THR:CG2	2.40	0.67
2:S:43:GLU:OE1	2:S:100:ARG:NH1	2.27	0.67
2:U:92:LYS:O	2:U:93:ALA:HB3	1.93	0.67
1:B:414:ALA:O	1:B:418:VAL:HG23	1.94	0.67
1:A:431:ARG:HB2	1:A:437:LEU:HD21	1.75	0.67
1:D:293:ILE:HG21	1:D:318:LEU:HD11	1.77	0.67
1:D:90:VAL:HG21	1:D:96:GLN:HG2	1.75	0.67
1:C:209:GLN:HB3	1:C:210:PRO:CD	2.24	0.67
1:D:435:ARG:HD2	1:D:440:GLU:OE1	1.95	0.67
2:S:33:LEU:CD1	2:S:38:TRP:HB2	2.25	0.66
1:B:333:GLY:O	1:C:128:LYS:NZ	2.26	0.66
1:C:339:ARG:O	1:C:343:LEU:HG	1.95	0.66
1:D:176:PRO:HD2	1:D:180:LEU:CD2	2.23	0.66
1:D:466:VAL:HG23	1:D:468:ASN:H	1.59	0.66
1:A:194:ARG:NH2	2:S:4:TRP:O	2.27	0.66
1:A:436:ASP:OD1	1:A:438:ALA:N	2.28	0.66
2:S:92:LYS:O	2:S:93:ALA:CB	2.43	0.66
1:B:195:GLY:HA3	1:B:417:ALA:HB3	1.76	0.66
1:C:89:ARG:HB2	1:C:89:ARG:NH1	2.09	0.66
2:U:43:GLU:OE1	2:U:100:ARG:NH1	2.26	0.66
1:C:293:ILE:HG21	1:C:318:LEU:HD11	1.76	0.66
1:B:202:ASP:OD2	1:B:217:ARG:NH2	2.29	0.66
2:T:33:LEU:HD13	2:T:38:TRP:HB2	1.78	0.66
1:D:151:PRO:HG2	1:D:372:PRO:HB2	1.78	0.65
1:B:466:VAL:HG23	1:B:467:PHE:N	2.11	0.65
1:A:293:ILE:HG21	1:A:318:LEU:HD11	1.78	0.65
1:D:332:VAL:O	1:D:332:VAL:CG1	2.44	0.65
1:A:440:GLU:O	1:A:444:ILE:HG13	1.96	0.65
1:B:368:TRP:O	1:B:369:VAL:C	2.38	0.65
1:B:383:HIS:O	1:B:386:HIS:N	2.25	0.65
1:A:89:ARG:HB2	1:A:89:ARG:NH1	2.10	0.65
1:D:451:TRP:CH2	2:V:19:PRO:HD3	2.31	0.65
1:D:383:HIS:N	1:D:386:HIS:HD2	1.92	0.65
1:C:71:THR:O	1:C:74:LEU:HB2	1.96	0.64
1:D:455:LEU:O	1:D:455:LEU:HD12	1.96	0.64
1:A:383:HIS:H	1:A:386:HIS:CD2	2.13	0.64
1:B:142:PRO:HB3	1:B:369:VAL:HG11	1.79	0.64
2:V:43:GLU:HA	2:V:68:THR:O	1.96	0.64
2:T:22:SER:H	2:T:25:GLN:HE21	1.45	0.64
1:C:436:ASP:OD1	1:C:438:ALA:N	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:LEU:HD13	1:D:200:THR:HG23	1.79	0.64
1:C:457:ALA:O	1:C:461:VAL:HG23	1.98	0.64
2:U:56:ASN:HB3	2:U:61:TYR:CD1	2.33	0.64
1:D:79:ARG:HH11	1:D:79:ARG:CG	1.85	0.64
1:B:176:PRO:HD2	1:B:180:LEU:HD22	1.78	0.64
1:B:304:GLN:NE2	1:B:304:GLN:CA	2.60	0.64
1:C:202:ASP:OD1	1:C:238:HIS:HE1	1.81	0.64
1:C:292:HIS:HA	1:C:325:HIS:HB2	1.80	0.64
1:C:440:GLU:O	1:C:444:ILE:HG13	1.96	0.64
1:B:297:MET:CG	1:B:297:MET:O	2.46	0.64
1:B:79:ARG:HG2	1:B:79:ARG:NH1	2.13	0.64
2:T:79:ASP:HB3	2:T:82:GLN:NE2	2.02	0.64
2:U:27:LEU:O	2:U:31:GLU:HB2	1.97	0.64
1:D:29:TYR:OH	1:D:35:ASP:OD2	2.14	0.64
1:D:443:GLU:O	1:D:446:ARG:HB3	1.97	0.64
2:T:56:ASN:HB3	2:T:61:TYR:CD1	2.33	0.64
1:D:195:GLY:HA3	1:D:417:ALA:HB3	1.80	0.64
1:B:29:TYR:CE2	1:B:31:THR:HA	2.33	0.63
2:T:75:PHE:CD1	1:D:9:ALA:HB1	2.27	0.63
1:D:251:ILE:O	1:D:255:VAL:HG23	1.98	0.63
1:A:19:GLU:HB3	1:A:52:GLU:CD	2.23	0.63
2:U:98:TRP:HD1	2:U:116:ILE:CD1	2.10	0.63
2:S:23:GLN:O	2:S:27:LEU:HB2	1.98	0.63
2:T:43:GLU:OE1	2:T:100:ARG:NH1	2.31	0.63
1:C:19:GLU:HB3	1:C:52:GLU:CD	2.23	0.63
1:C:19:GLU:HB3	1:C:52:GLU:OE1	1.98	0.63
2:V:99:ILE:O	2:V:116:ILE:HG13	1.98	0.63
1:B:305:LYS:HG2	1:B:305:LYS:O	1.99	0.63
1:A:29:TYR:CG	1:A:83:ARG:HD2	2.32	0.63
1:B:9:ALA:CB	2:V:75:PHE:HD1	2.12	0.63
2:U:98:TRP:CD1	2:U:116:ILE:HD11	2.32	0.63
2:V:71:LYS:O	2:V:72:LEU:HD12	1.98	0.63
1:C:414:ALA:HB3	1:C:415:PRO:CD	2.28	0.63
2:U:33:LEU:CD1	2:U:38:TRP:HB2	2.29	0.63
1:D:43:THR:HG22	1:D:131:ARG:HG3	1.81	0.63
1:A:435:ARG:HD2	1:A:440:GLU:OE1	1.99	0.63
1:C:379:SER:OG	1:C:401:GLN:HB2	1.99	0.63
1:C:90:VAL:HG23	1:C:96:GLN:O	1.99	0.62
1:C:425:GLU:OE1	2:U:17:TYR:HB2	1.99	0.62
1:A:176:PRO:HD2	1:A:180:LEU:HD22	1.79	0.62
1:C:332:VAL:HG13	1:C:332:VAL:O	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:ILE:HD12	1:C:390:LEU:CD1	2.29	0.62
1:C:23:THR:HG22	1:C:81:LYS:NZ	2.14	0.62
1:A:62:SER:O	1:D:178:LEU:HD22	2.00	0.62
1:B:151:PRO:HB3	1:B:323:GLY:O	1.99	0.62
1:B:435:ARG:HD2	1:B:440:GLU:OE1	2.00	0.62
1:C:51:GLU:HA	1:C:87:ILE:HD11	1.81	0.62
1:C:379:SER:HB3	4:C:490:CAP:O3	2.00	0.62
2:S:96:GLN:OE1	2:S:96:GLN:N	2.28	0.62
1:A:429:LYS:NZ	2:S:29:GLU:OE1	2.33	0.62
1:B:363:TYR:CD1	1:B:363:TYR:N	2.67	0.62
1:C:192:CYS:HB3	1:C:197:LEU:HD23	1.82	0.62
1:A:207:ASN:O	1:A:217:ARG:NH2	2.26	0.61
1:B:443:GLU:OE1	1:B:446:ARG:NH2	2.33	0.61
1:C:305:LYS:O	1:C:305:LYS:HG2	1.98	0.61
1:B:207:ASN:O	1:B:217:ARG:NH1	2.27	0.61
1:C:269:TYR:CD1	1:C:293:ILE:CG2	2.84	0.61
1:A:195:GLY:HA3	1:A:417:ALA:HB3	1.81	0.61
2:U:60:GLY:O	2:U:65:ARG:NH2	2.33	0.61
2:U:117:ALA:O	2:U:118:TYR:HB2	2.00	0.61
1:D:166:GLY:O	1:D:167:ARG:HB3	1.99	0.61
1:A:134:ARG:HG3	1:A:135:LEU:N	2.15	0.61
1:B:440:GLU:O	1:B:444:ILE:HG13	2.00	0.61
1:B:90:VAL:HG21	1:B:96:GLN:HG2	1.82	0.61
2:U:84:LEU:HD23	2:U:84:LEU:O	2.00	0.61
1:B:297:MET:O	1:B:297:MET:HG3	1.99	0.61
2:T:75:PHE:CE1	1:D:9:ALA:HB2	2.36	0.61
1:D:387:MET:N	1:D:388:PRO:HD2	2.16	0.61
2:V:33:LEU:C	2:V:33:LEU:HD12	2.25	0.61
2:T:77:CYS:CB	2:T:82:GLN:OE1	2.48	0.61
1:C:158:GLU:OE2	1:C:325:HIS:NE2	2.28	0.61
1:D:199:PHE:HA	1:D:237:GLY:O	2.00	0.61
1:A:449:CYS:CB	1:A:459:CYS:SG	2.88	0.61
1:D:430:ALA:HB1	1:D:444:ILE:HD13	1.81	0.61
1:C:304:GLN:HA	1:C:304:GLN:HE21	1.65	0.61
1:D:38:ALA:HB2	1:D:138:LEU:HD23	1.82	0.61
1:A:45:GLN:OE1	1:A:131:ARG:HB3	2.01	0.60
1:C:382:ILE:HD12	1:C:390:LEU:HD13	1.83	0.60
1:D:430:ALA:CB	1:D:444:ILE:HD13	2.30	0.60
1:C:90:VAL:CG2	1:C:96:GLN:HG2	2.24	0.60
1:C:193:LEU:HD13	1:C:200:THR:HG23	1.82	0.60
2:V:11:LYS:HG3	2:V:17:TYR:CE1	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:VAL:O	1:B:61:SER:HB2	2.02	0.60
2:T:79:ASP:H	2:T:82:GLN:NE2	2.00	0.60
1:C:66:TRP:CE3	1:C:67:THR:HB	2.36	0.60
1:A:429:LYS:CE	2:S:29:GLU:OE1	2.50	0.60
1:D:26:THR:CG2	1:D:26:THR:O	2.49	0.60
1:A:181:SER:HB2	1:B:156:GLN:HE22	1.67	0.60
1:A:425:GLU:OE1	2:S:17:TYR:HB2	2.02	0.60
2:S:83:VAL:O	2:S:86:GLU:HB2	2.02	0.60
1:B:363:TYR:N	1:B:363:TYR:HD1	2.00	0.60
2:U:79:ASP:H	2:U:82:GLN:NE2	1.99	0.60
1:D:120:ILE:HG22	1:D:121:VAL:HG23	1.84	0.60
2:V:113:ILE:O	2:V:114:SER:HB2	2.02	0.60
2:S:60:GLY:O	2:S:65:ARG:NH2	2.35	0.59
1:C:383:HIS:NE2	1:C:465:ILE:HB	2.17	0.59
1:D:155:ILE:HG12	1:D:375:LEU:HD13	1.84	0.59
1:B:271:THR:HG1	1:C:118:THR:HG1	1.50	0.59
1:C:385:TRP:CZ2	1:C:459:CYS:HB3	2.37	0.59
2:U:6:PRO:HG3	2:V:44:PHE:CE2	2.37	0.59
2:U:79:ASP:H	2:U:82:GLN:HE22	1.50	0.59
2:U:92:LYS:O	2:U:93:ALA:CB	2.49	0.59
1:D:190:TYR:O	1:D:194:ARG:HG2	2.02	0.59
1:D:295:ARG:O	1:D:298:HIS:HB3	2.01	0.59
1:B:9:ALA:CB	2:V:75:PHE:CD1	2.84	0.59
1:B:381:GLY:HA2	1:C:66:TRP:CD1	2.37	0.59
1:D:190:TYR:CE1	1:D:227:LYS:HD3	2.38	0.59
1:A:101:VAL:HG12	1:A:102:ALA:N	2.16	0.59
1:C:462:TRP:O	1:C:465:ILE:HG12	2.02	0.59
1:B:208:SER:O	1:C:109:GLU:HB2	2.02	0.59
1:C:387:MET:HB3	1:C:388:PRO:CD	2.31	0.59
2:V:60:GLY:O	2:V:65:ARG:NH2	2.36	0.59
1:B:443:GLU:O	1:B:447:GLU:HG3	2.01	0.59
2:V:27:LEU:O	2:V:31:GLU:HB2	2.03	0.59
1:A:452:SER:HB3	1:A:455:LEU:HB3	1.84	0.59
2:S:79:ASP:H	2:S:82:GLN:NE2	2.01	0.59
2:T:96:GLN:OE1	2:T:96:GLN:N	2.28	0.58
1:C:454:GLU:CD	1:C:454:GLU:H	2.10	0.58
1:D:234:GLU:O	1:D:236:LYS:HG2	2.03	0.58
1:D:440:GLU:O	1:D:444:ILE:HG13	2.02	0.58
2:V:56:ASN:ND2	2:V:58:SER:OG	2.36	0.58
1:B:171:GLY:O	1:B:401:GLN:HA	2.03	0.58
1:D:385:TRP:CZ2	1:D:459:CYS:HB3	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:69:MET:HE3	2:S:72:LEU:HD12	1.83	0.58
1:B:378:ALA:HB3	1:B:400:LEU:HD23	1.86	0.58
1:D:32:LYS:NZ	1:D:35:ASP:OD1	2.25	0.58
1:D:368:TRP:O	1:D:369:VAL:C	2.46	0.58
1:D:436:ASP:OD1	1:D:438:ALA:N	2.36	0.58
1:B:66:TRP:CE3	1:B:67:THR:HB	2.38	0.58
1:B:79:ARG:HH11	1:B:79:ARG:CG	2.15	0.58
1:C:448:ALA:HA	1:C:451:TRP:HD1	1.65	0.58
1:D:94:LYS:O	1:D:95:ASP:C	2.45	0.58
2:V:27:LEU:HD12	2:V:84:LEU:CD1	2.33	0.58
1:A:137:ASP:OD1	1:A:138:LEU:N	2.35	0.58
1:D:97:TYR:O	1:D:98:ILE:HD13	2.03	0.58
2:U:23:GLN:O	2:U:27:LEU:HB2	2.04	0.58
2:V:33:LEU:CD1	2:V:38:TRP:HB2	2.31	0.58
1:C:10:SER:O	1:C:11:VAL:HB	2.04	0.58
1:C:459:CYS:O	1:C:463:LYS:HB2	2.04	0.58
1:B:209:GLN:HB3	1:B:210:PRO:CD	2.34	0.58
2:V:56:ASN:HB3	2:V:61:TYR:CG	2.39	0.58
1:C:443:GLU:O	1:C:447:GLU:N	2.32	0.58
1:D:429:LYS:NZ	2:V:29:GLU:OE1	2.37	0.58
1:A:414:ALA:O	1:A:418:VAL:HG23	2.04	0.57
2:S:77:CYS:SG	2:S:82:GLN:NE2	2.77	0.57
1:B:387:MET:HE3	1:B:424:LEU:HB2	1.86	0.57
1:C:209:GLN:HB3	1:C:210:PRO:HD2	1.86	0.57
1:D:332:VAL:HG13	1:D:386:HIS:ND1	2.19	0.57
1:A:466:VAL:HG23	1:A:468:ASN:H	1.69	0.57
2:T:39:VAL:HG21	1:D:9:ALA:HB2	1.85	0.57
1:C:19:GLU:HB3	1:C:52:GLU:OE2	2.04	0.57
1:C:26:THR:HG22	1:C:29:TYR:CB	2.25	0.57
1:C:32:LYS:NZ	1:C:35:ASP:OD1	2.35	0.57
1:C:443:GLU:O	1:C:446:ARG:HB3	2.04	0.57
2:U:96:GLN:OE1	2:U:96:GLN:N	2.31	0.57
1:D:23:THR:HB	1:D:24:TYR:CD1	2.39	0.57
1:D:71:THR:O	1:D:74:LEU:HB2	2.05	0.57
1:D:133:LEU:O	1:D:307:HIS:HA	2.04	0.57
1:A:94:LYS:O	1:A:95:ASP:C	2.47	0.57
1:A:443:GLU:O	1:A:447:GLU:N	2.37	0.57
1:B:127:PHE:CE1	1:C:335:LEU:HD21	2.40	0.57
1:D:378:ALA:HB3	1:D:400:LEU:HD23	1.85	0.57
2:V:92:LYS:O	2:V:93:ALA:HB3	2.05	0.57
2:T:27:LEU:HD12	2:T:84:LEU:CD1	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:VAL:O	1:C:61:SER:HB2	2.04	0.57
1:C:94:LYS:O	1:C:96:GLN:N	2.38	0.57
1:C:317:ALA:HA	1:C:320:MET:HE3	1.86	0.57
2:U:43:GLU:HA	2:U:68:THR:O	2.04	0.57
2:U:119:LYS:HD2	2:U:123:TYR:C	2.29	0.57
1:D:202:ASP:OD1	1:D:238:HIS:CE1	2.55	0.57
1:B:250:MET:HE1	1:B:276:ALA:O	2.05	0.57
1:B:429:LYS:HE3	2:T:21:LEU:HD22	1.87	0.57
1:D:89:ARG:HB2	1:D:89:ARG:NH1	2.16	0.57
1:D:304:GLN:HA	1:D:304:GLN:NE2	2.19	0.57
2:T:94:TYR:HB3	2:T:97:ALA:HB2	1.85	0.57
1:C:155:ILE:HG12	1:C:375:LEU:CD1	2.31	0.57
1:C:293:ILE:HG13	1:C:318:LEU:HD11	1.85	0.56
1:A:120:ILE:HD13	1:A:138:LEU:HD21	1.86	0.56
1:A:193:LEU:HD13	1:A:200:THR:HG23	1.87	0.56
1:B:387:MET:HB3	1:B:388:PRO:CD	2.35	0.56
2:T:77:CYS:SG	2:T:82:GLN:CD	2.88	0.56
1:C:94:LYS:O	1:C:95:ASP:C	2.49	0.56
1:C:264:ILE:HG13	1:C:290:LEU:O	2.05	0.56
2:U:94:TYR:N	2:U:95:PRO:HD3	2.20	0.56
1:D:19:GLU:HB3	1:D:52:GLU:CD	2.31	0.56
1:D:383:HIS:NE2	1:D:465:ILE:HB	2.20	0.56
1:A:449:CYS:HB3	1:A:459:CYS:SG	2.45	0.56
1:B:425:GLU:OE1	2:T:17:TYR:N	2.36	0.56
2:T:86:GLU:OE1	2:T:86:GLU:HA	2.05	0.56
1:C:332:VAL:O	1:C:332:VAL:CG1	2.53	0.56
2:V:94:TYR:N	2:V:95:PRO:HD3	2.20	0.56
2:T:77:CYS:SG	2:T:78:THR:N	2.75	0.56
2:T:77:CYS:SG	2:T:82:GLN:NE2	2.79	0.56
1:C:26:THR:CG2	1:C:26:THR:O	2.51	0.56
1:D:181:SER:O	1:D:182:ALA:C	2.49	0.56
1:C:90:VAL:HG23	1:C:96:GLN:C	2.31	0.56
1:A:305:LYS:O	1:A:305:LYS:HG2	2.06	0.56
2:S:26:LEU:C	2:S:26:LEU:HD23	2.31	0.56
2:T:101:ILE:HG13	2:T:117:ALA:HB2	1.87	0.56
1:C:447:GLU:O	1:C:450:LYS:HB2	2.06	0.56
1:A:181:SER:CB	1:B:156:GLN:HE22	2.18	0.56
1:B:466:VAL:HG23	1:B:468:ASN:H	1.71	0.56
1:C:431:ARG:CB	1:C:437:LEU:HD21	2.34	0.56
2:S:34:LEU:O	2:S:35:LYS:C	2.48	0.55
1:B:387:MET:N	1:B:388:PRO:HD2	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:VAL:HG23	1:D:97:TYR:HA	1.87	0.55
1:D:331:VAL:HG12	1:D:332:VAL:N	2.20	0.55
1:C:45:GLN:OE1	1:C:131:ARG:HB3	2.07	0.55
1:C:306:ASN:OD1	1:C:306:ASN:N	2.33	0.55
1:D:387:MET:HE2	1:D:423:ALA:HB3	1.89	0.55
1:C:383:HIS:O	1:C:386:HIS:N	2.36	0.55
1:C:443:GLU:O	1:C:447:GLU:HG3	2.06	0.55
1:A:209:GLN:HB3	1:A:210:PRO:HD2	1.88	0.55
1:C:378:ALA:HB3	1:C:400:LEU:HD23	1.87	0.55
1:A:63:THR:HA	1:D:177:LYS:HB2	1.89	0.55
1:A:440:GLU:O	1:A:441:GLY:C	2.49	0.55
2:S:103:GLY:HA3	2:S:113:ILE:HG22	1.88	0.55
1:B:19:GLU:HB3	1:B:52:GLU:CD	2.31	0.55
1:B:173:THR:HA	1:B:201:LYS:HG2	1.88	0.55
1:B:422:VAL:O	1:B:423:ALA:C	2.48	0.55
1:C:466:VAL:HG23	1:C:468:ASN:H	1.72	0.55
2:U:83:VAL:O	2:U:86:GLU:HB2	2.06	0.55
1:B:60:GLU:OE2	1:B:65:THR:HA	2.07	0.55
2:T:42:LEU:HB3	2:T:70:TRP:HB3	1.88	0.55
1:C:214:TRP:CD2	1:C:253:ARG:HG2	2.42	0.55
2:U:26:LEU:C	2:U:26:LEU:HD23	2.32	0.55
1:D:304:GLN:HA	1:D:304:GLN:HE21	1.72	0.55
1:B:293:ILE:HG21	1:B:318:LEU:HD11	1.88	0.55
1:B:436:ASP:OD1	1:B:436:ASP:C	2.50	0.55
1:C:234:GLU:OE2	1:C:421:ARG:NH2	2.38	0.55
1:D:166:GLY:O	1:D:167:ARG:CB	2.54	0.55
1:A:94:LYS:O	1:A:96:GLN:N	2.40	0.55
1:C:298:HIS:CG	1:C:299:ALA:N	2.75	0.55
1:D:173:THR:HA	1:D:201:LYS:HG2	1.88	0.55
1:D:448:ALA:HA	1:D:451:TRP:HD1	1.70	0.55
1:A:190:TYR:O	1:A:194:ARG:HG2	2.06	0.54
2:S:33:LEU:C	2:S:33:LEU:HD12	2.32	0.54
1:B:445:ILE:HG13	1:B:446:ARG:N	2.22	0.54
2:U:56:ASN:HD21	2:U:58:SER:CB	2.19	0.54
1:A:42:VAL:HG13	1:A:97:TYR:HB2	1.90	0.54
1:B:201:LYS:HE2	1:B:202:ASP:O	2.07	0.54
2:U:33:LEU:C	2:U:33:LEU:CD1	2.79	0.54
1:A:295:ARG:O	1:A:298:HIS:HB3	2.08	0.54
2:T:39:VAL:CG2	1:D:9:ALA:CB	2.85	0.54
2:V:77:CYS:SG	2:V:78:THR:N	2.80	0.54
2:U:6:PRO:HG3	2:V:44:PHE:HE2	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:94:TYR:N	2:S:95:PRO:HD3	2.21	0.54
1:B:425:GLU:OE1	2:T:17:TYR:HB2	2.07	0.54
1:D:94:LYS:O	1:D:96:GLN:N	2.40	0.54
1:A:181:SER:O	1:A:182:ALA:C	2.51	0.54
1:C:201:LYS:HE2	1:C:202:ASP:O	2.08	0.54
1:D:29:TYR:CG	1:D:83:ARG:HD2	2.43	0.54
1:D:190:TYR:CZ	1:D:194:ARG:HD2	2.43	0.54
2:U:79:ASP:CB	2:U:82:GLN:NE2	2.61	0.54
1:B:454:GLU:H	1:B:454:GLU:CD	2.16	0.54
1:C:382:ILE:HG13	1:C:402:PHE:CE1	2.43	0.54
1:D:449:CYS:HA	1:D:455:LEU:HG	1.89	0.54
1:A:138:LEU:O	1:A:316:LYS:NZ	2.40	0.54
1:D:298:HIS:ND1	1:D:302:ASP:OD2	2.21	0.54
2:U:56:ASN:ND2	2:U:58:SER:OG	2.41	0.53
1:D:45:GLN:OE1	1:D:131:ARG:HB3	2.09	0.53
2:S:77:CYS:CB	2:S:82:GLN:OE1	2.55	0.53
2:U:3:VAL:HG22	2:V:71:LYS:H	1.74	0.53
1:A:79:ARG:HH11	1:A:79:ARG:CG	1.97	0.53
1:A:319:ARG:HD2	1:A:371:LEU:HD23	1.89	0.53
1:B:9:ALA:HB3	2:V:39:VAL:HG21	1.91	0.53
1:B:43:THR:O	1:B:43:THR:HG22	2.06	0.53
1:C:29:TYR:CE2	1:C:31:THR:HA	2.43	0.53
1:C:251:ILE:O	1:C:255:VAL:HG23	2.09	0.53
1:D:101:VAL:HG12	1:D:102:ALA:N	2.24	0.53
1:D:214:TRP:CD2	1:D:253:ARG:HG2	2.44	0.53
1:D:383:HIS:O	1:D:386:HIS:N	2.41	0.53
2:V:79:ASP:HB3	2:V:82:GLN:HB3	1.89	0.53
1:B:190:TYR:CE1	1:B:227:LYS:HD3	2.44	0.53
1:B:443:GLU:O	1:B:447:GLU:N	2.39	0.53
2:T:69:MET:CE	2:T:72:LEU:HD12	2.38	0.53
1:C:454:GLU:CD	1:C:454:GLU:N	2.66	0.53
2:U:79:ASP:O	2:U:82:GLN:N	2.42	0.53
1:B:298:HIS:ND1	1:B:302:ASP:OD2	2.33	0.53
2:V:113:ILE:HG13	2:V:114:SER:N	2.23	0.53
1:A:368:TRP:O	1:A:369:VAL:C	2.49	0.53
2:V:84:LEU:O	2:V:84:LEU:HD23	2.09	0.53
1:A:383:HIS:NE2	1:A:465:ILE:HB	2.23	0.53
1:C:23:THR:HG22	1:C:81:LYS:HZ3	1.74	0.53
1:C:411:TRP:CH2	2:U:2:GLN:OE1	2.62	0.53
1:A:202:ASP:OD1	1:A:238:HIS:HE1	1.92	0.53
1:A:209:GLN:HB3	1:A:210:PRO:CD	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:ASP:OD2	2:T:108:ARG:NH2	2.42	0.53
1:A:9:ALA:N	1:A:73:GLY:O	2.42	0.52
1:A:97:TYR:C	1:A:98:ILE:HD13	2.33	0.52
2:S:77:CYS:SG	2:S:82:GLN:CD	2.92	0.52
1:C:29:TYR:CG	1:C:83:ARG:HD2	2.44	0.52
1:C:133:LEU:O	1:C:307:HIS:HA	2.10	0.52
1:C:429:LYS:HE3	2:U:21:LEU:HD22	1.90	0.52
1:C:429:LYS:NZ	2:U:29:GLU:OE1	2.42	0.52
2:U:84:LEU:HD23	2:U:84:LEU:C	2.34	0.52
1:D:178:LEU:HD21	1:D:205:ASN:ND2	2.25	0.52
1:B:69:VAL:HA	1:C:407:LEU:O	2.09	0.52
1:B:94:LYS:O	1:B:95:ASP:C	2.50	0.52
1:C:332:VAL:CG1	1:C:386:HIS:ND1	2.71	0.52
2:S:86:GLU:OE1	2:S:86:GLU:HA	2.08	0.52
1:C:76:SER:O	1:C:76:SER:OG	2.23	0.52
1:C:430:ALA:CB	1:C:444:ILE:HD13	2.39	0.52
1:D:134:ARG:HA	1:D:308:GLY:O	2.10	0.52
2:V:89:GLU:O	2:V:92:LYS:NZ	2.35	0.52
2:V:113:ILE:HG13	2:V:114:SER:H	1.73	0.52
2:S:34:LEU:O	2:S:36:ASN:N	2.42	0.52
1:B:214:TRP:CD2	1:B:253:ARG:HG2	2.44	0.52
1:B:410:PRO:HD3	1:B:461:VAL:HG21	1.90	0.52
2:T:75:PHE:CD1	1:D:9:ALA:HB2	2.43	0.52
1:D:192:CYS:SG	1:D:413:ASN:ND2	2.83	0.52
1:A:155:ILE:HG12	1:A:375:LEU:CD1	2.38	0.52
1:B:335:LEU:HD21	1:C:127:PHE:CE1	2.45	0.52
1:B:466:VAL:HG23	1:B:468:ASN:N	2.25	0.52
1:D:190:TYR:HB2	1:D:224:ALA:HB1	1.92	0.52
1:A:397:ASP:OD2	2:S:108:ARG:NH2	2.43	0.52
2:S:27:LEU:O	2:S:31:GLU:HB2	2.10	0.52
1:B:32:LYS:O	1:B:35:ASP:HB2	2.10	0.52
2:T:22:SER:OG	2:T:25:GLN:HB2	2.09	0.52
1:C:214:TRP:CE3	1:C:253:ARG:HG2	2.45	0.52
2:U:107:VAL:HG12	2:U:107:VAL:O	2.08	0.52
1:B:440:GLU:O	1:B:441:GLY:C	2.52	0.52
1:C:227:LYS:HE2	2:V:66:TYR:O	2.10	0.52
1:A:50:PRO:HG3	1:A:97:TYR:CZ	2.45	0.52
1:A:241:ASN:ND2	1:A:243:THR:H	2.08	0.52
1:A:387:MET:HB3	1:A:388:PRO:HD3	1.92	0.52
1:C:153:HIS:N	1:C:324:ASP:OD1	2.41	0.52
1:D:10:SER:O	1:D:11:VAL:HB	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:TYR:C	1:D:98:ILE:HD13	2.34	0.52
2:S:56:ASN:ND2	2:S:58:SER:OG	2.42	0.52
1:C:449:CYS:HA	1:C:455:LEU:HG	1.92	0.52
2:U:106:ASN:OD1	2:U:106:ASN:C	2.52	0.52
2:S:98:TRP:HD1	2:S:116:ILE:HD11	1.74	0.51
1:B:9:ALA:HB2	2:V:75:PHE:CE1	2.45	0.51
1:C:60:GLU:OE2	1:C:65:THR:HA	2.09	0.51
1:C:166:GLY:O	1:C:167:ARG:HB3	2.09	0.51
1:D:214:TRP:CE3	1:D:253:ARG:HG2	2.45	0.51
2:V:27:LEU:HD12	2:V:84:LEU:HD12	1.92	0.51
1:B:318:LEU:C	1:B:320:MET:N	2.66	0.51
1:C:436:ASP:OD1	1:C:436:ASP:C	2.53	0.51
2:V:77:CYS:CB	2:V:82:GLN:OE1	2.58	0.51
1:C:153:HIS:CD2	1:C:290:LEU:HD23	2.45	0.51
1:C:178:LEU:HD21	1:C:205:ASN:ND2	2.26	0.51
2:U:89:GLU:O	2:U:92:LYS:HB3	2.09	0.51
1:A:21:LYS:HB2	1:A:52:GLU:OE1	2.10	0.51
1:A:24:TYR:HB2	1:A:55:ALA:HB1	1.93	0.51
1:B:418:VAL:O	1:B:419:ALA:C	2.52	0.51
1:B:442:ASN:OD1	1:B:446:ARG:NH1	2.40	0.51
1:B:443:GLU:OE2	1:B:446:ARG:NE	2.42	0.51
2:T:23:GLN:O	2:T:27:LEU:HB2	2.09	0.51
1:C:269:TYR:CD1	1:C:293:ILE:HG21	2.46	0.51
1:B:93:GLU:OE1	1:B:93:GLU:HA	2.10	0.51
1:C:331:VAL:HG12	1:C:332:VAL:N	2.24	0.51
1:B:411:TRP:CH2	2:T:2:GLN:OE1	2.63	0.51
2:V:26:LEU:C	2:V:26:LEU:HD23	2.36	0.51
1:A:43:THR:HG22	1:A:131:ARG:CG	2.38	0.51
1:B:133:LEU:O	1:B:307:HIS:HA	2.11	0.51
1:D:209:GLN:HB3	1:D:210:PRO:HD2	1.93	0.51
1:D:459:CYS:O	1:D:463:LYS:HB2	2.11	0.51
2:S:19:PRO:O	2:S:20:ASP:C	2.53	0.51
1:B:59:ALA:C	1:B:61:SER:H	2.19	0.51
2:U:35:LYS:HD2	2:U:35:LYS:O	2.11	0.51
1:D:446:ARG:HG3	1:D:446:ARG:O	2.11	0.51
2:V:25:GLN:O	2:V:28:SER:HB2	2.11	0.51
1:D:189:VAL:HG13	1:D:200:THR:OG1	2.10	0.51
1:D:269:TYR:CD1	1:D:293:ILE:CG2	2.94	0.51
2:V:86:GLU:O	2:V:89:GLU:HB3	2.11	0.51
1:A:412:GLY:HA3	2:T:72:LEU:HD11	1.93	0.50
1:D:385:TRP:HZ2	1:D:459:CYS:HB3	1.75	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:ASP:OD1	1:D:436:ASP:C	2.53	0.50
1:B:17:VAL:HG12	1:B:18:LYS:N	2.27	0.50
1:B:26:THR:HG22	1:B:26:THR:O	2.11	0.50
1:B:190:TYR:HB2	1:B:224:ALA:HB1	1.94	0.50
1:B:229:GLN:HE21	1:B:236:LYS:H	1.58	0.50
1:C:241:ASN:HD22	1:C:242:ALA:N	2.09	0.50
1:C:250:MET:HE1	1:C:276:ALA:O	2.11	0.50
1:C:330:THR:O	1:C:331:VAL:HB	2.11	0.50
1:A:72:ASP:HB3	1:A:77:LEU:HD21	1.94	0.50
2:S:84:LEU:HD23	2:S:84:LEU:C	2.36	0.50
1:B:283:TYR:CD1	1:B:283:TYR:C	2.88	0.50
1:B:363:TYR:HD1	1:B:363:TYR:H	1.57	0.50
2:U:11:LYS:HG3	2:U:17:TYR:HE1	1.73	0.50
1:D:299:ALA:HA	1:D:302:ASP:OD1	2.12	0.50
1:A:26:THR:HG22	1:A:29:TYR:CB	2.29	0.50
1:B:455:LEU:HD12	1:B:455:LEU:O	2.12	0.50
1:C:190:TYR:CE1	1:C:227:LYS:HD3	2.46	0.50
1:A:60:GLU:OE1	1:D:334:LYS:HE3	2.12	0.50
1:C:43:THR:HG22	1:C:43:THR:O	2.10	0.50
1:C:336:GLU:OE2	1:C:472:VAL:HB	2.12	0.50
1:D:9:ALA:N	1:D:73:GLY:O	2.45	0.50
2:V:83:VAL:O	2:V:86:GLU:HB2	2.12	0.50
2:T:12:TYR:HE2	2:T:98:TRP:NE1	2.10	0.50
1:C:304:GLN:NE2	1:C:304:GLN:CA	2.73	0.50
2:U:79:ASP:O	2:U:80:ALA:C	2.54	0.50
1:D:19:GLU:HB3	1:D:52:GLU:OE2	2.12	0.50
1:A:60:GLU:O	1:D:177:LYS:HE3	2.11	0.50
1:A:151:PRO:O	1:A:285:ARG:NH1	2.45	0.50
2:S:44:PHE:HA	2:S:98:TRP:O	2.11	0.50
1:B:127:PHE:CD1	1:C:335:LEU:HD23	2.47	0.50
1:B:436:ASP:OD1	1:B:438:ALA:N	2.44	0.50
1:C:9:ALA:N	1:C:73:GLY:O	2.45	0.50
1:C:345:PHE:HA	1:C:348:LEU:HB2	1.92	0.50
1:B:120:ILE:HG22	1:B:121:VAL:HG23	1.94	0.50
1:C:442:ASN:O	1:C:446:ARG:HB2	2.12	0.50
1:C:455:LEU:HD12	1:C:455:LEU:C	2.36	0.50
1:A:60:GLU:OE2	1:A:65:THR:HA	2.11	0.50
1:A:317:ALA:HA	1:A:320:MET:HE3	1.94	0.50
2:T:31:GLU:OE2	2:T:80:ALA:HB2	2.12	0.50
1:C:158:GLU:CD	1:C:325:HIS:HE2	2.18	0.50
1:A:151:PRO:HB3	1:A:323:GLY:O	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:TYR:CZ	1:A:194:ARG:HD2	2.47	0.49
1:A:378:ALA:HB3	1:A:400:LEU:HD23	1.92	0.49
1:C:41:ARG:O	1:C:41:ARG:HG2	2.12	0.49
1:B:157:VAL:O	1:B:161:LYS:HG2	2.13	0.49
1:D:313:VAL:O	1:D:314:LEU:C	2.55	0.49
1:A:336:GLU:OE2	1:A:472:VAL:HB	2.12	0.49
1:C:194:ARG:NH2	2:U:4:TRP:O	2.39	0.49
2:U:72:LEU:HG	2:U:73:PRO:HD2	1.94	0.49
1:A:51:GLU:HA	1:A:87:ILE:HD11	1.95	0.49
1:A:127:PHE:HA	1:D:335:LEU:HD23	1.94	0.49
1:D:98:ILE:HG22	1:D:100:TYR:CE1	2.47	0.49
1:A:158:GLU:CD	1:A:325:HIS:HE2	2.16	0.49
1:A:185:TYR:O	1:A:189:VAL:HG23	2.12	0.49
1:A:436:ASP:OD1	1:A:436:ASP:C	2.55	0.49
1:C:423:ALA:O	1:C:426:ALA:HB3	2.11	0.49
1:C:429:LYS:CE	2:U:29:GLU:OE1	2.61	0.49
1:D:207:ASN:O	1:D:217:ARG:NH2	2.30	0.49
2:V:26:LEU:O	2:V:29:GLU:HB2	2.12	0.49
2:V:56:ASN:HD21	2:V:58:SER:CB	2.25	0.49
2:V:79:ASP:CB	2:V:82:GLN:NE2	2.65	0.49
1:A:60:GLU:HG3	1:A:127:PHE:CZ	2.47	0.49
1:B:134:ARG:HA	1:B:308:GLY:O	2.12	0.49
1:B:332:VAL:CG1	1:B:386:HIS:ND1	2.73	0.49
1:C:43:THR:HG22	1:C:131:ARG:CG	2.40	0.49
1:D:26:THR:HG22	1:D:29:TYR:CB	2.34	0.49
1:D:29:TYR:CE2	1:D:31:THR:HA	2.48	0.49
2:V:23:GLN:O	2:V:27:LEU:HB2	2.13	0.49
1:A:298:HIS:CG	1:A:299:ALA:N	2.81	0.49
1:A:466:VAL:HG23	1:A:467:PHE:N	2.28	0.49
2:T:56:ASN:HD21	2:T:58:SER:CB	2.25	0.49
1:D:86:ARG:HG3	1:D:86:ARG:HH11	1.78	0.49
1:A:66:TRP:CE3	1:A:67:THR:HB	2.48	0.49
2:S:91:LYS:HD2	2:S:118:TYR:CD2	2.48	0.49
1:C:142:PRO:HB3	1:C:369:VAL:HG11	1.94	0.49
1:D:455:LEU:O	1:D:458:ALA:HB3	2.13	0.49
1:A:142:PRO:HB3	1:A:369:VAL:HG11	1.94	0.49
1:A:190:TYR:HB2	1:A:224:ALA:HB1	1.95	0.49
1:B:138:LEU:O	1:B:316:LYS:NZ	2.44	0.49
1:B:190:TYR:CZ	1:B:227:LYS:HD3	2.47	0.49
1:D:167:ARG:O	1:D:167:ARG:HG3	2.12	0.49
1:D:193:LEU:CD1	1:D:200:THR:HG23	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:ARG:O	1:D:343:LEU:HG	2.12	0.49
2:V:86:GLU:OE1	2:V:86:GLU:HA	2.12	0.49
1:A:118:THR:HG21	1:D:204:GLU:O	2.13	0.49
1:A:190:TYR:CE1	1:A:227:LYS:HD3	2.48	0.49
1:A:202:ASP:OD2	1:A:217:ARG:NH1	2.46	0.49
1:B:24:TYR:CD2	1:B:59:ALA:HB2	2.48	0.49
1:B:26:THR:CG2	1:B:29:TYR:HB2	2.38	0.49
1:B:42:VAL:HG13	1:B:97:TYR:HB2	1.95	0.49
1:B:251:ILE:O	1:B:255:VAL:HG23	2.13	0.49
1:D:60:GLU:OE2	1:D:65:THR:HA	2.13	0.49
1:D:331:VAL:HG21	1:D:339:ARG:HA	1.95	0.49
2:V:79:ASP:N	2:V:82:GLN:NE2	2.61	0.49
1:A:97:TYR:O	1:A:98:ILE:HD13	2.12	0.48
1:A:336:GLU:OE2	1:A:473:ASP:N	2.46	0.48
1:A:436:ASP:O	1:A:440:GLU:HB2	2.12	0.48
2:V:33:LEU:HD22	2:V:113:ILE:HG21	1.94	0.48
1:A:223:GLU:OE1	2:T:65:ARG:HD3	2.12	0.48
1:A:61:SER:HB3	1:A:103:TYR:HE1	1.78	0.48
1:B:429:LYS:NZ	2:T:29:GLU:OE1	2.46	0.48
1:C:202:ASP:OD1	1:C:238:HIS:CE1	2.64	0.48
1:C:229:GLN:HE21	1:C:236:LYS:H	1.60	0.48
2:U:86:GLU:O	2:U:89:GLU:HB3	2.12	0.48
1:D:203:ASP:HA	5:D:492:FMT:O1	2.13	0.48
1:B:52:GLU:O	1:B:53:ALA:C	2.56	0.48
1:D:42:VAL:HG23	1:D:130:LEU:HD22	1.95	0.48
2:V:11:LYS:HE3	2:V:17:TYR:CZ	2.48	0.48
1:A:153:HIS:CD2	1:A:290:LEU:HD23	2.48	0.48
1:A:414:ALA:O	1:A:417:ALA:HB3	2.13	0.48
1:A:462:TRP:O	1:A:465:ILE:HG12	2.13	0.48
1:B:295:ARG:O	1:B:298:HIS:HB3	2.14	0.48
1:D:311:PHE:O	1:D:312:ARG:C	2.55	0.48
2:S:58:SER:O	2:S:59:PRO:C	2.55	0.48
1:B:177:LYS:HB2	1:C:63:THR:HA	1.95	0.48
1:B:192:CYS:HB3	1:B:197:LEU:HD23	1.96	0.48
1:D:23:THR:HB	1:D:24:TYR:CE1	2.49	0.48
1:D:440:GLU:O	1:D:441:GLY:C	2.56	0.48
1:A:162:LEU:O	1:A:164:LYS:HG3	2.13	0.48
1:A:339:ARG:O	1:A:343:LEU:HG	2.14	0.48
1:B:97:TYR:C	1:B:98:ILE:HD13	2.38	0.48
1:B:167:ARG:O	1:B:167:ARG:HG3	2.13	0.48
2:T:44:PHE:HA	2:T:98:TRP:O	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:MET:HB3	1:D:388:PRO:HD3	1.95	0.48
2:V:22:SER:H	2:V:25:GLN:NE2	1.98	0.48
1:B:86:ARG:NH1	1:B:86:ARG:HG3	2.29	0.48
1:B:331:VAL:HG12	1:B:332:VAL:N	2.29	0.48
1:B:454:GLU:CD	1:B:454:GLU:N	2.72	0.48
1:D:202:ASP:OD2	1:D:217:ARG:NH1	2.46	0.48
1:B:48:VAL:HA	1:B:49:PRO:HD2	1.78	0.48
1:B:120:ILE:HD13	1:B:138:LEU:CD2	2.44	0.48
2:T:98:TRP:HD1	2:T:116:ILE:HD11	1.78	0.48
2:U:69:MET:HE3	2:U:72:LEU:HD12	1.96	0.48
2:U:73:PRO:HG2	2:U:75:PHE:CE2	2.49	0.48
2:U:77:CYS:SG	2:U:78:THR:N	2.86	0.48
1:D:175:LYS:NZ	4:D:490:CAP:O1	2.41	0.48
1:A:90:VAL:HG23	1:A:97:TYR:HA	1.96	0.48
1:B:141:PRO:O	1:B:142:PRO:C	2.56	0.48
1:C:295:ARG:O	1:C:296:ALA:C	2.56	0.48
1:D:239:TYR:CE2	1:D:292:HIS:CD2	3.02	0.48
1:A:133:LEU:O	1:A:307:HIS:HA	2.14	0.47
1:C:445:ILE:HD12	1:C:449:CYS:SG	2.53	0.47
1:D:164:LYS:NZ	1:D:198:ASP:OD1	2.38	0.47
2:T:39:VAL:CG2	1:D:9:ALA:HB3	2.44	0.47
1:C:389:ALA:O	1:C:392:GLU:HB3	2.13	0.47
2:U:15:LEU:C	2:U:17:TYR:H	2.22	0.47
1:B:43:THR:HG22	1:B:131:ARG:HG3	1.96	0.47
1:B:327:HIS:HA	1:B:377:VAL:HB	1.97	0.47
2:T:82:GLN:O	2:T:85:ALA:HB3	2.15	0.47
1:C:181:SER:HB2	1:D:156:GLN:NE2	2.23	0.47
1:C:414:ALA:O	1:C:417:ALA:HB3	2.14	0.47
1:D:50:PRO:HB2	1:D:87:ILE:HG21	1.96	0.47
1:A:158:GLU:OE2	1:A:325:HIS:NE2	2.29	0.47
1:A:332:VAL:HG13	1:A:332:VAL:O	2.14	0.47
1:D:19:GLU:HB3	1:D:52:GLU:OE1	2.13	0.47
1:D:41:ARG:NH1	1:D:96:GLN:OE1	2.44	0.47
2:S:77:CYS:SG	2:S:78:THR:N	2.84	0.47
1:C:52:GLU:O	1:C:55:ALA:N	2.48	0.47
1:C:154:GLY:N	1:C:324:ASP:OD1	2.45	0.47
1:D:425:GLU:OE1	2:V:17:TYR:N	2.43	0.47
1:D:429:LYS:CE	2:V:29:GLU:OE1	2.63	0.47
1:A:165:TYR:CD1	2:S:111:GLN:HB2	2.50	0.47
1:A:443:GLU:OE1	1:A:446:ARG:NH2	2.48	0.47
1:B:293:ILE:HG13	1:B:318:LEU:HD11	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:69:MET:HE3	2:T:72:LEU:HA	1.96	0.47
1:C:98:ILE:HG22	1:C:100:TYR:CE1	2.50	0.47
1:C:187:ARG:NH2	2:V:111:GLN:OE1	2.39	0.47
1:C:190:TYR:HB2	1:C:224:ALA:HB1	1.95	0.47
1:C:234:GLU:O	1:C:235:ILE:C	2.58	0.47
1:C:363:TYR:CD1	1:C:363:TYR:N	2.82	0.47
1:C:411:TRP:O	1:C:415:PRO:HG2	2.15	0.47
1:D:43:THR:HG22	1:D:43:THR:O	2.13	0.47
1:D:200:THR:OG1	1:D:238:HIS:HD2	1.98	0.47
1:D:410:PRO:HD3	1:D:461:VAL:HG21	1.97	0.47
1:D:454:GLU:H	1:D:454:GLU:CD	2.23	0.47
1:A:71:THR:HA	1:A:74:LEU:HD22	1.97	0.47
1:A:93:GLU:HG2	1:A:96:GLN:OE1	2.15	0.47
1:A:295:ARG:HG3	1:A:298:HIS:CD2	2.49	0.47
2:S:2:GLN:OE1	2:S:2:GLN:N	2.47	0.47
1:C:151:PRO:HB3	1:C:323:GLY:O	2.14	0.47
1:C:204:GLU:HB3	1:C:294:HIS:CD2	2.50	0.47
1:B:382:ILE:HG13	1:B:402:PHE:CE1	2.49	0.47
1:C:298:HIS:ND1	1:C:302:ASP:OD2	2.38	0.47
1:D:167:ARG:H	1:D:396:ASP:HB3	1.80	0.47
1:A:121:VAL:HG22	1:A:125:PHE:CE1	2.50	0.47
1:A:60:GLU:OE1	1:A:127:PHE:HZ	1.97	0.46
1:A:101:VAL:CG1	1:A:102:ALA:N	2.78	0.46
2:T:12:TYR:CE2	2:T:98:TRP:NE1	2.83	0.46
2:T:77:CYS:SG	2:T:82:GLN:OE1	2.74	0.46
1:C:436:ASP:O	1:C:437:LEU:C	2.57	0.46
1:D:229:GLN:HE21	1:D:236:LYS:H	1.62	0.46
1:D:397:ASP:OD2	2:V:108:ARG:NH2	2.48	0.46
2:V:108:ARG:HB3	2:V:110:VAL:HG13	1.96	0.46
1:A:19:GLU:HB3	1:A:52:GLU:OE2	2.15	0.46
2:S:22:SER:H	2:S:25:GLN:NE2	2.04	0.46
1:B:239:TYR:HE2	1:B:292:HIS:CE1	2.33	0.46
1:B:239:TYR:CE2	1:B:292:HIS:CE1	3.03	0.46
1:C:385:TRP:HZ2	1:C:459:CYS:HB3	1.80	0.46
1:A:318:LEU:C	1:A:320:MET:N	2.70	0.46
1:B:214:TRP:CE3	1:B:253:ARG:HG2	2.50	0.46
1:B:269:TYR:CD1	1:B:293:ILE:CG2	2.98	0.46
1:B:317:ALA:HA	1:B:320:MET:CE	2.43	0.46
2:U:77:CYS:CB	2:U:82:GLN:OE1	2.61	0.46
1:D:407:LEU:HG	1:D:413:ASN:OD1	2.16	0.46
1:B:225:LEU:HD12	1:B:225:LEU:C	2.40	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:VAL:HG23	1:C:97:TYR:HA	1.98	0.46
1:C:105:LEU:O	1:C:107:LEU:N	2.48	0.46
1:C:291:LEU:HG	1:C:293:ILE:HD11	1.97	0.46
1:D:336:GLU:OE2	1:D:472:VAL:HB	2.16	0.46
1:A:17:VAL:C	1:A:18:LYS:HG3	2.39	0.46
1:A:41:ARG:HA	1:A:97:TYR:O	2.15	0.46
1:B:90:VAL:HG23	1:B:97:TYR:HA	1.96	0.46
1:C:315:ALA:HB1	1:C:349:LEU:CD1	2.46	0.46
1:D:414:ALA:HB3	1:D:415:PRO:CD	2.35	0.46
2:S:42:LEU:HB3	2:S:70:TRP:HB3	1.98	0.46
1:B:50:PRO:HB2	1:B:87:ILE:HG21	1.97	0.46
1:B:204:GLU:HB3	1:B:294:HIS:CD2	2.50	0.46
1:B:331:VAL:HG21	1:B:339:ARG:HA	1.96	0.46
1:B:387:MET:CB	1:B:388:PRO:CD	2.91	0.46
1:D:296:ALA:O	1:D:297:MET:HB3	2.15	0.46
1:D:376:PRO:O	1:D:376:PRO:HG2	2.14	0.46
2:V:101:ILE:O	2:V:114:SER:HA	2.15	0.46
1:B:178:LEU:HD22	1:B:205:ASN:HD21	1.79	0.46
1:C:134:ARG:HG3	1:C:135:LEU:N	2.27	0.46
1:C:425:GLU:OE1	2:U:17:TYR:N	2.47	0.46
1:C:436:ASP:CG	1:C:439:GLN:H	2.23	0.46
2:V:92:LYS:O	2:V:93:ALA:CB	2.62	0.46
1:A:331:VAL:HG12	1:A:332:VAL:N	2.31	0.46
1:A:429:LYS:HE2	2:S:29:GLU:OE1	2.15	0.46
1:A:435:ARG:HH22	1:A:447:GLU:CD	2.24	0.46
1:A:466:VAL:HG23	1:A:468:ASN:N	2.31	0.46
1:B:381:GLY:HA2	1:C:66:TRP:NE1	2.31	0.46
2:T:33:LEU:HD22	2:T:113:ILE:HG21	1.97	0.46
1:C:388:PRO:HD3	1:C:445:ILE:HG21	1.97	0.46
2:V:19:PRO:O	2:V:20:ASP:C	2.58	0.46
2:V:105:ASP:HB2	2:V:112:CYS:SG	2.56	0.46
1:A:312:ARG:HH11	1:A:312:ARG:HD3	1.55	0.46
1:D:295:ARG:HD3	4:D:490:CAP:O6P	2.16	0.46
1:D:317:ALA:HA	1:D:320:MET:CE	2.41	0.46
1:D:466:VAL:HG23	1:D:468:ASN:N	2.28	0.46
1:A:239:TYR:HB3	1:A:266:MET:HB2	1.98	0.46
1:A:387:MET:HE3	1:A:424:LEU:HB2	1.98	0.46
1:B:463:LYS:HE2	1:B:463:LYS:HB3	1.44	0.46
1:C:181:SER:O	1:C:182:ALA:C	2.59	0.46
1:C:440:GLU:O	1:C:441:GLY:C	2.59	0.46
1:D:41:ARG:HD3	1:D:96:GLN:OE1	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:VAL:O	1:A:61:SER:HB2	2.15	0.45
1:B:383:HIS:N	1:B:386:HIS:HD2	2.01	0.45
1:C:195:GLY:HA3	1:C:417:ALA:CB	2.41	0.45
1:C:357:ASP:C	1:C:359:SER:N	2.73	0.45
1:D:192:CYS:HB3	1:D:197:LEU:HD23	1.97	0.45
1:A:244:ALA:HB1	1:A:249:GLU:HB3	1.98	0.45
1:A:269:TYR:CD1	1:A:293:ILE:CG2	2.99	0.45
1:C:463:LYS:HE2	1:C:463:LYS:HB3	1.39	0.45
2:U:96:GLN:H	2:U:96:GLN:CD	2.16	0.45
2:T:79:ASP:HB3	2:T:82:GLN:HB3	1.98	0.45
1:C:203:ASP:HA	5:C:492:FMT:O1	2.16	0.45
1:C:455:LEU:O	1:C:458:ALA:HB3	2.16	0.45
1:D:153:HIS:CD2	1:D:290:LEU:HD23	2.50	0.45
1:A:120:ILE:HG22	1:A:121:VAL:HG23	1.99	0.45
1:B:200:THR:OG1	1:B:238:HIS:CD2	2.63	0.45
2:T:33:LEU:C	2:T:33:LEU:HD12	2.41	0.45
1:C:97:TYR:O	1:C:98:ILE:HD13	2.16	0.45
1:C:283:TYR:C	1:C:283:TYR:CD2	2.94	0.45
2:U:91:LYS:HD2	2:U:118:TYR:CD2	2.52	0.45
1:D:291:LEU:HG	1:D:293:ILE:HD11	1.98	0.45
1:C:363:TYR:N	1:C:363:TYR:HD1	2.14	0.45
1:D:151:PRO:HB3	1:D:323:GLY:O	2.16	0.45
1:B:20:TYR:CD2	1:B:56:ALA:HA	2.51	0.45
1:B:26:THR:C	1:B:28:GLU:H	2.24	0.45
2:T:12:TYR:OH	2:T:123:TYR:HB3	2.16	0.45
1:C:383:HIS:N	1:C:386:HIS:HD2	2.12	0.45
1:A:20:TYR:CD2	1:A:56:ALA:HA	2.51	0.45
1:B:429:LYS:CE	2:T:29:GLU:OE1	2.65	0.45
2:T:91:LYS:H	2:T:91:LYS:HG2	1.63	0.45
1:A:120:ILE:HD13	1:A:138:LEU:CD2	2.47	0.45
1:B:451:TRP:CH2	2:T:19:PRO:HD3	2.52	0.45
2:T:75:PHE:HE1	1:D:9:ALA:HB2	1.82	0.45
1:C:368:TRP:O	1:C:369:VAL:C	2.59	0.45
1:D:301:ILE:CG2	1:D:309:ILE:HB	2.46	0.45
2:T:79:ASP:O	2:T:80:ALA:C	2.59	0.45
1:C:183:LYS:O	2:V:66:TYR:OH	2.30	0.45
1:D:421:ARG:NH1	1:D:425:GLU:OE2	2.50	0.45
1:D:455:LEU:HD12	1:D:455:LEU:C	2.40	0.45
1:A:335:LEU:HD23	1:D:127:PHE:CD1	2.51	0.45
1:B:66:TRP:CZ3	1:B:67:THR:HB	2.51	0.45
1:B:215:ARG:HH11	1:B:215:ARG:HD2	1.34	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:LEU:O	1:B:458:ALA:HB3	2.17	0.45
1:C:190:TYR:CZ	1:C:194:ARG:HD2	2.52	0.45
1:C:370:SER:O	1:C:371:LEU:C	2.58	0.45
2:U:2:GLN:OE1	2:U:2:GLN:N	2.50	0.45
2:U:68:THR:HG22	2:U:69:MET:O	2.17	0.45
1:D:169:LEU:HB2	1:D:399:VAL:HG22	1.99	0.45
2:U:44:PHE:HA	2:U:98:TRP:O	2.17	0.44
1:D:334:LYS:HB3	1:D:381:GLY:HA3	1.98	0.44
1:A:105:LEU:HA	1:A:105:LEU:HD12	1.79	0.44
1:A:407:LEU:HG	1:A:413:ASN:OD1	2.18	0.44
4:A:490:CAP:O4	5:A:492:FMT:O2	2.35	0.44
1:B:66:TRP:CD1	1:C:381:GLY:HA2	2.53	0.44
1:B:76:SER:O	1:B:76:SER:OG	2.36	0.44
2:T:27:LEU:HD12	2:T:84:LEU:HD12	1.99	0.44
2:T:45:GLU:OE2	2:T:48:HIS:N	2.44	0.44
1:C:451:TRP:CH2	2:U:19:PRO:HD3	2.52	0.44
1:D:141:PRO:HA	1:D:142:PRO:HD3	1.87	0.44
2:V:34:LEU:O	2:V:35:LYS:C	2.61	0.44
1:A:239:TYR:CE2	1:A:292:HIS:CE1	3.05	0.44
1:B:10:SER:OG	1:B:11:VAL:HG23	2.17	0.44
1:B:61:SER:HB3	1:B:103:TYR:HE1	1.82	0.44
1:B:239:TYR:CE2	1:B:292:HIS:CD2	3.06	0.44
1:B:264:ILE:HD13	1:B:264:ILE:HG21	1.52	0.44
2:U:12:TYR:OH	2:U:123:TYR:HB3	2.18	0.44
1:D:90:VAL:HG23	1:D:97:TYR:CA	2.48	0.44
1:D:165:TYR:CD1	2:V:111:GLN:HB2	2.52	0.44
1:D:194:ARG:NH2	2:V:4:TRP:O	2.45	0.44
1:D:414:ALA:CB	1:D:415:PRO:HD3	2.34	0.44
4:D:490:CAP:O2	4:D:490:CAP:O4	2.33	0.44
1:A:157:VAL:O	1:A:161:LYS:HG2	2.18	0.44
1:A:387:MET:HG2	1:A:424:LEU:HA	1.99	0.44
1:B:421:ARG:HH11	1:B:421:ARG:HD2	1.58	0.44
1:C:204:GLU:HG3	1:C:294:HIS:CE1	2.53	0.44
1:D:452:SER:CB	1:D:455:LEU:HB3	2.35	0.44
1:B:45:GLN:OE1	1:B:131:ARG:HB3	2.18	0.44
1:C:387:MET:CB	1:C:388:PRO:CD	2.93	0.44
1:A:127:PHE:CE1	1:D:335:LEU:HD21	2.52	0.44
1:B:150:GLY:HA3	1:B:371:LEU:HD11	1.99	0.44
1:C:191:GLU:O	1:C:194:ARG:HG2	2.18	0.44
2:U:41:CYS:HB3	2:U:102:ILE:HD11	2.00	0.44
1:D:90:VAL:HG23	1:D:96:GLN:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:THR:HA	1:A:201:LYS:HG2	1.99	0.44
1:A:214:TRP:CD2	1:A:253:ARG:HG2	2.52	0.44
2:S:41:CYS:SG	2:S:42:LEU:N	2.90	0.44
1:B:118:THR:HG21	1:C:204:GLU:O	2.17	0.44
1:B:176:PRO:O	1:B:177:LYS:C	2.61	0.44
1:C:239:TYR:HB3	1:C:266:MET:HB2	2.00	0.44
1:A:214:TRP:CD2	1:A:215:ARG:N	2.86	0.44
2:S:61:TYR:CD1	2:S:61:TYR:C	2.96	0.44
1:B:291:LEU:HG	1:B:293:ILE:HD11	2.00	0.44
1:C:23:THR:CG2	1:C:81:LYS:HZ3	2.31	0.44
1:C:435:ARG:HH22	1:C:447:GLU:CD	2.26	0.44
1:D:241:ASN:ND2	1:D:243:THR:H	2.16	0.44
1:D:318:LEU:HD22	1:D:326:ILE:HD12	2.00	0.44
1:A:177:LYS:HB2	1:D:63:THR:HA	2.00	0.44
1:A:311:PHE:O	1:A:312:ARG:C	2.61	0.44
1:B:239:TYR:CE2	1:B:292:HIS:CG	3.06	0.44
1:C:414:ALA:CB	1:C:415:PRO:HD3	2.37	0.44
2:U:84:LEU:O	2:U:87:VAL:HB	2.17	0.44
1:D:142:PRO:HB3	1:D:369:VAL:HG11	2.00	0.44
1:A:227:LYS:HE2	2:T:66:TYR:O	2.18	0.43
1:A:331:VAL:HG21	1:A:339:ARG:HA	2.00	0.43
1:B:127:PHE:CD1	1:C:335:LEU:CD2	3.01	0.43
1:B:138:LEU:HD12	1:B:313:VAL:HG13	1.99	0.43
1:B:382:ILE:HD12	1:B:390:LEU:HD13	1.99	0.43
1:C:10:SER:OG	1:C:11:VAL:HG23	2.17	0.43
1:C:101:VAL:HG12	1:C:102:ALA:N	2.33	0.43
1:C:310:HIS:CE1	1:C:312:ARG:CZ	3.00	0.43
2:U:56:ASN:ND2	2:U:58:SER:N	2.55	0.43
2:U:77:CYS:SG	2:U:82:GLN:CD	3.01	0.43
2:U:102:ILE:HG22	2:U:114:SER:HB2	2.00	0.43
1:D:63:THR:OG1	1:D:77:LEU:HD13	2.17	0.43
1:D:411:TRP:CH2	2:V:2:GLN:OE1	2.70	0.43
1:D:443:GLU:O	1:D:447:GLU:N	2.48	0.43
2:S:43:GLU:HA	2:S:68:THR:O	2.18	0.43
1:B:86:ARG:HG3	1:B:86:ARG:HH11	1.83	0.43
1:B:112:SER:O	1:B:113:VAL:C	2.57	0.43
1:B:264:ILE:HG13	1:B:290:LEU:O	2.17	0.43
1:B:336:GLU:OE2	1:B:472:VAL:HB	2.18	0.43
1:B:435:ARG:HH22	1:B:447:GLU:CD	2.26	0.43
2:T:101:ILE:O	2:T:114:SER:HA	2.17	0.43
2:U:79:ASP:N	2:U:82:GLN:NE2	2.64	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:PRO:O	1:D:285:ARG:NH1	2.51	0.43
1:D:443:GLU:OE2	1:D:446:ARG:NE	2.50	0.43
1:A:41:ARG:O	1:A:41:ARG:HG2	2.18	0.43
1:A:183:LYS:O	2:T:66:TYR:OH	2.33	0.43
1:B:331:VAL:HA	1:B:337:GLY:O	2.18	0.43
1:B:343:LEU:HD21	1:B:393:ILE:HG23	2.00	0.43
2:V:44:PHE:HA	2:V:98:TRP:O	2.18	0.43
2:V:113:ILE:CG1	2:V:114:SER:N	2.81	0.43
2:T:39:VAL:HG21	1:D:9:ALA:HB3	1.96	0.43
2:T:79:ASP:H	2:T:82:GLN:HE22	1.64	0.43
1:C:23:THR:CG2	1:C:81:LYS:NZ	2.80	0.43
1:D:264:ILE:HG13	1:D:290:LEU:O	2.19	0.43
2:T:29:GLU:HB3	2:T:115:PHE:CZ	2.53	0.43
2:U:10:LYS:HB3	2:U:50:PHE:CZ	2.53	0.43
2:U:11:LYS:HG3	2:U:17:TYR:CZ	2.53	0.43
2:V:33:LEU:C	2:V:33:LEU:CD1	2.91	0.43
1:B:24:TYR:CG	1:B:59:ALA:HB2	2.54	0.43
1:B:153:HIS:N	1:B:324:ASP:OD1	2.38	0.43
1:B:389:ALA:O	1:B:393:ILE:HG13	2.19	0.43
1:C:215:ARG:HH11	1:C:215:ARG:HD2	1.30	0.43
1:D:190:TYR:CZ	1:D:227:LYS:HD3	2.52	0.43
1:D:269:TYR:CD1	1:D:293:ILE:HG21	2.53	0.43
1:A:421:ARG:HH11	1:A:421:ARG:HD2	1.58	0.43
1:C:375:LEU:HD12	1:C:375:LEU:HA	1.80	0.43
2:U:41:CYS:HB2	2:U:104:PHE:HE2	1.82	0.43
1:D:383:HIS:N	1:D:386:HIS:CD2	2.71	0.43
1:D:463:LYS:HB3	1:D:463:LYS:HE2	1.40	0.43
2:V:30:VAL:O	2:V:34:LEU:HB2	2.19	0.43
1:A:298:HIS:ND1	1:A:302:ASP:OD2	2.35	0.43
1:A:343:LEU:HD23	1:A:343:LEU:HA	1.72	0.43
2:S:86:GLU:O	2:S:89:GLU:HB3	2.18	0.43
1:D:86:ARG:HG3	1:D:86:ARG:NH1	2.34	0.43
1:D:387:MET:HB3	1:D:388:PRO:CD	2.48	0.43
2:V:103:GLY:HA3	2:V:113:ILE:HG22	2.00	0.43
1:A:410:PRO:HD3	1:A:461:VAL:HG21	2.01	0.43
1:B:29:TYR:CG	1:B:83:ARG:HD2	2.54	0.43
1:B:94:LYS:HB2	1:B:94:LYS:NZ	2.34	0.43
1:B:101:VAL:HG12	1:B:102:ALA:N	2.32	0.43
1:B:185:TYR:O	1:B:189:VAL:HG23	2.18	0.43
1:B:293:ILE:HA	1:B:293:ILE:HD13	1.79	0.43
1:C:42:VAL:HG23	1:C:130:LEU:HD22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ARG:HG2	2:U:14:THR:OG1	2.18	0.43
1:C:178:LEU:CD2	1:C:205:ASN:ND2	2.81	0.43
1:C:410:PRO:HD3	1:C:461:VAL:HG21	2.00	0.43
2:U:117:ALA:O	2:U:118:TYR:CB	2.60	0.43
1:D:144:TYR:O	1:D:145:VAL:C	2.61	0.43
1:D:193:LEU:HD13	1:D:200:THR:CG2	2.47	0.43
2:V:11:LYS:HE3	2:V:17:TYR:CE1	2.54	0.43
2:V:82:GLN:O	2:V:85:ALA:CB	2.59	0.43
2:V:98:TRP:HD1	2:V:116:ILE:CD1	2.32	0.43
1:A:212:MET:HE2	1:A:212:MET:HB3	1.89	0.43
1:A:463:LYS:HE2	1:A:463:LYS:HB3	1.36	0.43
1:B:190:TYR:O	1:B:194:ARG:HG2	2.19	0.43
1:C:36:ILE:N	1:C:36:ILE:HD12	2.34	0.43
1:C:44:PRO:O	1:C:131:ARG:HG2	2.19	0.43
1:C:429:LYS:HZ3	1:C:429:LYS:HG3	1.75	0.43
1:D:163:ASN:HD22	1:D:163:ASN:HA	1.61	0.43
1:D:293:ILE:CG1	1:D:318:LEU:HD11	2.42	0.43
1:D:435:ARG:HH22	1:D:447:GLU:CD	2.27	0.43
1:A:457:ALA:O	1:A:461:VAL:HG23	2.18	0.42
2:T:14:THR:HG22	2:T:15:LEU:HG	2.01	0.42
2:U:89:GLU:O	2:U:92:LYS:O	2.37	0.42
1:D:280:LEU:HA	1:D:280:LEU:HD12	1.81	0.42
1:D:336:GLU:OE2	1:D:473:ASP:N	2.52	0.42
2:V:42:LEU:HB3	2:V:70:TRP:HB3	2.01	0.42
1:A:268:ASP:HA	1:A:294:HIS:O	2.19	0.42
1:A:332:VAL:O	1:A:332:VAL:CG1	2.66	0.42
2:S:34:LEU:C	2:S:36:ASN:N	2.74	0.42
1:B:239:TYR:CD2	1:B:292:HIS:CD2	3.07	0.42
1:C:86:ARG:HG3	1:C:86:ARG:NH1	2.33	0.42
1:C:315:ALA:HB1	1:C:349:LEU:HD11	2.01	0.42
2:U:101:ILE:O	2:U:114:SER:HA	2.19	0.42
1:A:45:GLN:HA	1:A:46:PRO:HD2	1.78	0.42
2:S:98:TRP:CD1	2:S:116:ILE:HD11	2.54	0.42
1:B:435:ARG:HD2	1:B:435:ARG:HH11	1.61	0.42
2:U:41:CYS:SG	2:U:42:LEU:N	2.92	0.42
2:U:79:ASP:HB3	2:U:82:GLN:HB3	2.01	0.42
1:D:295:ARG:O	1:D:296:ALA:C	2.61	0.42
2:V:29:GLU:HB3	2:V:115:PHE:CZ	2.53	0.42
2:V:43:GLU:OE2	2:V:100:ARG:NH1	2.45	0.42
1:A:215:ARG:HH11	1:A:215:ARG:HD2	1.34	0.42
1:B:106:ASP:O	1:C:210:PRO:HD2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:TYR:CZ	1:B:194:ARG:HD2	2.55	0.42
2:T:33:LEU:HD22	2:T:113:ILE:CG2	2.49	0.42
2:T:69:MET:HE1	1:D:70:TRP:CH2	2.54	0.42
1:C:204:GLU:HA	1:C:266:MET:HE1	2.02	0.42
1:D:264:ILE:HA	1:D:290:LEU:O	2.19	0.42
1:A:425:GLU:OE1	2:S:17:TYR:N	2.47	0.42
1:B:73:GLY:HA3	2:V:75:PHE:CE1	2.55	0.42
1:B:94:LYS:O	1:B:96:GLN:N	2.52	0.42
1:C:295:ARG:CZ	1:C:298:HIS:CE1	3.03	0.42
2:U:1:MET:SD	2:V:71:LYS:HB3	2.59	0.42
1:D:59:ALA:C	1:D:61:SER:H	2.27	0.42
1:D:293:ILE:CG2	1:D:318:LEU:HD11	2.45	0.42
2:V:113:ILE:O	2:V:114:SER:CB	2.66	0.42
1:A:318:LEU:HD22	1:A:326:ILE:HB	2.01	0.42
1:A:345:PHE:O	1:A:348:LEU:HB2	2.18	0.42
2:T:2:GLN:OE1	2:T:2:GLN:N	2.52	0.42
2:T:56:ASN:ND2	2:T:58:SER:OG	2.49	0.42
1:C:41:ARG:NH1	1:C:96:GLN:OE1	2.52	0.42
1:C:192:CYS:SG	1:C:413:ASN:ND2	2.93	0.42
1:C:368:TRP:C	1:C:369:VAL:HG22	2.44	0.42
1:D:443:GLU:O	1:D:447:GLU:HG3	2.19	0.42
2:V:110:VAL:HG23	2:V:111:GLN:C	2.45	0.42
1:A:318:LEU:HD22	1:A:326:ILE:HD12	2.00	0.42
2:S:3:VAL:HG22	2:T:71:LYS:H	1.84	0.42
1:B:26:THR:C	1:B:28:GLU:N	2.77	0.42
1:B:85:TYR:O	1:B:86:ARG:HB3	2.19	0.42
1:B:318:LEU:C	1:B:320:MET:H	2.27	0.42
1:C:238:HIS:O	1:C:239:TYR:C	2.62	0.42
1:C:442:ASN:O	1:C:446:ARG:CB	2.68	0.42
1:D:66:TRP:CE3	1:D:67:THR:HB	2.54	0.42
1:D:154:GLY:HA2	1:D:373:GLY:O	2.20	0.42
1:A:292:HIS:NE2	1:A:327:HIS:NE2	2.68	0.42
1:B:89:ARG:HB2	1:B:89:ARG:NH1	2.25	0.42
2:T:84:LEU:HD23	2:T:84:LEU:O	2.20	0.42
1:C:150:GLY:HA3	1:C:371:LEU:HD11	2.01	0.42
1:D:167:ARG:HA	1:D:168:PRO:HD3	1.79	0.42
1:D:421:ARG:O	1:D:425:GLU:HG3	2.19	0.42
1:A:167:ARG:HG2	2:S:14:THR:OG1	2.20	0.42
1:A:283:TYR:CD2	1:A:283:TYR:C	2.98	0.42
2:S:26:LEU:O	2:S:29:GLU:HB2	2.20	0.42
1:B:9:ALA:N	1:B:73:GLY:O	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:26:LEU:HD23	2:T:26:LEU:C	2.45	0.42
1:C:151:PRO:O	1:C:285:ARG:NH1	2.53	0.42
1:C:190:TYR:CZ	1:C:227:LYS:HD3	2.55	0.42
1:C:441:GLY:O	1:C:444:ILE:HB	2.19	0.42
1:D:239:TYR:HB3	1:D:266:MET:HB2	2.02	0.42
1:D:454:GLU:CD	1:D:454:GLU:N	2.78	0.42
1:A:465:ILE:HG12	1:A:465:ILE:H	1.37	0.42
1:C:330:THR:HG21	1:C:382:ILE:HG23	2.01	0.42
1:A:68:THR:O	1:D:408:GLY:HA2	2.19	0.41
1:A:429:LYS:NZ	1:A:433:GLU:OE1	2.53	0.41
2:S:3:VAL:HG21	2:T:70:TRP:CE3	2.55	0.41
1:C:41:ARG:HH11	1:C:41:ARG:HD3	1.43	0.41
2:U:30:VAL:O	2:U:34:LEU:HD12	2.20	0.41
1:D:423:ALA:O	1:D:426:ALA:HB3	2.20	0.41
1:A:77:LEU:N	1:A:77:LEU:HD23	2.35	0.41
1:A:280:LEU:HD12	1:A:280:LEU:HA	1.82	0.41
2:S:22:SER:OG	2:S:25:GLN:HB2	2.20	0.41
2:S:33:LEU:HD13	2:S:38:TRP:CB	2.45	0.41
1:B:229:GLN:HG3	1:B:234:GLU:O	2.20	0.41
1:B:411:TRP:CZ3	2:T:2:GLN:OE1	2.74	0.41
1:C:269:TYR:CD1	1:C:293:ILE:HG22	2.55	0.41
2:U:105:ASP:HB2	2:U:112:CYS:SG	2.59	0.41
1:D:409:HIS:HA	1:D:410:PRO:HD2	1.74	0.41
2:V:119:LYS:HD2	2:V:123:TYR:C	2.45	0.41
1:B:251:ILE:HD13	1:B:251:ILE:HA	1.73	0.41
2:U:79:ASP:C	2:U:81:THR:N	2.77	0.41
1:D:151:PRO:O	1:D:152:PRO:C	2.61	0.41
1:A:304:GLN:NE2	1:A:304:GLN:HA	2.35	0.41
2:S:113:ILE:O	2:S:114:SER:HB2	2.20	0.41
1:B:295:ARG:HG3	1:B:298:HIS:CD2	2.55	0.41
1:C:27:PRO:HD2	1:C:28:GLU:OE2	2.20	0.41
1:C:387:MET:HE3	1:C:424:LEU:CB	2.42	0.41
1:C:452:SER:HA	1:C:453:PRO:HD3	1.91	0.41
2:U:3:VAL:HG21	2:V:70:TRP:CZ3	2.55	0.41
1:D:465:ILE:H	1:D:465:ILE:HG12	1.67	0.41
2:V:96:GLN:OE1	2:V:96:GLN:N	2.41	0.41
2:S:101:ILE:HG13	2:S:117:ALA:HB2	2.01	0.41
1:B:407:LEU:HG	1:B:413:ASN:OD1	2.20	0.41
1:C:45:GLN:HA	1:C:46:PRO:HD2	1.80	0.41
1:C:225:LEU:C	1:C:225:LEU:HD12	2.46	0.41
2:U:34:LEU:C	2:U:36:ASN:N	2.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:ARG:HE	1:D:360:ARG:HB2	1.59	0.41
1:D:363:TYR:N	1:D:363:TYR:CD1	2.89	0.41
2:V:55:ASN:N	2:V:63:ASP:OD2	2.45	0.41
1:A:24:TYR:CD2	1:A:59:ALA:HB2	2.55	0.41
1:A:304:GLN:HA	1:A:304:GLN:HE21	1.84	0.41
1:A:363:TYR:CD1	1:A:363:TYR:N	2.88	0.41
1:A:451:TRP:CH2	2:S:19:PRO:HD3	2.56	0.41
1:C:311:PHE:O	1:C:312:ARG:C	2.63	0.41
2:U:30:VAL:HG11	2:U:83:VAL:HG22	2.01	0.41
2:U:113:ILE:CG1	2:U:114:SER:N	2.83	0.41
1:D:382:ILE:HG13	1:D:402:PHE:CE1	2.56	0.41
1:A:318:LEU:C	1:A:320:MET:H	2.28	0.41
2:S:29:GLU:HB3	2:S:115:PHE:CZ	2.56	0.41
1:C:312:ARG:HH11	1:C:312:ARG:HD3	1.55	0.41
1:C:397:ASP:OD2	2:U:108:ARG:NH2	2.53	0.41
1:C:449:CYS:HB3	1:C:456:ALA:HA	2.01	0.41
2:U:35:LYS:NZ	2:U:36:ASN:ND2	2.69	0.41
1:D:442:ASN:O	1:D:446:ARG:HB2	2.20	0.41
1:A:128:LYS:HD2	1:D:333:GLY:O	2.20	0.41
1:A:264:ILE:HD13	1:A:264:ILE:HG21	1.88	0.41
1:A:335:LEU:HD21	1:D:127:PHE:CE1	2.55	0.41
1:A:387:MET:N	1:A:388:PRO:HD2	2.36	0.41
1:C:71:THR:HA	1:C:74:LEU:HD22	2.02	0.41
1:C:448:ALA:C	1:C:450:LYS:N	2.78	0.41
1:D:388:PRO:HD3	1:D:445:ILE:HG21	2.03	0.41
1:A:171:GLY:O	1:A:401:GLN:HA	2.21	0.41
1:B:17:VAL:O	1:B:18:LYS:HG3	2.21	0.41
1:B:105:LEU:O	1:B:107:LEU:N	2.54	0.41
1:B:213:ARG:HH11	1:B:213:ARG:HD2	1.60	0.41
1:B:447:GLU:O	1:B:450:LYS:HB2	2.21	0.41
2:T:98:TRP:HD1	2:T:116:ILE:CD1	2.34	0.41
2:T:105:ASP:OD1	2:T:105:ASP:C	2.63	0.41
1:C:105:LEU:C	1:C:107:LEU:N	2.79	0.41
1:C:192:CYS:HB2	1:C:200:THR:HG21	2.03	0.41
1:C:201:LYS:HG3	1:C:202:ASP:O	2.21	0.41
1:C:310:HIS:ND1	1:C:312:ARG:CZ	2.84	0.41
1:C:357:ASP:C	1:C:359:SER:H	2.29	0.41
1:C:388:PRO:O	1:C:392:GLU:HB2	2.21	0.41
2:U:11:LYS:HE3	2:U:17:TYR:CZ	2.56	0.41
2:U:13:GLU:HB3	2:U:14:THR:H	1.67	0.41
2:U:35:LYS:HD2	2:U:35:LYS:C	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:119:LYS:HD2	2:U:123:TYR:OXT	2.20	0.41
1:D:17:VAL:C	1:D:18:LYS:HG3	2.46	0.41
1:D:431:ARG:HG3	1:D:437:LEU:CD2	2.51	0.41
1:A:239:TYR:HE2	1:A:292:HIS:CE1	2.39	0.41
1:A:310:HIS:HD1	1:A:312:ARG:H	1.69	0.41
1:B:171:GLY:HA2	1:B:199:PHE:O	2.20	0.41
2:T:11:LYS:HG3	2:T:17:TYR:CZ	2.56	0.41
1:C:200:THR:OG1	1:C:238:HIS:HD2	2.04	0.41
2:U:15:LEU:O	2:U:17:TYR:N	2.54	0.41
1:D:215:ARG:HH11	1:D:215:ARG:HD2	1.66	0.41
1:D:304:GLN:NE2	1:D:304:GLN:CA	2.84	0.41
1:D:451:TRP:CZ2	2:V:19:PRO:HD3	2.56	0.41
1:B:121:VAL:HG13	1:C:300:VAL:HG21	2.01	0.40
1:C:371:LEU:HD12	1:C:371:LEU:HA	1.94	0.40
1:D:343:LEU:HD23	1:D:343:LEU:HA	1.70	0.40
1:A:440:GLU:O	1:A:441:GLY:O	2.39	0.40
1:C:51:GLU:HA	1:C:87:ILE:CD1	2.48	0.40
1:D:152:PRO:O	1:D:285:ARG:NH1	2.51	0.40
1:A:173:THR:HG21	4:A:490:CAP:O2	2.21	0.40
1:B:9:ALA:HB2	2:V:75:PHE:CD1	2.56	0.40
1:C:175:LYS:HA	1:C:176:PRO:C	2.47	0.40
1:A:48:VAL:HA	1:A:49:PRO:HD2	1.71	0.40
1:A:152:PRO:HA	1:A:285:ARG:HD3	2.03	0.40
1:A:448:ALA:HA	1:A:451:TRP:HD1	1.82	0.40
2:S:105:ASP:OD2	2:S:108:ARG:HD3	2.21	0.40
1:B:51:GLU:HA	1:B:87:ILE:CD1	2.51	0.40
1:B:105:LEU:HA	1:B:105:LEU:HD12	1.75	0.40
1:B:163:ASN:HD22	1:B:163:ASN:HA	1.53	0.40
1:B:165:TYR:CD1	2:T:111:GLN:HB2	2.56	0.40
1:B:429:LYS:HE2	2:T:29:GLU:OE1	2.22	0.40
1:C:45:GLN:O	1:C:46:PRO:C	2.63	0.40
1:C:146:LYS:HA	1:C:146:LYS:HD2	1.83	0.40
2:U:53:ARG:HD3	2:U:57:LYS:HG2	2.03	0.40
2:V:77:CYS:SG	2:V:82:GLN:CD	3.04	0.40
2:V:107:VAL:O	2:V:107:VAL:HG12	2.21	0.40
1:A:17:VAL:HG21	1:D:465:ILE:HD12	2.03	0.40
1:A:157:VAL:HA	1:A:160:ASP:HB2	2.04	0.40
2:S:14:THR:HG22	2:S:15:LEU:HG	2.04	0.40
1:C:357:ASP:OD2	1:C:360:ARG:HB2	2.21	0.40
1:C:466:VAL:HG23	1:C:468:ASN:N	2.37	0.40
1:D:86:ARG:HH11	1:D:86:ARG:CG	2.33	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:ARG:NH2	1:C:30:GLN:NE2[3_654]	2.00	0.20

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	463/477 (97%)	402 (87%)	48 (10%)	13 (3%)	4	9
1	B	463/477 (97%)	399 (86%)	52 (11%)	12 (3%)	4	11
1	C	463/477 (97%)	388 (84%)	63 (14%)	12 (3%)	4	11
1	D	463/477 (97%)	400 (86%)	52 (11%)	11 (2%)	4	12
2	S	121/123 (98%)	104 (86%)	14 (12%)	3 (2%)	4	11
2	T	121/123 (98%)	102 (84%)	17 (14%)	2 (2%)	7	19
2	U	121/123 (98%)	99 (82%)	19 (16%)	3 (2%)	4	11
2	V	121/123 (98%)	100 (83%)	19 (16%)	2 (2%)	7	19
All	All	2336/2400 (97%)	1994 (85%)	284 (12%)	58 (2%)	4	11

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	PRO
1	A	95	ASP
1	A	167	ARG
2	S	93	ALA
1	B	46	PRO
1	B	95	ASP
1	B	167	ARG
2	T	93	ALA
1	C	46	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	95	ASP
1	C	167	ARG
2	U	93	ALA
1	D	46	PRO
1	D	95	ASP
1	D	167	ARG
2	V	93	ALA
1	A	106	ASP
1	A	441	GLY
1	A	442	ASN
1	B	10	SER
1	B	106	ASP
1	B	441	GLY
1	B	442	ASN
1	C	86	ARG
1	C	106	ASP
1	C	441	GLY
1	C	442	ASN
2	U	16	SER
1	D	369	VAL
1	D	441	GLY
1	D	442	ASN
1	A	86	ARG
1	B	86	ARG
2	T	76	GLY
2	U	76	GLY
1	D	10	SER
1	D	86	ARG
1	A	10	SER
2	S	35	LYS
2	S	76	GLY
1	B	21	LYS
1	C	10	SER
1	A	11	VAL
1	B	11	VAL
1	B	369	VAL
1	C	11	VAL
1	C	384	VAL
1	C	385	TRP
1	D	11	VAL
1	D	166	GLY
2	V	16	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	155	ILE
1	D	384	VAL
1	A	384	VAL
1	B	384	VAL
1	A	403	GLY
1	C	369	VAL
1	A	369	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	373/386 (97%)	320 (86%)	53 (14%)	3	8
1	B	373/386 (97%)	318 (85%)	55 (15%)	3	8
1	C	373/386 (97%)	320 (86%)	53 (14%)	3	8
1	D	373/386 (97%)	320 (86%)	53 (14%)	3	8
2	S	109/109 (100%)	86 (79%)	23 (21%)	1	3
2	T	109/109 (100%)	86 (79%)	23 (21%)	1	3
2	U	109/109 (100%)	87 (80%)	22 (20%)	1	4
2	V	109/109 (100%)	83 (76%)	26 (24%)	1	2
All	All	1928/1980 (97%)	1620 (84%)	308 (16%)	2	6

All (308) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	21	LYS
1	A	22	LEU
1	A	23	THR
1	A	26	THR
1	A	28	GLU
1	A	32	LYS
1	A	37	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	46	PRO
1	A	61	SER
1	A	74	LEU
1	A	77	LEU
1	A	79	ARG
1	A	89	ARG
1	A	94	LYS
1	A	121	VAL
1	A	134	ARG
1	A	139	ARG
1	A	142	PRO
1	A	152	PRO
1	A	163	ASN
1	A	169	LEU
1	A	172	CYS
1	A	178	LEU
1	A	193	LEU
1	A	197	LEU
1	A	201	LYS
1	A	213	ARG
1	A	215	ARG
1	A	225	LEU
1	A	285	ARG
1	A	295	ARG
1	A	312	ARG
1	A	314	LEU
1	A	318	LEU
1	A	319	ARG
1	A	331	VAL
1	A	332	VAL
1	A	338	GLU
1	A	349	LEU
1	A	356	GLN
1	A	363	TYR
1	A	379	SER
1	A	384	VAL
1	A	429	LYS
1	A	433	GLU
1	A	437	LEU
1	A	442	ASN
1	A	445	ILE
1	A	463	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	464	GLU
1	A	465	ILE
1	A	466	VAL
2	S	2	GLN
2	S	6	PRO
2	S	23	GLN
2	S	26	LEU
2	S	27	LEU
2	S	29	GLU
2	S	31	GLU
2	S	33	LEU
2	S	35	LYS
2	S	42	LEU
2	S	54	GLU
2	S	77	CYS
2	S	78	THR
2	S	81	THR
2	S	82	GLN
2	S	83	VAL
2	S	91	LYS
2	S	92	LYS
2	S	96	GLN
2	S	100	ARG
2	S	110	VAL
2	S	119	LYS
2	S	121	GLU
1	B	10	SER
1	B	21	LYS
1	B	22	LEU
1	B	28	GLU
1	B	32	LYS
1	B	45	GLN
1	B	46	PRO
1	B	61	SER
1	B	74	LEU
1	B	77	LEU
1	B	79	ARG
1	B	89	ARG
1	B	93	GLU
1	B	94	LYS
1	B	121	VAL
1	B	131	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	134	ARG
1	B	139	ARG
1	B	163	ASN
1	B	169	LEU
1	B	173	THR
1	B	178	LEU
1	B	193	LEU
1	B	197	LEU
1	B	201	LYS
1	B	213	ARG
1	B	215	ARG
1	B	225	LEU
1	B	239	TYR
1	B	285	ARG
1	B	295	ARG
1	B	304	GLN
1	B	312	ARG
1	B	314	LEU
1	B	318	LEU
1	B	319	ARG
1	B	331	VAL
1	B	332	VAL
1	B	335	LEU
1	B	338	GLU
1	B	349	LEU
1	B	356	GLN
1	B	359	SER
1	B	363	TYR
1	B	384	VAL
1	B	421	ARG
1	B	429	LYS
1	B	433	GLU
1	B	437	LEU
1	B	442	ASN
1	B	445	ILE
1	B	463	LYS
1	B	464	GLU
1	B	465	ILE
1	B	466	VAL
2	T	2	GLN
2	T	14	THR
2	T	23	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	T	27	LEU
2	T	28	SER
2	T	29	GLU
2	T	33	LEU
2	T	35	LYS
2	T	42	LEU
2	T	54	GLU
2	T	65	ARG
2	T	72	LEU
2	T	77	CYS
2	T	78	THR
2	T	81	THR
2	T	82	GLN
2	T	83	VAL
2	T	91	LYS
2	T	92	LYS
2	T	96	GLN
2	T	101	ILE
2	T	110	VAL
2	T	121	GLU
1	C	10	SER
1	C	21	LYS
1	C	23	THR
1	C	26	THR
1	C	32	LYS
1	C	45	GLN
1	C	46	PRO
1	C	61	SER
1	C	74	LEU
1	C	76	SER
1	C	77	LEU
1	C	79	ARG
1	C	87	ILE
1	C	89	ARG
1	C	93	GLU
1	C	94	LYS
1	C	121	VAL
1	C	131	ARG
1	C	134	ARG
1	C	139	ARG
1	C	142	PRO
1	C	163	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	169	LEU
1	C	178	LEU
1	C	193	LEU
1	C	197	LEU
1	C	200	THR
1	C	201	LYS
1	C	213	ARG
1	C	215	ARG
1	C	239	TYR
1	C	278	THR
1	C	285	ARG
1	C	295	ARG
1	C	314	LEU
1	C	318	LEU
1	C	319	ARG
1	C	331	VAL
1	C	332	VAL
1	C	338	GLU
1	C	349	LEU
1	C	356	GLN
1	C	363	TYR
1	C	379	SER
1	C	384	VAL
1	C	437	LEU
1	C	442	ASN
1	C	445	ILE
1	C	454	GLU
1	C	463	LYS
1	C	464	GLU
1	C	465	ILE
1	C	466	VAL
2	U	2	GLN
2	U	6	PRO
2	U	7	ILE
2	U	23	GLN
2	U	27	LEU
2	U	28	SER
2	U	29	GLU
2	U	31	GLU
2	U	33	LEU
2	U	35	LYS
2	U	42	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	U	74	MET
2	U	77	CYS
2	U	78	THR
2	U	81	THR
2	U	82	GLN
2	U	83	VAL
2	U	91	LYS
2	U	92	LYS
2	U	96	GLN
2	U	101	ILE
2	U	110	VAL
1	D	10	SER
1	D	21	LYS
1	D	22	LEU
1	D	23	THR
1	D	26	THR
1	D	28	GLU
1	D	32	LYS
1	D	37	LEU
1	D	43	THR
1	D	46	PRO
1	D	61	SER
1	D	74	LEU
1	D	77	LEU
1	D	79	ARG
1	D	89	ARG
1	D	93	GLU
1	D	94	LYS
1	D	121	VAL
1	D	134	ARG
1	D	139	ARG
1	D	163	ASN
1	D	169	LEU
1	D	172	CYS
1	D	178	LEU
1	D	180	LEU
1	D	193	LEU
1	D	197	LEU
1	D	200	THR
1	D	201	LYS
1	D	213	ARG
1	D	215	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	225	LEU
1	D	285	ARG
1	D	295	ARG
1	D	298	HIS
1	D	312	ARG
1	D	314	LEU
1	D	319	ARG
1	D	331	VAL
1	D	332	VAL
1	D	338	GLU
1	D	349	LEU
1	D	356	GLN
1	D	379	SER
1	D	384	VAL
1	D	429	LYS
1	D	433	GLU
1	D	437	LEU
1	D	442	ASN
1	D	445	ILE
1	D	464	GLU
1	D	465	ILE
1	D	466	VAL
2	V	2	GLN
2	V	6	PRO
2	V	23	GLN
2	V	27	LEU
2	V	29	GLU
2	V	31	GLU
2	V	33	LEU
2	V	35	LYS
2	V	42	LEU
2	V	43	GLU
2	V	52	TYR
2	V	54	GLU
2	V	65	ARG
2	V	74	MET
2	V	77	CYS
2	V	78	THR
2	V	81	THR
2	V	82	GLN
2	V	83	VAL
2	V	91	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	V	92	LYS
2	V	96	GLN
2	V	100	ARG
2	V	110	VAL
2	V	119	LYS
2	V	121	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	153	HIS
1	A	163	ASN
1	A	207	ASN
1	A	238	HIS
1	A	241	ASN
1	A	277	ASN
1	A	304	GLN
1	A	356	GLN
2	S	25	GLN
2	S	36	ASN
2	S	55	ASN
2	S	56	ASN
2	S	82	GLN
1	B	149	GLN
1	B	153	HIS
1	B	156	GLN
1	B	163	ASN
1	B	207	ASN
1	B	229	GLN
1	B	238	HIS
1	B	241	ASN
1	B	304	GLN
1	B	356	GLN
2	T	23	GLN
2	T	25	GLN
2	T	36	ASN
2	T	55	ASN
2	T	56	ASN
2	T	82	GLN
1	C	115	ASN
1	C	153	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	163	ASN
1	C	229	GLN
1	C	238	HIS
1	C	241	ASN
1	C	277	ASN
1	C	304	GLN
1	C	356	GLN
1	C	401	GLN
2	U	23	GLN
2	U	25	GLN
2	U	36	ASN
2	U	55	ASN
2	U	56	ASN
2	U	82	GLN
2	U	111	GLN
1	D	115	ASN
1	D	156	GLN
1	D	163	ASN
1	D	229	GLN
1	D	238	HIS
1	D	241	ASN
1	D	304	GLN
1	D	386	HIS
2	V	23	GLN
2	V	25	GLN
2	V	36	ASN
2	V	55	ASN
2	V	56	ASN
2	V	82	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FMT	B	492	1,3	2,2,2	0.48	0	1,1,1	0.27	0
5	FMT	C	492	1,3	2,2,2	1.24	0	1,1,1	0.69	0
5	FMT	D	492	1,3	2,2,2	1.06	0	1,1,1	0.31	0
4	CAP	C	490	3	18,20,20	2.49	10 (55%)	23,31,31	6.19	13 (56%)
4	CAP	A	490	3	18,20,20	2.94	10 (55%)	23,31,31	4.78	12 (52%)
4	CAP	D	490	3	18,20,20	1.86	4 (22%)	23,31,31	4.80	11 (47%)
5	FMT	A	492	1,3	2,2,2	0.74	0	1,1,1	1.52	0
4	CAP	B	490	3	18,20,20	3.10	8 (44%)	23,31,31	5.05	12 (52%)

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
4	CAP	B	490	3	-	16/29/29/29	-
4	CAP	D	490	3	-	11/29/29/29	-
4	CAP	A	490	3	-	15/29/29/29	-
4	CAP	C	490	3	-	11/29/29/29	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	490	CAP	C5-C4	-7.52	1.41	1.51
4	A	490	CAP	C4-C3	-6.23	1.48	1.54
4	C	490	CAP	C4-C3	-5.96	1.48	1.54
4	B	490	CAP	O2-C2	-5.01	1.32	1.43
4	B	490	CAP	P1-O1P	4.66	1.65	1.50
4	A	490	CAP	O2-C2	-4.52	1.33	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	490	CAP	P1-O1P	4.31	1.63	1.50
4	A	490	CAP	P1-O1P	4.29	1.63	1.50
4	B	490	CAP	C4-C3	-4.18	1.50	1.54
4	A	490	CAP	C5-C4	-3.92	1.46	1.51
4	B	490	CAP	O5-C5	-3.68	1.30	1.44
4	D	490	CAP	O2-C2	-3.41	1.36	1.43
4	B	490	CAP	O3-C3	-3.34	1.36	1.42
4	A	490	CAP	P2-O5P	3.22	1.66	1.54
4	C	490	CAP	P1-O1P	3.16	1.60	1.50
4	D	490	CAP	P2-O5P	3.08	1.66	1.54
4	C	490	CAP	O2-C2	-2.94	1.37	1.43
4	C	490	CAP	C5-C4	-2.89	1.47	1.51
4	D	490	CAP	O5-C5	-2.73	1.34	1.44
4	A	490	CAP	O1-C1	-2.72	1.35	1.43
4	A	490	CAP	O5-C5	-2.69	1.34	1.44
4	C	490	CAP	O5-C5	-2.69	1.34	1.44
4	A	490	CAP	P1-O3P	-2.68	1.44	1.54
4	C	490	CAP	P1-O2P	-2.62	1.45	1.54
4	A	490	CAP	P1-O2P	-2.61	1.45	1.54
4	C	490	CAP	P2-O4P	-2.54	1.42	1.50
4	C	490	CAP	P2-O5P	2.47	1.64	1.54
4	C	490	CAP	C2-C	-2.39	1.51	1.53
4	A	490	CAP	O7-C	-2.36	1.22	1.30
4	B	490	CAP	P2-O5P	2.35	1.63	1.54
4	C	490	CAP	O7-C	-2.30	1.22	1.30
4	B	490	CAP	P2-O6P	-2.03	1.47	1.54

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	490	CAP	O3-C3-C4	-15.43	76.08	109.13
4	C	490	CAP	C5-C4-C3	-14.98	81.95	111.96
4	C	490	CAP	O2-C2-C	-14.04	82.72	109.07
4	D	490	CAP	C5-C4-C3	-13.36	85.20	111.96
4	A	490	CAP	O2-C2-C	-12.55	85.51	109.07
4	B	490	CAP	C5-C4-C3	-11.99	87.95	111.96
4	B	490	CAP	O3-C3-C4	-11.88	83.68	109.13
4	A	490	CAP	C5-C4-C3	-11.72	88.49	111.96
4	D	490	CAP	O3-C3-C4	-11.25	85.02	109.13
4	B	490	CAP	O2-C2-C	-10.79	88.81	109.07
4	A	490	CAP	O3-C3-C4	-9.62	88.52	109.13
4	D	490	CAP	O2-C2-C	-8.73	92.68	109.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	490	CAP	O4-C4-C5	8.07	127.78	109.99
4	D	490	CAP	O4-C4-C5	7.45	126.42	109.99
4	C	490	CAP	O7-C-C2	7.09	125.94	114.06
4	C	490	CAP	O4-C4-C5	6.98	125.39	109.99
4	C	490	CAP	O4-C4-C3	-6.32	96.16	108.78
4	B	490	CAP	O4-C4-C3	-6.22	96.35	108.78
4	A	490	CAP	O4-C4-C5	6.14	123.53	109.99
4	A	490	CAP	O3P-P1-O2P	5.67	129.05	107.80
4	D	490	CAP	O4-C4-C3	-5.07	98.65	108.78
4	C	490	CAP	O3P-P1-O1	-4.54	94.82	106.67
4	B	490	CAP	O3P-P1-O2P	4.53	124.79	107.80
4	C	490	CAP	O6P-P2-O5P	-4.01	92.75	107.80
4	B	490	CAP	O7-C-C2	3.80	120.42	114.06
4	D	490	CAP	O3P-P1-O2P	3.74	121.83	107.80
4	C	490	CAP	O6-C-C2	-3.62	115.58	122.32
4	B	490	CAP	O6P-P2-O4P	3.34	123.85	110.83
4	D	490	CAP	O6P-P2-O5P	-3.28	95.49	107.80
4	A	490	CAP	O6P-P2-O4P	3.27	123.59	110.83
4	A	490	CAP	O7-C-C2	2.91	118.93	114.06
4	C	490	CAP	O3P-P1-O2P	2.88	118.59	107.80
4	D	490	CAP	O2P-P1-O1	-2.85	99.23	106.67
4	A	490	CAP	O4-C4-C3	-2.82	103.15	108.78
4	B	490	CAP	O5-C5-C4	2.80	116.84	109.36
4	D	490	CAP	O7-C-C2	2.74	118.64	114.06
4	A	490	CAP	O5-P2-O4P	2.61	113.48	106.44
4	A	490	CAP	O5P-P2-O4P	-2.59	100.73	110.83
4	D	490	CAP	O6P-P2-O4P	2.59	120.91	110.83
4	C	490	CAP	O5P-P2-O4P	2.58	120.87	110.83
4	A	490	CAP	O6P-P2-O5	-2.53	100.07	106.67
4	A	490	CAP	O6-C-C2	-2.50	117.66	122.32
4	B	490	CAP	O6P-P2-O5P	-2.28	99.26	107.80
4	D	490	CAP	O7-C-O6	-2.22	116.74	123.86
4	C	490	CAP	O2P-P1-O1P	2.21	119.46	110.83
4	B	490	CAP	O3P-P1-O1	-2.21	100.91	106.67
4	C	490	CAP	O5-P2-O4P	2.12	112.17	106.44
4	B	490	CAP	O1-P1-O1P	-2.00	101.02	106.44

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	490	CAP	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	490	CAP	O2-C2-C3-C4
4	A	490	CAP	O2-C2-C3-O3
4	A	490	CAP	C2-C3-C4-C5
4	A	490	CAP	C2-C3-C4-O4
4	A	490	CAP	O3-C3-C4-O4
4	A	490	CAP	O4-C4-C5-O5
4	B	490	CAP	O1-C1-C2-C
4	B	490	CAP	C1-C2-C3-C4
4	B	490	CAP	C1-C2-C3-O3
4	B	490	CAP	O2-C2-C3-C4
4	B	490	CAP	O2-C2-C3-O3
4	B	490	CAP	O6-C-C2-C3
4	B	490	CAP	C2-C3-C4-O4
4	B	490	CAP	O3-C3-C4-O4
4	B	490	CAP	O4-C4-C5-O5
4	B	490	CAP	C5-O5-P2-O4P
4	B	490	CAP	C5-O5-P2-O5P
4	B	490	CAP	C5-O5-P2-O6P
4	C	490	CAP	C1-C2-C3-C4
4	C	490	CAP	O2-C2-C3-C4
4	C	490	CAP	C2-C3-C4-C5
4	C	490	CAP	C2-C3-C4-O4
4	C	490	CAP	O3-C3-C4-O4
4	C	490	CAP	O4-C4-C5-O5
4	C	490	CAP	C4-C5-O5-P2
4	C	490	CAP	C5-O5-P2-O5P
4	D	490	CAP	C1-C2-C3-C4
4	D	490	CAP	C1-C2-C3-O3
4	D	490	CAP	O2-C2-C3-C4
4	D	490	CAP	O2-C2-C3-O3
4	D	490	CAP	C2-C3-C4-O4
4	D	490	CAP	O3-C3-C4-O4
4	D	490	CAP	C3-C4-C5-O5
4	D	490	CAP	O4-C4-C5-O5
4	D	490	CAP	C5-O5-P2-O5P
4	A	490	CAP	C3-C4-C5-O5
4	B	490	CAP	C3-C4-C5-O5
4	C	490	CAP	C3-C4-C5-O5
4	A	490	CAP	C4-C5-O5-P2
4	B	490	CAP	C4-C5-O5-P2
4	D	490	CAP	C4-C5-O5-P2
4	A	490	CAP	O7-C-C2-O2

Continued on next page...

Continued from previous page...

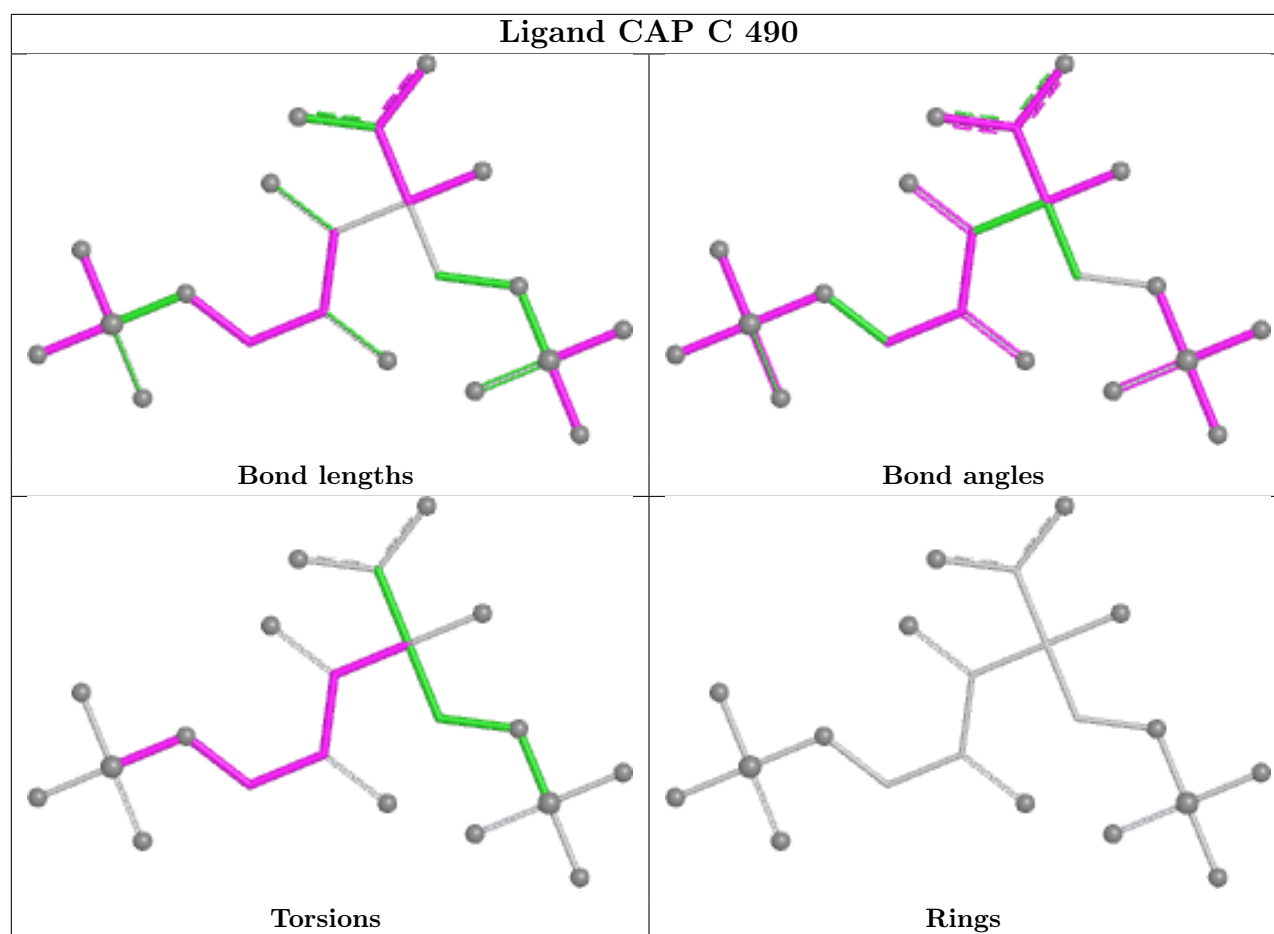
Mol	Chain	Res	Type	Atoms
4	A	490	CAP	O6-C-C2-O2
4	C	490	CAP	C5-O5-P2-O6P
4	D	490	CAP	C2-C3-C4-C5
4	B	490	CAP	O1-C1-C2-C3
4	A	490	CAP	O6-C-C2-C1
4	A	490	CAP	O7-C-C2-C1
4	A	490	CAP	C5-O5-P2-O4P
4	A	490	CAP	C5-O5-P2-O6P
4	C	490	CAP	O3-C3-C4-C5
4	B	490	CAP	C2-C3-C4-C5

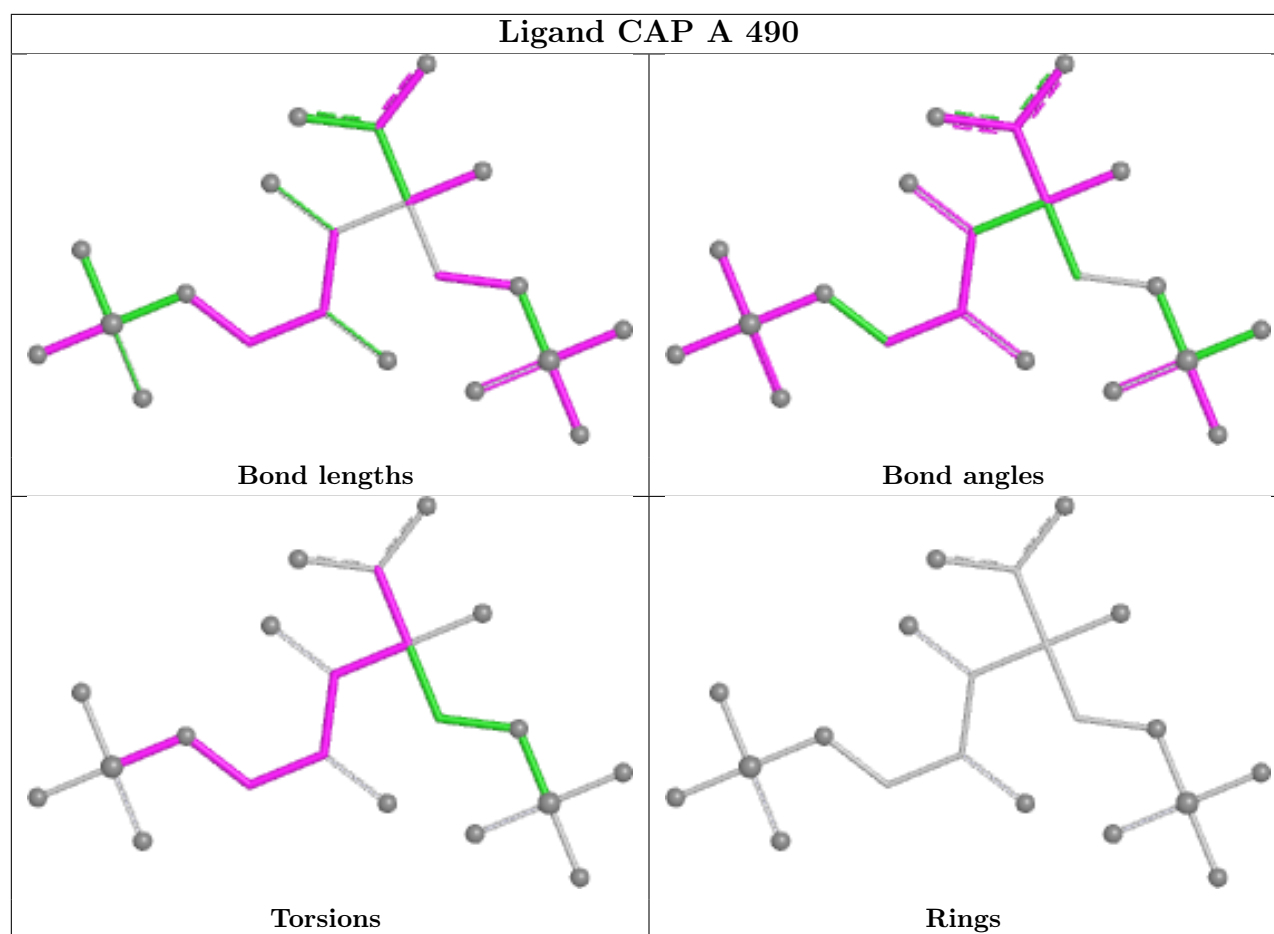
There are no ring outliers.

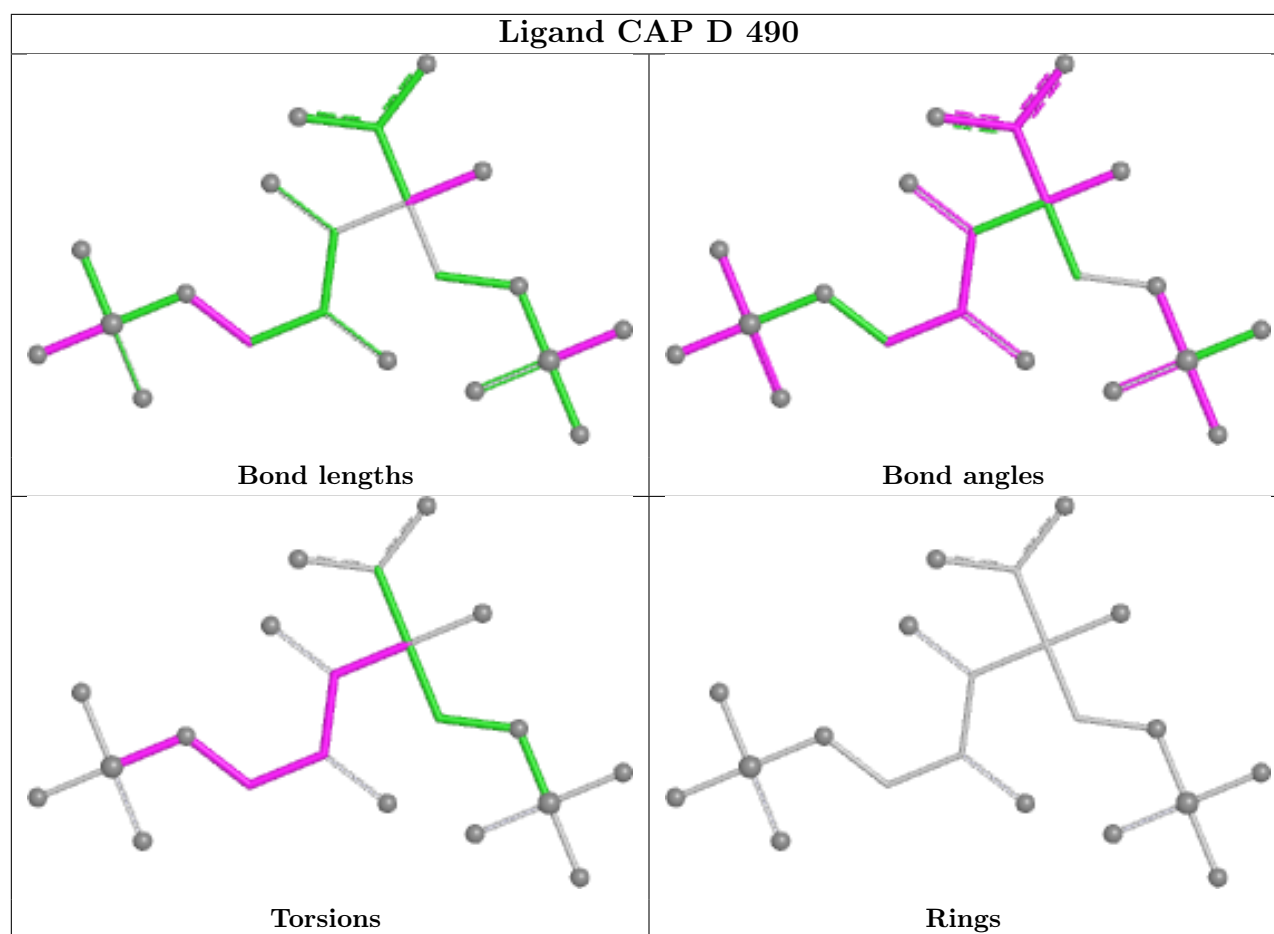
6 monomers are involved in 8 short contacts:

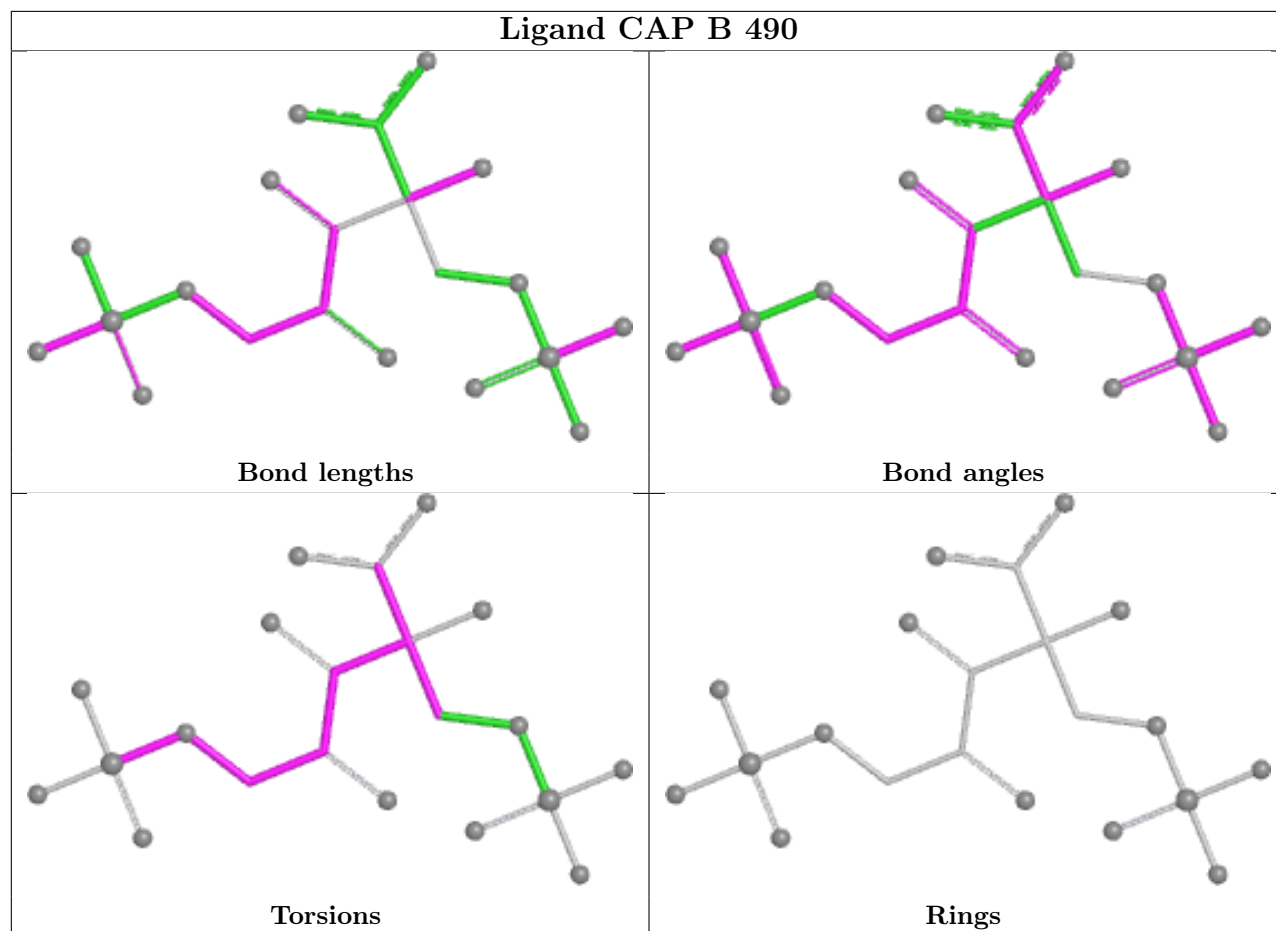
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	492	FMT	1	0
5	D	492	FMT	1	0
4	C	490	CAP	1	0
4	A	490	CAP	2	0
4	D	490	CAP	3	0
5	A	492	FMT	1	0

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









5.7 Other polymers [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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.