



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:57 PM UTC

PDB ID : 2R5I / pdb_00002r5i
Title : Pentamer Structure of Major Capsid Protein L1 of Human Papilloma Virus type 18
Authors : Bishop, B.; Dasgupta, J.; Chen, X.S.
Deposited on : 2007-09-03
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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:

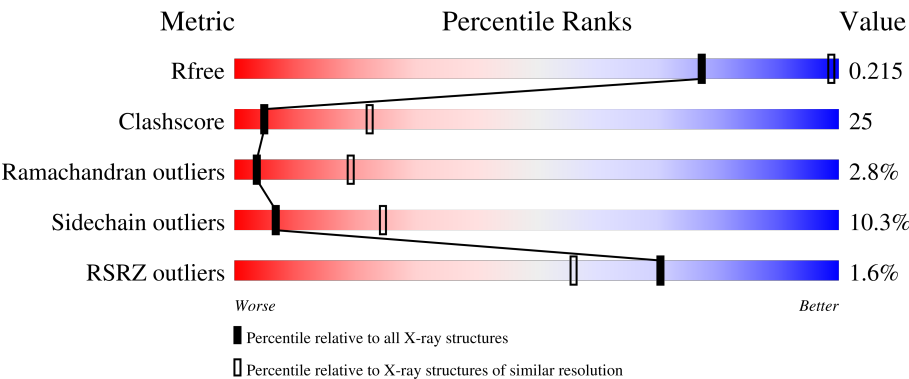
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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

Mol	Chain	Length	Quality of chain
1	A	428	39%40%17%..
1	B	428	37%43%16%..
1	C	428	43%37%17%..
1	D	428	38%44%15%..
1	E	428	2%38%41%17%..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	428	
1	G	428	
1	H	428	
1	I	428	
1	J	428	
1	K	428	
1	L	428	
1	M	428	
1	N	428	
1	O	428	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 49845 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 L1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	0	0	0
			3323	2098	562	643	20			
1	B	423	Total	C	N	O	S	0	0	0
			3323	2098	562	643	20			
1	C	423	Total	C	N	O	S	0	0	0
			3323	2098	562	643	20			
1	D	423	Total	C	N	O	S	0	0	0
			3323	2098	562	643	20			
1	E	423	Total	C	N	O	S	0	0	0
			3323	2098	562	643	20			
1	F	423	Total	C	N	O	S	0	0	0
			3323	2098	562	643	20			
1	G	423	Total	C	N	O	S	0	0	0
			3323	2098	562	643	20			
1	H	423	Total	C	N	O	S	0	0	0
			3323	2098	562	643	20			
1	I	423	Total	C	N	O	S	0	0	0
			3323	2098	562	643	20			
1	J	423	Total	C	N	O	S	0	0	0
			3323	2098	562	643	20			
1	K	423	Total	C	N	O	S	0	0	0
			3323	2098	562	643	20			
1	L	423	Total	C	N	O	S	0	0	0
			3323	2098	562	643	20			
1	M	423	Total	C	N	O	S	0	0	0
			3323	2098	562	643	20			
1	N	423	Total	C	N	O	S	0	0	0
			3323	2098	562	643	20			
1	O	423	Total	C	N	O	S	0	0	0
			3323	2098	562	643	20			

There are 135 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ALA	-	expression tag	UNP Q80B70
A	47	ASP	ASN	engineered mutation	UNP Q80B70
A	175	SER	CYS	engineered mutation	UNP Q80B70
A	393	GLN	HIS	engineered mutation	UNP Q80B70
A	405	GLY	-	linker	UNP Q80B70
A	406	GLY	-	linker	UNP Q80B70
A	407	SER	-	linker	UNP Q80B70
A	408	GLY	-	linker	UNP Q80B70
A	409	GLY	-	linker	UNP Q80B70
B	20	ALA	-	expression tag	UNP Q80B70
B	47	ASP	ASN	engineered mutation	UNP Q80B70
B	175	SER	CYS	engineered mutation	UNP Q80B70
B	393	GLN	HIS	engineered mutation	UNP Q80B70
B	405	GLY	-	linker	UNP Q80B70
B	406	GLY	-	linker	UNP Q80B70
B	407	SER	-	linker	UNP Q80B70
B	408	GLY	-	linker	UNP Q80B70
B	409	GLY	-	linker	UNP Q80B70
C	20	ALA	-	expression tag	UNP Q80B70
C	47	ASP	ASN	engineered mutation	UNP Q80B70
C	175	SER	CYS	engineered mutation	UNP Q80B70
C	393	GLN	HIS	engineered mutation	UNP Q80B70
C	405	GLY	-	linker	UNP Q80B70
C	406	GLY	-	linker	UNP Q80B70
C	407	SER	-	linker	UNP Q80B70
C	408	GLY	-	linker	UNP Q80B70
C	409	GLY	-	linker	UNP Q80B70
D	20	ALA	-	expression tag	UNP Q80B70
D	47	ASP	ASN	engineered mutation	UNP Q80B70
D	175	SER	CYS	engineered mutation	UNP Q80B70
D	393	GLN	HIS	engineered mutation	UNP Q80B70
D	405	GLY	-	linker	UNP Q80B70
D	406	GLY	-	linker	UNP Q80B70
D	407	SER	-	linker	UNP Q80B70
D	408	GLY	-	linker	UNP Q80B70
D	409	GLY	-	linker	UNP Q80B70
E	20	ALA	-	expression tag	UNP Q80B70
E	47	ASP	ASN	engineered mutation	UNP Q80B70
E	175	SER	CYS	engineered mutation	UNP Q80B70
E	393	GLN	HIS	engineered mutation	UNP Q80B70
E	405	GLY	-	linker	UNP Q80B70
E	406	GLY	-	linker	UNP Q80B70
E	407	SER	-	linker	UNP Q80B70

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	408	GLY	-	linker	UNP Q80B70
E	409	GLY	-	linker	UNP Q80B70
F	20	ALA	-	expression tag	UNP Q80B70
F	47	ASP	ASN	engineered mutation	UNP Q80B70
F	175	SER	CYS	engineered mutation	UNP Q80B70
F	393	GLN	HIS	engineered mutation	UNP Q80B70
F	405	GLY	-	linker	UNP Q80B70
F	406	GLY	-	linker	UNP Q80B70
F	407	SER	-	linker	UNP Q80B70
F	408	GLY	-	linker	UNP Q80B70
F	409	GLY	-	linker	UNP Q80B70
G	20	ALA	-	expression tag	UNP Q80B70
G	47	ASP	ASN	engineered mutation	UNP Q80B70
G	175	SER	CYS	engineered mutation	UNP Q80B70
G	393	GLN	HIS	engineered mutation	UNP Q80B70
G	405	GLY	-	linker	UNP Q80B70
G	406	GLY	-	linker	UNP Q80B70
G	407	SER	-	linker	UNP Q80B70
G	408	GLY	-	linker	UNP Q80B70
G	409	GLY	-	linker	UNP Q80B70
H	20	ALA	-	expression tag	UNP Q80B70
H	47	ASP	ASN	engineered mutation	UNP Q80B70
H	175	SER	CYS	engineered mutation	UNP Q80B70
H	393	GLN	HIS	engineered mutation	UNP Q80B70
H	405	GLY	-	linker	UNP Q80B70
H	406	GLY	-	linker	UNP Q80B70
H	407	SER	-	linker	UNP Q80B70
H	408	GLY	-	linker	UNP Q80B70
H	409	GLY	-	linker	UNP Q80B70
I	20	ALA	-	expression tag	UNP Q80B70
I	47	ASP	ASN	engineered mutation	UNP Q80B70
I	175	SER	CYS	engineered mutation	UNP Q80B70
I	393	GLN	HIS	engineered mutation	UNP Q80B70
I	405	GLY	-	linker	UNP Q80B70
I	406	GLY	-	linker	UNP Q80B70
I	407	SER	-	linker	UNP Q80B70
I	408	GLY	-	linker	UNP Q80B70
I	409	GLY	-	linker	UNP Q80B70
J	20	ALA	-	expression tag	UNP Q80B70
J	47	ASP	ASN	engineered mutation	UNP Q80B70
J	175	SER	CYS	engineered mutation	UNP Q80B70
J	393	GLN	HIS	engineered mutation	UNP Q80B70

Continued on next page...

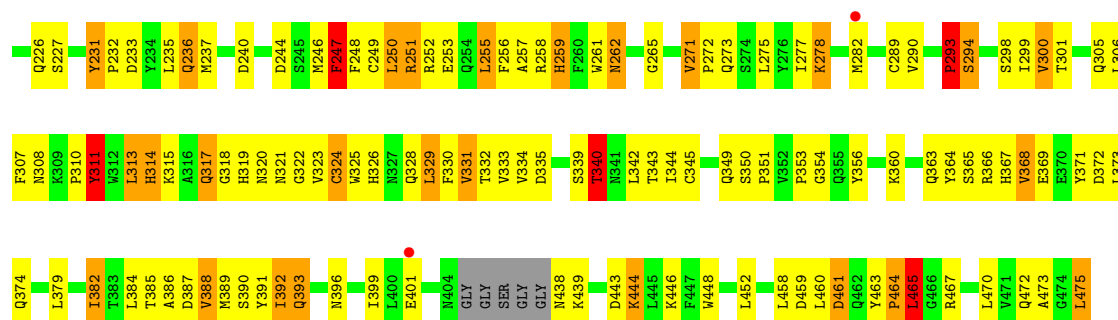
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	405	GLY	-	linker	UNP Q80B70
J	406	GLY	-	linker	UNP Q80B70
J	407	SER	-	linker	UNP Q80B70
J	408	GLY	-	linker	UNP Q80B70
J	409	GLY	-	linker	UNP Q80B70
K	20	ALA	-	expression tag	UNP Q80B70
K	47	ASP	ASN	engineered mutation	UNP Q80B70
K	175	SER	CYS	engineered mutation	UNP Q80B70
K	393	GLN	HIS	engineered mutation	UNP Q80B70
K	405	GLY	-	linker	UNP Q80B70
K	406	GLY	-	linker	UNP Q80B70
K	407	SER	-	linker	UNP Q80B70
K	408	GLY	-	linker	UNP Q80B70
K	409	GLY	-	linker	UNP Q80B70
L	20	ALA	-	expression tag	UNP Q80B70
L	47	ASP	ASN	engineered mutation	UNP Q80B70
L	175	SER	CYS	engineered mutation	UNP Q80B70
L	393	GLN	HIS	engineered mutation	UNP Q80B70
L	405	GLY	-	linker	UNP Q80B70
L	406	GLY	-	linker	UNP Q80B70
L	407	SER	-	linker	UNP Q80B70
L	408	GLY	-	linker	UNP Q80B70
L	409	GLY	-	linker	UNP Q80B70
M	20	ALA	-	expression tag	UNP Q80B70
M	47	ASP	ASN	engineered mutation	UNP Q80B70
M	175	SER	CYS	engineered mutation	UNP Q80B70
M	393	GLN	HIS	engineered mutation	UNP Q80B70
M	405	GLY	-	linker	UNP Q80B70
M	406	GLY	-	linker	UNP Q80B70
M	407	SER	-	linker	UNP Q80B70
M	408	GLY	-	linker	UNP Q80B70
M	409	GLY	-	linker	UNP Q80B70
N	20	ALA	-	expression tag	UNP Q80B70
N	47	ASP	ASN	engineered mutation	UNP Q80B70
N	175	SER	CYS	engineered mutation	UNP Q80B70
N	393	GLN	HIS	engineered mutation	UNP Q80B70
N	405	GLY	-	linker	UNP Q80B70
N	406	GLY	-	linker	UNP Q80B70
N	407	SER	-	linker	UNP Q80B70
N	408	GLY	-	linker	UNP Q80B70
N	409	GLY	-	linker	UNP Q80B70
O	20	ALA	-	expression tag	UNP Q80B70

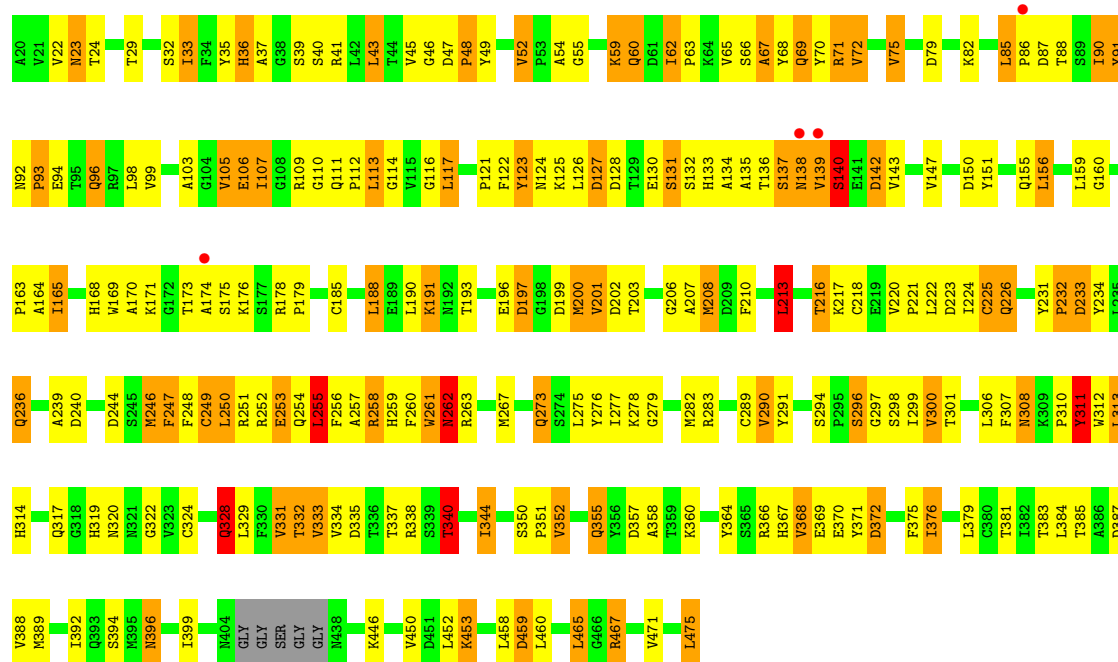
Continued on next page...

Continued from previous page...

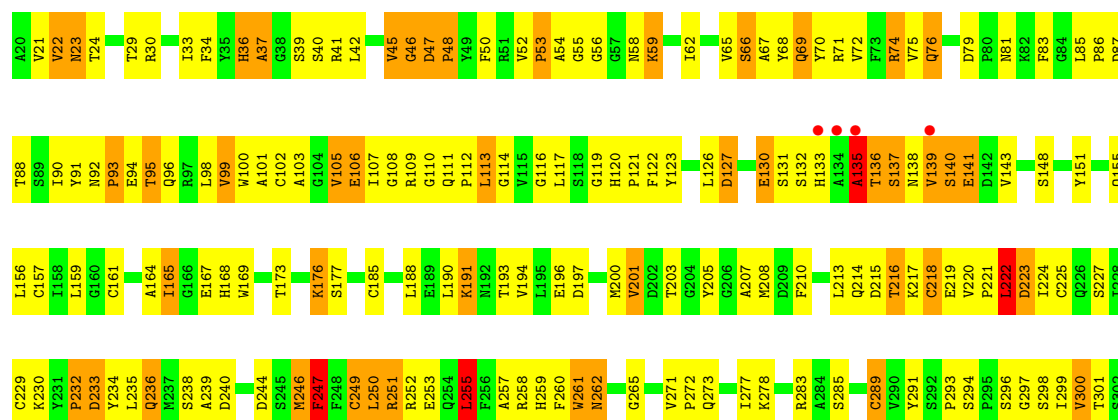
Chain	Residue	Modelled	Actual	Comment	Reference
O	47	ASP	ASN	engineered mutation	UNP Q80B70
O	175	SER	CYS	engineered mutation	UNP Q80B70
O	393	GLN	HIS	engineered mutation	UNP Q80B70
O	405	GLY	-	linker	UNP Q80B70
O	406	GLY	-	linker	UNP Q80B70
O	407	SER	-	linker	UNP Q80B70
O	408	GLY	-	linker	UNP Q80B70
O	409	GLY	-	linker	UNP Q80B70

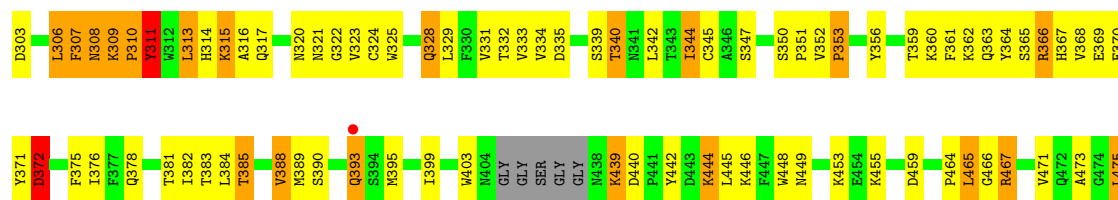


• Molecule 1: L1 protein

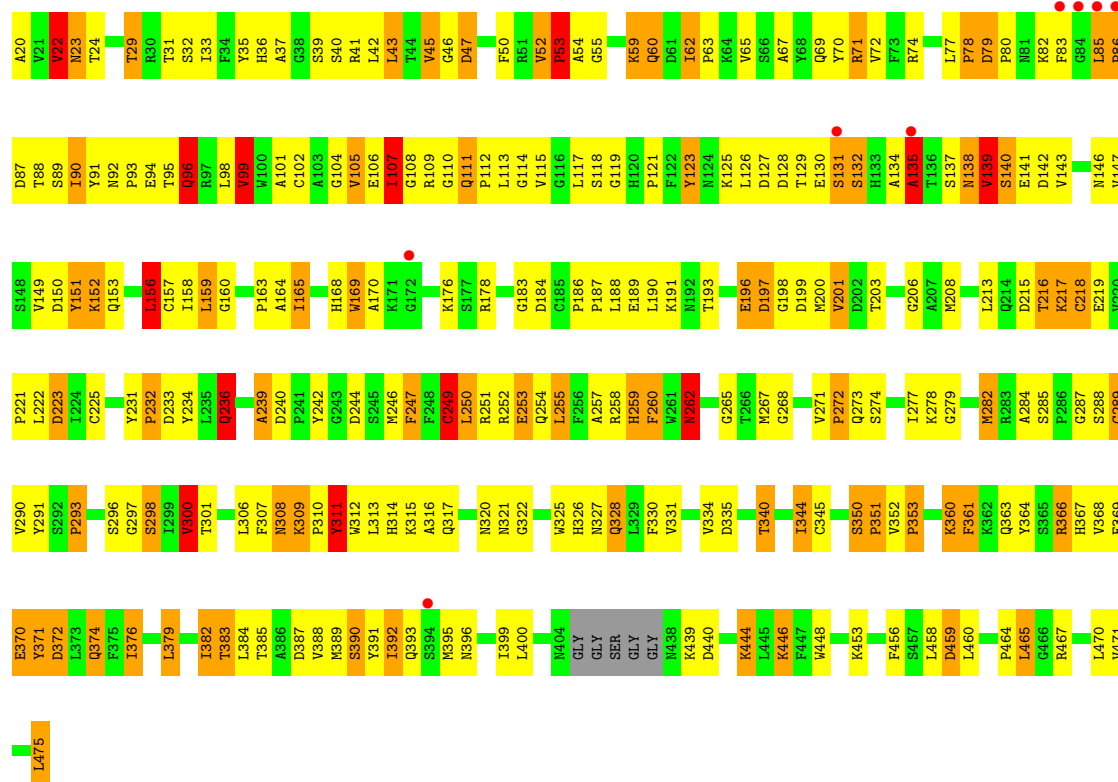


• Molecule 1: L1 protein

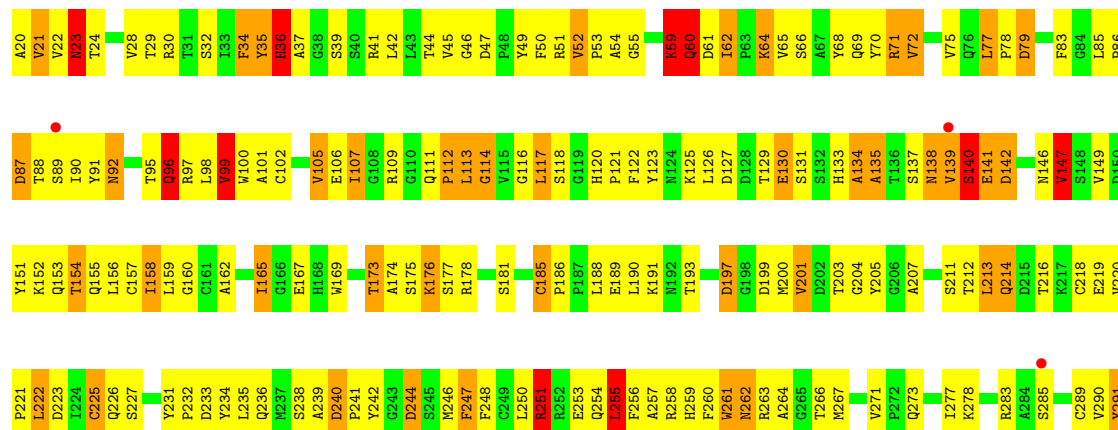




• Molecule 1: L1 protein

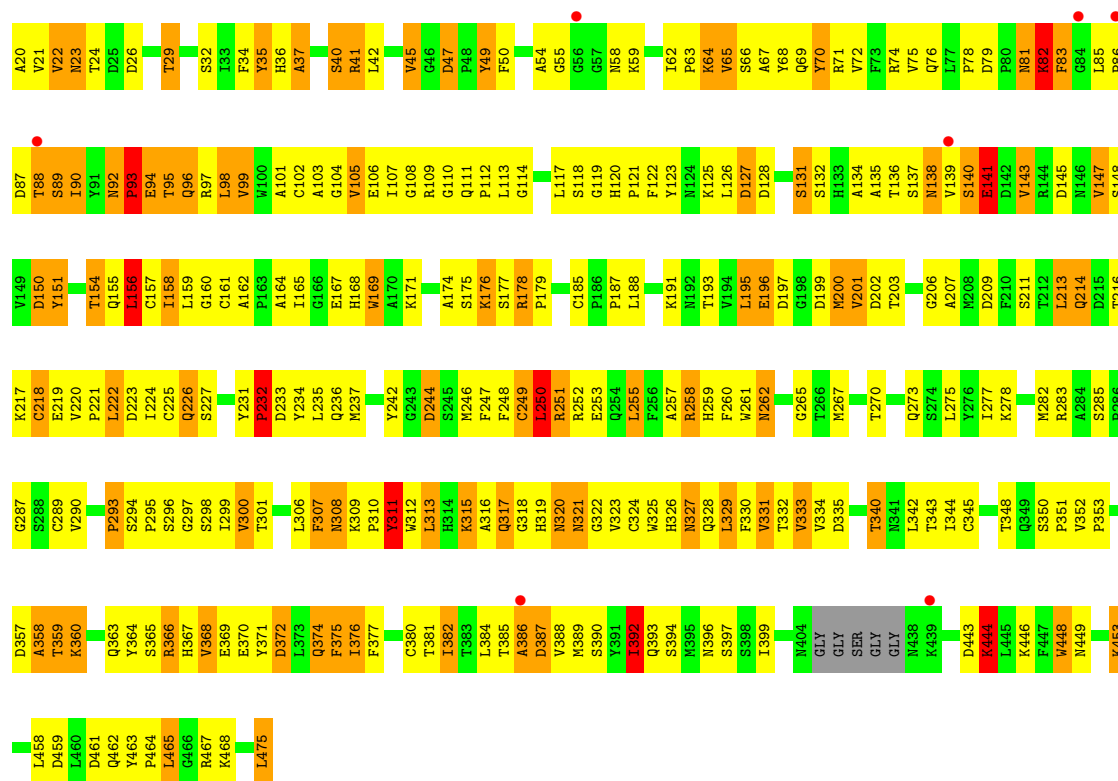


• Molecule 1: L1 protein

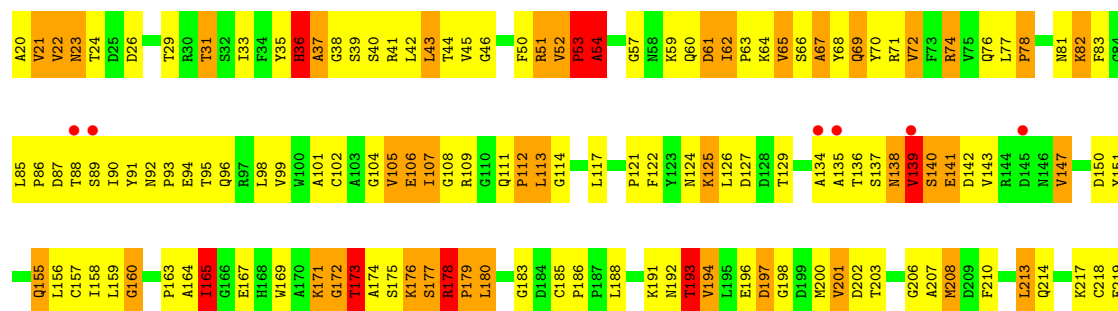


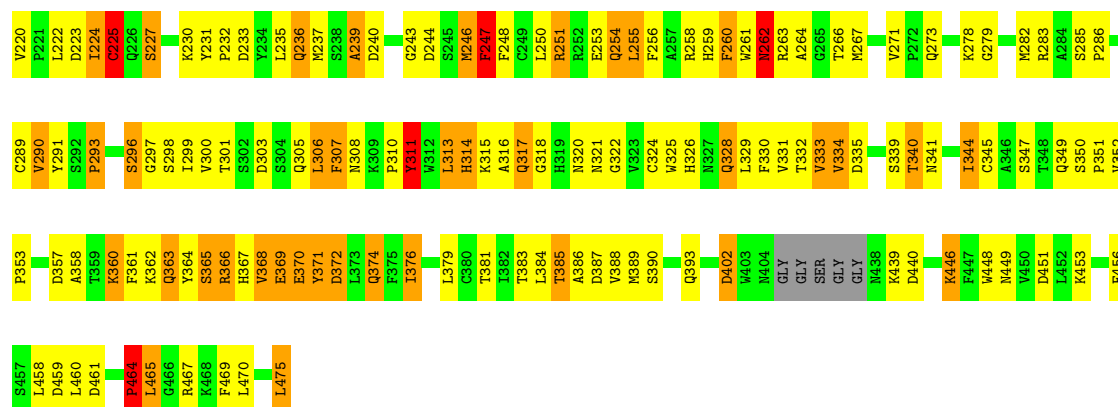


• Molecule 1: L1 protein

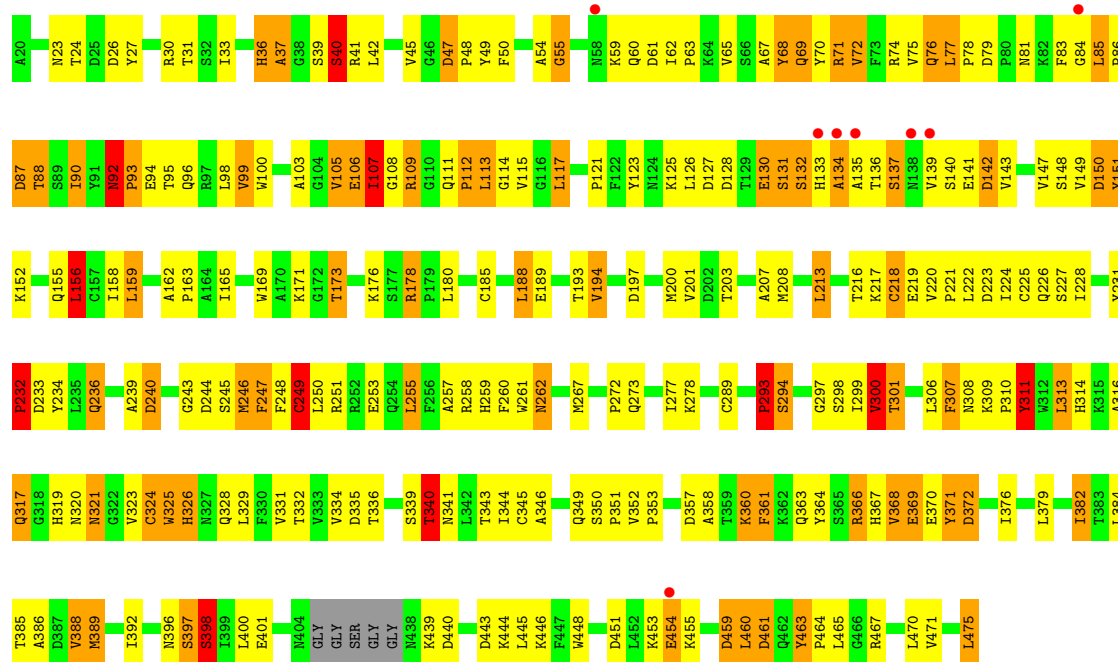


• Molecule 1: L1 protein

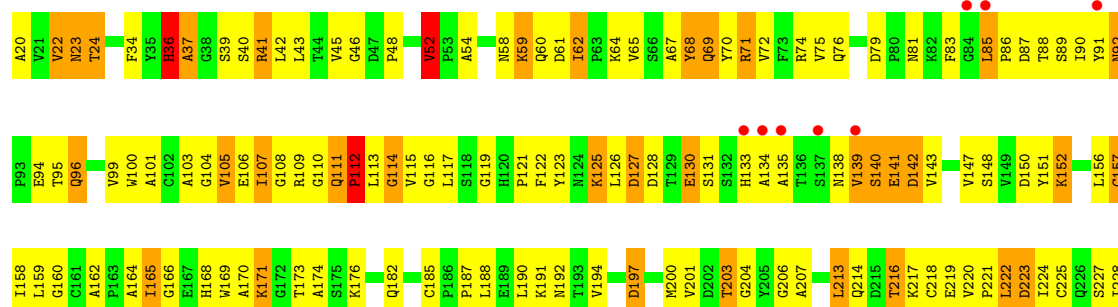


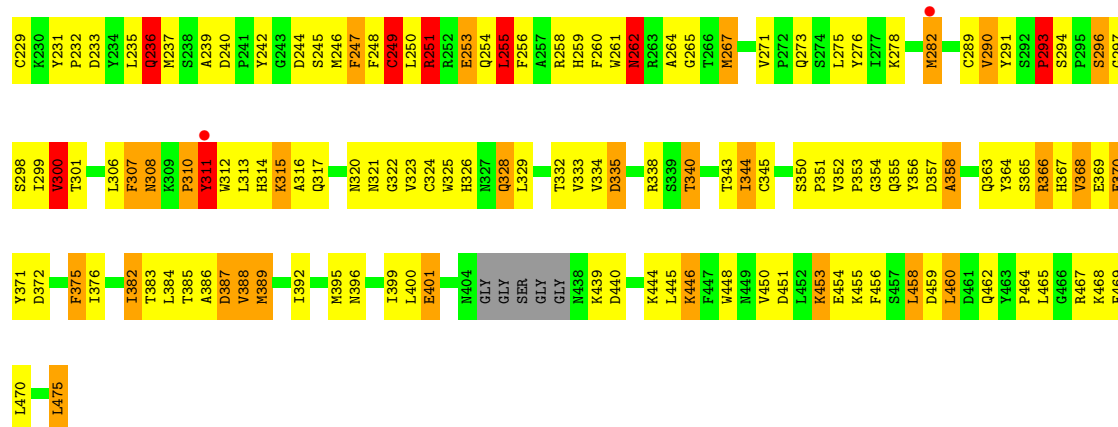


• Molecule 1: L1 protein

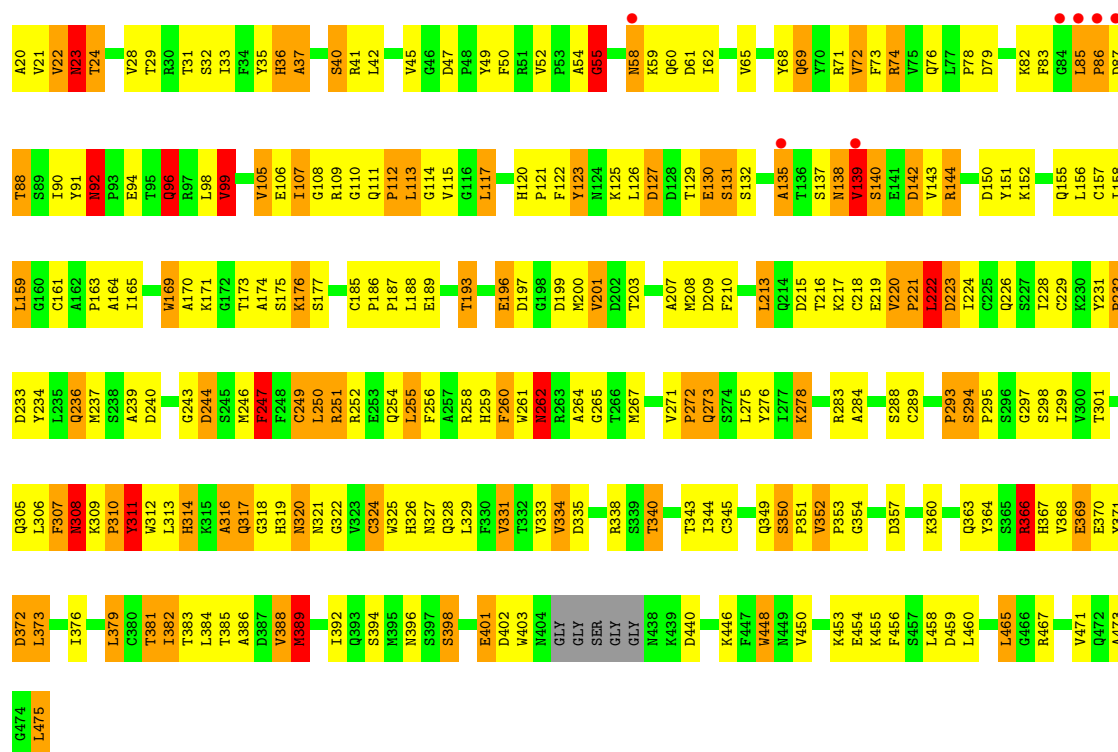


• Molecule 1: L1 protein

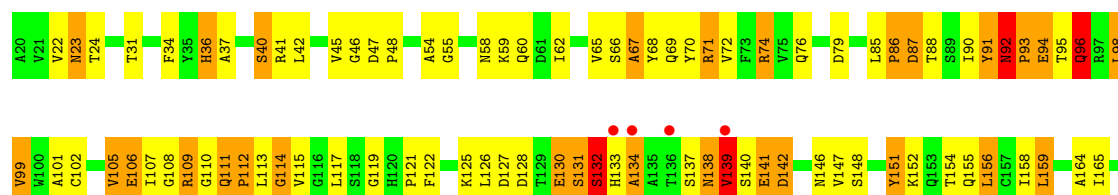


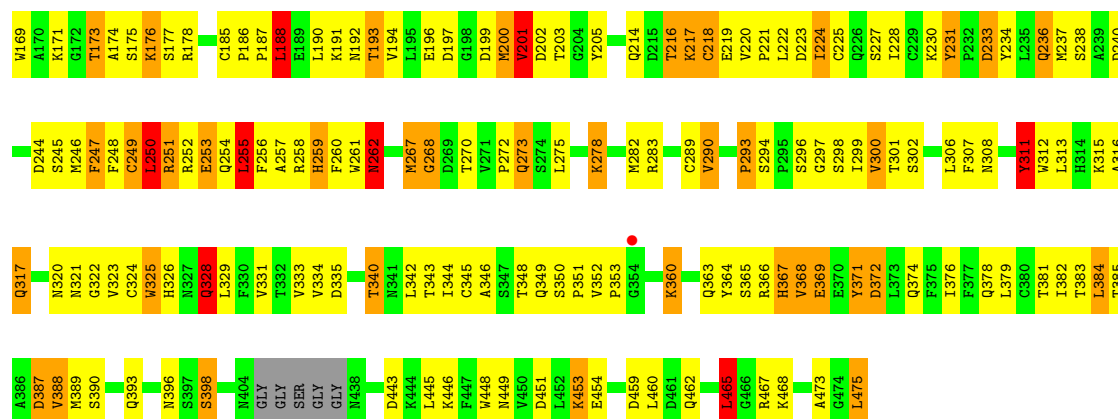


• Molecule 1: L1 protein

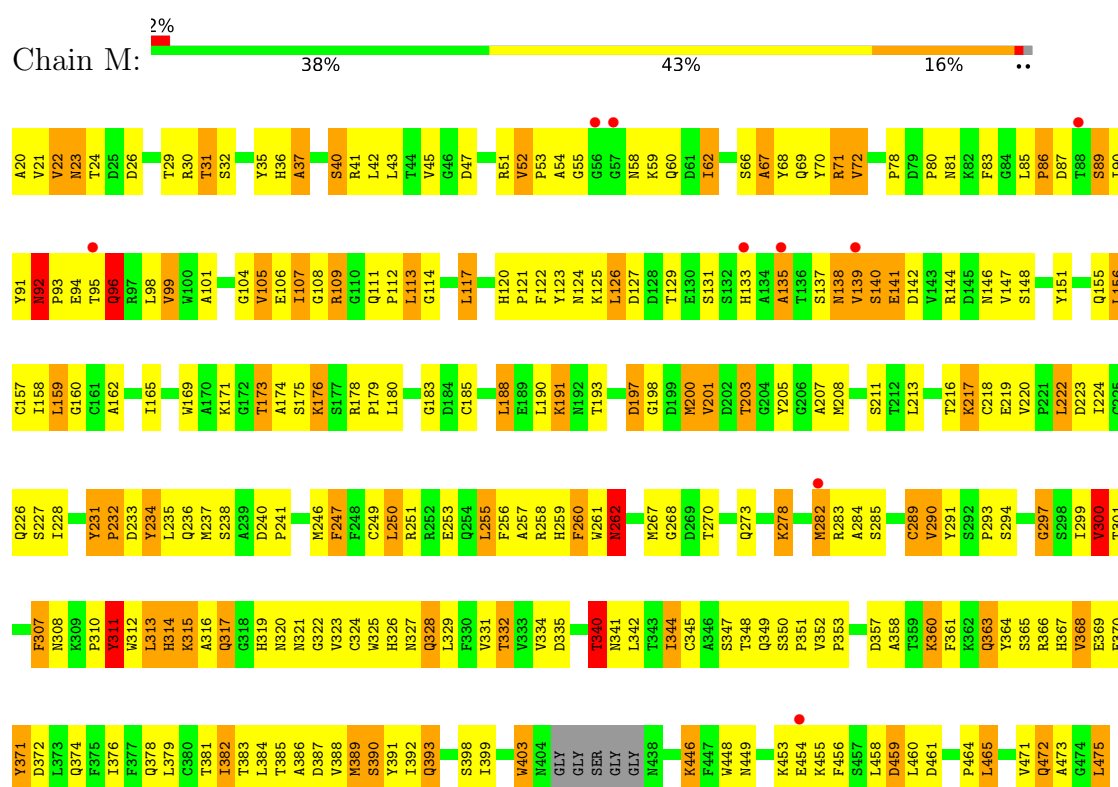


• Molecule 1: L1 protein

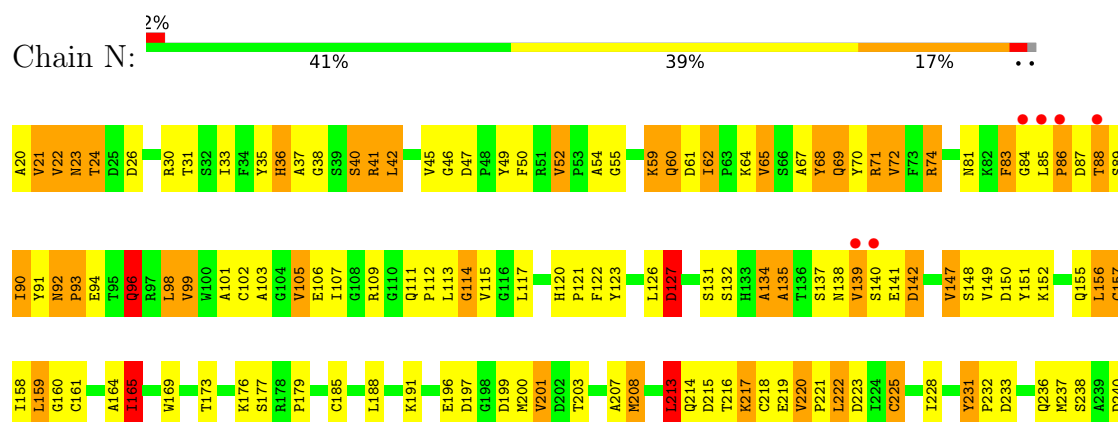


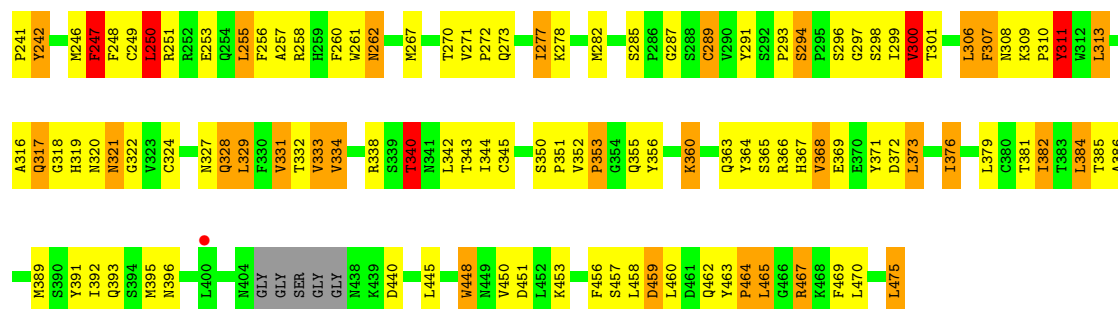


• Molecule 1: L1 protein

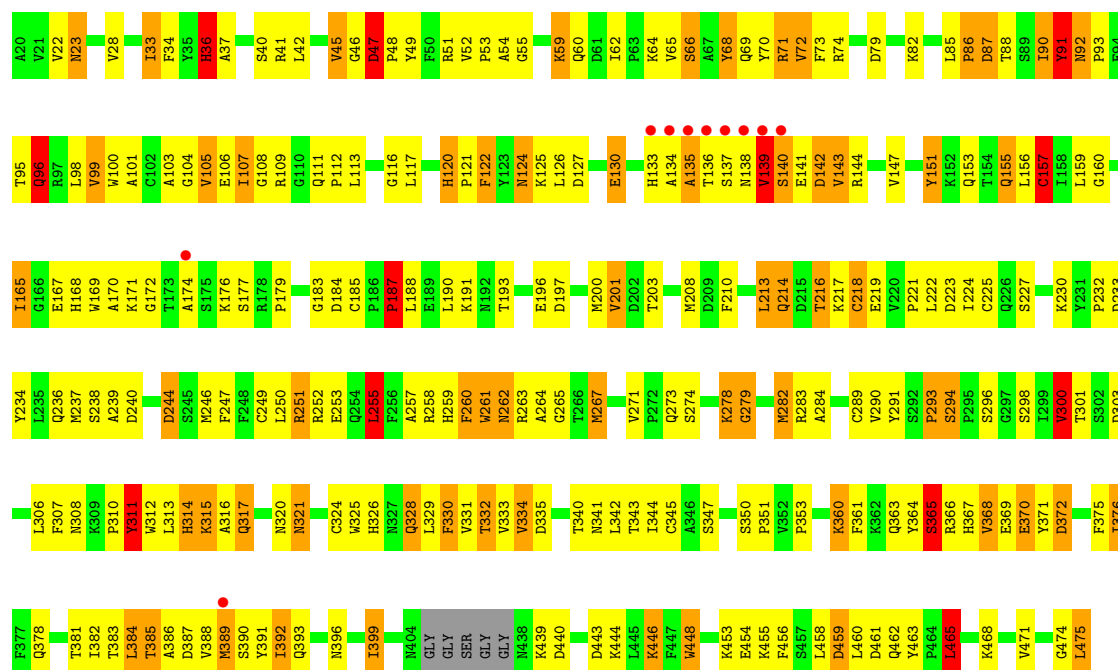


• Molecule 1: L1 protein





• Molecule 1: L1 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	81.16Å 105.04Å 235.75Å 87.56° 85.66° 68.16°	Depositor
Resolution (Å)	40.00 – 3.40 40.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-3.40) 99.6 (40.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	19.60	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.214 , 0.260 0.204 , 0.215	Depositor DCC
R_{free} test set	11857 reflections (7.47%)	wwPDB-VP
Wilson B-factor (Å ²)	63.4	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	49845	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	109/3408 (3.2%)	1.81	74/4633 (1.6%)
1	B	2.25	113/3408 (3.3%)	1.72	53/4633 (1.1%)
1	C	2.20	99/3408 (2.9%)	1.75	59/4633 (1.3%)
1	D	2.30	118/3408 (3.5%)	1.76	49/4633 (1.1%)
1	E	2.33	139/3408 (4.1%)	1.75	51/4633 (1.1%)
1	F	2.28	130/3408 (3.8%)	1.73	58/4633 (1.3%)
1	G	2.32	131/3408 (3.8%)	1.82	67/4633 (1.4%)
1	H	2.22	127/3408 (3.7%)	1.82	84/4633 (1.8%)
1	I	2.17	104/3408 (3.1%)	1.69	46/4633 (1.0%)
1	J	2.25	118/3408 (3.5%)	1.75	56/4633 (1.2%)
1	K	2.26	121/3408 (3.6%)	1.78	74/4633 (1.6%)
1	L	2.23	117/3408 (3.4%)	1.77	56/4633 (1.2%)
1	M	2.26	117/3408 (3.4%)	1.75	51/4633 (1.1%)
1	N	2.23	102/3408 (3.0%)	1.70	47/4633 (1.0%)
1	O	2.24	112/3408 (3.3%)	1.77	54/4633 (1.2%)
All	All	2.25	1757/51120 (3.4%)	1.76	879/69495 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (1757) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	207	ALA	CA-CB	-15.49	1.32	1.53
1	M	257	ALA	CA-CB	-14.13	1.34	1.52
1	G	160	GLY	C-O	13.29	1.38	1.23
1	D	439	LYS	CE-NZ	13.26	1.89	1.49
1	F	89	SER	C-O	13.11	1.38	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	164	ALA	CA-CB	-12.99	1.31	1.53
1	K	334	VAL	CA-CB	-12.49	1.38	1.54
1	M	207	ALA	CA-CB	-12.43	1.36	1.52
1	H	88	THR	CA-CB	12.25	1.69	1.52
1	D	101	ALA	CA-CB	-11.75	1.32	1.53
1	N	69	GLN	C-O	-11.68	1.09	1.24
1	M	299	ILE	CA-CB	-11.62	1.41	1.54
1	O	103	ALA	CA-CB	-11.59	1.37	1.54
1	J	164	ALA	CA-CB	-11.55	1.35	1.53
1	J	101	ALA	CA-CB	-11.44	1.37	1.53
1	B	101	ALA	CA-CB	-11.44	1.36	1.53
1	L	257	ALA	CA-CB	-11.25	1.38	1.53
1	K	72	VAL	C-O	-11.24	1.11	1.24
1	O	170	ALA	CA-CB	-11.14	1.34	1.54
1	A	257	ALA	CA-CB	-10.99	1.39	1.53
1	E	164	ALA	CA-CB	-10.84	1.35	1.53
1	L	453	LYS	CD-CE	10.78	1.84	1.52
1	N	89	SER	C-O	10.75	1.34	1.23
1	N	52	VAL	CA-CB	-10.43	1.42	1.53
1	E	52	VAL	CA-CB	-10.42	1.43	1.53
1	I	162	ALA	CA-CB	-10.37	1.41	1.53
1	E	186	PRO	CA-C	-10.36	1.42	1.52
1	O	168	HIS	C-O	-10.22	1.11	1.23
1	H	67	ALA	CA-CB	-10.20	1.35	1.53
1	M	282	MET	SD-CE	10.11	2.04	1.79
1	F	139	VAL	CA-CB	10.07	1.68	1.54
1	E	201	VAL	CA-C	-10.06	1.44	1.52
1	B	197	ASP	C-O	-10.05	1.12	1.24
1	N	368	VAL	C-O	-10.00	1.12	1.23
1	F	381	THR	C-O	9.93	1.36	1.23
1	B	52	VAL	CA-CB	-9.88	1.43	1.53
1	A	67	ALA	CA-CB	-9.79	1.36	1.53
1	O	218	CYS	C-O	-9.78	1.14	1.24
1	B	231	TYR	CA-C	-9.77	1.43	1.52
1	K	55	GLY	C-O	9.76	1.37	1.23
1	K	155	GLN	C-O	-9.74	1.12	1.23
1	D	251	ARG	CA-C	-9.70	1.40	1.52
1	J	207	ALA	CA-CB	-9.69	1.40	1.52
1	E	83	PHE	C-O	9.68	1.36	1.23
1	H	285	SER	CA-C	9.65	1.60	1.52
1	K	37	ALA	CA-CB	-9.61	1.37	1.53
1	B	207	ALA	CA-CB	-9.60	1.40	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	116	GLY	C-O	9.58	1.34	1.24
1	A	101	ALA	CA-CB	-9.54	1.39	1.53
1	G	64	LYS	CD-CE	9.50	1.80	1.52
1	D	133	HIS	CA-C	9.47	1.65	1.52
1	G	187	PRO	C-O	9.43	1.33	1.23
1	D	103	ALA	CA-CB	-9.43	1.40	1.54
1	I	299	ILE	CA-CB	-9.42	1.43	1.54
1	D	88	THR	CA-CB	9.39	1.65	1.52
1	L	453	LYS	CG-CD	9.39	1.80	1.52
1	G	206	GLY	C-O	9.24	1.35	1.23
1	E	186	PRO	C-O	-9.22	1.14	1.24
1	C	156	LEU	CA-C	-9.19	1.41	1.52
1	K	307	PHE	C-O	-9.19	1.12	1.23
1	D	255	LEU	C-O	-9.18	1.14	1.24
1	H	207	ALA	CA-CB	-9.13	1.41	1.53
1	A	267	MET	SD-CE	9.12	2.02	1.79
1	O	238	SER	CA-C	-9.10	1.41	1.52
1	G	315	LYS	CD-CE	9.08	1.79	1.52
1	G	285	SER	CA-C	9.02	1.60	1.52
1	B	388	VAL	CA-CB	-9.02	1.44	1.54
1	E	20	ALA	N-CA	9.02	1.63	1.46
1	G	174	ALA	CA-CB	8.99	1.66	1.53
1	L	194	VAL	CA-CB	-8.99	1.43	1.54
1	E	249	CYS	C-O	-8.98	1.14	1.23
1	K	161	CYS	CA-C	-8.97	1.41	1.53
1	O	88	THR	CA-CB	8.96	1.65	1.52
1	J	300	VAL	C-O	-8.94	1.14	1.24
1	I	165	ILE	CA-CB	-8.90	1.43	1.54
1	O	342	LEU	C-O	8.88	1.34	1.23
1	B	42	LEU	C-O	-8.85	1.12	1.23
1	E	85	LEU	C-O	8.85	1.34	1.23
1	L	192	ASN	C-O	-8.84	1.13	1.23
1	O	72	VAL	CA-CB	-8.83	1.43	1.54
1	E	446	LYS	CD-CE	8.82	1.78	1.52
1	F	88	THR	CA-CB	8.82	1.63	1.53
1	D	252	ARG	CZ-NH2	8.81	1.45	1.33
1	D	315	LYS	CG-CD	8.81	1.78	1.52
1	G	93	PRO	C-O	8.80	1.35	1.24
1	M	197	ASP	C-O	-8.80	1.13	1.23
1	E	86	PRO	C-O	8.80	1.35	1.24
1	N	88	THR	CA-CB	8.75	1.63	1.53
1	E	101	ALA	CA-CB	-8.73	1.41	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	360	LYS	CD-CE	8.71	1.78	1.52
1	O	315	LYS	CE-NZ	8.66	1.75	1.49
1	G	330	PHE	C-O	8.66	1.34	1.24
1	L	88	THR	CA-CB	8.64	1.65	1.53
1	N	310	PRO	C-O	-8.63	1.14	1.23
1	N	52	VAL	N-CA	-8.60	1.40	1.46
1	N	101	ALA	CA-CB	-8.55	1.41	1.53
1	N	285	SER	CA-C	8.54	1.60	1.52
1	E	201	VAL	C-O	-8.53	1.14	1.23
1	H	456	PHE	C-O	-8.53	1.13	1.23
1	E	90	ILE	C-O	8.52	1.34	1.24
1	B	135	ALA	CA-CB	8.51	1.67	1.53
1	K	139	VAL	N-CA	8.49	1.56	1.46
1	G	140	SER	N-CA	-8.47	1.36	1.46
1	M	173	THR	C-O	8.46	1.33	1.24
1	L	282	MET	SD-CE	8.45	2.00	1.79
1	O	190	LEU	C-O	-8.45	1.13	1.24
1	I	72	VAL	CA-CB	-8.44	1.43	1.53
1	M	135	ALA	CA-CB	8.41	1.67	1.53
1	D	218	CYS	CA-C	-8.41	1.43	1.53
1	F	257	ALA	CA-CB	-8.34	1.42	1.53
1	A	245	SER	CB-OG	8.33	1.58	1.42
1	C	253	GLU	C-O	-8.31	1.13	1.23
1	D	191	LYS	CE-NZ	8.31	1.74	1.49
1	K	123	TYR	C-O	-8.31	1.14	1.23
1	C	138	ASN	CA-C	8.31	1.63	1.52
1	K	260	PHE	C-O	-8.30	1.14	1.24
1	B	52	VAL	N-CA	-8.29	1.40	1.46
1	F	72	VAL	C-O	-8.28	1.15	1.24
1	D	190	LEU	C-O	-8.28	1.14	1.24
1	L	311	TYR	CE2-CZ	8.28	1.58	1.38
1	B	153	GLN	C-O	-8.27	1.14	1.24
1	O	311	TYR	CE2-CZ	8.27	1.58	1.38
1	O	105	VAL	CA-C	-8.26	1.42	1.52
1	N	134	ALA	CA-CB	8.26	1.67	1.53
1	G	310	PRO	C-O	-8.24	1.15	1.23
1	E	225	CYS	C-O	-8.23	1.14	1.24
1	E	257	ALA	CA-CB	-8.23	1.41	1.53
1	A	186	PRO	C-O	-8.22	1.15	1.24
1	B	139	VAL	CA-CB	8.21	1.65	1.54
1	C	62	ILE	C-O	-8.21	1.14	1.24
1	L	164	ALA	CA-CB	-8.20	1.40	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	62	ILE	CA-CB	-8.17	1.45	1.53
1	O	174	ALA	CA-CB	8.16	1.66	1.53
1	D	388	VAL	C-O	-8.16	1.15	1.24
1	B	158	ILE	CA-CB	-8.16	1.44	1.54
1	A	174	ALA	CA-CB	8.14	1.65	1.53
1	F	242	TYR	C-O	8.14	1.33	1.24
1	A	285	SER	CA-C	8.14	1.59	1.52
1	H	158	ILE	C-O	8.13	1.32	1.24
1	M	472	GLN	CG-CD	8.13	1.72	1.52
1	E	374	GLN	C-O	-8.11	1.14	1.23
1	B	439	LYS	N-CA	8.11	1.56	1.46
1	D	41	ARG	CZ-NH1	8.10	1.44	1.32
1	B	140	SER	CB-OG	8.10	1.58	1.42
1	E	366	ARG	CZ-NH1	8.10	1.44	1.32
1	B	472	GLN	C-O	8.09	1.34	1.24
1	H	344	ILE	CA-CB	-8.09	1.44	1.54
1	J	396	ASN	CA-C	-8.07	1.45	1.53
1	C	191	LYS	CD-CE	8.06	1.76	1.52
1	A	272	PRO	N-CA	-8.06	1.37	1.47
1	E	311	TYR	CE2-CZ	8.05	1.57	1.38
1	L	366	ARG	CZ-NH1	8.05	1.44	1.32
1	L	282	MET	CG-SD	8.04	2.00	1.80
1	B	293	PRO	CA-CB	-8.04	1.45	1.54
1	E	300	VAL	C-O	-8.04	1.15	1.24
1	G	41	ARG	CA-C	-8.04	1.44	1.53
1	I	311	TYR	CE2-CZ	8.04	1.57	1.38
1	M	446	LYS	CG-CD	8.03	1.76	1.52
1	G	257	ALA	CA-CB	-8.02	1.43	1.53
1	H	81	ASN	CA-C	-8.02	1.43	1.52
1	B	323	VAL	CA-CB	-8.02	1.44	1.54
1	A	62	ILE	CA-CB	-8.01	1.48	1.54
1	B	105	VAL	C-O	-8.01	1.15	1.23
1	D	47	ASP	C-O	7.99	1.34	1.23
1	H	141	GLU	CA-C	-7.98	1.49	1.53
1	M	191	LYS	CD-CE	7.97	1.76	1.52
1	G	293	PRO	N-CA	-7.95	1.38	1.46
1	J	197	ASP	C-O	-7.95	1.14	1.23
1	I	87	ASP	CA-C	7.93	1.61	1.52
1	J	103	ALA	CA-CB	-7.93	1.39	1.54
1	D	132	SER	C-O	7.93	1.33	1.23
1	N	26	ASP	C-O	-7.93	1.14	1.24
1	D	277	ILE	CA-CB	-7.93	1.44	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	257	ALA	CA-CB	-7.91	1.43	1.53
1	O	255	LEU	C-O	-7.91	1.15	1.23
1	F	101	ALA	C-O	7.91	1.33	1.24
1	D	136	THR	C-O	7.90	1.33	1.23
1	G	187	PRO	CA-C	7.90	1.60	1.52
1	B	343	THR	CA-C	-7.88	1.43	1.52
1	B	168	HIS	C-O	-7.88	1.14	1.23
1	O	183	GLY	C-O	-7.87	1.13	1.24
1	N	36	HIS	C-O	-7.87	1.14	1.23
1	M	340	THR	CA-CB	7.87	1.65	1.53
1	A	158	ILE	C-O	7.84	1.32	1.24
1	B	278	LYS	C-O	-7.84	1.14	1.23
1	A	76	GLN	C-O	-7.79	1.14	1.24
1	G	169	TRP	C-O	7.78	1.33	1.24
1	L	250	LEU	N-CA	7.78	1.55	1.46
1	C	155	GLN	CA-C	-7.77	1.43	1.52
1	C	255	LEU	C-O	-7.77	1.15	1.23
1	A	458	LEU	CA-C	-7.76	1.42	1.52
1	K	366	ARG	CZ-NH1	7.73	1.43	1.32
1	F	153	GLN	C-O	-7.73	1.14	1.24
1	J	446	LYS	CG-CD	7.72	1.75	1.52
1	F	162	ALA	CA-CB	-7.71	1.42	1.54
1	M	109	ARG	C-O	-7.71	1.14	1.24
1	C	453	LYS	CE-NZ	7.71	1.72	1.49
1	M	289	CYS	CA-C	-7.69	1.42	1.52
1	E	239	ALA	CA-CB	-7.69	1.40	1.53
1	B	141	GLU	CB-CG	7.68	1.75	1.52
1	E	253	GLU	C-O	-7.66	1.14	1.23
1	G	277	ILE	CA-CB	-7.64	1.45	1.54
1	L	175	SER	CA-C	7.62	1.62	1.52
1	E	165	ILE	CA-CB	-7.61	1.45	1.54
1	M	382	ILE	CA-CB	-7.61	1.45	1.54
1	I	446	LYS	C-O	-7.60	1.14	1.23
1	E	67	ALA	CA-CB	-7.60	1.40	1.53
1	J	382	ILE	CA-CB	-7.59	1.44	1.54
1	B	271	VAL	CA-CB	7.58	1.64	1.54
1	C	140	SER	C-O	7.58	1.33	1.24
1	K	373	LEU	C-O	-7.57	1.14	1.24
1	D	52	VAL	CA-CB	-7.57	1.45	1.53
1	D	240	ASP	C-O	7.56	1.33	1.24
1	H	311	TYR	CE2-CZ	7.56	1.56	1.38
1	K	220	VAL	C-O	-7.56	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	123	TYR	C-O	-7.56	1.14	1.23
1	D	135	ALA	C-O	7.56	1.33	1.24
1	G	214	GLN	C-O	7.56	1.32	1.23
1	N	207	ALA	CA-CB	-7.55	1.43	1.52
1	E	89	SER	C-O	7.55	1.30	1.24
1	F	190	LEU	C-O	-7.55	1.15	1.24
1	D	177	SER	N-CA	7.54	1.55	1.46
1	O	458	LEU	CA-C	-7.53	1.42	1.52
1	N	103	ALA	CA-CB	-7.51	1.43	1.54
1	E	344	ILE	CA-CB	-7.50	1.45	1.54
1	E	170	ALA	CA-CB	-7.50	1.40	1.53
1	E	310	PRO	C-O	-7.49	1.15	1.23
1	F	138	ASN	CA-C	7.49	1.62	1.52
1	M	323	VAL	CA-CB	-7.49	1.44	1.53
1	I	463	TYR	CA-CB	-7.46	1.44	1.54
1	C	165	ILE	CA-CB	-7.46	1.45	1.54
1	N	331	VAL	CA-CB	-7.45	1.43	1.53
1	F	315	LYS	CA-C	-7.45	1.45	1.53
1	M	363	GLN	C-O	-7.45	1.15	1.24
1	C	258	ARG	C-O	-7.44	1.15	1.24
1	G	95	THR	C-O	7.44	1.33	1.23
1	D	207	ALA	CA-CB	-7.44	1.43	1.53
1	C	43	LEU	C-O	-7.43	1.14	1.23
1	J	388	VAL	CA-CB	-7.43	1.45	1.54
1	C	133	HIS	CA-C	7.42	1.63	1.52
1	N	114	GLY	C-O	7.42	1.31	1.23
1	E	168	HIS	C-O	-7.42	1.14	1.23
1	B	331	VAL	CA-CB	-7.41	1.44	1.53
1	N	396	ASN	CA-C	-7.41	1.46	1.53
1	K	310	PRO	CA-C	-7.41	1.44	1.52
1	G	88	THR	CA-CB	7.41	1.61	1.53
1	N	102	CYS	C-O	-7.41	1.15	1.23
1	K	252	ARG	CZ-NH1	7.40	1.43	1.32
1	H	54	ALA	N-CA	-7.40	1.36	1.46
1	J	125	LYS	CE-NZ	7.40	1.71	1.49
1	K	308	ASN	C-O	-7.40	1.13	1.23
1	L	67	ALA	CA-CB	-7.40	1.41	1.53
1	M	262	ASN	C-O	-7.40	1.14	1.23
1	I	310	PRO	C-O	-7.39	1.16	1.23
1	B	257	ALA	CA-CB	-7.38	1.43	1.53
1	G	151	TYR	N-CA	7.38	1.55	1.45
1	J	239	ALA	CA-CB	-7.36	1.41	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	365	SER	CB-OG	7.36	1.56	1.42
1	A	380	CYS	C-O	7.36	1.32	1.23
1	G	97	ARG	CZ-NH1	7.35	1.43	1.32
1	D	135	ALA	CA-CB	7.35	1.65	1.53
1	A	282	MET	SD-CE	7.34	1.98	1.79
1	B	93	PRO	C-O	-7.34	1.14	1.24
1	C	261	TRP	C-O	-7.32	1.14	1.23
1	D	222	LEU	C-O	-7.32	1.15	1.24
1	D	113	LEU	CA-C	-7.32	1.43	1.52
1	F	21	VAL	CA-CB	-7.31	1.45	1.54
1	E	272	PRO	N-CA	-7.30	1.38	1.47
1	M	352	VAL	CA-CB	7.30	1.63	1.54
1	B	392	ILE	CA-CB	-7.30	1.42	1.54
1	E	312	TRP	C-O	-7.29	1.15	1.24
1	E	382	ILE	CA-CB	-7.29	1.45	1.54
1	C	174	ALA	CA-CB	7.28	1.62	1.53
1	A	87	ASP	C-O	7.27	1.33	1.24
1	N	201	VAL	CA-CB	-7.26	1.44	1.54
1	B	170	ALA	CA-CB	-7.25	1.41	1.54
1	F	199	ASP	CA-C	7.25	1.62	1.52
1	B	149	VAL	C-O	-7.25	1.15	1.24
1	E	63	PRO	N-CA	-7.25	1.38	1.47
1	M	323	VAL	C-O	-7.25	1.17	1.24
1	N	384	LEU	C-O	-7.25	1.15	1.24
1	N	282	MET	SD-CE	7.24	1.97	1.79
1	G	135	ALA	CA-CB	7.23	1.65	1.53
1	A	138	ASN	CA-C	7.23	1.62	1.52
1	F	62	ILE	CA-CB	-7.22	1.46	1.53
1	A	164	ALA	CA-CB	-7.22	1.41	1.53
1	E	105	VAL	CA-CB	-7.21	1.44	1.55
1	G	323	VAL	C-O	7.21	1.31	1.24
1	I	386	ALA	CA-CB	-7.21	1.42	1.53
1	G	252	ARG	CZ-NH1	7.21	1.42	1.32
1	B	340	THR	N-CA	7.21	1.55	1.46
1	D	105	VAL	CA-C	-7.19	1.44	1.52
1	N	257	ALA	CA-CB	-7.19	1.44	1.52
1	B	202	ASP	N-CA	-7.18	1.37	1.46
1	B	52	VAL	CA-C	-7.17	1.47	1.53
1	N	65	VAL	C-O	-7.17	1.16	1.24
1	A	60	GLN	CA-C	-7.16	1.43	1.52
1	E	108	GLY	C-O	-7.16	1.15	1.23
1	N	165	ILE	CA-CB	-7.15	1.45	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	134	ALA	CA-CB	7.15	1.65	1.53
1	O	303	ASP	C-O	-7.14	1.15	1.24
1	K	139	VAL	CA-C	7.13	1.61	1.52
1	O	72	VAL	C-O	-7.13	1.16	1.24
1	M	53	PRO	C-O	7.12	1.32	1.23
1	D	232	PRO	C-O	-7.12	1.13	1.23
1	F	376	ILE	C-O	7.12	1.31	1.24
1	J	133	HIS	C-O	7.12	1.32	1.24
1	M	260	PHE	C-O	-7.11	1.15	1.24
1	D	165	ILE	C-O	-7.11	1.16	1.24
1	E	153	GLN	C-O	-7.11	1.15	1.24
1	K	473	ALA	CA-CB	-7.10	1.41	1.53
1	F	20	ALA	N-CA	7.09	1.59	1.46
1	C	296	SER	CA-C	-7.09	1.43	1.52
1	E	85	LEU	CA-C	7.08	1.62	1.53
1	M	138	ASN	CA-C	7.08	1.61	1.52
1	L	152	LYS	N-CA	-7.08	1.37	1.46
1	M	162	ALA	C-O	7.08	1.31	1.24
1	D	471	VAL	CA-CB	-7.07	1.46	1.54
1	J	20	ALA	N-CA	7.07	1.59	1.46
1	N	333	VAL	CA-CB	-7.07	1.45	1.54
1	F	186	PRO	CA-C	-7.06	1.45	1.52
1	H	339	SER	C-O	-7.05	1.14	1.23
1	J	282	MET	SD-CE	7.05	1.97	1.79
1	L	252	ARG	CG-CD	7.05	1.73	1.52
1	J	401	GLU	CA-C	-7.04	1.43	1.52
1	N	228	ILE	CA-CB	-7.04	1.45	1.54
1	K	450	VAL	CA-CB	-7.03	1.45	1.53
1	D	247	PHE	N-CA	-7.03	1.38	1.46
1	A	56	GLY	N-CA	7.02	1.55	1.45
1	M	101	ALA	CA-CB	-7.02	1.41	1.53
1	J	54	ALA	CA-CB	7.01	1.65	1.53
1	I	372	ASP	CA-C	7.01	1.60	1.52
1	H	251	ARG	NE-CZ	7.00	1.40	1.33
1	H	141	GLU	N-CA	-7.00	1.40	1.46
1	L	191	LYS	CD-CE	6.99	1.73	1.52
1	K	448	TRP	C-O	-6.99	1.15	1.24
1	A	52	VAL	C-N	6.99	1.41	1.33
1	A	222	LEU	C-O	-6.99	1.15	1.24
1	J	71	ARG	CZ-NH1	6.99	1.42	1.32
1	N	62	ILE	N-CA	-6.96	1.40	1.46
1	I	231	TYR	C-O	-6.96	1.15	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	251	ARG	CA-C	-6.96	1.44	1.52
1	F	127	ASP	C-O	6.95	1.31	1.23
1	H	283	ARG	N-CA	6.95	1.55	1.46
1	J	75	VAL	CA-CB	-6.95	1.45	1.54
1	O	136	THR	C-O	6.95	1.32	1.23
1	O	140	SER	C-O	6.95	1.32	1.24
1	C	103	ALA	CA-CB	-6.94	1.44	1.54
1	O	68	TYR	N-CA	-6.94	1.38	1.46
1	C	175	SER	C-O	6.93	1.32	1.23
1	J	453	LYS	CD-CE	6.93	1.73	1.52
1	K	187	PRO	CA-C	6.93	1.59	1.52
1	E	52	VAL	N-CA	-6.92	1.41	1.46
1	E	260	PHE	C-O	-6.92	1.15	1.24
1	F	75	VAL	C-O	6.92	1.31	1.24
1	C	107	ILE	C-O	-6.92	1.15	1.23
1	N	67	ALA	CA-CB	-6.91	1.41	1.53
1	I	220	VAL	C-O	-6.91	1.18	1.24
1	N	72	VAL	C-O	-6.91	1.16	1.24
1	K	207	ALA	CA-CB	-6.90	1.44	1.53
1	L	388	VAL	CA-CB	-6.90	1.46	1.54
1	K	92	ASN	C-O	-6.89	1.16	1.24
1	K	311	TYR	CE2-CZ	6.89	1.54	1.38
1	F	315	LYS	CG-CD	6.89	1.73	1.52
1	B	306	LEU	C-O	-6.88	1.15	1.24
1	B	460	LEU	N-CA	-6.88	1.37	1.46
1	C	197	ASP	C-O	-6.88	1.15	1.24
1	D	116	GLY	C-O	6.88	1.31	1.24
1	I	62	ILE	CA-CB	6.87	1.60	1.53
1	M	68	TYR	CA-C	-6.86	1.43	1.52
1	B	174	ALA	CA-CB	6.86	1.62	1.53
1	K	169	TRP	C-O	-6.86	1.15	1.24
1	H	464	PRO	C-O	-6.86	1.15	1.24
1	L	112	PRO	N-CA	6.86	1.54	1.46
1	D	359	THR	C-O	-6.85	1.15	1.24
1	J	368	VAL	C-O	6.85	1.32	1.23
1	A	162	ALA	CA-CB	-6.85	1.42	1.53
1	A	105	VAL	CA-CB	-6.85	1.45	1.55
1	O	95	THR	CA-CB	-6.84	1.44	1.54
1	E	62	ILE	CA-C	-6.84	1.47	1.53
1	O	191	LYS	CD-CE	6.84	1.73	1.52
1	G	206	GLY	N-CA	6.83	1.52	1.45
1	M	51	ARG	CG-CD	6.83	1.73	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	311	TYR	C-O	-6.83	1.16	1.24
1	A	139	VAL	N-CA	6.83	1.54	1.46
1	D	62	ILE	C-O	-6.83	1.16	1.24
1	H	191	LYS	CD-CE	6.82	1.73	1.52
1	M	32	SER	C-O	-6.82	1.14	1.24
1	F	207	ALA	CA-CB	-6.81	1.44	1.52
1	G	83	PHE	C-O	6.80	1.32	1.23
1	J	228	ILE	C-O	6.80	1.31	1.24
1	O	130	GLU	CA-C	-6.79	1.44	1.52
1	I	451	ASP	C-O	-6.79	1.15	1.24
1	G	98	LEU	C-O	6.79	1.32	1.24
1	K	165	ILE	CA-CB	-6.79	1.46	1.54
1	M	155	GLN	CA-C	-6.78	1.44	1.52
1	N	220	VAL	C-O	-6.78	1.19	1.24
1	G	140	SER	CA-C	-6.78	1.44	1.52
1	H	134	ALA	CA-CB	6.78	1.65	1.53
1	G	332	THR	CA-C	6.77	1.61	1.52
1	I	88	THR	CA-CB	6.77	1.62	1.52
1	L	371	TYR	CA-C	-6.76	1.44	1.52
1	E	105	VAL	C-O	-6.76	1.15	1.23
1	L	71	ARG	CZ-NH1	6.76	1.42	1.32
1	L	154	THR	CA-CB	6.76	1.66	1.54
1	I	397	SER	C-O	6.75	1.32	1.24
1	N	467	ARG	CZ-NH2	6.75	1.42	1.33
1	K	174	ALA	CA-CB	6.75	1.61	1.53
1	D	449	ASN	C-O	-6.74	1.15	1.24
1	H	136	THR	C-O	6.74	1.32	1.23
1	F	191	LYS	CG-CD	6.74	1.72	1.52
1	B	82	LYS	CA-C	6.73	1.61	1.52
1	H	192	ASN	C-O	-6.73	1.15	1.23
1	J	439	LYS	N-CA	6.73	1.54	1.46
1	D	130	GLU	CA-C	-6.72	1.44	1.53
1	L	293	PRO	N-CA	-6.72	1.39	1.46
1	N	340	THR	N-CA	6.72	1.54	1.46
1	G	218	CYS	CA-C	-6.72	1.45	1.53
1	M	162	ALA	CA-CB	-6.71	1.44	1.54
1	A	311	TYR	CE2-CZ	6.71	1.54	1.38
1	C	311	TYR	CE2-CZ	6.71	1.54	1.38
1	I	156	LEU	CA-C	-6.71	1.44	1.52
1	J	139	VAL	CA-CB	6.71	1.63	1.54
1	B	105	VAL	CA-CB	-6.70	1.43	1.55
1	D	75	VAL	N-CA	-6.69	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	375	PHE	C-O	6.69	1.32	1.23
1	H	69	GLN	C-O	-6.69	1.15	1.23
1	I	26	ASP	C-O	-6.69	1.15	1.24
1	L	138	ASN	CA-C	6.69	1.61	1.52
1	F	99	VAL	C-O	6.68	1.30	1.23
1	F	174	ALA	CA-CB	6.68	1.63	1.53
1	H	82	LYS	CE-NZ	6.68	1.69	1.49
1	D	439	LYS	CD-CE	6.67	1.72	1.52
1	B	446	LYS	CD-CE	6.67	1.72	1.52
1	C	140	SER	CA-C	6.67	1.61	1.52
1	O	157	CYS	N-CA	-6.67	1.38	1.46
1	O	386	ALA	CA-CB	-6.67	1.42	1.53
1	O	213	LEU	CG-CD1	-6.67	1.30	1.52
1	L	130	GLU	CA-C	-6.66	1.43	1.52
1	A	165	ILE	C-O	-6.66	1.16	1.24
1	D	252	ARG	CZ-NH1	6.66	1.42	1.32
1	J	36	HIS	C-O	-6.66	1.15	1.23
1	B	144	ARG	N-CA	-6.66	1.38	1.46
1	F	465	LEU	CG-CD1	6.65	1.74	1.52
1	I	325	TRP	C-O	-6.65	1.16	1.23
1	G	311	TYR	CE2-CZ	6.65	1.54	1.38
1	N	149	VAL	CB-CG1	-6.65	1.30	1.52
1	B	473	ALA	CA-CB	-6.65	1.42	1.53
1	I	439	LYS	N-CA	6.64	1.54	1.46
1	F	197	ASP	C-O	-6.64	1.15	1.23
1	K	135	ALA	CA-CB	6.64	1.64	1.53
1	L	102	CYS	CA-C	6.63	1.61	1.52
1	F	461	ASP	CG-OD2	6.63	1.38	1.25
1	H	193	THR	CB-CG2	6.63	1.74	1.52
1	L	174	ALA	C-O	6.63	1.32	1.24
1	O	62	ILE	CA-CB	-6.62	1.46	1.53
1	C	134	ALA	CA-CB	6.62	1.60	1.54
1	J	95	THR	C-O	6.62	1.32	1.23
1	L	346	ALA	CA-C	6.62	1.60	1.52
1	A	61	ASP	CA-C	6.61	1.61	1.52
1	N	83	PHE	CA-C	-6.61	1.44	1.52
1	E	360	LYS	CD-CE	6.61	1.72	1.52
1	M	344	ILE	CA-C	-6.61	1.44	1.52
1	N	156	LEU	C-O	6.61	1.31	1.23
1	C	376	ILE	C-O	6.61	1.31	1.24
1	M	133	HIS	CA-C	6.61	1.62	1.52
1	O	453	LYS	CG-CD	6.61	1.72	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	74	ARG	CA-CB	-6.60	1.44	1.53
1	M	446	LYS	C-O	-6.60	1.16	1.24
1	N	238	SER	CA-C	-6.60	1.43	1.52
1	H	363	GLN	CA-C	6.60	1.60	1.52
1	C	282	MET	SD-CE	6.59	1.96	1.79
1	E	82	LYS	CD-CE	6.59	1.72	1.52
1	M	78	PRO	C-O	-6.59	1.16	1.23
1	G	90	ILE	C-O	6.59	1.31	1.24
1	G	82	LYS	CE-NZ	6.59	1.69	1.49
1	N	105	VAL	CA-C	-6.59	1.44	1.52
1	A	52	VAL	N-CA	6.59	1.51	1.46
1	I	98	LEU	C-O	6.59	1.31	1.23
1	G	161	CYS	CA-C	-6.58	1.44	1.53
1	L	315	LYS	CA-C	-6.58	1.46	1.53
1	G	209	ASP	C-O	6.58	1.32	1.23
1	N	213	LEU	C-O	-6.58	1.15	1.24
1	J	89	SER	C-O	6.58	1.30	1.23
1	D	388	VAL	CA-CB	-6.57	1.46	1.54
1	H	248	PHE	CD1-CE1	6.57	1.58	1.38
1	L	139	VAL	CB-CG2	6.56	1.74	1.52
1	G	143	VAL	CA-C	6.56	1.61	1.52
1	I	103	ALA	CA-C	-6.56	1.43	1.52
1	D	140	SER	C-O	6.56	1.32	1.24
1	D	191	LYS	CD-CE	6.56	1.72	1.52
1	A	295	PRO	CA-CB	-6.55	1.44	1.53
1	G	98	LEU	CA-C	6.55	1.60	1.52
1	K	335	ASP	CA-C	-6.55	1.46	1.53
1	D	53	PRO	CA-C	-6.54	1.43	1.52
1	J	69	GLN	C-O	-6.54	1.16	1.23
1	O	251	ARG	C-O	-6.54	1.15	1.23
1	K	401	GLU	C-O	-6.53	1.16	1.24
1	K	88	THR	CA-CB	6.53	1.61	1.52
1	H	310	PRO	C-O	-6.53	1.17	1.23
1	C	107	ILE	N-CA	-6.52	1.38	1.46
1	D	93	PRO	CA-C	-6.51	1.43	1.52
1	G	64	LYS	CG-CD	6.51	1.72	1.52
1	O	306	LEU	C-O	-6.51	1.15	1.24
1	M	107	ILE	N-CA	-6.51	1.38	1.46
1	O	321	ASN	N-CA	-6.51	1.38	1.46
1	E	321	ASN	N-CA	-6.50	1.38	1.46
1	H	178	ARG	CA-C	6.50	1.61	1.52
1	L	453	LYS	CE-NZ	6.50	1.68	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	391	TYR	C-O	-6.50	1.16	1.24
1	O	79	ASP	C-O	-6.50	1.16	1.24
1	D	473	ALA	CA-CB	-6.50	1.43	1.53
1	J	344	ILE	CA-CB	-6.49	1.46	1.54
1	K	247	PHE	N-CA	-6.49	1.38	1.46
1	M	41	ARG	C-O	-6.49	1.16	1.23
1	N	160	GLY	C-O	6.49	1.31	1.24
1	L	278	LYS	CE-NZ	6.49	1.68	1.49
1	O	446	LYS	CG-CD	6.49	1.72	1.52
1	A	231	TYR	CA-C	-6.49	1.46	1.52
1	B	356	TYR	C-O	-6.49	1.16	1.23
1	M	159	LEU	C-O	-6.49	1.15	1.23
1	G	360	LYS	CD-CE	6.48	1.72	1.52
1	M	344	ILE	CA-CB	-6.47	1.46	1.54
1	D	215	ASP	C-O	-6.47	1.16	1.24
1	K	105	VAL	CA-CB	-6.47	1.44	1.54
1	A	62	ILE	CA-C	-6.47	1.48	1.52
1	O	28	VAL	C-O	-6.47	1.17	1.24
1	B	132	SER	C-O	6.46	1.32	1.24
1	N	40	SER	C-O	-6.46	1.15	1.24
1	K	196	GLU	C-O	-6.46	1.15	1.23
1	M	460	LEU	N-CA	-6.46	1.38	1.46
1	A	159	LEU	CA-C	-6.45	1.44	1.52
1	F	323	VAL	CA-CB	-6.45	1.46	1.53
1	J	467	ARG	CZ-NH1	6.45	1.41	1.32
1	D	334	VAL	CA-CB	-6.45	1.45	1.54
1	I	368	VAL	CA-CB	-6.45	1.44	1.54
1	E	178	ARG	CA-C	6.45	1.59	1.52
1	J	446	LYS	C-O	-6.45	1.16	1.24
1	J	114	GLY	C-O	6.44	1.30	1.23
1	H	314	HIS	CA-C	6.43	1.61	1.52
1	I	232	PRO	C-O	-6.43	1.14	1.23
1	A	20	ALA	N-CA	6.43	1.58	1.46
1	E	80	PRO	C-O	-6.43	1.15	1.24
1	G	34	PHE	C-O	6.43	1.32	1.24
1	B	72	VAL	C-O	-6.42	1.17	1.24
1	F	311	TYR	CE2-CZ	6.42	1.53	1.38
1	L	325	TRP	CA-C	-6.42	1.44	1.52
1	C	333	VAL	CA-C	-6.42	1.44	1.52
1	O	224	ILE	C-O	6.41	1.32	1.24
1	D	220	VAL	C-O	-6.41	1.16	1.24
1	K	284	ALA	CA-C	-6.41	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	71	ARG	CZ-NH1	6.41	1.41	1.32
1	E	287	GLY	C-O	6.41	1.29	1.24
1	G	37	ALA	C-O	6.40	1.32	1.23
1	C	105	VAL	CA-C	-6.40	1.45	1.52
1	E	37	ALA	CA-CB	-6.40	1.43	1.53
1	A	140	SER	C-O	6.40	1.32	1.24
1	G	138	ASN	CA-CB	6.39	1.62	1.53
1	H	175	SER	C-O	6.39	1.31	1.23
1	J	62	ILE	N-CA	-6.39	1.41	1.46
1	C	200	MET	C-O	-6.39	1.15	1.23
1	E	470	LEU	CA-C	-6.39	1.44	1.52
1	C	43	LEU	CA-C	-6.39	1.44	1.52
1	F	368	VAL	CA-CB	-6.39	1.45	1.54
1	H	125	LYS	C-O	6.39	1.31	1.24
1	E	62	ILE	C-O	-6.38	1.17	1.24
1	I	77	LEU	CG-CD1	-6.38	1.31	1.52
1	J	107	ILE	C-O	-6.38	1.16	1.23
1	L	177	SER	CB-OG	6.38	1.54	1.42
1	B	30	ARG	CZ-NH1	6.38	1.41	1.32
1	I	178	ARG	CA-C	6.38	1.60	1.52
1	F	175	SER	CA-C	6.38	1.61	1.52
1	F	341	ASN	C-O	6.38	1.31	1.24
1	J	79	ASP	C-O	-6.37	1.16	1.24
1	O	135	ALA	C-O	6.37	1.31	1.23
1	O	456	PHE	C-O	-6.37	1.16	1.23
1	J	203	THR	C-O	-6.37	1.15	1.24
1	F	190	LEU	N-CA	-6.36	1.38	1.46
1	H	81	ASN	C-O	-6.36	1.16	1.24
1	M	459	ASP	CA-C	-6.36	1.45	1.53
1	N	20	ALA	CA-CB	6.36	1.73	1.52
1	A	77	LEU	C-O	6.36	1.32	1.23
1	F	175	SER	C-O	6.36	1.31	1.23
1	L	176	LYS	CA-C	6.36	1.61	1.52
1	J	267	MET	C-O	-6.36	1.16	1.24
1	B	96	GLN	C-O	-6.36	1.15	1.23
1	D	252	ARG	NE-CZ	6.36	1.40	1.33
1	E	45	VAL	C-O	-6.36	1.16	1.23
1	N	343	THR	C-O	-6.36	1.16	1.24
1	J	237	MET	N-CA	-6.35	1.38	1.46
1	B	294	SER	CA-C	-6.35	1.46	1.52
1	F	88	THR	N-CA	6.35	1.55	1.46
1	M	241	PRO	CA-CB	-6.35	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	321	ASN	N-CA	-6.35	1.38	1.46
1	J	171	LYS	CE-NZ	6.34	1.68	1.49
1	D	123	TYR	C-O	-6.34	1.16	1.23
1	O	439	LYS	C-O	6.34	1.31	1.24
1	M	282	MET	C-O	6.33	1.32	1.24
1	F	175	SER	N-CA	6.33	1.53	1.45
1	B	299	ILE	CA-C	-6.33	1.45	1.52
1	M	178	ARG	C-N	6.32	1.41	1.33
1	A	278	LYS	CD-CE	6.32	1.71	1.52
1	M	317	GLN	CG-CD	6.32	1.67	1.52
1	C	446	LYS	CG-CD	6.32	1.71	1.52
1	K	170	ALA	CA-CB	-6.32	1.43	1.54
1	M	310	PRO	C-O	-6.32	1.17	1.23
1	J	162	ALA	CA-CB	-6.32	1.44	1.54
1	F	238	SER	C-O	6.31	1.31	1.24
1	K	105	VAL	C-O	-6.31	1.17	1.23
1	J	165	ILE	CA-CB	-6.31	1.46	1.54
1	J	168	HIS	C-O	-6.31	1.16	1.23
1	H	53	PRO	N-CA	-6.30	1.39	1.47
1	A	177	SER	N-CA	6.30	1.54	1.46
1	A	111	GLN	CA-CB	-6.30	1.43	1.53
1	H	453	LYS	CA-C	-6.30	1.44	1.52
1	H	157	CYS	N-CA	-6.30	1.38	1.46
1	L	299	ILE	CA-CB	-6.30	1.46	1.54
1	K	139	VAL	C-O	6.29	1.31	1.24
1	A	177	SER	CA-C	6.29	1.61	1.52
1	I	360	LYS	CE-NZ	6.28	1.68	1.49
1	K	369	GLU	C-O	-6.28	1.16	1.23
1	E	156	LEU	CA-CB	-6.28	1.42	1.53
1	H	112	PRO	CA-CB	-6.27	1.45	1.53
1	J	174	ALA	C-O	6.27	1.31	1.24
1	J	248	PHE	CE2-CZ	6.27	1.57	1.38
1	M	52	VAL	CA-CB	-6.26	1.47	1.53
1	E	361	PHE	C-O	6.26	1.31	1.23
1	E	252	ARG	N-CA	-6.26	1.38	1.46
1	K	78	PRO	N-CA	-6.26	1.39	1.47
1	K	139	VAL	CA-CB	6.26	1.62	1.54
1	F	398	SER	C-O	6.25	1.32	1.24
1	F	266	THR	CA-CB	6.25	1.62	1.53
1	H	39	SER	CA-C	-6.25	1.44	1.53
1	O	139	VAL	CA-CB	6.25	1.62	1.54
1	M	456	PHE	C-O	-6.25	1.16	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	88	THR	CA-CB	6.25	1.61	1.52
1	E	282	MET	CG-SD	6.25	1.96	1.80
1	O	62	ILE	C-O	-6.25	1.17	1.24
1	E	309	LYS	CE-NZ	6.24	1.68	1.49
1	M	147	VAL	CA-C	-6.24	1.45	1.52
1	A	86	PRO	CA-C	6.23	1.60	1.52
1	E	123	TYR	C-O	-6.23	1.16	1.23
1	O	453	LYS	CD-CE	6.23	1.71	1.52
1	G	177	SER	N-CA	6.23	1.53	1.46
1	K	159	LEU	CA-C	-6.22	1.45	1.52
1	M	89	SER	C-O	6.22	1.30	1.24
1	D	296	SER	C-O	-6.22	1.16	1.24
1	A	232	PRO	N-CD	-6.22	1.39	1.47
1	L	165	ILE	CA-CB	-6.22	1.46	1.54
1	M	360	LYS	CG-CD	6.22	1.71	1.52
1	A	176	LYS	N-CA	6.21	1.53	1.46
1	H	37	ALA	C-O	6.21	1.31	1.23
1	K	40	SER	C-O	-6.21	1.16	1.24
1	D	220	VAL	CA-CB	-6.21	1.46	1.54
1	F	189	GLU	CD-OE1	6.21	1.37	1.25
1	A	344	ILE	CA-CB	-6.21	1.46	1.54
1	G	315	LYS	CA-C	-6.20	1.46	1.53
1	N	365	SER	C-O	-6.20	1.17	1.24
1	I	112	PRO	N-CA	6.20	1.53	1.46
1	E	216	THR	N-CA	-6.19	1.39	1.46
1	A	176	LYS	CA-C	6.19	1.60	1.52
1	L	173	THR	C-O	6.19	1.31	1.23
1	F	134	ALA	CA-CB	6.19	1.64	1.53
1	B	93	PRO	CA-C	-6.18	1.43	1.52
1	E	219	GLU	N-CA	-6.18	1.37	1.46
1	F	369	GLU	CD-OE2	6.18	1.37	1.25
1	D	260	PHE	C-O	-6.18	1.17	1.24
1	J	68	TYR	C-O	-6.18	1.13	1.23
1	C	163	PRO	CB-CG	-6.17	1.18	1.49
1	J	76	GLN	CD-OE1	6.17	1.35	1.23
1	B	277	ILE	CA-CB	-6.17	1.46	1.54
1	G	20	ALA	N-CA	6.17	1.57	1.46
1	J	206	GLY	N-CA	6.17	1.52	1.45
1	E	85	LEU	C-N	6.17	1.41	1.33
1	E	223	ASP	C-O	-6.17	1.15	1.24
1	M	453	LYS	CD-CE	6.17	1.71	1.52
1	C	179	PRO	CA-C	6.16	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	393	GLN	C-O	6.16	1.31	1.24
1	N	68	TYR	N-CA	-6.16	1.39	1.46
1	E	139	VAL	C-O	6.16	1.31	1.24
1	O	239	ALA	CA-CB	-6.16	1.43	1.53
1	C	136	THR	CA-CB	6.15	1.63	1.53
1	D	272	PRO	C-O	-6.15	1.16	1.23
1	E	138	ASN	CA-C	6.15	1.60	1.52
1	L	186	PRO	CA-C	-6.15	1.46	1.52
1	O	293	PRO	N-CA	-6.15	1.40	1.46
1	L	251	ARG	CA-C	-6.15	1.45	1.52
1	D	40	SER	CB-OG	6.14	1.54	1.42
1	D	105	VAL	C-O	-6.14	1.17	1.23
1	G	318	GLY	C-O	6.14	1.29	1.23
1	C	216	THR	C-O	-6.14	1.17	1.24
1	E	236	GLN	C-O	-6.14	1.16	1.24
1	I	27	TYR	CA-C	-6.13	1.44	1.52
1	D	291	TYR	CA-C	-6.13	1.45	1.52
1	G	444	LYS	CD-CE	6.13	1.70	1.52
1	M	231	TYR	CA-C	-6.13	1.46	1.52
1	E	96	GLN	C-O	-6.13	1.16	1.23
1	M	311	TYR	CE2-CZ	6.12	1.52	1.38
1	M	267	MET	C-O	-6.12	1.16	1.23
1	A	393	GLN	CB-CG	6.11	1.70	1.52
1	N	59	LYS	CG-CD	6.11	1.70	1.52
1	H	107	ILE	N-CA	-6.11	1.39	1.46
1	L	268	GLY	C-O	-6.11	1.15	1.23
1	M	37	ALA	CA-CB	-6.11	1.43	1.53
1	F	139	VAL	CA-C	6.11	1.60	1.52
1	G	368	VAL	C-O	-6.11	1.16	1.23
1	J	158	ILE	CA-CB	-6.11	1.46	1.54
1	J	456	PHE	C-O	-6.10	1.16	1.24
1	O	153	GLN	C-O	-6.10	1.16	1.24
1	O	260	PHE	C-O	-6.10	1.17	1.24
1	E	232	PRO	CA-C	-6.10	1.44	1.52
1	H	155	GLN	CA-C	-6.10	1.45	1.52
1	I	339	SER	N-CA	-6.10	1.38	1.46
1	D	353	PRO	CB-CG	6.09	1.80	1.49
1	I	173	THR	C-O	6.09	1.31	1.23
1	C	60	GLN	CA-C	6.09	1.60	1.52
1	D	297	GLY	CA-C	-6.09	1.44	1.52
1	H	104	GLY	N-CA	6.09	1.51	1.45
1	F	71	ARG	CZ-NH1	6.08	1.41	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	75	VAL	CA-CB	-6.08	1.46	1.53
1	I	245	SER	C-O	-6.08	1.16	1.24
1	F	311	TYR	CG-CD2	6.08	1.52	1.39
1	E	439	LYS	CG-CD	6.07	1.70	1.52
1	I	173	THR	CA-CB	6.07	1.63	1.53
1	N	270	THR	C-O	-6.07	1.16	1.24
1	O	90	ILE	CA-CB	6.07	1.63	1.54
1	D	385	THR	CA-C	-6.07	1.44	1.53
1	F	54	ALA	C-O	6.07	1.31	1.23
1	B	150	ASP	CA-C	-6.06	1.45	1.52
1	O	317	GLN	C-O	6.06	1.31	1.24
1	G	138	ASN	N-CA	6.06	1.53	1.46
1	K	158	ILE	CA-C	6.06	1.60	1.52
1	D	135	ALA	CA-C	6.06	1.60	1.52
1	I	105	VAL	CA-C	-6.06	1.45	1.52
1	M	62	ILE	C-O	-6.06	1.17	1.24
1	E	169	TRP	C-O	-6.05	1.16	1.23
1	L	106	GLU	CD-OE1	6.05	1.36	1.25
1	H	63	PRO	CA-CB	-6.05	1.45	1.53
1	H	72	VAL	C-O	-6.05	1.17	1.24
1	C	255	LEU	CA-C	-6.04	1.45	1.52
1	C	453	LYS	CD-CE	6.04	1.70	1.52
1	F	199	ASP	C-O	6.04	1.31	1.23
1	O	252	ARG	CZ-NH1	6.04	1.41	1.32
1	C	252	ARG	CZ-NH1	6.04	1.41	1.32
1	J	112	PRO	CA-C	6.04	1.59	1.52
1	F	160	GLY	C-O	6.03	1.30	1.24
1	L	94	GLU	CG-CD	6.03	1.67	1.52
1	K	401	GLU	CD-OE1	6.03	1.36	1.25
1	B	147	VAL	C-O	-6.03	1.16	1.23
1	A	53	PRO	N-CD	6.03	1.56	1.47
1	J	227	SER	CA-C	-6.03	1.44	1.52
1	M	228	ILE	C-O	6.03	1.30	1.24
1	G	54	ALA	C-O	6.02	1.31	1.23
1	O	282	MET	SD-CE	6.02	1.94	1.79
1	B	290	VAL	CA-CB	-6.02	1.46	1.53
1	K	262	ASN	CA-C	-6.02	1.45	1.52
1	C	72	VAL	CA-CB	-6.02	1.46	1.54
1	J	125	LYS	CD-CE	6.02	1.70	1.52
1	N	334	VAL	CA-CB	-6.02	1.46	1.54
1	E	446	LYS	CG-CD	6.01	1.70	1.52
1	C	116	GLY	C-O	6.01	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	376	ILE	C-O	6.01	1.30	1.24
1	J	192	ASN	C-O	-6.01	1.16	1.23
1	N	191	LYS	CG-CD	6.01	1.70	1.52
1	E	390	SER	CB-OG	6.00	1.54	1.42
1	B	311	TYR	C-O	-6.00	1.16	1.24
1	G	374	GLN	CA-C	-6.00	1.45	1.52
1	A	290	VAL	CA-CB	-6.00	1.46	1.53
1	F	264	ALA	C-O	5.99	1.31	1.23
1	G	88	THR	CB-OG1	5.99	1.53	1.43
1	H	374	GLN	CD-OE1	5.99	1.34	1.23
1	L	228	ILE	CA-CB	-5.99	1.47	1.54
1	N	21	VAL	CA-CB	-5.99	1.47	1.54
1	L	253	GLU	C-O	-5.98	1.16	1.23
1	H	186	PRO	CA-C	-5.98	1.46	1.52
1	J	335	ASP	CA-C	-5.98	1.47	1.53
1	M	299	ILE	N-CA	-5.98	1.38	1.46
1	K	99	VAL	CA-CB	-5.98	1.44	1.55
1	G	282	MET	C-O	5.97	1.31	1.24
1	I	389	MET	SD-CE	5.97	1.94	1.79
1	C	188	LEU	N-CA	-5.96	1.38	1.46
1	E	107	ILE	CA-C	-5.96	1.46	1.52
1	K	186	PRO	CA-C	-5.96	1.46	1.52
1	N	107	ILE	C-O	-5.96	1.17	1.23
1	A	252	ARG	NE-CZ	5.96	1.39	1.33
1	C	138	ASN	C-O	5.96	1.31	1.24
1	A	315	LYS	CA-C	-5.96	1.46	1.52
1	B	90	ILE	CG1-CD1	5.95	1.75	1.51
1	C	344	ILE	CA-CB	-5.95	1.46	1.54
1	E	446	LYS	CE-NZ	5.95	1.67	1.49
1	J	152	LYS	CG-CD	5.95	1.70	1.52
1	A	147	VAL	CA-C	-5.95	1.45	1.52
1	M	160	GLY	C-O	5.95	1.30	1.23
1	M	398	SER	C-O	-5.95	1.16	1.24
1	C	396	ASN	CA-C	-5.95	1.48	1.53
1	H	260	PHE	C-O	-5.94	1.17	1.24
1	B	251	ARG	CD-NE	5.94	1.54	1.46
1	E	95	THR	CA-CB	5.94	1.63	1.54
1	G	34	PHE	CE1-CZ	5.94	1.56	1.38
1	K	338	ARG	CZ-NH1	5.94	1.41	1.32
1	J	225	CYS	N-CA	-5.94	1.39	1.46
1	M	165	ILE	CA-CB	-5.94	1.47	1.54
1	F	146	ASN	C-O	5.94	1.31	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	371	TYR	C-O	-5.94	1.15	1.23
1	C	168	HIS	C-O	-5.94	1.16	1.23
1	I	376	ILE	CG1-CD1	-5.94	1.28	1.51
1	I	323	VAL	C-O	-5.93	1.17	1.24
1	I	132	SER	C-O	5.93	1.31	1.23
1	O	191	LYS	CE-NZ	5.93	1.67	1.49
1	A	75	VAL	C-O	-5.93	1.17	1.24
1	J	311	TYR	CE2-CZ	5.93	1.52	1.38
1	F	327	ASN	C-O	5.93	1.31	1.23
1	B	382	ILE	CA-CB	-5.93	1.46	1.54
1	A	404	ASN	C-O	5.92	1.35	1.23
1	F	277	ILE	CA-CB	-5.92	1.47	1.54
1	F	354	GLY	C-O	5.92	1.31	1.23
1	N	360	LYS	CD-CE	5.92	1.70	1.52
1	K	23	ASN	C-O	-5.92	1.16	1.23
1	E	371	TYR	C-O	-5.92	1.16	1.23
1	J	24	THR	N-CA	-5.92	1.39	1.46
1	M	232	PRO	CA-C	-5.92	1.45	1.52
1	I	309	LYS	CA-C	-5.92	1.46	1.52
1	A	53	PRO	C-O	5.91	1.30	1.23
1	F	248	PHE	CD1-CE1	5.91	1.56	1.38
1	H	254	GLN	CD-NE2	5.91	1.45	1.33
1	O	170	ALA	CA-C	-5.91	1.45	1.52
1	G	394	SER	C-O	5.91	1.30	1.24
1	M	341	ASN	CA-CB	-5.91	1.45	1.53
1	I	133	HIS	CA-C	5.91	1.60	1.52
1	O	155	GLN	CA-C	-5.91	1.45	1.52
1	I	105	VAL	CA-CB	-5.91	1.45	1.54
1	C	123	TYR	C-O	-5.91	1.16	1.23
1	D	46	GLY	C-O	-5.90	1.17	1.23
1	J	105	VAL	CA-C	-5.90	1.45	1.52
1	I	332	THR	CA-CB	-5.90	1.45	1.53
1	J	375	PHE	C-O	5.90	1.31	1.23
1	M	176	LYS	CA-C	5.90	1.60	1.52
1	B	142	ASP	CA-C	-5.90	1.46	1.52
1	G	29	THR	C-O	5.90	1.31	1.23
1	J	264	ALA	C-O	-5.90	1.16	1.23
1	C	357	ASP	CG-OD2	5.89	1.36	1.25
1	I	366	ARG	CZ-NH2	5.89	1.41	1.33
1	J	224	ILE	C-O	5.89	1.31	1.24
1	I	37	ALA	CA-CB	-5.89	1.44	1.53
1	D	157	CYS	C-O	-5.89	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	165	ILE	C-O	-5.88	1.17	1.24
1	K	52	VAL	CA-CB	-5.88	1.48	1.53
1	D	81	ASN	CA-CB	-5.88	1.43	1.53
1	L	349	GLN	N-CA	5.88	1.52	1.45
1	O	368	VAL	CA-CB	-5.88	1.46	1.54
1	G	251	ARG	NE-CZ	5.88	1.39	1.33
1	H	446	LYS	CG-CD	5.88	1.70	1.52
1	I	382	ILE	C-O	-5.88	1.17	1.24
1	N	155	GLN	C-O	-5.88	1.17	1.23
1	M	200	MET	N-CA	-5.87	1.38	1.45
1	M	365	SER	CA-C	-5.87	1.45	1.52
1	B	80	PRO	C-O	-5.87	1.16	1.24
1	D	311	TYR	CE2-CZ	5.87	1.52	1.38
1	F	36	HIS	C-O	-5.86	1.16	1.23
1	I	277	ILE	CA-CB	-5.86	1.47	1.54
1	L	188	LEU	N-CA	-5.86	1.38	1.46
1	A	90	ILE	N-CA	5.86	1.53	1.46
1	O	468	LYS	CE-NZ	5.86	1.67	1.49
1	E	157	CYS	N-CA	-5.86	1.39	1.46
1	C	191	LYS	CG-CD	5.86	1.70	1.52
1	O	71	ARG	CZ-NH1	5.86	1.41	1.32
1	J	91	TYR	C-O	-5.85	1.16	1.23
1	F	72	VAL	CA-CB	-5.85	1.46	1.53
1	A	90	ILE	CA-CB	5.85	1.62	1.54
1	C	133	HIS	C-O	5.84	1.30	1.24
1	D	230	LYS	CA-C	-5.84	1.45	1.52
1	E	149	VAL	C-O	-5.84	1.17	1.23
1	J	220	VAL	N-CA	-5.84	1.39	1.46
1	D	246	MET	SD-CE	-5.84	1.65	1.79
1	F	23	ASN	C-O	5.84	1.30	1.23
1	E	62	ILE	C-N	-5.84	1.26	1.33
1	H	239	ALA	CA-CB	5.84	1.62	1.53
1	K	465	LEU	CG-CD2	-5.84	1.33	1.52
1	C	171	LYS	N-CA	-5.83	1.38	1.46
1	C	337	THR	CB-CG2	-5.83	1.33	1.52
1	K	175	SER	N-CA	5.83	1.53	1.46
1	K	189	GLU	C-O	-5.83	1.16	1.23
1	A	236	GLN	C-O	-5.83	1.16	1.24
1	D	133	HIS	C-O	5.83	1.31	1.24
1	J	299	ILE	C-O	5.83	1.31	1.24
1	K	251	ARG	CA-C	-5.83	1.45	1.52
1	E	293	PRO	CA-CB	-5.83	1.47	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	THR	C-O	-5.82	1.17	1.23
1	B	299	ILE	C-O	-5.82	1.16	1.24
1	G	392	ILE	C-O	5.82	1.31	1.24
1	K	130	GLU	CA-C	-5.82	1.44	1.52
1	I	307	PHE	C-O	-5.82	1.16	1.23
1	N	311	TYR	CE2-CZ	5.82	1.52	1.38
1	H	439	LYS	CG-CD	5.82	1.70	1.52
1	J	37	ALA	CA-CB	-5.82	1.44	1.53
1	O	332	THR	CA-CB	-5.82	1.45	1.53
1	C	165	ILE	C-O	5.82	1.30	1.24
1	D	289	CYS	CA-C	-5.82	1.45	1.53
1	K	276	TYR	C-O	-5.82	1.17	1.23
1	O	64	LYS	N-CA	-5.82	1.39	1.46
1	D	194	VAL	CA-CB	-5.81	1.47	1.54
1	F	461	ASP	CG-OD1	5.81	1.36	1.25
1	I	369	GLU	C-O	-5.81	1.17	1.23
1	I	388	VAL	CA-CB	-5.81	1.47	1.54
1	J	24	THR	C-O	-5.81	1.16	1.24
1	E	196	GLU	C-O	-5.81	1.16	1.23
1	A	239	ALA	C-O	-5.81	1.16	1.24
1	G	468	LYS	CD-CE	5.81	1.69	1.52
1	H	147	VAL	CA-C	-5.81	1.45	1.52
1	H	446	LYS	CD-CE	5.81	1.69	1.52
1	O	113	LEU	CA-C	-5.81	1.45	1.53
1	O	124	ASN	CA-C	-5.81	1.46	1.53
1	L	41	ARG	N-CA	-5.81	1.39	1.46
1	M	316	ALA	CA-C	-5.80	1.45	1.53
1	J	293	PRO	CA-CB	-5.80	1.47	1.54
1	O	332	THR	CA-C	5.80	1.59	1.52
1	H	164	ALA	CA-CB	-5.79	1.43	1.53
1	I	39	SER	CA-C	-5.79	1.45	1.53
1	C	273	GLN	CD-OE1	5.79	1.34	1.23
1	D	58	ASN	N-CA	5.79	1.53	1.46
1	K	386	ALA	CA-C	-5.78	1.45	1.52
1	E	274	SER	C-O	-5.78	1.16	1.24
1	M	179	PRO	C-O	5.78	1.30	1.23
1	J	249	CYS	CA-C	-5.78	1.46	1.52
1	K	398	SER	C-O	-5.78	1.17	1.24
1	C	249	CYS	C-O	-5.78	1.17	1.23
1	L	296	SER	CA-C	-5.78	1.45	1.52
1	O	133	HIS	CA-C	5.78	1.60	1.52
1	B	45	VAL	C-O	-5.78	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	299	ILE	C-O	5.78	1.31	1.24
1	H	38	GLY	CA-C	-5.77	1.46	1.51
1	N	179	PRO	C-O	5.77	1.30	1.23
1	A	399	ILE	CA-CB	5.77	1.61	1.54
1	J	446	LYS	CD-CE	5.77	1.69	1.52
1	M	129	THR	C-O	-5.77	1.16	1.24
1	C	226	GLN	C-O	-5.77	1.15	1.23
1	B	107	ILE	CA-CB	-5.77	1.47	1.53
1	E	306	LEU	C-O	-5.77	1.16	1.24
1	L	328	GLN	C-O	5.77	1.31	1.23
1	N	139	VAL	N-CA	5.77	1.53	1.46
1	N	277	ILE	C-O	5.77	1.30	1.24
1	D	177	SER	CA-CB	5.77	1.62	1.53
1	D	362	LYS	CE-NZ	5.76	1.66	1.49
1	H	248	PHE	CE2-CZ	5.76	1.55	1.38
1	H	461	ASP	N-CA	-5.76	1.38	1.46
1	J	306	LEU	CA-C	-5.76	1.44	1.52
1	J	358	ALA	CA-CB	5.76	1.62	1.53
1	L	114	GLY	C-O	5.76	1.29	1.23
1	F	379	LEU	C-O	5.76	1.30	1.23
1	I	228	ILE	CA-CB	-5.76	1.47	1.54
1	J	194	VAL	N-CA	5.76	1.53	1.46
1	N	36	HIS	N-CA	-5.76	1.39	1.45
1	C	261	TRP	CA-C	-5.76	1.45	1.52
1	M	179	PRO	CA-C	5.76	1.59	1.52
1	G	444	LYS	CG-CD	5.76	1.69	1.52
1	A	123	TYR	C-O	-5.75	1.16	1.23
1	N	38	GLY	C-O	-5.75	1.16	1.23
1	G	224	ILE	CA-CB	5.75	1.62	1.54
1	L	446	LYS	CG-CD	5.75	1.69	1.52
1	G	101	ALA	CA-CB	-5.74	1.44	1.53
1	O	66	SER	CA-C	-5.74	1.45	1.52
1	K	320	ASN	CA-C	-5.74	1.45	1.52
1	I	103	ALA	CA-CB	-5.74	1.45	1.54
1	K	144	ARG	CA-C	-5.74	1.45	1.52
1	N	309	LYS	CA-C	-5.74	1.46	1.52
1	G	252	ARG	CD-NE	5.74	1.54	1.46
1	G	164	ALA	C-O	5.74	1.31	1.23
1	G	397	SER	CA-C	5.74	1.60	1.52
1	N	74	ARG	CA-CB	-5.74	1.45	1.52
1	C	178	ARG	CZ-NH1	5.73	1.40	1.32
1	D	444	LYS	CD-CE	5.73	1.69	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	107	ILE	C-O	-5.73	1.17	1.23
1	A	61	ASP	N-CA	-5.73	1.38	1.46
1	G	128	ASP	CA-CB	5.73	1.59	1.52
1	N	456	PHE	C-O	-5.73	1.16	1.23
1	A	239	ALA	CA-CB	-5.73	1.44	1.53
1	B	191	LYS	CA-C	-5.73	1.45	1.52
1	K	152	LYS	C-O	-5.73	1.17	1.23
1	L	76	GLN	CD-NE2	5.72	1.45	1.33
1	N	267	MET	C-O	-5.72	1.17	1.24
1	B	247	PHE	N-CA	-5.72	1.39	1.46
1	B	443	ASP	CA-C	-5.72	1.44	1.52
1	N	149	VAL	C-O	-5.72	1.17	1.24
1	B	438	ASN	N-CA	5.71	1.57	1.46
1	L	252	ARG	CD-NE	5.71	1.54	1.46
1	E	383	THR	N-CA	5.71	1.53	1.46
1	L	134	ALA	CA-CB	5.71	1.63	1.53
1	H	155	GLN	C-O	-5.71	1.17	1.23
1	I	84	GLY	C-O	5.71	1.31	1.23
1	K	267	MET	C-O	-5.71	1.17	1.24
1	G	160	GLY	N-CA	5.71	1.51	1.45
1	N	373	LEU	CG-CD2	-5.71	1.33	1.52
1	O	384	LEU	C-O	-5.71	1.17	1.24
1	F	191	LYS	CD-CE	5.70	1.69	1.52
1	H	165	ILE	C-O	5.70	1.30	1.24
1	I	321	ASN	N-CA	-5.70	1.39	1.46
1	L	225	CYS	C-O	-5.70	1.17	1.24
1	O	465	LEU	C-O	-5.70	1.17	1.24
1	K	72	VAL	CA-CB	-5.70	1.47	1.54
1	L	105	VAL	CA-C	-5.70	1.46	1.52
1	I	398	SER	C-O	-5.69	1.17	1.24
1	K	37	ALA	N-CA	-5.69	1.39	1.46
1	L	70	TYR	C-O	-5.69	1.17	1.23
1	L	133	HIS	CA-C	5.69	1.60	1.52
1	O	184	ASP	CA-C	-5.69	1.45	1.53
1	J	61	ASP	CG-OD1	5.69	1.36	1.25
1	K	41	ARG	CA-C	-5.69	1.47	1.53
1	K	82	LYS	C-O	-5.69	1.16	1.24
1	D	310	PRO	C-O	-5.69	1.17	1.23
1	A	63	PRO	N-CA	-5.69	1.40	1.47
1	F	377	PHE	C-O	5.69	1.30	1.23
1	A	446	LYS	CG-CD	5.69	1.69	1.52
1	B	310	PRO	CA-C	-5.69	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	294	SER	CA-C	-5.68	1.46	1.52
1	J	72	VAL	CA-C	-5.68	1.45	1.52
1	A	158	ILE	N-CA	-5.68	1.39	1.46
1	H	303	ASP	CG-OD2	5.68	1.36	1.25
1	F	291	TYR	C-O	5.67	1.30	1.23
1	A	331	VAL	C-O	5.67	1.30	1.24
1	C	257	ALA	CA-CB	-5.67	1.45	1.53
1	G	134	ALA	CA-CB	5.67	1.63	1.53
1	I	454	GLU	CD-OE2	5.67	1.36	1.25
1	B	136	THR	C-O	5.67	1.30	1.23
1	C	331	VAL	C-O	-5.67	1.18	1.24
1	H	368	VAL	CA-CB	-5.67	1.45	1.54
1	J	310	PRO	CA-C	-5.67	1.45	1.52
1	H	74	ARG	CA-CB	-5.67	1.45	1.53
1	A	260	PHE	C-O	-5.66	1.17	1.24
1	I	30	ARG	C-O	-5.66	1.17	1.23
1	I	194	VAL	CA-CB	-5.66	1.47	1.54
1	L	72	VAL	C-O	-5.66	1.18	1.24
1	G	70	TYR	CA-C	5.66	1.60	1.52
1	F	59	LYS	C-O	5.66	1.31	1.24
1	G	201	VAL	C-O	5.66	1.29	1.23
1	D	76	GLN	CD-NE2	5.66	1.45	1.33
1	F	167	GLU	CD-OE2	5.65	1.36	1.25
1	M	368	VAL	CA-CB	-5.65	1.45	1.54
1	D	75	VAL	CA-CB	-5.65	1.47	1.54
1	H	167	GLU	CA-C	-5.65	1.45	1.52
1	B	248	PHE	CD1-CE1	5.65	1.55	1.38
1	M	374	GLN	CD-NE2	5.65	1.45	1.33
1	J	22	VAL	CA-CB	-5.64	1.47	1.54
1	N	177	SER	N-CA	5.64	1.53	1.46
1	E	135	ALA	C-O	5.64	1.31	1.24
1	E	374	GLN	CD-NE2	5.64	1.45	1.33
1	L	224	ILE	CG1-CD1	-5.64	1.29	1.51
1	E	288	SER	C-O	-5.64	1.17	1.23
1	K	115	VAL	CB-CG1	-5.64	1.33	1.52
1	G	200	MET	C-O	5.64	1.31	1.23
1	C	173	THR	C-O	5.64	1.30	1.23
1	D	100	TRP	CA-C	5.63	1.60	1.52
1	G	377	PHE	CA-CB	-5.63	1.43	1.53
1	K	193	THR	CA-C	5.63	1.59	1.52
1	L	233	ASP	N-CA	-5.63	1.39	1.46
1	A	236	GLN	CD-OE1	5.63	1.34	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	79	ASP	C-O	-5.63	1.17	1.24
1	M	446	LYS	CD-CE	5.63	1.69	1.52
1	A	29	THR	C-O	5.63	1.30	1.23
1	I	130	GLU	CA-C	-5.63	1.45	1.53
1	O	86	PRO	C-O	5.63	1.31	1.24
1	B	186	PRO	CA-CB	-5.62	1.46	1.54
1	H	262	ASN	CA-C	-5.62	1.45	1.52
1	G	138	ASN	CA-C	5.62	1.60	1.52
1	L	214	GLN	C-O	5.62	1.30	1.23
1	E	78	PRO	CA-C	-5.62	1.45	1.52
1	M	328	GLN	CA-C	-5.62	1.46	1.52
1	F	366	ARG	CZ-NH1	5.61	1.40	1.32
1	G	75	VAL	C-O	5.61	1.30	1.24
1	J	116	GLY	N-CA	5.61	1.53	1.45
1	J	458	LEU	CG-CD2	-5.61	1.34	1.52
1	D	466	GLY	C-O	-5.61	1.17	1.23
1	I	336	THR	CB-CG2	-5.61	1.34	1.52
1	H	460	LEU	CG-CD2	-5.61	1.34	1.52
1	K	381	THR	C-O	-5.60	1.17	1.23
1	D	37	ALA	CA-C	-5.60	1.45	1.52
1	E	135	ALA	CA-C	5.60	1.60	1.52
1	I	75	VAL	CA-CB	-5.60	1.47	1.54
1	D	315	LYS	CA-C	-5.60	1.46	1.52
1	H	138	ASN	CA-C	5.60	1.60	1.52
1	M	191	LYS	CG-CD	5.60	1.69	1.52
1	E	37	ALA	C-O	-5.60	1.16	1.23
1	N	241	PRO	N-CA	-5.59	1.40	1.47
1	A	389	MET	SD-CE	5.59	1.93	1.79
1	G	178	ARG	C-N	5.59	1.40	1.33
1	D	403	TRP	N-CA	-5.59	1.38	1.46
1	H	89	SER	CA-C	5.59	1.61	1.52
1	N	450	VAL	CA-CB	-5.59	1.46	1.54
1	D	39	SER	N-CA	5.59	1.53	1.45
1	E	158	ILE	C-O	5.59	1.29	1.24
1	H	376	ILE	CB-CG2	-5.59	1.34	1.52
1	L	48	PRO	C-O	-5.59	1.17	1.24
1	L	369	GLU	CA-CB	-5.59	1.44	1.53
1	I	76	GLN	CD-OE1	5.59	1.34	1.23
1	K	138	ASN	C-O	5.59	1.30	1.24
1	O	444	LYS	C-O	-5.58	1.16	1.24
1	D	168	HIS	C-O	-5.58	1.17	1.23
1	O	87	ASP	C-O	5.58	1.30	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	165	ILE	C-O	5.58	1.30	1.24
1	O	341	ASN	C-O	-5.58	1.17	1.24
1	E	105	VAL	CA-C	-5.58	1.45	1.52
1	E	262	ASN	N-CA	-5.58	1.39	1.45
1	C	124	ASN	N-CA	-5.58	1.39	1.46
1	I	72	VAL	C-O	-5.58	1.18	1.24
1	A	459	ASP	N-CA	5.57	1.53	1.46
1	F	205	TYR	CA-C	-5.57	1.45	1.52
1	K	240	ASP	CA-C	-5.57	1.47	1.53
1	A	262	ASN	CA-CB	-5.57	1.44	1.53
1	M	268	GLY	C-O	5.57	1.31	1.23
1	K	69	GLN	C-O	-5.57	1.16	1.23
1	L	323	VAL	CB-CG2	-5.57	1.34	1.52
1	L	446	LYS	CD-CE	5.57	1.69	1.52
1	O	177	SER	CA-C	5.57	1.59	1.52
1	C	52	VAL	N-CA	-5.57	1.41	1.46
1	M	237	MET	N-CA	-5.57	1.38	1.46
1	F	285	SER	CB-OG	5.57	1.53	1.42
1	H	61	ASP	N-CA	-5.57	1.39	1.46
1	L	128	ASP	C-O	-5.57	1.17	1.24
1	L	190	LEU	CA-C	-5.56	1.45	1.52
1	F	211	SER	N-CA	5.56	1.53	1.46
1	A	339	SER	N-CA	-5.56	1.39	1.46
1	C	174	ALA	C-O	5.56	1.30	1.24
1	H	29	THR	CA-CB	-5.56	1.45	1.53
1	I	112	PRO	C-O	5.56	1.30	1.23
1	F	456	PHE	C-O	-5.56	1.17	1.23
1	J	222	LEU	C-O	-5.56	1.17	1.24
1	H	101	ALA	CA-CB	-5.56	1.40	1.53
1	M	321	ASN	N-CA	-5.55	1.38	1.46
1	J	72	VAL	CB-CG1	-5.55	1.34	1.52
1	I	257	ALA	CA-CB	5.55	1.60	1.53
1	H	263	ARG	C-O	-5.54	1.17	1.24
1	O	187	PRO	CA-C	5.54	1.58	1.52
1	J	450	VAL	CA-CB	-5.54	1.46	1.53
1	L	94	GLU	CD-OE2	5.54	1.35	1.25
1	O	335	ASP	CA-C	-5.54	1.46	1.52
1	H	88	THR	N-CA	5.54	1.53	1.46
1	K	288	SER	C-O	-5.54	1.17	1.23
1	O	51	ARG	CZ-NH2	5.54	1.40	1.33
1	E	284	ALA	CA-CB	-5.53	1.45	1.53
1	J	468	LYS	CD-CE	5.53	1.69	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	220	VAL	C-O	-5.53	1.17	1.24
1	G	103	ALA	CA-CB	-5.53	1.44	1.54
1	G	387	ASP	C-O	5.53	1.30	1.24
1	G	150	ASP	CG-OD2	5.53	1.35	1.25
1	H	76	GLN	CG-CD	5.53	1.65	1.52
1	O	386	ALA	C-O	5.53	1.30	1.24
1	F	105	VAL	CA-C	-5.53	1.46	1.52
1	I	371	TYR	C-O	-5.53	1.16	1.23
1	F	116	GLY	C-O	5.52	1.29	1.24
1	B	134	ALA	CA-CB	5.52	1.59	1.54
1	N	299	ILE	CA-CB	-5.52	1.47	1.54
1	O	101	ALA	CA-CB	-5.52	1.44	1.53
1	G	333	VAL	CA-C	-5.52	1.45	1.52
1	G	365	SER	N-CA	-5.52	1.39	1.46
1	H	369	GLU	C-O	-5.52	1.17	1.23
1	H	372	ASP	CG-OD2	5.52	1.35	1.25
1	G	321	ASN	CA-C	5.52	1.59	1.53
1	B	99	VAL	CA-CB	-5.51	1.45	1.55
1	C	85	LEU	C-N	5.51	1.40	1.34
1	C	299	ILE	N-CA	-5.51	1.39	1.46
1	F	390	SER	C-O	5.51	1.30	1.24
1	I	150	ASP	C-O	5.51	1.30	1.24
1	O	474	GLY	C-O	5.51	1.31	1.23
1	I	326	HIS	CA-C	-5.51	1.45	1.52
1	J	191	LYS	CG-CD	5.51	1.69	1.52
1	H	370	GLU	CD-OE2	5.51	1.35	1.25
1	K	471	VAL	C-O	-5.51	1.18	1.24
1	B	43	LEU	C-O	-5.51	1.16	1.23
1	F	214	GLN	C-O	5.51	1.30	1.24
1	F	89	SER	CA-C	5.51	1.60	1.52
1	F	328	GLN	C-O	5.51	1.30	1.23
1	G	88	THR	CB-CG2	5.51	1.70	1.52
1	B	100	TRP	CA-C	5.50	1.59	1.52
1	G	293	PRO	CA-CB	-5.50	1.47	1.54
1	H	247	PHE	CA-C	-5.50	1.45	1.52
1	I	366	ARG	CZ-NH1	5.50	1.40	1.32
1	N	90	ILE	CG1-CD1	5.50	1.73	1.51
1	G	282	MET	SD-CE	5.50	1.93	1.79
1	H	129	THR	CA-C	-5.50	1.45	1.52
1	B	115	VAL	CA-CB	-5.50	1.46	1.55
1	D	446	LYS	CD-CE	5.50	1.69	1.52
1	N	469	PHE	N-CA	-5.50	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	26	ASP	C-O	-5.50	1.17	1.24
1	M	140	SER	N-CA	5.50	1.53	1.46
1	B	28	VAL	C-O	-5.49	1.18	1.24
1	B	282	MET	C-O	5.49	1.31	1.24
1	D	229	CYS	CA-CB	-5.49	1.46	1.53
1	G	265	GLY	N-CA	5.49	1.50	1.45
1	I	158	ILE	CB-CG2	-5.49	1.34	1.52
1	H	105	VAL	CA-CB	-5.49	1.47	1.55
1	M	278	LYS	C-O	-5.49	1.17	1.23
1	A	290	VAL	C-O	-5.49	1.18	1.24
1	E	63	PRO	CB-CG	-5.49	1.22	1.49
1	O	310	PRO	CA-C	-5.49	1.46	1.52
1	D	299	ILE	CA-C	-5.49	1.46	1.52
1	F	248	PHE	CE2-CZ	5.49	1.55	1.38
1	B	69	GLN	C-O	-5.49	1.17	1.24
1	I	446	LYS	CG-CD	5.49	1.69	1.52
1	C	90	ILE	C-O	5.48	1.30	1.24
1	G	81	ASN	CA-C	5.48	1.59	1.52
1	E	460	LEU	N-CA	-5.48	1.39	1.46
1	M	332	THR	N-CA	5.48	1.52	1.46
1	C	69	GLN	C-O	-5.48	1.16	1.23
1	E	134	ALA	CA-C	5.48	1.60	1.52
1	F	451	ASP	CG-OD1	5.48	1.35	1.25
1	J	236	GLN	CA-C	-5.48	1.45	1.52
1	L	255	LEU	C-O	-5.48	1.17	1.23
1	L	40	SER	CA-C	5.48	1.60	1.52
1	L	443	ASP	CG-OD2	5.48	1.35	1.25
1	K	58	ASN	CA-C	5.47	1.59	1.52
1	K	299	ILE	CA-CB	-5.47	1.48	1.54
1	J	52	VAL	N-CA	-5.47	1.42	1.46
1	K	173	THR	C-O	5.47	1.30	1.23
1	L	47	ASP	C-N	-5.47	1.27	1.34
1	G	226	GLN	CD-OE1	5.47	1.33	1.23
1	D	393	GLN	CA-C	-5.47	1.46	1.52
1	J	366	ARG	CZ-NH1	5.47	1.40	1.32
1	K	243	GLY	C-O	-5.47	1.16	1.23
1	D	33	ILE	C-O	5.47	1.30	1.23
1	N	88	THR	N-CA	5.47	1.54	1.46
1	J	204	GLY	N-CA	-5.46	1.37	1.45
1	D	41	ARG	CA-C	-5.46	1.45	1.52
1	H	44	THR	CA-CB	5.46	1.62	1.53
1	H	282	MET	CA-C	5.46	1.60	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	264	ALA	C-O	-5.46	1.16	1.23
1	M	67	ALA	CA-CB	-5.46	1.44	1.53
1	M	72	VAL	CB-CG1	-5.46	1.34	1.52
1	L	171	LYS	N-CA	-5.46	1.39	1.46
1	E	32	SER	CA-C	5.46	1.60	1.52
1	E	102	CYS	CA-C	5.46	1.59	1.52
1	H	20	ALA	N-CA	5.46	1.56	1.46
1	A	86	PRO	C-O	5.45	1.30	1.24
1	L	200	MET	SD-CE	5.45	1.93	1.79
1	N	98	LEU	CG-CD1	-5.45	1.34	1.52
1	N	247	PHE	C-O	-5.45	1.16	1.24
1	E	360	LYS	CG-CD	5.45	1.68	1.52
1	L	323	VAL	N-CA	-5.45	1.39	1.46
1	I	293	PRO	CA-CB	-5.45	1.47	1.54
1	F	173	THR	C-O	5.45	1.30	1.24
1	G	156	LEU	CA-C	-5.45	1.45	1.52
1	I	207	ALA	CA-CB	-5.45	1.45	1.52
1	M	158	ILE	C-O	5.45	1.29	1.24
1	N	379	LEU	C-O	-5.45	1.17	1.23
1	O	278	LYS	N-CA	5.45	1.52	1.46
1	F	137	SER	C-O	5.44	1.30	1.23
1	F	326	HIS	N-CA	5.44	1.53	1.46
1	J	160	GLY	CA-C	-5.44	1.45	1.51
1	L	449	ASN	CA-C	-5.44	1.46	1.52
1	O	135	ALA	CA-CB	5.44	1.60	1.53
1	L	317	GLN	N-CA	-5.44	1.39	1.46
1	M	262	ASN	CA-C	-5.44	1.45	1.53
1	E	218	CYS	C-O	-5.44	1.18	1.24
1	H	251	ARG	CZ-NH1	5.43	1.40	1.32
1	E	132	SER	C-O	5.43	1.30	1.23
1	O	306	LEU	N-CA	-5.43	1.39	1.46
1	K	271	VAL	CA-C	-5.43	1.47	1.52
1	F	174	ALA	C-O	5.43	1.30	1.24
1	N	40	SER	CB-OG	5.43	1.53	1.42
1	K	62	ILE	CA-C	-5.43	1.48	1.53
1	E	350	SER	CA-C	5.42	1.58	1.52
1	H	83	PHE	CA-C	-5.42	1.46	1.52
1	H	137	SER	CA-C	5.42	1.59	1.52
1	L	465	LEU	CG-CD2	-5.42	1.34	1.52
1	M	217	LYS	CD-CE	5.42	1.68	1.52
1	B	130	GLU	CA-C	-5.42	1.45	1.52
1	C	52	VAL	CA-CB	-5.42	1.47	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	139	VAL	CA-CB	5.42	1.61	1.54
1	M	171	LYS	CD-CE	5.42	1.68	1.52
1	C	135	ALA	CA-CB	5.42	1.61	1.53
1	E	351	PRO	CA-C	5.42	1.61	1.52
1	G	358	ALA	CA-CB	-5.42	1.45	1.53
1	M	386	ALA	C-O	5.42	1.30	1.24
1	B	256	PHE	CA-C	-5.42	1.46	1.52
1	F	87	ASP	C-O	5.42	1.30	1.24
1	J	64	LYS	CA-CB	-5.42	1.46	1.53
1	A	177	SER	CB-OG	5.41	1.52	1.42
1	A	247	PHE	CA-C	-5.41	1.46	1.53
1	C	137	SER	C-O	5.41	1.30	1.24
1	G	175	SER	C-O	5.41	1.30	1.23
1	K	273	GLN	CD-OE1	5.41	1.33	1.23
1	A	112	PRO	C-O	-5.41	1.17	1.23
1	A	156	LEU	CA-C	-5.41	1.46	1.52
1	B	452	LEU	CA-CB	-5.41	1.46	1.53
1	H	201	VAL	CA-C	-5.41	1.45	1.52
1	F	105	VAL	CA-CB	-5.41	1.45	1.55
1	F	255	LEU	CA-C	-5.41	1.46	1.52
1	J	34	PHE	CA-C	-5.40	1.46	1.52
1	L	74	ARG	CA-C	-5.40	1.46	1.53
1	C	29	THR	CA-C	-5.40	1.46	1.52
1	D	196	GLU	C-O	-5.40	1.17	1.23
1	I	231	TYR	CA-C	-5.40	1.48	1.52
1	J	52	VAL	CA-CB	-5.40	1.48	1.53
1	C	39	SER	C-O	5.39	1.30	1.23
1	D	218	CYS	C-O	-5.39	1.18	1.24
1	G	329	LEU	C-O	5.39	1.30	1.24
1	L	251	ARG	NE-CZ	5.39	1.39	1.33
1	A	254	GLN	C-O	-5.39	1.17	1.24
1	I	249	CYS	CA-C	5.39	1.58	1.52
1	D	339	SER	C-O	-5.39	1.16	1.23
1	F	52	VAL	CA-CB	-5.39	1.48	1.53
1	G	76	GLN	C-O	5.39	1.30	1.24
1	I	324	CYS	CA-C	-5.39	1.46	1.53
1	E	197	ASP	C-O	-5.39	1.17	1.24
1	H	31	THR	CA-CB	-5.39	1.44	1.53
1	J	128	ASP	CA-C	-5.39	1.46	1.52
1	E	159	LEU	CA-C	-5.38	1.46	1.52
1	H	402	ASP	CB-CG	5.38	1.65	1.52
1	I	128	ASP	CA-C	-5.38	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	341	ASN	C-O	-5.38	1.17	1.24
1	O	62	ILE	N-CA	-5.38	1.42	1.46
1	G	95	THR	CA-C	5.38	1.59	1.52
1	M	224	ILE	CA-C	-5.38	1.46	1.52
1	F	85	LEU	C-N	5.38	1.40	1.33
1	J	276	TYR	CB-CG	5.38	1.63	1.51
1	M	175	SER	CA-C	5.38	1.59	1.52
1	B	79	ASP	C-N	-5.38	1.27	1.33
1	B	36	HIS	C-O	-5.38	1.17	1.23
1	H	136	THR	CA-CB	5.37	1.63	1.53
1	N	277	ILE	CA-CB	-5.37	1.47	1.54
1	N	89	SER	C-N	5.37	1.38	1.33
1	O	90	ILE	N-CA	5.37	1.53	1.46
1	E	291	TYR	C-O	5.37	1.30	1.23
1	G	35	TYR	C-O	5.37	1.30	1.23
1	O	300	VAL	CA-CB	-5.37	1.48	1.54
1	E	376	ILE	C-O	5.37	1.30	1.24
1	N	287	GLY	N-CA	5.37	1.51	1.45
1	B	222	LEU	C-O	-5.37	1.17	1.24
1	F	134	ALA	C-O	5.37	1.30	1.24
1	I	68	TYR	CA-C	-5.37	1.46	1.53
1	F	79	ASP	CG-OD2	5.36	1.35	1.25
1	F	390	SER	CA-C	5.36	1.59	1.52
1	N	319	HIS	C-O	-5.36	1.17	1.24
1	A	49	TYR	CA-CB	-5.36	1.46	1.53
1	F	71	ARG	C-O	5.36	1.30	1.24
1	A	191	LYS	CA-C	-5.36	1.46	1.52
1	I	189	GLU	CD-OE1	5.36	1.35	1.25
1	J	130	GLU	CA-C	-5.36	1.46	1.52
1	M	113	LEU	CA-C	-5.36	1.45	1.52
1	D	106	GLU	CG-CD	5.36	1.65	1.52
1	K	158	ILE	C-O	5.36	1.29	1.24
1	G	453	LYS	CD-CE	5.36	1.68	1.52
1	J	368	VAL	CA-CB	-5.35	1.46	1.54
1	G	196	GLU	C-O	-5.35	1.17	1.23
1	H	439	LYS	N-CA	5.35	1.53	1.46
1	D	353	PRO	N-CA	5.35	1.53	1.47
1	E	453	LYS	CE-NZ	5.35	1.65	1.49
1	G	207	ALA	CA-CB	-5.35	1.46	1.53
1	K	392	ILE	C-O	-5.35	1.17	1.24
1	B	193	THR	C-O	-5.35	1.17	1.23
1	D	344	ILE	CA-CB	-5.35	1.47	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	375	PHE	N-CA	5.35	1.52	1.45
1	H	202	ASP	CA-CB	-5.35	1.45	1.53
1	K	21	VAL	C-O	-5.35	1.17	1.24
1	L	293	PRO	CA-CB	-5.35	1.48	1.54
1	L	323	VAL	CA-CB	-5.35	1.47	1.54
1	M	284	ALA	CA-CB	-5.35	1.44	1.53
1	E	316	ALA	CA-CB	-5.34	1.45	1.53
1	I	243	GLY	C-O	-5.34	1.16	1.24
1	O	385	THR	C-O	5.34	1.30	1.24
1	F	309	LYS	CA-C	-5.34	1.47	1.52
1	C	290	VAL	CA-CB	-5.34	1.47	1.53
1	G	287	GLY	C-O	5.34	1.30	1.24
1	H	243	GLY	C-O	-5.34	1.16	1.24
1	D	223	ASP	N-CA	-5.34	1.39	1.46
1	B	401	GLU	CD-OE1	5.33	1.35	1.25
1	G	49	TYR	C-O	5.33	1.31	1.23
1	G	107	ILE	CA-CB	-5.33	1.47	1.53
1	J	275	LEU	CG-CD2	-5.33	1.34	1.52
1	A	339	SER	C-O	-5.33	1.16	1.23
1	I	445	LEU	N-CA	-5.33	1.39	1.45
1	M	20	ALA	N-CA	5.33	1.56	1.46
1	H	227	SER	CA-C	-5.32	1.45	1.53
1	C	202	ASP	N-CA	-5.32	1.39	1.46
1	E	129	THR	CA-C	-5.32	1.45	1.52
1	D	344	ILE	CA-C	-5.32	1.46	1.52
1	M	183	GLY	C-O	-5.32	1.17	1.24
1	O	107	ILE	CG1-CD1	-5.32	1.30	1.51
1	O	179	PRO	C-O	5.32	1.30	1.23
1	C	48	PRO	C-O	-5.32	1.17	1.24
1	I	128	ASP	CG-OD1	5.32	1.35	1.25
1	M	117	LEU	C-O	-5.32	1.17	1.23
1	F	113	LEU	C-O	-5.32	1.17	1.23
1	G	385	THR	C-O	5.31	1.30	1.23
1	H	192	ASN	CA-C	-5.31	1.45	1.52
1	C	368	VAL	CA-CB	-5.31	1.46	1.54
1	K	389	MET	CA-C	-5.31	1.46	1.52
1	K	402	ASP	CG-OD1	5.31	1.35	1.25
1	L	72	VAL	N-CA	5.31	1.52	1.46
1	J	166	GLY	C-O	-5.31	1.16	1.24
1	A	116	GLY	C-O	5.31	1.29	1.24
1	G	360	LYS	CG-CD	5.31	1.68	1.52
1	N	231	TYR	CA-C	-5.31	1.47	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	122	PHE	C-O	-5.30	1.17	1.23
1	K	382	ILE	C-O	-5.30	1.18	1.24
1	H	202	ASP	N-CA	-5.30	1.39	1.46
1	B	218	CYS	CA-C	-5.30	1.46	1.53
1	I	226	GLN	CA-C	-5.30	1.45	1.52
1	E	189	GLU	CD-OE1	5.30	1.35	1.25
1	F	446	LYS	C-O	-5.30	1.17	1.24
1	I	69	GLN	C-O	-5.30	1.17	1.23
1	L	216	THR	CA-CB	-5.30	1.45	1.53
1	L	132	SER	C-O	5.29	1.30	1.24
1	O	140	SER	CA-C	5.29	1.59	1.52
1	G	196	GLU	CA-C	-5.29	1.46	1.52
1	J	469	PHE	N-CA	-5.29	1.40	1.46
1	M	179	PRO	N-CA	5.29	1.53	1.47
1	A	158	ILE	CA-CB	-5.29	1.47	1.54
1	G	309	LYS	CE-NZ	5.29	1.65	1.49
1	G	446	LYS	CA-C	-5.29	1.46	1.52
1	O	45	VAL	C-O	-5.29	1.18	1.24
1	F	347	SER	C-O	5.29	1.30	1.23
1	G	348	THR	CB-CG2	5.29	1.70	1.52
1	O	267	MET	C-O	-5.29	1.17	1.24
1	A	305	GLN	CA-C	-5.29	1.45	1.52
1	B	465	LEU	N-CA	-5.29	1.39	1.46
1	F	299	ILE	CG1-CD1	5.29	1.72	1.51
1	K	316	ALA	CA-CB	-5.29	1.45	1.53
1	M	62	ILE	N-CA	-5.29	1.42	1.46
1	C	299	ILE	CA-CB	-5.28	1.47	1.54
1	E	271	VAL	CB-CG2	-5.28	1.35	1.52
1	E	379	LEU	C-O	-5.28	1.17	1.24
1	A	173	THR	C-O	5.28	1.30	1.23
1	I	317	GLN	CG-CD	5.28	1.65	1.52
1	L	87	ASP	CA-C	5.27	1.58	1.52
1	M	282	MET	CG-SD	5.27	1.94	1.80
1	C	128	ASP	CG-OD1	5.27	1.35	1.25
1	N	242	TYR	C-O	-5.27	1.17	1.24
1	C	290	VAL	CA-C	-5.27	1.47	1.52
1	G	366	ARG	CZ-NH1	5.27	1.40	1.32
1	I	106	GLU	N-CA	-5.27	1.40	1.46
1	N	247	PHE	N-CA	-5.27	1.40	1.46
1	I	65	VAL	C-O	-5.27	1.18	1.24
1	K	295	PRO	CA-CB	-5.27	1.45	1.53
1	I	152	LYS	C-O	-5.27	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	170	ALA	CA-CB	-5.26	1.45	1.54
1	H	376	ILE	CA-CB	-5.26	1.47	1.54
1	M	104	GLY	N-CA	-5.26	1.40	1.45
1	E	140	SER	CA-C	5.26	1.59	1.52
1	A	23	ASN	N-CA	-5.26	1.39	1.46
1	K	276	TYR	N-CA	-5.26	1.39	1.46
1	K	305	GLN	N-CA	5.26	1.52	1.46
1	B	178	ARG	CZ-NH1	5.26	1.40	1.32
1	E	315	LYS	CG-CD	5.26	1.68	1.52
1	L	451	ASP	CG-OD1	5.26	1.35	1.25
1	M	238	SER	CA-C	-5.26	1.45	1.52
1	N	208	MET	CA-CB	-5.26	1.44	1.53
1	N	256	PHE	C-O	5.26	1.29	1.23
1	O	46	GLY	C-O	5.26	1.29	1.23
1	D	127	ASP	C-O	5.25	1.29	1.23
1	B	311	TYR	CE2-CZ	5.25	1.50	1.38
1	J	400	LEU	CA-C	-5.25	1.45	1.52
1	A	391	TYR	C-O	5.25	1.30	1.24
1	K	222	LEU	C-O	-5.25	1.18	1.24
1	K	310	PRO	C-O	-5.25	1.18	1.23
1	O	116	GLY	N-CA	-5.25	1.40	1.45
1	D	289	CYS	C-O	-5.25	1.16	1.23
1	J	229	CYS	CA-CB	-5.25	1.46	1.53
1	J	236	GLN	C-O	-5.25	1.17	1.24
1	E	140	SER	C-O	5.24	1.30	1.24
1	E	370	GLU	C-O	-5.24	1.18	1.24
1	L	473	ALA	C-O	5.24	1.30	1.24
1	E	129	THR	CA-CB	-5.24	1.46	1.53
1	A	473	ALA	CA-CB	-5.24	1.44	1.53
1	L	194	VAL	CB-CG1	-5.24	1.35	1.52
1	A	257	ALA	C-O	-5.24	1.17	1.24
1	F	39	SER	C-O	5.24	1.31	1.23
1	B	77	LEU	C-O	5.24	1.29	1.23
1	C	328	GLN	CA-C	-5.24	1.46	1.52
1	E	206	GLY	N-CA	5.24	1.50	1.45
1	L	259	HIS	C-O	-5.24	1.17	1.23
1	M	312	TRP	CE2-CZ2	-5.23	1.28	1.39
1	G	312	TRP	CA-CB	-5.23	1.46	1.53
1	K	278	LYS	C-O	5.23	1.30	1.23
1	D	233	ASP	CG-OD1	5.23	1.35	1.25
1	L	155	GLN	CA-C	-5.23	1.46	1.52
1	G	45	VAL	CA-C	-5.23	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	188	LEU	C-O	-5.23	1.17	1.23
1	D	439	LYS	CA-CB	5.22	1.59	1.53
1	H	183	GLY	C-O	-5.22	1.16	1.24
1	J	253	GLU	C-O	-5.22	1.17	1.23
1	M	129	THR	CA-C	-5.22	1.45	1.52
1	N	318	GLY	C-O	5.22	1.28	1.23
1	B	202	ASP	CB-CG	5.22	1.65	1.52
1	H	324	CYS	CA-C	-5.22	1.46	1.53
1	I	151	TYR	CA-CB	-5.22	1.45	1.53
1	K	376	ILE	CA-CB	-5.22	1.48	1.54
1	E	215	ASP	C-O	-5.22	1.17	1.24
1	L	188	LEU	CG-CD2	-5.22	1.35	1.52
1	B	446	LYS	CG-CD	5.22	1.68	1.52
1	D	309	LYS	CA-CB	-5.22	1.47	1.54
1	F	334	VAL	CA-C	-5.22	1.46	1.52
1	K	309	LYS	CE-NZ	5.22	1.65	1.49
1	N	30	ARG	CA-C	-5.22	1.46	1.52
1	O	134	ALA	CA-CB	5.22	1.62	1.53
1	O	370	GLU	C-O	-5.22	1.18	1.24
1	H	254	GLN	CD-OE1	5.21	1.33	1.23
1	E	77	LEU	N-CA	5.21	1.52	1.45
1	L	454	GLU	CD-OE1	5.21	1.35	1.25
1	F	177	SER	N-CA	5.21	1.52	1.46
1	K	163	PRO	CA-C	-5.21	1.46	1.52
1	H	174	ALA	CA-C	-5.21	1.45	1.52
1	O	214	GLN	C-O	5.21	1.29	1.23
1	C	277	ILE	CA-CB	-5.21	1.48	1.54
1	D	236	GLN	C-O	-5.21	1.18	1.24
1	G	104	GLY	C-O	5.21	1.30	1.23
1	B	278	LYS	CA-C	-5.21	1.46	1.52
1	O	168	HIS	CA-C	-5.21	1.46	1.52
1	A	299	ILE	CG1-CD1	5.20	1.72	1.51
1	F	165	ILE	CA-CB	-5.20	1.48	1.54
1	K	73	PHE	N-CA	-5.20	1.39	1.46
1	L	101	ALA	CA-CB	-5.20	1.45	1.53
1	N	240	ASP	C-N	-5.20	1.27	1.34
1	H	341	ASN	CA-CB	-5.20	1.46	1.53
1	B	374	GLN	CD-OE1	5.20	1.33	1.23
1	G	209	ASP	CA-C	5.20	1.59	1.53
1	H	208	MET	CA-CB	-5.20	1.47	1.53
1	J	251	ARG	CZ-NH2	5.20	1.40	1.33
1	L	374	GLN	CD-OE1	5.20	1.33	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	ARG	CZ-NH2	5.20	1.40	1.33
1	H	360	LYS	CG-CD	5.20	1.68	1.52
1	J	61	ASP	CG-OD2	5.20	1.35	1.25
1	C	450	VAL	CA-C	-5.20	1.46	1.52
1	E	198	GLY	N-CA	-5.20	1.38	1.45
1	J	445	LEU	C-O	-5.19	1.17	1.23
1	O	171	LYS	C-O	5.19	1.30	1.24
1	B	368	VAL	CA-CB	-5.19	1.47	1.55
1	E	189	GLU	CD-OE2	5.19	1.35	1.25
1	F	340	THR	N-CA	5.19	1.52	1.46
1	H	65	VAL	CA-CB	-5.19	1.47	1.54
1	O	151	TYR	N-CA	5.19	1.52	1.45
1	K	357	ASP	N-CA	-5.19	1.40	1.46
1	A	332	THR	C-O	-5.18	1.17	1.24
1	G	145	ASP	CG-OD2	5.18	1.35	1.25
1	C	190	LEU	CA-CB	-5.18	1.46	1.53
1	G	377	PHE	CE1-CZ	5.18	1.54	1.38
1	H	362	LYS	C-O	-5.18	1.17	1.24
1	D	285	SER	CA-C	5.18	1.57	1.52
1	K	113	LEU	N-CA	-5.18	1.39	1.46
1	M	105	VAL	C-O	-5.18	1.18	1.23
1	K	74	ARG	CZ-NH1	5.18	1.40	1.32
1	L	387	ASP	CG-OD1	5.18	1.35	1.25
1	M	285	SER	CA-C	5.18	1.58	1.52
1	C	312	TRP	CE2-CZ2	-5.17	1.28	1.39
1	N	31	THR	CA-C	-5.17	1.45	1.53
1	K	24	THR	CA-C	5.17	1.59	1.52
1	N	448	TRP	CA-C	-5.17	1.46	1.52
1	B	374	GLN	CA-CB	-5.17	1.44	1.53
1	C	332	THR	CA-CB	-5.17	1.45	1.53
1	C	311	TYR	CG-CD2	5.17	1.50	1.39
1	H	470	LEU	C-O	-5.17	1.17	1.24
1	K	28	VAL	C-O	-5.17	1.18	1.24
1	L	273	GLN	CD-NE2	5.17	1.44	1.33
1	L	275	LEU	CG-CD2	-5.17	1.35	1.52
1	G	255	LEU	CA-C	-5.17	1.46	1.52
1	B	373	LEU	CG-CD2	-5.16	1.35	1.52
1	F	191	LYS	C-O	5.16	1.30	1.24
1	G	168	HIS	CA-C	-5.16	1.46	1.52
1	I	40	SER	C-O	-5.16	1.17	1.24
1	K	306	LEU	C-O	-5.16	1.17	1.24
1	B	180	LEU	N-CA	-5.16	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	311	TYR	CG-CD1	5.16	1.50	1.39
1	G	468	LYS	CE-NZ	5.16	1.64	1.49
1	F	451	ASP	CA-C	5.15	1.59	1.52
1	M	449	ASN	C-O	-5.15	1.17	1.24
1	L	302	SER	C-O	5.15	1.30	1.24
1	F	36	HIS	CA-CB	-5.15	1.45	1.53
1	F	398	SER	CA-C	5.15	1.59	1.52
1	L	231	TYR	C-O	-5.15	1.17	1.24
1	A	262	ASN	C-O	-5.15	1.17	1.23
1	F	359	THR	C-O	5.15	1.30	1.24
1	F	468	LYS	CE-NZ	5.15	1.64	1.49
1	G	162	ALA	CA-CB	5.15	1.61	1.53
1	F	386	ALA	CA-CB	5.14	1.62	1.53
1	L	165	ILE	CA-C	-5.14	1.46	1.52
1	G	232	PRO	CG-CD	5.14	1.68	1.50
1	J	222	LEU	CA-C	-5.14	1.45	1.52
1	N	24	THR	CB-CG2	-5.14	1.35	1.52
1	L	109	ARG	C-O	-5.14	1.17	1.24
1	I	382	ILE	CA-C	-5.14	1.45	1.52
1	O	167	GLU	CA-C	-5.14	1.46	1.52
1	B	106	GLU	N-CA	-5.14	1.40	1.46
1	K	309	LYS	CA-C	-5.14	1.47	1.52
1	G	179	PRO	C-O	5.14	1.29	1.23
1	B	339	SER	CA-C	-5.13	1.46	1.52
1	D	30	ARG	CA-C	-5.13	1.46	1.52
1	K	306	LEU	CA-CB	-5.13	1.45	1.53
1	M	393	GLN	CD-NE2	5.13	1.44	1.33
1	E	350	SER	C-O	5.13	1.29	1.24
1	H	78	PRO	N-CA	-5.13	1.41	1.46
1	L	105	VAL	C-O	-5.13	1.18	1.23
1	O	134	ALA	C-O	5.13	1.30	1.24
1	A	372	ASP	N-CA	-5.13	1.40	1.46
1	D	45	VAL	CB-CG2	-5.13	1.35	1.52
1	I	41	ARG	N-CA	-5.13	1.40	1.46
1	K	389	MET	SD-CE	5.13	1.92	1.79
1	M	371	TYR	CA-C	-5.13	1.46	1.52
1	M	378	GLN	CA-CB	-5.13	1.45	1.53
1	A	141	GLU	CD-OE2	5.12	1.35	1.25
1	A	403	TRP	C-O	5.12	1.30	1.24
1	B	140	SER	C-O	5.12	1.30	1.24
1	D	372	ASP	C-O	-5.12	1.17	1.23
1	I	220	VAL	CA-CB	-5.12	1.47	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	242	TYR	C-O	5.12	1.30	1.24
1	I	109	ARG	C-O	-5.12	1.17	1.23
1	I	133	HIS	C-O	5.12	1.30	1.24
1	K	55	GLY	CA-C	5.12	1.59	1.51
1	A	139	VAL	C-O	5.12	1.30	1.24
1	A	153	GLN	C-O	-5.12	1.17	1.24
1	F	92	ASN	N-CA	-5.12	1.40	1.46
1	M	234	TYR	N-CA	-5.12	1.40	1.46
1	H	139	VAL	C-O	5.11	1.30	1.24
1	I	361	PHE	C-O	5.11	1.29	1.23
1	F	51	ARG	NE-CZ	5.11	1.38	1.33
1	G	376	ILE	C-O	5.11	1.29	1.24
1	O	179	PRO	CA-C	5.11	1.58	1.52
1	D	102	CYS	C-O	-5.11	1.17	1.24
1	D	455	LYS	CE-NZ	5.11	1.64	1.49
1	K	379	LEU	C-O	-5.11	1.17	1.24
1	L	178	ARG	C-N	5.11	1.39	1.33
1	E	289	CYS	CA-C	-5.10	1.46	1.52
1	H	76	GLN	CD-OE1	5.10	1.33	1.23
1	C	71	ARG	CZ-NH1	5.10	1.39	1.32
1	J	24	THR	CB-CG2	-5.10	1.35	1.52
1	H	260	PHE	N-CA	5.10	1.52	1.46
1	D	137	SER	C-O	5.10	1.30	1.24
1	F	130	GLU	N-CA	-5.10	1.39	1.46
1	K	456	PHE	C-O	-5.10	1.17	1.23
1	M	389	MET	C-O	5.10	1.30	1.24
1	K	232	PRO	CA-C	-5.10	1.46	1.52
1	N	353	PRO	CA-C	-5.10	1.46	1.52
1	G	156	LEU	N-CA	-5.09	1.39	1.45
1	G	386	ALA	C-O	5.09	1.30	1.24
1	J	338	ARG	CZ-NH2	5.09	1.40	1.33
1	C	213	LEU	CG-CD1	-5.09	1.35	1.52
1	C	306	LEU	C-O	-5.09	1.17	1.24
1	M	40	SER	CB-OG	5.09	1.52	1.42
1	B	88	THR	N-CA	5.09	1.52	1.46
1	L	367	HIS	CA-C	-5.09	1.46	1.52
1	C	113	LEU	CA-C	-5.09	1.46	1.52
1	H	306	LEU	C-O	-5.09	1.17	1.24
1	F	382	ILE	CA-C	-5.09	1.46	1.52
1	F	389	MET	SD-CE	5.09	1.92	1.79
1	L	273	GLN	CD-OE1	5.09	1.33	1.23
1	M	222	LEU	CA-CB	-5.09	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	35	TYR	CE1-CZ	5.08	1.50	1.38
1	H	449	ASN	CA-C	-5.08	1.46	1.52
1	A	224	ILE	CA-CB	-5.08	1.48	1.54
1	H	370	GLU	C-O	-5.08	1.18	1.24
1	K	367	HIS	C-O	-5.08	1.17	1.23
1	O	330	PHE	C-O	5.08	1.29	1.23
1	B	145	ASP	CG-OD1	5.08	1.35	1.25
1	E	151	TYR	N-CA	5.08	1.52	1.45
1	F	139	VAL	CB-CG2	5.08	1.69	1.52
1	H	124	ASN	N-CA	-5.08	1.40	1.46
1	I	162	ALA	C-O	-5.08	1.19	1.24
1	L	467	ARG	CZ-NH2	5.08	1.40	1.33
1	F	28	VAL	C-O	5.08	1.29	1.24
1	F	142	ASP	C-O	5.08	1.30	1.23
1	F	322	GLY	N-CA	5.08	1.52	1.45
1	A	371	TYR	CZ-OH	5.08	1.48	1.38
1	C	355	GLN	C-O	5.08	1.30	1.24
1	D	205	TYR	N-CA	-5.08	1.40	1.46
1	H	293	PRO	CA-CB	-5.08	1.48	1.54
1	O	396	ASN	C-O	-5.08	1.18	1.23
1	E	353	PRO	N-CA	5.08	1.53	1.47
1	F	77	LEU	C-O	5.08	1.29	1.23
1	B	120	HIS	C-O	-5.07	1.17	1.25
1	H	290	VAL	CA-CB	-5.07	1.47	1.53
1	M	315	LYS	CA-C	-5.07	1.47	1.52
1	N	365	SER	CB-OG	5.07	1.52	1.42
1	N	450	VAL	N-CA	-5.07	1.39	1.46
1	F	204	GLY	C-O	5.07	1.29	1.24
1	H	54	ALA	CA-CB	-5.07	1.44	1.53
1	B	187	PRO	CG-CD	5.07	1.68	1.50
1	D	303	ASP	CG-OD1	5.07	1.34	1.25
1	K	20	ALA	N-CA	5.07	1.55	1.46
1	N	164	ALA	CA-CB	-5.07	1.45	1.53
1	O	334	VAL	C-O	5.07	1.29	1.24
1	A	179	PRO	C-O	5.07	1.30	1.24
1	G	344	ILE	CA-CB	-5.07	1.48	1.54
1	D	176	LYS	CD-CE	5.07	1.67	1.52
1	O	461	ASP	CG-OD2	5.07	1.34	1.25
1	M	399	ILE	C-O	-5.06	1.18	1.24
1	N	457	SER	CA-C	5.06	1.58	1.52
1	I	113	LEU	CA-CB	-5.06	1.44	1.53
1	I	346	ALA	C-O	5.06	1.30	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	367	HIS	C-O	-5.06	1.17	1.24
1	N	250	LEU	CA-CB	-5.06	1.45	1.53
1	O	120	HIS	CA-C	-5.06	1.46	1.52
1	A	206	GLY	N-CA	5.06	1.50	1.45
1	G	96	GLN	N-CA	5.06	1.52	1.45
1	J	387	ASP	CG-OD1	5.06	1.34	1.25
1	K	239	ALA	CA-CB	-5.06	1.45	1.53
1	J	251	ARG	CD-NE	5.06	1.53	1.46
1	B	116	GLY	C-O	5.05	1.29	1.24
1	D	167	GLU	CG-CD	5.05	1.64	1.52
1	J	290	VAL	C-O	-5.05	1.18	1.24
1	J	152	LYS	C-O	-5.05	1.17	1.23
1	J	182	GLN	C-O	5.05	1.30	1.24
1	C	262	ASN	CA-C	-5.05	1.46	1.52
1	C	450	VAL	C-O	-5.05	1.18	1.24
1	K	331	VAL	CA-CB	-5.05	1.47	1.53
1	A	103	ALA	CA-CB	-5.05	1.46	1.54
1	F	34	PHE	C-O	5.05	1.30	1.24
1	D	95	THR	CA-CB	5.04	1.61	1.54
1	G	64	LYS	CA-CB	-5.04	1.46	1.53
1	I	158	ILE	N-CA	-5.04	1.40	1.46
1	K	215	ASP	CG-OD1	5.04	1.34	1.25
1	N	215	ASP	C-O	-5.04	1.17	1.24
1	A	252	ARG	CZ-NH1	5.04	1.39	1.32
1	F	185	CYS	C-O	-5.04	1.17	1.24
1	H	106	GLU	C-O	-5.04	1.17	1.23
1	K	115	VAL	C-O	5.04	1.29	1.23
1	A	278	LYS	CE-NZ	5.04	1.64	1.49
1	E	119	GLY	C-O	-5.04	1.18	1.23
1	L	67	ALA	CA-C	-5.04	1.45	1.52
1	M	231	TYR	C-O	-5.04	1.18	1.24
1	B	158	ILE	CA-C	5.03	1.58	1.52
1	C	226	GLN	CA-C	-5.03	1.46	1.53
1	L	312	TRP	C-O	-5.03	1.18	1.24
1	H	311	TYR	N-CA	-5.03	1.39	1.46
1	E	178	ARG	C-N	5.03	1.39	1.33
1	F	359	THR	CA-C	5.03	1.59	1.52
1	H	63	PRO	CA-C	-5.02	1.45	1.52
1	K	164	ALA	CA-CB	-5.02	1.45	1.53
1	C	232	PRO	CA-C	-5.02	1.46	1.52
1	D	66	SER	CA-C	-5.02	1.46	1.52
1	E	400	LEU	CA-C	-5.02	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	22	VAL	CB-CG2	-5.02	1.35	1.52
1	B	252	ARG	CZ-NH1	5.02	1.39	1.32
1	J	315	LYS	CA-C	-5.02	1.47	1.52
1	N	329	LEU	C-O	5.02	1.30	1.24
1	C	467	ARG	CA-C	-5.02	1.46	1.52
1	E	31	THR	CA-C	-5.02	1.46	1.53
1	E	72	VAL	C-O	-5.02	1.18	1.24
1	I	218	CYS	N-CA	-5.02	1.41	1.46
1	L	218	CYS	CA-C	-5.02	1.45	1.52
1	L	467	ARG	CZ-NH1	5.02	1.39	1.32
1	M	123	TYR	N-CA	5.02	1.52	1.46
1	M	159	LEU	CA-C	-5.02	1.46	1.52
1	A	176	LYS	C-O	5.02	1.29	1.24
1	F	342	LEU	C-O	5.02	1.29	1.23
1	H	206	GLY	C-O	5.02	1.30	1.23
1	O	91	TYR	N-CA	-5.01	1.39	1.46
1	J	85	LEU	C-O	5.01	1.30	1.23
1	L	79	ASP	C-O	-5.01	1.18	1.24
1	E	43	LEU	C-O	5.01	1.29	1.23
1	G	443	ASP	CG-OD2	5.01	1.34	1.25
1	H	129	THR	C-O	-5.01	1.17	1.24
1	B	194	VAL	CA-C	5.01	1.58	1.52
1	E	392	ILE	CA-CB	-5.01	1.47	1.54
1	M	86	PRO	C-O	5.01	1.30	1.24
1	E	444	LYS	CG-CD	5.01	1.67	1.52
1	H	402	ASP	CG-OD2	5.01	1.34	1.25
1	N	135	ALA	C-O	5.01	1.30	1.24
1	E	53	PRO	N-CA	-5.00	1.41	1.47
1	F	455	LYS	C-O	5.00	1.30	1.24
1	H	372	ASP	C-O	-5.00	1.18	1.23

All (879) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	141	GLU	N-CA-C	13.91	122.11	108.75
1	G	140	SER	CA-C-N	-13.31	96.11	121.54
1	G	140	SER	C-N-CA	-13.31	96.11	121.54
1	D	54	ALA	N-CA-C	13.20	127.31	111.33
1	K	314	HIS	N-CA-C	-10.48	100.34	113.55
1	B	141	GLU	N-CA-C	10.22	132.57	110.80
1	L	109	ARG	NE-CZ-NH2	10.20	128.38	119.20
1	H	61	ASP	N-CA-CB	-10.14	94.51	109.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	109	ARG	NE-CZ-NH1	-9.95	111.55	121.50
1	A	314	HIS	N-CA-C	-9.87	100.78	113.12
1	H	175	SER	N-CA-C	9.79	124.05	110.24
1	C	39	SER	N-CA-C	-9.78	96.71	110.50
1	B	142	ASP	N-CA-C	-9.73	90.96	107.80
1	O	47	ASP	N-CA-C	-9.73	97.81	110.07
1	L	343	THR	N-CA-C	-9.36	94.00	109.07
1	A	185	CYS	CA-C-N	9.34	130.00	120.38
1	A	185	CYS	C-N-CA	9.34	130.00	120.38
1	O	244	ASP	N-CA-C	-9.30	102.06	113.50
1	C	279	GLY	N-CA-C	-9.14	101.83	112.79
1	K	86	PRO	N-CA-C	-9.06	102.89	114.03
1	N	333	VAL	N-CA-C	8.87	120.89	108.12
1	D	141	GLU	N-CA-C	8.80	129.55	110.80
1	E	141	GLU	N-CA-C	8.79	129.53	110.80
1	M	307	PHE	N-CA-C	8.78	123.97	110.36
1	L	453	LYS	CG-CD-CE	-8.75	91.17	111.30
1	O	314	HIS	N-CA-C	-8.74	103.20	114.04
1	N	343	THR	N-CA-C	-8.71	95.05	109.07
1	F	141	GLU	N-CA-C	8.63	129.18	110.80
1	N	297	GLY	N-CA-C	-8.62	94.63	112.04
1	H	60	GLN	CA-C-N	8.61	132.94	120.71
1	H	60	GLN	C-N-CA	8.61	132.94	120.71
1	K	32	SER	N-CA-C	-8.61	102.09	112.59
1	H	52	VAL	CA-C-N	8.47	130.43	119.84
1	H	52	VAL	C-N-CA	8.47	130.43	119.84
1	G	96	GLN	N-CA-C	8.47	123.23	109.85
1	J	141	GLU	CA-CB-CG	-8.43	97.25	114.10
1	C	62	ILE	CA-C-N	8.39	130.33	119.84
1	C	62	ILE	C-N-CA	8.39	130.33	119.84
1	K	47	ASP	N-CA-C	-8.39	99.50	110.07
1	K	271	VAL	CA-C-N	8.34	128.86	119.93
1	K	271	VAL	C-N-CA	8.34	128.86	119.93
1	F	297	GLY	N-CA-C	-8.34	97.62	112.54
1	C	206	GLY	CA-C-O	-8.33	114.64	122.39
1	A	60	GLN	O-C-N	8.28	133.60	122.59
1	O	96	GLN	N-CA-C	8.26	121.97	109.41
1	K	164	ALA	CA-C-N	-8.23	112.49	123.10
1	K	164	ALA	C-N-CA	-8.23	112.49	123.10
1	A	141	GLU	N-CA-C	8.22	128.31	110.80
1	G	47	ASP	N-CA-C	-8.22	99.71	110.07
1	B	71	ARG	N-CA-C	-8.18	94.93	108.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	212	THR	N-CA-C	8.18	123.25	113.28
1	F	263	ARG	NE-CZ-NH2	-8.13	111.89	119.20
1	K	165	ILE	CA-C-N	-8.12	113.73	122.67
1	K	165	ILE	C-N-CA	-8.12	113.73	122.67
1	E	265	GLY	CA-C-O	-8.06	115.55	122.16
1	N	62	ILE	N-CA-C	-8.03	99.01	107.60
1	J	244	ASP	N-CA-C	-8.02	103.64	113.50
1	F	261	TRP	N-CA-C	8.00	122.49	109.85
1	I	460	LEU	N-CA-C	-7.99	102.57	111.28
1	K	224	ILE	CA-C-O	7.98	125.68	119.46
1	H	224	ILE	N-CA-C	-7.96	105.56	113.20
1	A	223	ASP	N-CA-C	7.92	122.76	113.18
1	A	205	TYR	N-CA-C	-7.91	101.83	112.26
1	J	311	TYR	CA-C-O	-7.88	111.84	120.36
1	C	314	HIS	N-CA-C	-7.88	103.27	113.12
1	D	297	GLY	N-CA-C	-7.88	98.44	112.54
1	B	354	GLY	N-CA-C	-7.87	102.21	115.34
1	K	284	ALA	N-CA-C	-7.83	103.75	113.38
1	F	308	ASN	N-CA-C	-7.71	103.82	113.23
1	C	244	ASP	N-CA-C	-7.70	103.91	113.38
1	L	96	GLN	N-CA-C	7.68	121.08	109.41
1	J	354	GLY	N-CA-C	-7.64	103.21	115.66
1	G	71	ARG	CA-C-N	-7.60	112.94	123.13
1	G	71	ARG	C-N-CA	-7.60	112.94	123.13
1	K	164	ALA	N-CA-C	7.59	120.80	110.55
1	I	90	ILE	CB-CA-C	-7.58	100.96	111.65
1	J	297	GLY	N-CA-C	-7.56	99.00	112.54
1	H	177	SER	N-CA-C	7.56	119.16	111.07
1	I	61	ASP	N-CA-C	7.54	121.16	110.23
1	M	201	VAL	CB-CA-C	-7.53	100.84	111.38
1	I	107	ILE	CB-CA-C	-7.51	101.72	111.25
1	A	62	ILE	CA-C-N	7.50	127.46	120.03
1	A	62	ILE	C-N-CA	7.50	127.46	120.03
1	G	141	GLU	N-CA-C	7.50	126.78	110.80
1	E	285	SER	CA-C-N	7.50	127.51	119.78
1	E	285	SER	C-N-CA	7.50	127.51	119.78
1	I	314	HIS	N-CA-C	-7.46	103.79	113.12
1	A	56	GLY	N-CA-C	7.46	130.85	113.18
1	O	312	TRP	CA-C-N	-7.43	112.75	123.00
1	O	312	TRP	C-N-CA	-7.43	112.75	123.00
1	I	297	GLY	N-CA-C	-7.40	98.52	111.62
1	L	217	LYS	N-CA-C	-7.40	102.52	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	453	LYS	N-CA-C	-7.39	103.24	111.82
1	E	22	VAL	N-CA-C	7.39	119.46	108.46
1	K	343	THR	N-CA-C	-7.39	97.65	109.76
1	I	117	LEU	N-CA-C	7.36	121.83	110.42
1	K	33	ILE	CB-CA-C	-7.35	101.80	110.91
1	L	62	ILE	CA-C-N	7.35	127.79	119.92
1	L	62	ILE	C-N-CA	7.35	127.79	119.92
1	B	314	HIS	N-CA-C	-7.34	103.94	113.12
1	H	171	LYS	N-CA-C	-7.34	95.61	108.23
1	L	297	GLY	N-CA-C	-7.28	97.34	112.04
1	K	333	VAL	N-CA-C	7.27	119.30	108.46
1	N	352	VAL	CA-C-N	7.27	127.30	119.89
1	N	352	VAL	C-N-CA	7.27	127.30	119.89
1	A	224	ILE	N-CA-C	-7.25	106.15	113.47
1	G	140	SER	N-CA-C	-7.21	101.93	111.24
1	G	297	GLY	N-CA-C	-7.20	97.50	112.04
1	E	86	PRO	N-CA-C	-7.20	103.93	113.65
1	I	62	ILE	N-CA-C	-7.19	99.90	107.60
1	A	297	GLY	N-CA-C	-7.19	99.67	112.54
1	K	224	ILE	N-CA-C	-7.19	106.30	113.20
1	M	297	GLY	N-CA-C	-7.19	101.59	113.02
1	A	271	VAL	CA-C-N	7.18	128.81	119.84
1	A	271	VAL	C-N-CA	7.18	128.81	119.84
1	H	328	GLN	CB-CG-CD	-7.17	100.41	112.60
1	E	297	GLY	N-CA-C	-7.17	102.33	112.37
1	G	216	THR	N-CA-C	7.16	119.09	111.28
1	B	51	ARG	CA-C-N	-7.16	114.69	122.85
1	B	51	ARG	C-N-CA	-7.16	114.69	122.85
1	N	384	LEU	N-CA-C	7.14	119.44	109.15
1	C	261	TRP	N-CA-C	7.13	120.58	109.52
1	E	244	ASP	N-CA-C	-7.12	104.62	113.38
1	F	244	ASP	N-CA-C	-7.12	104.40	113.23
1	I	307	PHE	N-CA-C	7.10	121.37	110.36
1	I	85	LEU	CA-C-N	7.10	126.73	119.56
1	I	85	LEU	C-N-CA	7.10	126.73	119.56
1	B	244	ASP	N-CA-C	-7.07	104.26	113.17
1	H	172	GLY	CA-C-O	7.07	129.03	121.53
1	M	323	VAL	N-CA-C	7.06	118.16	108.84
1	N	271	VAL	CA-C-N	7.05	127.09	119.90
1	N	271	VAL	C-N-CA	7.05	127.09	119.90
1	C	340	THR	CA-C-N	-7.04	113.19	123.05
1	C	340	THR	C-N-CA	-7.04	113.19	123.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	198	GLY	N-CA-C	7.03	123.45	115.08
1	G	22	VAL	N-CA-C	7.02	119.66	108.85
1	G	448	TRP	N-CA-C	-7.00	94.73	107.75
1	C	52	VAL	CA-C-O	7.00	124.31	119.20
1	N	448	TRP	N-CA-C	-6.99	96.25	108.20
1	K	354	GLY	N-CA-C	-6.99	103.67	115.34
1	M	403	TRP	N-CA-C	-6.96	104.53	113.16
1	J	216	THR	N-CA-C	6.95	119.74	111.33
1	E	62	ILE	N-CA-C	-6.93	100.18	107.60
1	K	388	VAL	N-CA-C	-6.92	103.73	110.72
1	K	105	VAL	CB-CA-C	-6.89	100.07	110.55
1	C	54	ALA	N-CA-C	6.88	119.94	110.24
1	A	333	VAL	N-CA-C	6.85	117.39	108.35
1	E	67	ALA	N-CA-C	-6.84	104.90	113.18
1	A	53	PRO	N-CD-CG	-6.84	92.95	103.20
1	J	141	GLU	N-CA-C	6.83	119.56	109.24
1	L	333	VAL	N-CA-C	6.83	117.37	108.35
1	J	223	ASP	N-CA-C	6.82	121.19	113.01
1	B	90	ILE	N-CA-C	-6.81	103.38	113.39
1	I	165	ILE	CA-C-N	-6.81	116.41	122.47
1	I	165	ILE	C-N-CA	-6.81	116.41	122.47
1	B	343	THR	N-CA-C	-6.79	97.83	108.90
1	M	389	MET	N-CA-C	6.79	118.68	111.28
1	N	217	LYS	N-CA-C	-6.76	103.45	113.40
1	B	117	LEU	N-CA-C	6.76	120.53	110.52
1	K	62	ILE	CA-C-N	6.76	127.15	119.92
1	K	62	ILE	C-N-CA	6.76	127.15	119.92
1	N	26	ASP	N-CA-C	6.76	119.66	111.82
1	A	61	ASP	N-CA-CB	-6.74	99.11	110.49
1	L	262	ASN	CA-C-N	-6.73	112.84	122.94
1	L	262	ASN	C-N-CA	-6.73	112.84	122.94
1	C	71	ARG	N-CA-C	-6.73	97.55	108.52
1	M	47	ASP	N-CA-C	-6.73	101.59	110.07
1	M	96	GLN	N-CA-C	6.72	119.63	109.41
1	H	467	ARG	NE-CZ-NH2	6.72	125.25	119.20
1	H	197	ASP	CA-C-N	-6.69	116.21	123.30
1	H	197	ASP	C-N-CA	-6.69	116.21	123.30
1	H	141	GLU	CA-CB-CG	-6.68	100.73	114.10
1	H	141	GLU	CB-CA-C	-6.67	106.72	116.53
1	K	312	TRP	CA-C-N	-6.67	113.90	122.77
1	K	312	TRP	C-N-CA	-6.67	113.90	122.77
1	J	164	ALA	CA-C-N	-6.66	114.51	123.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	164	ALA	C-N-CA	-6.66	114.51	123.10
1	C	297	GLY	N-CA-C	-6.64	99.86	111.62
1	O	399	ILE	CB-CA-C	-6.64	103.18	112.14
1	G	26	ASP	N-CA-C	6.63	119.33	111.71
1	E	259	HIS	N-CA-C	6.62	119.97	109.50
1	L	151	TYR	N-CA-C	6.62	118.40	110.19
1	O	471	VAL	CB-CA-C	-6.62	103.50	111.97
1	C	368	VAL	CB-CA-C	-6.61	101.38	110.90
1	G	94	GLU	N-CA-C	-6.61	105.22	113.55
1	E	225	CYS	N-CA-CB	-6.59	100.18	110.06
1	D	236	GLN	N-CA-C	6.58	118.45	111.28
1	J	41	ARG	NE-CZ-NH2	6.57	125.11	119.20
1	O	143	VAL	N-CA-C	-6.57	106.39	112.43
1	C	338	ARG	NE-CZ-NH1	-6.56	114.94	121.50
1	K	244	ASP	N-CA-C	-6.56	105.31	113.38
1	I	294	SER	CA-C-O	6.56	124.51	119.46
1	E	191	LYS	N-CA-C	6.55	119.61	109.07
1	C	67	ALA	N-CA-C	-6.54	104.78	112.89
1	K	403	TRP	N-CA-C	-6.53	105.18	113.02
1	C	96	GLN	N-CA-C	6.52	119.09	109.24
1	K	297	GLY	N-CA-C	-6.52	100.87	112.54
1	E	108	GLY	CA-C-O	-6.51	115.65	121.64
1	M	89	SER	N-CA-C	-6.50	103.51	112.03
1	O	36	HIS	N-CA-C	-6.50	99.59	109.85
1	J	388	VAL	CB-CA-C	-6.49	103.67	111.97
1	B	265	GLY	N-CA-C	-6.49	104.97	111.85
1	F	471	VAL	CB-CA-C	-6.49	103.67	111.97
1	E	163	PRO	CB-CA-C	6.49	119.53	111.23
1	M	228	ILE	CA-C-N	-6.49	114.05	123.00
1	M	228	ILE	C-N-CA	-6.49	114.05	123.00
1	J	307	PHE	N-CA-C	6.48	120.20	109.96
1	D	314	HIS	N-CA-C	-6.48	105.02	113.12
1	J	71	ARG	N-CA-C	-6.46	98.67	109.07
1	O	460	LEU	N-CA-C	-6.46	104.24	111.28
1	C	197	ASP	N-CA-C	-6.46	99.37	109.25
1	C	299	ILE	CA-C-N	-6.46	115.18	123.19
1	C	299	ILE	C-N-CA	-6.46	115.18	123.19
1	L	200	MET	N-CA-C	6.45	120.03	110.48
1	J	201	VAL	CA-C-O	-6.45	116.59	121.68
1	G	96	GLN	CB-CG-CD	-6.44	101.66	112.60
1	B	310	PRO	CA-C-O	-6.43	113.44	120.97
1	E	140	SER	CA-C-N	-6.43	109.25	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	140	SER	C-N-CA	-6.43	109.25	121.54
1	D	62	ILE	CA-C-N	6.43	126.80	119.92
1	D	62	ILE	C-N-CA	6.43	126.80	119.92
1	A	354	GLY	N-CA-C	-6.42	105.19	115.66
1	E	165	ILE	CA-C-N	-6.42	116.75	122.47
1	E	165	ILE	C-N-CA	-6.42	116.75	122.47
1	H	62	ILE	CB-CA-C	-6.42	103.80	111.18
1	H	299	ILE	CA-C-N	-6.41	114.79	123.12
1	H	299	ILE	C-N-CA	-6.41	114.79	123.12
1	K	310	PRO	CA-C-O	-6.41	114.09	121.98
1	O	315	LYS	CD-CE-NZ	-6.41	91.39	111.90
1	H	171	LYS	CA-C-N	-6.41	111.24	123.29
1	H	171	LYS	C-N-CA	-6.41	111.24	123.29
1	J	389	MET	N-CA-C	6.40	117.92	111.07
1	F	32	SER	N-CA-C	-6.39	104.79	112.59
1	C	170	ALA	N-CA-C	6.38	119.11	109.41
1	L	366	ARG	NE-CZ-NH2	-6.38	113.45	119.20
1	B	460	LEU	N-CA-C	-6.38	104.40	111.36
1	H	62	ILE	CA-C-N	6.38	127.81	119.84
1	H	62	ILE	C-N-CA	6.38	127.81	119.84
1	E	360	LYS	N-CA-CB	-6.36	100.67	110.46
1	J	352	VAL	CA-C-N	6.36	126.33	119.78
1	J	352	VAL	C-N-CA	6.36	126.33	119.78
1	I	65	VAL	N-CA-C	6.34	116.76	107.37
1	J	240	ASP	CA-C-N	6.34	125.56	118.97
1	J	240	ASP	C-N-CA	6.34	125.56	118.97
1	M	300	VAL	N-CA-C	-6.34	98.61	107.80
1	N	71	ARG	N-CA-C	-6.33	98.08	108.41
1	G	250	LEU	CA-C-N	-6.33	112.17	122.81
1	G	250	LEU	C-N-CA	-6.33	112.17	122.81
1	H	137	SER	N-CA-C	6.31	119.19	110.35
1	L	205	TYR	N-CA-C	-6.30	104.91	112.59
1	N	391	TYR	N-CA-C	-6.30	103.72	111.40
1	L	323	VAL	CA-C-N	-6.29	113.46	122.77
1	L	323	VAL	C-N-CA	-6.29	113.46	122.77
1	B	82	LYS	CB-CG-CD	-6.29	96.84	111.30
1	A	107	ILE	CB-CA-C	-6.28	103.27	111.25
1	H	41	ARG	NE-CZ-NH2	6.28	124.85	119.20
1	L	453	LYS	CD-CE-NZ	-6.27	91.82	111.90
1	L	451	ASP	CA-C-N	-6.27	112.57	122.79
1	L	451	ASP	C-N-CA	-6.27	112.57	122.79
1	A	376	ILE	N-CA-C	-6.27	98.44	107.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	244	ASP	N-CA-C	-6.26	105.67	113.38
1	D	22	VAL	N-CA-C	6.26	119.07	108.86
1	H	102	CYS	CA-CB-SG	-6.25	100.02	114.40
1	K	352	VAL	CA-C-N	6.25	126.26	119.89
1	K	352	VAL	C-N-CA	6.25	126.26	119.89
1	D	393	GLN	N-CA-C	-6.24	104.40	111.14
1	H	36	HIS	N-CA-C	-6.24	99.74	109.72
1	B	113	LEU	N-CA-C	-6.24	101.25	110.48
1	E	99	VAL	CB-CA-C	-6.23	100.72	110.69
1	C	127	ASP	N-CA-C	6.23	117.69	108.60
1	B	240	ASP	CA-C-N	6.22	125.71	119.24
1	B	240	ASP	C-N-CA	6.22	125.71	119.24
1	K	62	ILE	N-CA-C	-6.22	101.39	107.55
1	B	168	HIS	N-CA-C	6.22	117.68	108.60
1	D	216	THR	N-CA-C	6.22	118.57	111.11
1	D	261	TRP	N-CA-C	6.22	119.16	109.52
1	M	290	VAL	CA-C-N	-6.21	111.98	122.92
1	M	290	VAL	C-N-CA	-6.21	111.98	122.92
1	E	31	THR	N-CA-C	-6.21	100.19	109.94
1	C	246	MET	N-CA-C	6.21	118.54	107.80
1	D	265	GLY	CA-C-O	-6.20	117.31	122.33
1	E	184	ASP	N-CA-C	-6.20	102.54	110.53
1	I	105	VAL	CB-CA-C	-6.19	101.14	110.55
1	D	310	PRO	CA-C-O	-6.19	113.72	120.97
1	G	155	GLN	CA-C-N	-6.19	111.04	121.75
1	G	155	GLN	C-N-CA	-6.19	111.04	121.75
1	I	63	PRO	CA-C-N	-6.19	114.19	122.42
1	I	63	PRO	C-N-CA	-6.19	114.19	122.42
1	H	201	VAL	CB-CA-C	-6.19	101.14	111.29
1	F	176	LYS	N-CA-C	-6.19	104.80	112.90
1	L	240	ASP	CA-C-N	6.18	125.59	118.85
1	L	240	ASP	C-N-CA	6.18	125.59	118.85
1	J	201	VAL	CB-CA-C	-6.17	102.46	112.03
1	F	391	TYR	N-CA-C	-6.17	104.18	111.03
1	G	54	ALA	N-CA-C	6.17	118.26	110.24
1	B	67	ALA	N-CA-C	-6.17	105.76	113.28
1	F	462	GLN	N-CA-C	6.17	120.66	113.20
1	A	52	VAL	CA-C-N	-6.16	114.27	120.31
1	A	52	VAL	C-N-CA	-6.16	114.27	120.31
1	D	48	PRO	N-CA-CB	-6.15	97.74	103.46
1	D	105	VAL	CB-CA-C	-6.14	101.22	110.55
1	L	86	PRO	N-CA-C	-6.12	106.21	113.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	92	ASN	CA-C-N	6.12	127.50	119.84
1	L	92	ASN	C-N-CA	6.12	127.50	119.84
1	F	376	ILE	N-CA-C	-6.12	98.66	107.78
1	G	265	GLY	CA-C-O	-6.12	117.37	122.33
1	F	96	GLN	N-CA-C	6.11	119.51	109.85
1	A	106	GLU	CA-C-N	-6.11	114.74	122.43
1	A	106	GLU	C-N-CA	-6.11	114.74	122.43
1	B	50	PHE	CA-C-O	-6.11	114.75	121.28
1	J	48	PRO	N-CA-C	6.10	121.49	113.86
1	N	294	SER	N-CA-C	-6.10	101.96	109.65
1	E	352	VAL	CA-C-N	6.09	126.11	119.89
1	E	352	VAL	C-N-CA	6.09	126.11	119.89
1	K	223	ASP	N-CA-C	6.09	120.32	113.01
1	O	252	ARG	NE-CZ-NH2	-6.08	113.72	119.20
1	K	58	ASN	N-CA-C	6.08	118.81	108.90
1	M	453	LYS	CD-CE-NZ	-6.08	92.45	111.90
1	F	294	SER	CA-C-N	-6.08	114.48	120.98
1	F	294	SER	C-N-CA	-6.08	114.48	120.98
1	B	259	HIS	N-CA-C	6.06	118.92	109.52
1	M	460	LEU	N-CA-C	-6.05	104.68	111.28
1	O	448	TRP	N-CA-C	-6.05	97.85	108.20
1	O	224	ILE	N-CA-C	-6.05	107.36	113.47
1	C	225	CYS	N-CA-CB	-6.05	100.99	110.06
1	O	47	ASP	CA-C-N	6.05	125.75	119.64
1	O	47	ASP	C-N-CA	6.05	125.75	119.64
1	L	348	THR	N-CA-C	-6.04	105.00	112.90
1	C	75	VAL	N-CA-C	6.03	117.09	107.98
1	F	137	SER	N-CA-C	6.03	118.08	110.24
1	H	469	PHE	N-CA-C	-6.03	104.27	111.69
1	F	201	VAL	CB-CA-C	-6.03	102.69	112.03
1	O	160	GLY	CA-C-N	-6.02	113.64	122.86
1	O	160	GLY	C-N-CA	-6.02	113.64	122.86
1	G	206	GLY	N-CA-C	-6.02	105.55	112.29
1	N	105	VAL	CB-CA-C	-6.02	99.64	110.48
1	F	102	CYS	CA-CB-SG	-6.01	100.57	114.40
1	H	236	GLN	N-CA-C	6.01	117.83	111.28
1	E	62	ILE	CA-C-N	6.01	126.35	119.92
1	E	62	ILE	C-N-CA	6.01	126.35	119.92
1	O	120	HIS	CA-C-N	5.99	125.87	119.28
1	O	120	HIS	C-N-CA	5.99	125.87	119.28
1	A	53	PRO	CA-C-N	5.99	132.97	121.54
1	A	53	PRO	C-N-CA	5.99	132.97	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	206	GLY	N-CA-C	-5.98	105.10	112.33
1	M	174	ALA	CA-C-N	-5.98	112.87	121.42
1	M	174	ALA	C-N-CA	-5.98	112.87	121.42
1	H	198	GLY	CA-C-O	-5.98	114.75	119.83
1	K	240	ASP	CA-C-N	5.98	125.37	118.85
1	K	240	ASP	C-N-CA	5.98	125.37	118.85
1	F	330	PHE	N-CA-C	5.97	119.79	110.17
1	G	65	VAL	N-CA-C	5.97	115.94	106.32
1	K	252	ARG	NE-CZ-NH2	-5.97	113.83	119.20
1	N	71	ARG	CA-C-N	-5.96	115.14	123.13
1	N	71	ARG	C-N-CA	-5.96	115.14	123.13
1	C	41	ARG	NE-CZ-NH1	-5.96	115.54	121.50
1	A	61	ASP	CA-C-N	-5.96	118.15	123.33
1	A	61	ASP	C-N-CA	-5.96	118.15	123.33
1	O	54	ALA	N-CA-C	5.95	118.63	110.24
1	O	33	ILE	CB-CA-C	-5.95	103.76	110.96
1	H	105	VAL	CB-CA-C	-5.94	100.49	111.18
1	H	246	MET	N-CA-C	5.93	119.16	108.48
1	E	89	SER	N-CA-C	-5.93	103.41	110.41
1	N	102	CYS	CA-CB-SG	-5.92	100.78	114.40
1	A	165	ILE	N-CA-C	5.92	117.11	108.53
1	H	224	ILE	CB-CA-C	-5.91	104.84	110.70
1	E	311	TYR	CA-C-O	-5.91	113.98	120.36
1	B	141	GLU	CA-CB-CG	-5.90	102.30	114.10
1	N	376	ILE	N-CA-C	-5.90	99.04	107.77
1	C	314	HIS	CB-CA-C	5.89	119.28	109.56
1	H	141	GLU	O-C-N	5.89	126.54	121.65
1	L	267	MET	N-CA-C	5.89	118.25	109.59
1	J	440	ASP	CA-C-N	5.89	125.51	119.56
1	J	440	ASP	C-N-CA	5.89	125.51	119.56
1	E	107	ILE	CB-CA-C	-5.88	103.78	111.25
1	B	96	GLN	N-CA-C	5.88	118.63	109.52
1	H	175	SER	CA-C-N	5.88	128.96	120.79
1	H	175	SER	C-N-CA	5.88	128.96	120.79
1	C	155	GLN	CB-CA-C	-5.86	101.68	110.24
1	A	55	GLY	N-CA-C	5.86	127.06	113.18
1	M	219	GLU	N-CA-C	5.85	120.42	113.28
1	O	216	THR	CB-CA-C	-5.85	101.69	110.88
1	D	161	CYS	N-CA-C	-5.85	103.62	111.87
1	D	239	ALA	N-CA-C	5.85	117.65	111.28
1	F	155	GLN	CB-CA-C	-5.85	101.14	110.14
1	D	105	VAL	CA-C-O	-5.84	115.54	121.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	213	LEU	CA-C-O	5.83	125.56	119.14
1	A	52	VAL	CB-CA-C	-5.83	104.47	111.18
1	O	453	LYS	CB-CG-CD	-5.83	97.88	111.30
1	G	137	SER	CA-C-N	5.83	129.64	121.24
1	G	137	SER	C-N-CA	5.83	129.64	121.24
1	M	108	GLY	CA-C-N	-5.83	114.19	122.94
1	M	108	GLY	C-N-CA	-5.83	114.19	122.94
1	B	75	VAL	CB-CA-C	-5.83	103.91	110.96
1	N	306	LEU	N-CA-C	5.82	119.57	112.23
1	G	222	LEU	N-CA-C	5.82	118.37	111.33
1	E	183	GLY	CA-C-O	5.81	125.14	119.27
1	G	21	VAL	CA-C-N	-5.81	112.92	122.67
1	G	21	VAL	C-N-CA	-5.81	112.92	122.67
1	G	102	CYS	CA-CB-SG	-5.81	101.04	114.40
1	D	291	TYR	CA-C-O	-5.80	114.56	120.71
1	I	382	ILE	CB-CA-C	-5.80	102.53	110.77
1	B	321	ASN	N-CA-CB	-5.80	103.86	110.35
1	H	50	PHE	N-CA-C	5.79	117.92	108.76
1	K	228	ILE	CA-C-N	-5.79	114.73	122.72
1	K	228	ILE	C-N-CA	-5.79	114.73	122.72
1	M	203	THR	N-CA-C	5.79	120.46	113.17
1	D	47	ASP	CA-C-N	5.78	125.47	119.64
1	D	47	ASP	C-N-CA	5.78	125.47	119.64
1	G	258	ARG	N-CA-C	-5.77	104.36	111.40
1	H	194	VAL	CB-CA-C	-5.77	103.65	111.15
1	F	450	VAL	CB-CA-C	-5.77	103.17	111.19
1	H	174	ALA	N-CA-C	-5.77	98.51	110.80
1	F	140	SER	CA-C-N	-5.76	110.53	121.54
1	F	140	SER	C-N-CA	-5.76	110.53	121.54
1	G	359	THR	OG1-CB-CG2	5.76	120.83	109.30
1	N	42	LEU	CA-CB-CG	-5.76	96.13	116.30
1	N	462	GLN	N-CA-C	5.76	119.92	113.01
1	F	307	PHE	N-CA-C	5.75	118.86	110.17
1	K	324	CYS	CA-C-O	-5.75	115.63	122.13
1	B	217	LYS	N-CA-C	-5.75	106.21	113.23
1	E	85	LEU	N-CA-C	5.75	118.48	110.20
1	F	30	ARG	N-CA-C	5.75	119.28	110.20
1	K	278	LYS	CA-C-N	-5.75	115.89	122.85
1	K	278	LYS	C-N-CA	-5.75	115.89	122.85
1	I	343	THR	N-CA-C	-5.74	99.54	108.90
1	H	57	GLY	N-CA-C	-5.74	105.54	112.49
1	H	64	LYS	CG-CD-CE	5.73	124.49	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	59	LYS	N-CA-C	5.73	123.01	110.80
1	A	201	VAL	CB-CA-C	-5.73	101.90	111.29
1	F	54	ALA	N-CA-C	5.73	118.37	110.35
1	N	160	GLY	CA-C-N	-5.73	113.45	122.79
1	N	160	GLY	C-N-CA	-5.73	113.45	122.79
1	H	107	ILE	CB-CA-C	-5.72	103.98	111.25
1	O	263	ARG	NE-CZ-NH2	-5.72	114.05	119.20
1	I	219	GLU	N-CA-C	-5.72	106.47	113.50
1	L	105	VAL	CB-CA-C	-5.72	100.64	110.30
1	G	64	LYS	CG-CD-CE	-5.70	98.19	111.30
1	B	70	TYR	CA-C-N	-5.70	114.73	122.77
1	B	70	TYR	C-N-CA	-5.70	114.73	122.77
1	F	271	VAL	CA-C-N	5.69	126.95	119.84
1	F	271	VAL	C-N-CA	5.69	126.95	119.84
1	G	331	VAL	N-CA-CB	-5.69	104.50	111.67
1	B	61	ASP	N-CA-C	5.69	118.26	110.24
1	F	341	ASN	N-CA-C	5.69	118.00	108.73
1	B	47	ASP	N-CA-C	-5.69	102.91	110.07
1	H	297	GLY	N-CA-C	-5.68	102.72	111.64
1	M	282	MET	CB-CG-SD	-5.68	95.67	112.70
1	H	279	GLY	N-CA-C	-5.67	99.73	113.18
1	C	202	ASP	CA-C-N	-5.67	113.70	122.49
1	C	202	ASP	C-N-CA	-5.67	113.70	122.49
1	H	51	ARG	NE-CZ-NH1	-5.67	115.83	121.50
1	G	290	VAL	CA-C-N	-5.67	113.74	122.87
1	G	290	VAL	C-N-CA	-5.67	113.74	122.87
1	L	468	LYS	O-C-N	5.67	128.13	122.12
1	A	53	PRO	O-C-N	5.66	130.05	123.14
1	C	217	LYS	N-CA-C	-5.66	105.07	113.40
1	H	62	ILE	N-CA-C	5.66	113.66	107.60
1	J	52	VAL	CA-C-O	5.66	123.55	119.25
1	C	32	SER	N-CA-C	-5.65	105.06	112.41
1	E	366	ARG	NE-CZ-NH2	-5.65	114.11	119.20
1	A	165	ILE	CA-C-N	-5.65	117.08	121.82
1	A	165	ILE	C-N-CA	-5.65	117.08	121.82
1	G	343	THR	N-CA-C	-5.65	99.32	108.52
1	H	334	VAL	CA-C-N	-5.65	113.23	121.76
1	H	334	VAL	C-N-CA	-5.65	113.23	121.76
1	K	21	VAL	CB-CA-C	-5.64	103.84	111.63
1	A	158	ILE	CB-CA-C	-5.64	102.10	110.33
1	O	65	VAL	N-CA-CB	-5.63	104.57	111.67
1	C	306	LEU	N-CA-C	5.63	119.32	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	61	ASP	N-CA-C	5.63	118.17	110.24
1	K	394	SER	N-CA-C	-5.62	104.77	111.69
1	D	52	VAL	O-C-N	5.62	124.91	121.37
1	A	209	ASP	N-CA-CB	-5.61	102.19	110.49
1	O	143	VAL	CB-CA-C	-5.60	104.81	111.65
1	D	201	VAL	CB-CA-C	-5.60	102.10	111.29
1	E	271	VAL	CA-C-N	5.60	125.61	119.90
1	E	271	VAL	C-N-CA	5.60	125.61	119.90
1	G	307	PHE	N-CA-C	5.60	118.62	110.17
1	K	117	LEU	N-CA-C	5.60	119.10	110.42
1	O	265	GLY	CA-C-O	-5.60	117.80	122.33
1	I	246	MET	CA-C-N	-5.60	113.70	122.49
1	I	246	MET	C-N-CA	-5.60	113.70	122.49
1	D	306	LEU	N-CA-C	5.59	119.28	112.23
1	L	41	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	M	348	THR	N-CA-C	-5.59	105.57	112.90
1	A	96	GLN	N-CA-C	5.59	117.91	109.41
1	G	171	LYS	CA-C-N	5.59	125.28	119.92
1	G	171	LYS	C-N-CA	5.59	125.28	119.92
1	N	86	PRO	N-CA-C	-5.59	107.16	114.03
1	O	463	TYR	CA-C-N	5.59	126.82	119.84
1	O	463	TYR	C-N-CA	5.59	126.82	119.84
1	H	217	LYS	N-CA-C	-5.58	106.42	113.23
1	L	368	VAL	CB-CA-C	-5.58	102.23	110.82
1	K	262	ASN	CA-C-N	-5.58	114.84	122.93
1	K	262	ASN	C-N-CA	-5.58	114.84	122.93
1	I	165	ILE	N-CA-C	5.58	115.98	108.17
1	H	385	THR	N-CA-C	-5.57	101.27	109.18
1	N	22	VAL	N-CA-C	5.57	117.94	108.86
1	O	240	ASP	CA-C-N	5.57	125.23	119.05
1	O	240	ASP	C-N-CA	5.57	125.23	119.05
1	H	160	GLY	CA-C-O	-5.57	116.20	121.60
1	C	233	ASP	N-CA-C	5.56	118.20	108.52
1	L	98	LEU	N-CA-C	5.56	118.55	109.59
1	M	179	PRO	CA-C-N	-5.56	114.96	123.07
1	M	179	PRO	C-N-CA	-5.56	114.96	123.07
1	A	227	SER	CA-C-N	-5.55	115.71	123.10
1	A	227	SER	C-N-CA	-5.55	115.71	123.10
1	J	256	PHE	CA-C-N	-5.55	115.03	122.42
1	J	256	PHE	C-N-CA	-5.55	115.03	122.42
1	C	113	LEU	CA-C-O	-5.55	115.51	121.56
1	C	47	ASP	N-CA-C	-5.55	103.07	110.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	176	LYS	CA-C-N	5.55	127.66	120.44
1	D	176	LYS	C-N-CA	5.55	127.66	120.44
1	L	251	ARG	NH1-CZ-NH2	-5.55	112.08	119.30
1	N	127	ASP	N-CA-C	5.55	116.70	108.60
1	O	224	ILE	CA-C-O	5.54	123.97	118.98
1	N	98	LEU	CB-CG-CD1	-5.54	94.08	110.70
1	I	247	PHE	N-CA-C	-5.54	105.21	112.41
1	A	329	LEU	CA-C-N	-5.54	114.90	122.93
1	A	329	LEU	C-N-CA	-5.54	114.90	122.93
1	I	33	ILE	N-CA-C	5.54	116.73	108.54
1	N	228	ILE	CA-C-N	-5.54	115.41	122.77
1	N	228	ILE	C-N-CA	-5.54	115.41	122.77
1	F	61	ASP	N-CA-C	5.53	118.04	110.24
1	M	282	MET	N-CA-C	-5.52	106.05	112.89
1	M	382	ILE	CB-CA-C	-5.52	102.90	110.96
1	B	179	PRO	CA-C-N	-5.52	115.22	123.00
1	B	179	PRO	C-N-CA	-5.52	115.22	123.00
1	C	117	LEU	N-CA-CB	-5.52	101.95	110.56
1	A	86	PRO	N-CA-C	-5.52	107.45	114.35
1	B	201	VAL	CB-CA-C	-5.51	103.48	112.03
1	L	47	ASP	N-CA-C	-5.51	103.12	110.07
1	O	389	MET	N-CA-C	5.51	117.37	111.36
1	O	453	LYS	CG-CD-CE	-5.51	98.63	111.30
1	E	279	GLY	N-CA-C	-5.50	106.18	112.79
1	M	391	TYR	N-CA-C	-5.50	104.92	111.03
1	O	261	TRP	N-CA-C	5.50	117.77	109.41
1	G	191	LYS	N-CA-C	5.50	118.44	109.59
1	O	360	LYS	N-CA-CB	-5.50	102.00	110.46
1	A	343	THR	N-CA-C	-5.50	100.22	109.07
1	A	290	VAL	N-CA-C	-5.49	99.24	107.37
1	D	307	PHE	N-CA-C	5.49	118.55	109.94
1	G	158	ILE	N-CA-C	5.49	116.63	108.46
1	N	300	VAL	N-CA-C	-5.49	99.85	107.80
1	B	105	VAL	CB-CA-C	-5.48	100.89	110.71
1	A	448	TRP	N-CA-C	-5.48	99.59	108.41
1	E	39	SER	N-CA-C	-5.48	103.25	110.43
1	C	47	ASP	CA-C-N	5.47	125.17	119.64
1	C	47	ASP	C-N-CA	5.47	125.17	119.64
1	F	147	VAL	N-CA-C	5.47	117.28	108.85
1	O	333	VAL	N-CA-C	5.47	116.55	108.45
1	G	108	GLY	CA-C-N	-5.47	114.22	122.81
1	G	108	GLY	C-N-CA	-5.47	114.22	122.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	202	ASP	CB-CA-C	-5.47	102.28	110.16
1	B	470	LEU	N-CA-C	5.47	117.95	111.33
1	A	105	VAL	CB-CA-C	-5.46	101.35	111.18
1	F	460	LEU	N-CA-C	-5.46	105.33	111.28
1	C	333	VAL	N-CA-C	5.46	115.55	108.35
1	M	211	SER	N-CA-C	-5.46	105.36	112.23
1	A	300	VAL	N-CA-C	-5.45	99.80	107.75
1	E	391	TYR	N-CA-C	-5.44	105.27	111.14
1	G	248	PHE	N-CA-C	-5.44	100.24	108.46
1	G	309	LYS	N-CA-C	-5.44	99.63	108.82
1	A	67	ALA	CA-C-O	5.43	125.65	119.18
1	C	201	VAL	CB-CA-C	-5.43	103.61	112.03
1	O	343	THR	N-CA-C	-5.43	100.33	109.07
1	D	439	LYS	CD-CE-NZ	-5.43	94.52	111.90
1	H	165	ILE	N-CA-C	5.43	115.77	108.17
1	B	108	GLY	O-C-N	-5.42	118.00	122.77
1	H	141	GLU	CB-CG-CD	5.42	121.82	112.60
1	D	165	ILE	N-CA-C	5.42	116.39	108.53
1	B	161	CYS	N-CA-C	-5.42	103.55	111.30
1	N	460	LEU	N-CA-C	-5.42	105.37	111.28
1	A	108	GLY	CA-C-N	-5.41	114.82	122.94
1	A	108	GLY	C-N-CA	-5.41	114.82	122.94
1	G	105	VAL	CB-CA-C	-5.41	102.32	110.55
1	J	271	VAL	CA-C-N	5.41	125.42	119.90
1	J	271	VAL	C-N-CA	5.41	125.42	119.90
1	B	41	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	D	246	MET	N-CA-C	5.41	117.43	108.13
1	G	32	SER	N-CA-C	-5.41	104.25	111.87
1	H	113	LEU	N-CA-C	-5.41	102.88	110.50
1	M	314	HIS	N-CA-C	-5.41	106.36	113.12
1	O	73	PHE	N-CA-C	-5.40	100.37	109.07
1	B	48	PRO	N-CA-CB	-5.40	98.07	103.20
1	G	65	VAL	CB-CA-C	-5.40	105.75	112.45
1	J	460	LEU	N-CA-C	-5.39	105.48	111.36
1	M	30	ARG	NE-CZ-NH2	5.39	124.06	119.20
1	F	158	ILE	CB-CA-C	-5.39	101.39	110.71
1	M	53	PRO	O-C-N	5.39	129.21	123.01
1	H	43	LEU	N-CA-CB	-5.39	102.66	111.66
1	H	333	VAL	N-CA-C	5.38	116.42	108.45
1	M	113	LEU	N-CA-C	-5.38	102.91	110.50
1	F	240	ASP	CA-C-N	5.38	124.57	118.97
1	F	240	ASP	C-N-CA	5.38	124.57	118.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	246	MET	N-CA-C	5.38	116.85	107.49
1	L	245	SER	N-CA-C	-5.38	105.08	111.69
1	H	271	VAL	CA-C-N	5.37	125.38	119.90
1	H	271	VAL	C-N-CA	5.37	125.38	119.90
1	K	150	ASP	O-C-N	-5.37	117.10	123.22
1	M	456	PHE	CA-C-O	-5.37	114.93	121.05
1	N	96	GLN	N-CA-C	5.37	117.57	109.41
1	N	161	CYS	N-CA-C	-5.37	104.30	111.87
1	J	125	LYS	CD-CE-NZ	-5.37	94.73	111.90
1	L	158	ILE	CB-CA-C	-5.37	101.80	110.28
1	H	225	CYS	N-CA-CB	-5.36	102.02	110.06
1	A	382	ILE	CB-CA-C	-5.36	103.17	110.77
1	C	33	ILE	CB-CA-C	-5.36	104.27	110.91
1	M	41	ARG	NE-CZ-NH1	-5.36	116.14	121.50
1	H	262	ASN	CB-CA-C	-5.35	100.97	109.80
1	M	260	PHE	O-C-N	-5.35	117.22	123.27
1	N	382	ILE	CB-CA-C	-5.35	104.36	110.73
1	F	129	THR	N-CA-C	-5.35	106.07	112.59
1	M	92	ASN	CA-CB-CG	-5.35	107.25	112.60
1	C	263	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	K	471	VAL	CB-CA-C	-5.35	104.86	111.70
1	J	265	GLY	CA-C-O	-5.34	118.00	122.33
1	A	298	SER	N-CA-C	-5.34	99.43	110.80
1	G	321	ASN	N-CA-CB	-5.34	103.72	110.45
1	L	333	VAL	CA-C-N	-5.34	115.03	122.71
1	L	333	VAL	C-N-CA	-5.34	115.03	122.71
1	K	107	ILE	CB-CA-C	-5.33	104.51	110.96
1	K	312	TRP	N-CA-C	5.33	117.44	108.96
1	F	305	GLN	CA-C-O	5.33	126.77	120.69
1	B	134	ALA	O-C-N	5.33	127.11	123.11
1	K	96	GLN	N-CA-C	5.33	118.27	109.85
1	L	111	GLN	CA-C-N	5.33	125.53	120.31
1	L	111	GLN	C-N-CA	5.33	125.53	120.31
1	E	223	ASP	N-CA-C	5.33	119.53	113.19
1	H	21	VAL	CB-CA-C	-5.33	104.28	111.63
1	H	224	ILE	CA-C-O	5.33	123.61	119.46
1	J	39	SER	N-CA-C	-5.33	103.45	110.43
1	I	225	CYS	N-CA-CB	-5.32	101.50	110.49
1	I	47	ASP	N-CA-C	-5.32	103.37	110.07
1	C	106	GLU	CA-C-N	-5.32	115.73	122.43
1	C	106	GLU	C-N-CA	-5.32	115.73	122.43
1	G	89	SER	N-CA-C	-5.32	102.45	110.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	41	ARG	NE-CZ-NH1	-5.32	116.18	121.50
1	A	99	VAL	CB-CA-C	-5.32	102.19	110.69
1	G	232	PRO	CA-C-N	-5.32	114.18	122.05
1	G	232	PRO	C-N-CA	-5.32	114.18	122.05
1	M	32	SER	N-CA-C	-5.31	106.02	112.88
1	G	449	ASN	N-CA-C	5.31	117.40	109.59
1	F	64	LYS	CG-CD-CE	-5.31	99.10	111.30
1	I	109	ARG	CB-CG-CD	-5.30	99.10	111.30
1	O	105	VAL	CA-CB-CG2	-5.30	101.39	110.40
1	H	339	SER	N-CA-C	5.30	119.25	112.26
1	L	384	LEU	N-CA-C	5.30	116.78	109.15
1	M	105	VAL	CB-CA-C	-5.30	101.23	110.71
1	I	55	GLY	N-CA-C	5.30	125.73	113.18
1	L	238	SER	N-CA-C	-5.30	106.32	112.89
1	H	286	PRO	CA-C-N	-5.29	115.97	122.75
1	H	286	PRO	C-N-CA	-5.29	115.97	122.75
1	E	310	PRO	CA-C-O	-5.29	115.13	121.48
1	I	240	ASP	CA-C-N	5.29	125.10	119.28
1	I	240	ASP	C-N-CA	5.29	125.10	119.28
1	M	22	VAL	N-CA-C	5.29	117.48	108.86
1	B	387	ASP	N-CA-C	5.29	117.46	111.11
1	K	129	THR	N-CA-C	-5.29	106.69	112.72
1	B	374	GLN	N-CA-C	5.29	118.36	109.95
1	M	238	SER	N-CA-C	-5.29	106.34	112.89
1	A	52	VAL	O-C-N	5.28	125.78	120.92
1	J	306	LEU	CA-C-O	-5.28	113.42	119.60
1	B	202	ASP	CB-CA-C	-5.28	102.34	110.26
1	N	453	LYS	N-CA-C	-5.28	105.69	111.82
1	J	356	TYR	N-CA-C	5.28	117.35	109.59
1	G	320	ASN	N-CA-C	-5.27	100.57	108.96
1	A	352	VAL	CA-C-N	5.27	125.27	119.89
1	A	352	VAL	C-N-CA	5.27	125.27	119.89
1	G	141	GLU	CA-C-N	5.27	131.60	121.54
1	G	141	GLU	C-N-CA	5.27	131.60	121.54
1	D	52	VAL	CA-C-N	5.27	126.42	119.84
1	D	52	VAL	C-N-CA	5.27	126.42	119.84
1	H	208	MET	N-CA-C	5.26	115.08	108.45
1	I	71	ARG	CA-C-N	-5.26	116.08	123.13
1	I	71	ARG	C-N-CA	-5.26	116.08	123.13
1	E	118	SER	N-CA-C	-5.26	100.12	109.06
1	F	450	VAL	N-CA-C	5.26	115.16	107.37
1	J	64	LYS	CA-C-N	-5.26	116.08	123.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	64	LYS	C-N-CA	-5.26	116.08	123.13
1	B	282	MET	N-CA-C	-5.26	105.72	111.82
1	C	224	ILE	N-CA-C	-5.25	108.01	113.10
1	M	144	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	F	370	GLU	CA-C-O	5.25	126.00	120.33
1	M	71	ARG	N-CA-C	-5.25	100.17	108.73
1	N	50	PHE	N-CA-C	5.25	116.82	108.79
1	J	365	SER	CA-C-N	-5.24	114.23	122.73
1	J	365	SER	C-N-CA	-5.24	114.23	122.73
1	J	396	ASN	CB-CA-C	-5.24	104.93	111.43
1	A	60	GLN	N-CA-CB	5.24	119.35	110.49
1	L	58	ASN	N-CA-C	5.24	116.87	107.80
1	I	301	THR	N-CA-C	5.24	117.15	109.24
1	A	202	ASP	CA-C-N	-5.24	113.90	122.54
1	A	202	ASP	C-N-CA	-5.24	113.90	122.54
1	D	240	ASP	CA-C-N	5.24	125.29	119.32
1	D	240	ASP	C-N-CA	5.24	125.29	119.32
1	A	390	SER	N-CA-C	-5.23	105.76	111.82
1	A	141	GLU	CA-C-N	-5.22	114.63	122.47
1	A	141	GLU	C-N-CA	-5.22	114.63	122.47
1	K	85	LEU	CB-CG-CD1	-5.22	95.03	110.70
1	O	279	GLY	N-CA-C	-5.22	100.81	113.18
1	A	231	TYR	CA-C-N	5.21	125.22	119.90
1	A	231	TYR	C-N-CA	5.21	125.22	119.90
1	D	445	LEU	N-CA-C	5.21	118.20	110.48
1	F	160	GLY	CA-C-N	-5.21	114.16	122.66
1	F	160	GLY	C-N-CA	-5.21	114.16	122.66
1	O	165	ILE	CA-C-N	-5.21	117.83	122.47
1	O	165	ILE	C-N-CA	-5.21	117.83	122.47
1	A	262	ASN	N-CA-CB	-5.21	102.50	110.42
1	F	51	ARG	CA-C-N	-5.21	116.91	122.85
1	F	51	ARG	C-N-CA	-5.21	116.91	122.85
1	F	387	ASP	CA-C-N	-5.21	113.88	120.60
1	F	387	ASP	C-N-CA	-5.21	113.88	120.60
1	E	47	ASP	N-CA-C	-5.20	103.51	110.07
1	E	71	ARG	CA-C-N	-5.20	116.16	123.13
1	E	71	ARG	C-N-CA	-5.20	116.16	123.13
1	L	201	VAL	CB-CA-C	-5.20	102.76	111.29
1	C	352	VAL	CB-CA-C	-5.20	101.90	111.36
1	J	67	ALA	N-CA-C	-5.19	106.45	112.89
1	H	22	VAL	N-CA-C	5.19	117.32	108.86
1	L	155	GLN	CB-CA-C	-5.19	102.66	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	41	ARG	NE-CZ-NH1	-5.19	116.31	121.50
1	L	325	TRP	N-CA-C	-5.19	102.00	110.20
1	B	461	ASP	N-CA-CB	-5.19	101.73	110.49
1	I	92	ASN	CA-C-N	5.19	126.32	119.84
1	I	92	ASN	C-N-CA	5.19	126.32	119.84
1	D	235	LEU	N-CA-C	5.18	116.74	111.14
1	J	58	ASN	N-CA-C	5.18	116.84	108.34
1	G	160	GLY	CA-C-N	-5.18	114.93	122.86
1	G	160	GLY	C-N-CA	-5.18	114.93	122.86
1	H	33	ILE	CA-C-N	-5.18	115.17	122.94
1	H	33	ILE	C-N-CA	-5.18	115.17	122.94
1	E	152	LYS	N-CA-C	-5.17	103.70	110.53
1	K	446	LYS	N-CA-C	5.17	117.98	109.76
1	A	140	SER	CA-C-N	-5.17	111.67	121.54
1	A	140	SER	C-N-CA	-5.17	111.67	121.54
1	I	228	ILE	N-CA-C	5.17	115.29	107.80
1	I	366	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	E	160	GLY	CA-C-O	-5.17	116.56	121.62
1	O	290	VAL	CA-C-N	-5.16	114.56	122.87
1	O	290	VAL	C-N-CA	-5.16	114.56	122.87
1	B	342	LEU	N-CA-C	-5.16	102.11	110.32
1	H	175	SER	CA-C-O	5.16	126.82	121.15
1	I	471	VAL	CB-CA-C	-5.16	105.36	111.81
1	D	108	GLY	O-C-N	-5.16	119.53	123.35
1	D	74	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	D	365	SER	N-CA-CB	-5.15	102.61	110.65
1	G	195	LEU	CA-C-N	-5.15	113.85	122.92
1	G	195	LEU	C-N-CA	-5.15	113.85	122.92
1	J	74	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	J	262	ASN	CA-C-N	-5.15	115.89	123.00
1	J	262	ASN	C-N-CA	-5.15	115.89	123.00
1	N	191	LYS	CG-CD-CE	-5.15	99.45	111.30
1	I	226	GLN	CB-CA-C	-5.14	102.66	111.46
1	C	276	TYR	N-CA-C	5.14	115.32	108.38
1	J	275	LEU	CD1-CG-CD2	-5.14	99.48	110.80
1	D	110	GLY	O-C-N	-5.14	116.02	122.70
1	B	324	CYS	CB-CA-C	-5.13	104.02	112.03
1	H	307	PHE	N-CA-C	5.13	118.32	110.36
1	A	62	ILE	N-CA-CB	-5.13	106.93	112.37
1	N	307	PHE	N-CA-C	5.13	117.81	109.86
1	K	177	SER	N-CA-C	5.13	117.54	111.33
1	K	216	THR	CB-CA-C	-5.13	102.61	110.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	LEU	N-CA-C	5.12	118.69	112.23
1	F	330	PHE	CA-C-N	-5.12	116.04	123.11
1	F	330	PHE	C-N-CA	-5.12	116.04	123.11
1	B	79	ASP	CA-C-O	5.12	124.21	119.24
1	C	105	VAL	CB-CA-C	-5.12	101.64	110.30
1	C	394	SER	N-CA-C	-5.12	105.61	111.14
1	N	289	CYS	CA-CB-SG	-5.12	102.63	114.40
1	E	190	LEU	CA-C-N	-5.12	115.94	123.00
1	E	190	LEU	C-N-CA	-5.12	115.94	123.00
1	K	294	SER	CA-C-N	-5.11	115.46	120.52
1	K	294	SER	C-N-CA	-5.11	115.46	120.52
1	K	467	ARG	N-CA-C	-5.11	105.62	111.14
1	M	31	THR	N-CA-C	-5.11	102.01	109.63
1	A	175	SER	CA-C-N	5.11	127.39	120.44
1	A	175	SER	C-N-CA	5.11	127.39	120.44
1	M	26	ASP	N-CA-C	5.11	119.23	112.89
1	O	271	VAL	CA-C-N	5.11	125.10	119.89
1	O	271	VAL	C-N-CA	5.11	125.10	119.89
1	M	240	ASP	CA-C-N	5.11	124.61	119.19
1	M	240	ASP	C-N-CA	5.11	124.61	119.19
1	J	343	THR	N-CA-C	-5.11	100.92	109.24
1	N	338	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	O	462	GLN	N-CA-C	5.11	119.14	113.01
1	C	208	MET	N-CA-C	5.10	116.56	108.96
1	K	201	VAL	CB-CA-C	-5.10	102.92	111.29
1	K	350	SER	O-C-N	5.10	123.79	120.27
1	D	238	SER	N-CA-C	-5.10	105.80	111.36
1	J	400	LEU	N-CA-C	-5.10	106.57	112.89
1	K	52	VAL	CB-CA-C	-5.10	105.32	111.18
1	L	299	ILE	CA-C-N	-5.09	116.87	123.19
1	L	299	ILE	C-N-CA	-5.09	116.87	123.19
1	G	331	VAL	CA-C-N	-5.09	115.01	122.19
1	G	331	VAL	C-N-CA	-5.09	115.01	122.19
1	L	248	PHE	N-CA-C	-5.09	99.95	110.80
1	B	329	LEU	CB-CG-CD2	-5.09	95.43	110.70
1	J	312	TRP	CA-C-N	-5.09	116.22	122.84
1	J	312	TRP	C-N-CA	-5.09	116.22	122.84
1	O	210	PHE	N-CA-C	5.09	118.27	111.75
1	B	141	GLU	CA-C-O	-5.09	113.23	120.51
1	H	264	ALA	N-CA-C	-5.09	103.33	110.50
1	N	451	ASP	CA-C-N	-5.08	114.50	122.79
1	N	451	ASP	C-N-CA	-5.08	114.50	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	300	VAL	N-CA-C	-5.08	101.06	108.17
1	D	467	ARG	N-CA-C	-5.08	105.66	111.14
1	K	130	GLU	N-CA-C	-5.08	105.39	112.45
1	H	310	PRO	CA-C-O	-5.08	115.74	121.98
1	N	41	ARG	NE-CZ-NH2	5.07	123.77	119.20
1	C	63	PRO	CB-CA-C	-5.07	103.19	111.56
1	B	158	ILE	CB-CA-C	-5.07	102.93	110.33
1	K	47	ASP	CA-C-O	5.07	124.45	120.19
1	O	100	TRP	O-C-N	-5.07	117.30	123.13
1	D	271	VAL	CA-C-N	5.07	125.07	119.90
1	D	271	VAL	C-N-CA	5.07	125.07	119.90
1	C	90	ILE	N-CA-C	-5.07	105.21	112.35
1	L	158	ILE	N-CA-C	5.07	115.56	108.17
1	K	265	GLY	N-CA-C	-5.06	106.48	111.85
1	G	32	SER	CA-C-N	-5.06	116.54	123.12
1	G	32	SER	C-N-CA	-5.06	116.54	123.12
1	C	338	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	K	217	LYS	N-CA-C	-5.05	105.97	113.40
1	A	190	LEU	CA-C-O	-5.05	114.93	120.69
1	K	216	THR	N-CA-C	5.05	117.17	111.11
1	K	221	PRO	CA-C-N	5.05	127.30	120.38
1	K	221	PRO	C-N-CA	5.05	127.30	120.38
1	I	340	THR	CA-C-N	-5.05	116.05	122.77
1	I	340	THR	C-N-CA	-5.05	116.05	122.77
1	C	60	GLN	N-CA-C	5.04	121.54	110.80
1	M	58	ASN	N-CA-C	5.04	116.99	108.02
1	H	365	SER	CA-C-N	-5.04	115.38	122.94
1	H	365	SER	C-N-CA	-5.04	115.38	122.94
1	H	467	ARG	N-CA-C	-5.04	105.70	111.14
1	M	390	SER	O-C-N	5.04	128.46	122.27
1	F	334	VAL	N-CA-C	-5.03	100.87	108.12
1	F	463	TYR	N-CA-C	5.03	117.78	109.58
1	L	47	ASP	CA-C-N	5.03	124.64	119.56
1	L	47	ASP	C-N-CA	5.03	124.64	119.56
1	F	344	ILE	CA-C-N	-5.03	115.89	122.99
1	F	344	ILE	C-N-CA	-5.03	115.89	122.99
1	K	318	GLY	CA-C-O	-5.03	116.64	121.92
1	C	85	LEU	CA-C-N	5.03	125.10	119.87
1	C	85	LEU	C-N-CA	5.03	125.10	119.87
1	H	179	PRO	CA-C-N	-5.03	115.68	122.77
1	H	179	PRO	C-N-CA	-5.03	115.68	122.77
1	K	144	ARG	N-CA-C	-5.03	102.25	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	324	CYS	CB-CA-C	-5.03	104.41	112.05
1	D	54	ALA	CA-C-N	-5.03	111.56	121.41
1	D	54	ALA	C-N-CA	-5.03	111.56	121.41
1	F	114	GLY	CA-C-N	-5.03	114.28	122.57
1	F	114	GLY	C-N-CA	-5.03	114.28	122.57
1	J	356	TYR	CA-C-O	5.03	126.41	120.58
1	H	180	LEU	CA-C-N	-5.02	113.92	120.95
1	H	180	LEU	C-N-CA	-5.02	113.92	120.95
1	J	61	ASP	N-CA-C	5.02	117.32	110.24
1	J	370	GLU	O-C-N	-5.02	117.39	123.27
1	F	225	CYS	N-CA-CB	-5.02	102.00	110.49
1	A	392	ILE	N-CA-C	-5.02	105.01	112.04
1	D	47	ASP	N-CA-C	-5.02	103.71	109.93
1	H	112	PRO	CA-C-O	-5.02	115.90	122.12
1	N	62	ILE	CA-C-N	5.02	125.29	119.92
1	N	62	ILE	C-N-CA	5.02	125.29	119.92
1	F	71	ARG	NE-CZ-NH1	-5.02	116.48	121.50
1	C	213	LEU	CD1-CG-CD2	-5.02	99.76	110.80
1	E	471	VAL	CB-CA-C	-5.02	105.54	111.81
1	J	255	LEU	CA-C-O	-5.01	115.91	121.28
1	O	71	ARG	N-CA-C	-5.01	100.35	108.52
1	D	56	GLY	O-C-N	5.01	127.55	122.24
1	E	29	THR	CB-CA-C	-5.01	101.26	109.53
1	J	260	PHE	CA-C-N	-5.01	114.73	122.59
1	J	260	PHE	C-N-CA	-5.01	114.73	122.59
1	K	283	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	L	290	VAL	N-CA-C	-5.01	99.96	107.37
1	F	117	LEU	N-CA-C	5.01	117.93	110.52
1	G	255	LEU	CA-C-O	-5.01	115.65	121.26
1	I	173	THR	N-CA-CB	5.00	117.35	109.69
1	H	235	LEU	N-CA-C	-5.00	105.74	111.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	53	PRO	Peptide

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	3323	0	3192	200	1
1	B	3323	0	3192	184	0
1	C	3323	0	3192	157	1
1	D	3323	0	3192	159	0
1	E	3323	0	3192	173	0
1	F	3323	0	3192	207	0
1	G	3323	0	3192	216	0
1	H	3323	0	3192	211	0
1	I	3323	0	3192	181	0
1	J	3323	0	3192	171	0
1	K	3323	0	3192	164	0
1	L	3323	0	3192	183	0
1	M	3323	0	3192	168	0
1	N	3323	0	3192	179	0
1	O	3323	0	3192	168	0
All	All	49845	0	47880	2464	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 25.

All (2464) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:446:LYS:CG	1:J:446:LYS:CD	1.75	1.63
1:B:141:GLU:CB	1:B:141:GLU:CG	1.75	1.63
1:C:191:LYS:CE	1:C:191:LYS:CD	1.76	1.62
1:L:360:LYS:CD	1:L:360:LYS:CE	1.78	1.61
1:F:465:LEU:CG	1:F:465:LEU:CD1	1.74	1.61
1:D:315:LYS:CG	1:D:315:LYS:CD	1.78	1.60
1:M:446:LYS:CD	1:M:446:LYS:CG	1.76	1.59
1:G:64:LYS:CD	1:G:64:LYS:CE	1.80	1.59
1:M:191:LYS:CD	1:M:191:LYS:CE	1.76	1.59
1:E:446:LYS:CE	1:E:446:LYS:CD	1.78	1.57
1:B:90:ILE:CD1	1:B:90:ILE:CG1	1.75	1.57
1:J:171:LYS:NZ	1:J:171:LYS:CE	1.68	1.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:453:LYS:CG	1:L:453:LYS:CD	1.80	1.56
1:G:315:LYS:CD	1:G:315:LYS:CE	1.79	1.56
1:G:82:LYS:NZ	1:G:82:LYS:CE	1.69	1.54
1:H:82:LYS:NZ	1:H:82:LYS:CE	1.69	1.53
1:L:453:LYS:NZ	1:L:453:LYS:CE	1.68	1.53
1:L:278:LYS:NZ	1:L:278:LYS:CE	1.68	1.53
1:L:453:LYS:CD	1:L:453:LYS:CE	1.84	1.53
1:E:309:LYS:NZ	1:E:309:LYS:CE	1.68	1.51
1:C:453:LYS:NZ	1:C:453:LYS:CE	1.72	1.50
1:D:191:LYS:NZ	1:D:191:LYS:CE	1.74	1.49
1:I:360:LYS:NZ	1:I:360:LYS:CE	1.68	1.49
1:J:125:LYS:NZ	1:J:125:LYS:CE	1.71	1.49
1:D:353:PRO:CB	1:D:353:PRO:CG	1.80	1.48
1:O:315:LYS:NZ	1:O:315:LYS:CE	1.75	1.48
1:A:267:MET:CE	1:A:267:MET:SD	2.02	1.48
1:B:138:ASN:ND2	1:B:140:SER:HB3	1.28	1.45
1:M:282:MET:CE	1:M:282:MET:SD	2.04	1.45
1:G:58:ASN:HB2	1:H:178:ARG:NH1	1.11	1.39
1:D:439:LYS:NZ	1:D:439:LYS:CE	1.89	1.35
1:A:57:GLY:HA3	1:B:184:ASP:OD2	1.29	1.29
1:B:138:ASN:HD21	1:B:140:SER:CB	1.48	1.24
1:L:353:PRO:CD	1:L:360:LYS:HZ2	1.49	1.24
1:G:58:ASN:CB	1:H:178:ARG:HH12	1.52	1.22
1:L:353:PRO:HD2	1:L:360:LYS:NZ	1.56	1.20
1:F:181:SER:HB2	1:M:89:SER:HB2	1.17	1.16
1:A:353:PRO:HD2	1:A:360:LYS:HZ2	1.11	1.16
1:F:384:LEU:HB3	1:F:389:MET:HE2	1.20	1.15
1:G:58:ASN:CB	1:H:178:ARG:NH1	2.05	1.14
1:A:57:GLY:CA	1:B:184:ASP:OD2	1.94	1.14
1:N:353:PRO:HG2	1:N:360:LYS:HZ2	1.05	1.13
1:H:273:GLN:HE22	1:H:278:LYS:HE2	1.00	1.12
1:N:384:LEU:HB3	1:N:389:MET:HE2	1.27	1.10
1:B:273:GLN:HE22	1:B:278:LYS:HE2	1.09	1.09
1:M:273:GLN:HE22	1:M:278:LYS:HE2	1.05	1.09
1:A:282:MET:HG2	1:G:89:SER:HB2	1.27	1.09
1:J:384:LEU:HB3	1:J:389:MET:HE2	1.30	1.09
1:L:121:PRO:HG3	1:M:289:CYS:SG	1.93	1.08
1:H:353:PRO:HD2	1:H:360:LYS:HZ2	1.13	1.08
1:H:141:GLU:HG2	1:H:142:ASP:N	1.68	1.07
1:L:273:GLN:HE22	1:L:278:LYS:HE2	1.07	1.07
1:C:273:GLN:HE22	1:C:278:LYS:HE2	1.12	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:353:PRO:CD	1:E:360:LYS:HZ2	1.68	1.07
1:G:353:PRO:HD2	1:G:360:LYS:HZ2	0.94	1.06
1:J:273:GLN:HE22	1:J:278:LYS:HE2	1.19	1.06
1:D:475:LEU:HD23	1:D:475:LEU:H	1.20	1.05
1:G:353:PRO:HD2	1:G:360:LYS:NZ	1.71	1.05
1:E:353:PRO:HD2	1:E:360:LYS:NZ	1.69	1.05
1:N:475:LEU:H	1:N:475:LEU:HD23	1.16	1.05
1:B:353:PRO:HG2	1:B:360:LYS:HZ2	1.14	1.05
1:H:141:GLU:CG	1:H:142:ASP:N	2.18	1.04
1:H:353:PRO:HD2	1:H:360:LYS:NZ	1.71	1.04
1:H:121:PRO:HG3	1:I:289:CYS:SG	1.97	1.04
1:H:51:ARG:NH1	1:H:61:ASP:OD2	1.92	1.03
1:N:273:GLN:HE22	1:N:278:LYS:HE2	1.18	1.03
1:G:353:PRO:CD	1:G:360:LYS:HZ2	1.72	1.02
1:F:353:PRO:HG2	1:F:360:LYS:HZ2	1.25	1.01
1:E:353:PRO:HD2	1:E:360:LYS:HZ2	0.88	1.01
1:O:353:PRO:HD2	1:O:360:LYS:HZ2	1.20	1.00
1:L:273:GLN:NE2	1:L:278:LYS:HE2	1.76	1.00
1:H:384:LEU:HB3	1:H:389:MET:HE2	1.44	1.00
1:A:216:THR:HG22	1:A:218:CYS:HB2	1.44	0.99
1:H:273:GLN:NE2	1:H:278:LYS:HE2	1.76	0.99
1:K:353:PRO:HD2	1:K:360:LYS:HZ1	1.24	0.99
1:D:384:LEU:HB3	1:D:389:MET:HE2	1.42	0.99
1:H:141:GLU:HG2	1:H:142:ASP:H	1.24	0.99
1:F:273:GLN:HE22	1:F:278:LYS:HE2	1.24	0.99
1:A:353:PRO:HG2	1:A:360:LYS:HZ3	1.27	0.97
1:K:384:LEU:HB3	1:K:389:MET:HE2	1.43	0.97
1:C:384:LEU:HB3	1:C:389:MET:HE2	1.45	0.97
1:A:273:GLN:HE22	1:A:278:LYS:HE2	1.30	0.96
1:I:136:THR:O	1:I:137:SER:O	1.83	0.96
1:N:111:GLN:HB3	1:N:112:PRO:HD2	1.44	0.96
1:L:353:PRO:CD	1:L:360:LYS:NZ	2.23	0.95
1:G:58:ASN:HB2	1:H:178:ARG:HH11	1.32	0.94
1:F:289:CYS:SG	1:J:121:PRO:HG3	2.08	0.94
1:N:353:PRO:HG2	1:N:360:LYS:NZ	1.80	0.94
1:A:289:CYS:SG	1:E:121:PRO:HG3	2.07	0.94
1:M:126:LEU:HB3	1:M:262:ASN:HB3	1.48	0.94
1:L:353:PRO:HD2	1:L:360:LYS:HZ2	0.78	0.94
1:I:353:PRO:HD2	1:I:360:LYS:HZ2	1.32	0.94
1:L:126:LEU:HB3	1:L:262:ASN:HB3	1.51	0.93
1:I:353:PRO:HD2	1:I:360:LYS:NZ	1.84	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:PRO:HD2	1:A:360:LYS:NZ	1.86	0.91
1:F:181:SER:CB	1:M:89:SER:HB2	1.99	0.91
1:G:353:PRO:HG2	1:G:360:LYS:HZ3	1.34	0.91
1:B:121:PRO:HG3	1:C:289:CYS:SG	2.11	0.90
1:L:111:GLN:HB3	1:L:112:PRO:HD2	1.52	0.90
1:F:475:LEU:H	1:F:475:LEU:HD23	1.35	0.90
1:D:273:GLN:HE22	1:D:278:LYS:HE2	1.35	0.90
1:K:475:LEU:HD23	1:K:475:LEU:H	1.37	0.90
1:O:329:LEU:HD23	1:O:329:LEU:C	1.98	0.89
1:E:273:GLN:HE22	1:E:278:LYS:HE2	1.36	0.89
1:H:350:SER:HB3	1:H:351:PRO:HD3	1.55	0.89
1:O:143:VAL:O	1:O:143:VAL:HG12	1.73	0.88
1:E:138:ASN:HD22	1:E:140:SER:HB3	1.38	0.88
1:I:273:GLN:HE22	1:I:278:LYS:HE2	1.37	0.88
1:D:45:VAL:HG12	1:D:368:VAL:HG22	1.52	0.88
1:K:353:PRO:HD2	1:K:360:LYS:NZ	1.88	0.87
1:K:273:GLN:HE22	1:K:278:LYS:HE2	1.38	0.87
1:M:273:GLN:NE2	1:M:278:LYS:HE2	1.89	0.87
1:O:353:PRO:HD2	1:O:360:LYS:NZ	1.88	0.87
1:A:353:PRO:CD	1:A:360:LYS:HZ2	1.87	0.87
1:D:121:PRO:HG3	1:E:289:CYS:SG	2.14	0.87
1:O:70:TYR:OH	1:O:232:PRO:HD3	1.75	0.87
1:E:384:LEU:HB3	1:E:389:MET:HE2	1.54	0.87
1:J:247:PHE:CE2	1:J:322:GLY:HA2	2.10	0.86
1:I:344:ILE:HD11	1:J:188:LEU:HD11	1.56	0.86
1:H:353:PRO:HG2	1:H:360:LYS:HZ3	1.37	0.86
1:E:111:GLN:HB3	1:E:112:PRO:HD2	1.56	0.85
1:F:384:LEU:CB	1:F:389:MET:HE2	2.06	0.85
1:E:353:PRO:HG2	1:E:360:LYS:HZ3	1.39	0.85
1:B:273:GLN:NE2	1:B:278:LYS:HE2	1.91	0.85
1:G:353:PRO:CD	1:G:360:LYS:NZ	2.36	0.85
1:M:313:LEU:H	1:M:313:LEU:HD23	1.40	0.84
1:F:111:GLN:HB3	1:F:112:PRO:HD2	1.58	0.84
1:O:138:ASN:HD22	1:O:140:SER:HB3	1.43	0.84
1:A:324:CYS:HB3	1:A:328:GLN:O	1.77	0.83
1:F:126:LEU:HB3	1:F:262:ASN:HB3	1.59	0.83
1:N:353:PRO:CG	1:N:360:LYS:HZ2	1.90	0.83
1:G:368:VAL:HG11	1:H:169:TRP:CZ2	2.14	0.83
1:B:364:TYR:CD2	1:C:185:CYS:HB2	2.14	0.83
1:G:388:VAL:O	1:G:392:ILE:HG13	1.79	0.83
1:M:105:VAL:HG21	1:M:159:LEU:HD11	1.59	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:GLN:NE2	1:C:278:LYS:HE2	1.92	0.83
1:B:353:PRO:CG	1:B:360:LYS:HZ2	1.92	0.82
1:C:350:SER:HB3	1:C:351:PRO:HD3	1.61	0.82
1:H:353:PRO:CD	1:H:360:LYS:NZ	2.42	0.82
1:F:313:LEU:HD23	1:F:313:LEU:H	1.43	0.82
1:L:353:PRO:HG2	1:L:360:LYS:HZ3	1.44	0.82
1:E:475:LEU:HD23	1:E:475:LEU:H	1.44	0.82
1:G:350:SER:HB3	1:G:351:PRO:HD3	1.61	0.81
1:O:315:LYS:NZ	1:O:315:LYS:CD	2.43	0.81
1:G:111:GLN:HB3	1:G:112:PRO:HD2	1.62	0.81
1:J:138:ASN:HD22	1:J:140:SER:HB3	1.45	0.81
1:A:51:ARG:NH1	1:A:61:ASP:OD2	2.14	0.81
1:G:105:VAL:HG21	1:G:159:LEU:HD11	1.62	0.81
1:J:171:LYS:NZ	1:J:171:LYS:CD	2.43	0.81
1:H:141:GLU:HG2	1:H:142:ASP:HB2	1.59	0.81
1:C:105:VAL:HG21	1:C:159:LEU:HD11	1.61	0.80
1:D:105:VAL:HG21	1:D:159:LEU:HD11	1.63	0.80
1:J:99:VAL:HG21	1:J:382:ILE:HD11	1.64	0.80
1:B:141:GLU:CG	1:B:141:GLU:CA	2.58	0.80
1:B:344:ILE:HD11	1:C:188:LEU:HD11	1.64	0.80
1:H:307:PHE:HE1	1:H:335:ASP:HB2	1.46	0.80
1:H:159:LEU:CD2	1:H:331:VAL:HG22	2.11	0.80
1:K:121:PRO:HG3	1:L:289:CYS:SG	2.22	0.80
1:N:368:VAL:HG11	1:O:169:TRP:CZ2	2.16	0.80
1:A:282:MET:HG2	1:G:89:SER:CB	2.09	0.80
1:E:353:PRO:CD	1:E:360:LYS:NZ	2.37	0.80
1:F:105:VAL:HG21	1:F:159:LEU:HD11	1.62	0.80
1:H:45:VAL:HG12	1:H:368:VAL:HG22	1.64	0.80
1:E:345:CYS:HB3	1:E:363:GLN:NE2	1.96	0.80
1:F:141:GLU:HG2	1:F:141:GLU:O	1.81	0.80
1:K:353:PRO:HG2	1:K:360:LYS:HZ2	1.46	0.80
1:O:475:LEU:HD23	1:O:475:LEU:H	1.47	0.80
1:B:353:PRO:HG2	1:B:360:LYS:NZ	1.95	0.80
1:N:353:PRO:CG	1:N:360:LYS:NZ	2.45	0.80
1:E:45:VAL:HG12	1:E:368:VAL:HG22	1.63	0.79
1:A:121:PRO:HG3	1:B:289:CYS:SG	2.23	0.79
1:E:216:THR:O	1:E:217:LYS:HB2	1.82	0.79
1:H:345:CYS:HB3	1:H:363:GLN:NE2	1.97	0.79
1:L:105:VAL:HG12	1:L:106:GLU:N	1.97	0.79
1:N:353:PRO:HD2	1:N:360:LYS:HZ1	1.47	0.79
1:F:121:PRO:HG3	1:G:289:CYS:SG	2.22	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:ASN:ND2	1:E:140:SER:HB3	1.98	0.79
1:I:111:GLN:HB3	1:I:112:PRO:HD2	1.63	0.79
1:L:453:LYS:CG	1:L:453:LYS:CE	2.60	0.79
1:A:216:THR:CG2	1:A:218:CYS:HB2	2.12	0.79
1:H:246:MET:O	1:H:246:MET:HG3	1.83	0.79
1:J:111:GLN:HB3	1:J:112:PRO:HD2	1.64	0.78
1:M:111:GLN:HB3	1:M:112:PRO:HD2	1.63	0.78
1:O:345:CYS:HB3	1:O:363:GLN:NE2	1.98	0.78
1:A:313:LEU:HD23	1:A:313:LEU:H	1.49	0.78
1:A:345:CYS:HB3	1:A:363:GLN:NE2	1.97	0.78
1:C:368:VAL:HG12	1:C:369:GLU:N	1.99	0.78
1:C:111:GLN:HB3	1:C:112:PRO:HD2	1.64	0.78
1:F:307:PHE:HE1	1:F:335:ASP:HB2	1.46	0.78
1:C:475:LEU:HD23	1:C:475:LEU:H	1.49	0.78
1:E:273:GLN:NE2	1:E:278:LYS:HE2	1.97	0.78
1:I:246:MET:HG3	1:I:246:MET:O	1.83	0.78
1:F:181:SER:HB2	1:M:89:SER:CB	2.09	0.78
1:H:51:ARG:O	1:H:53:PRO:HD3	1.83	0.78
1:K:87:ASP:O	1:K:90:ILE:HG12	1.83	0.78
1:F:345:CYS:HB3	1:F:363:GLN:NE2	1.99	0.78
1:G:70:TYR:OH	1:G:232:PRO:HD3	1.84	0.78
1:N:345:CYS:HB3	1:N:363:GLN:NE2	1.98	0.78
1:G:300:VAL:CG1	1:H:255:LEU:HD13	2.14	0.77
1:H:353:PRO:CG	1:H:360:LYS:HZ3	1.96	0.77
1:G:121:PRO:HG3	1:H:289:CYS:SG	2.24	0.77
1:D:151:TYR:CG	1:D:203:THR:HB	2.19	0.77
1:K:105:VAL:HG21	1:K:159:LEU:HD11	1.65	0.77
1:N:353:PRO:CD	1:N:360:LYS:HZ1	1.97	0.77
1:E:126:LEU:HB3	1:E:262:ASN:HB3	1.67	0.76
1:G:214:GLN:OE1	1:G:219:GLU:HB2	1.86	0.76
1:A:111:GLN:HB3	1:A:112:PRO:HD2	1.67	0.76
1:A:353:PRO:CD	1:A:360:LYS:NZ	2.46	0.76
1:G:78:PRO:HD3	1:G:453:LYS:HA	1.67	0.76
1:O:353:PRO:CD	1:O:360:LYS:HZ2	1.98	0.76
1:G:140:SER:O	1:G:141:GLU:HB2	1.85	0.75
1:K:353:PRO:CD	1:K:360:LYS:HZ1	1.99	0.75
1:G:368:VAL:HG11	1:H:169:TRP:HZ2	1.51	0.75
1:I:324:CYS:HB3	1:I:328:GLN:O	1.87	0.75
1:J:273:GLN:NE2	1:J:278:LYS:HE2	2.00	0.75
1:N:99:VAL:HG21	1:N:382:ILE:HD11	1.68	0.75
1:B:45:VAL:HG12	1:B:368:VAL:HG22	1.67	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:LEU:HB3	1:B:262:ASN:HB3	1.67	0.75
1:B:247:PHE:CE2	1:B:322:GLY:HA2	2.20	0.75
1:D:313:LEU:HD23	1:D:313:LEU:H	1.51	0.75
1:I:105:VAL:HG21	1:I:159:LEU:HD11	1.67	0.75
1:E:247:PHE:CE2	1:E:322:GLY:HA2	2.21	0.75
1:I:273:GLN:NE2	1:I:278:LYS:HE2	2.02	0.75
1:N:111:GLN:HB3	1:N:112:PRO:CD	2.15	0.75
1:O:85:LEU:HB3	1:O:86:PRO:HD2	1.69	0.75
1:H:54:ALA:HB2	1:H:61:ASP:HB2	1.67	0.74
1:O:109:ARG:H	1:O:308:ASN:HD21	1.34	0.74
1:B:105:VAL:HG21	1:B:159:LEU:HD11	1.69	0.74
1:C:45:VAL:HG12	1:C:368:VAL:HG22	1.67	0.74
1:B:105:VAL:HG12	1:B:106:GLU:N	2.00	0.74
1:C:126:LEU:HB3	1:C:262:ASN:HB3	1.69	0.74
1:N:273:GLN:NE2	1:N:278:LYS:HE2	1.99	0.74
1:A:475:LEU:HD23	1:A:475:LEU:H	1.52	0.74
1:H:353:PRO:CD	1:H:360:LYS:HZ2	1.96	0.74
1:B:384:LEU:HB3	1:B:389:MET:HE2	1.70	0.74
1:E:200:MET:HE2	1:E:223:ASP:O	1.87	0.74
1:K:368:VAL:HG11	1:L:169:TRP:CZ2	2.23	0.74
1:O:126:LEU:HB3	1:O:262:ASN:HB3	1.69	0.74
1:E:105:VAL:HG12	1:E:106:GLU:N	2.02	0.73
1:I:216:THR:HG22	1:I:218:CYS:HB2	1.69	0.73
1:J:138:ASN:ND2	1:J:140:SER:HB3	2.01	0.73
1:N:353:PRO:HD2	1:N:360:LYS:NZ	2.02	0.73
1:B:329:LEU:HD23	1:B:329:LEU:C	2.13	0.73
1:C:246:MET:HG3	1:C:246:MET:O	1.87	0.73
1:L:453:LYS:CD	1:L:453:LYS:CB	2.65	0.73
1:O:138:ASN:ND2	1:O:140:SER:HB3	2.03	0.73
1:B:368:VAL:HG12	1:B:369:GLU:N	2.03	0.73
1:L:396:ASN:ND2	1:L:398:SER:OG	2.21	0.73
1:M:92:ASN:O	1:M:94:GLU:N	2.20	0.73
1:G:64:LYS:CE	1:G:64:LYS:CG	2.66	0.73
1:N:353:PRO:CD	1:N:360:LYS:NZ	2.51	0.73
1:H:368:VAL:HG11	1:I:169:TRP:CZ2	2.24	0.73
1:L:87:ASP:O	1:L:90:ILE:HG12	1.89	0.73
1:N:105:VAL:HG12	1:N:106:GLU:N	2.04	0.73
1:O:314:HIS:O	1:O:315:LYS:HG3	1.89	0.73
1:I:105:VAL:HG12	1:I:106:GLU:N	2.02	0.73
1:N:384:LEU:HB3	1:N:389:MET:CE	2.13	0.73
1:A:105:VAL:HG21	1:A:159:LEU:HD11	1.71	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:250:LEU:HB3	1:L:306:LEU:HD21	1.71	0.73
1:N:350:SER:HB3	1:N:351:PRO:HD3	1.69	0.73
1:D:273:GLN:NE2	1:D:278:LYS:HE2	2.04	0.72
1:H:46:GLY:HA3	1:H:65:VAL:HG23	1.69	0.72
1:I:475:LEU:HD23	1:I:475:LEU:H	1.54	0.72
1:J:126:LEU:HB3	1:J:262:ASN:HB3	1.71	0.72
1:G:64:LYS:CD	1:G:64:LYS:NZ	2.52	0.72
1:A:353:PRO:CG	1:A:360:LYS:HZ3	2.01	0.72
1:F:353:PRO:HG2	1:F:360:LYS:NZ	2.02	0.72
1:K:369:GLU:HG3	1:K:371:TYR:HE1	1.54	0.72
1:B:216:THR:O	1:B:217:LYS:HB2	1.89	0.72
1:D:368:VAL:HG11	1:E:169:TRP:CZ2	2.23	0.72
1:J:125:LYS:NZ	1:J:125:LYS:CD	2.51	0.72
1:N:114:GLY:HA3	1:N:340:THR:HG23	1.70	0.72
1:D:126:LEU:HB3	1:D:262:ASN:HB3	1.71	0.72
1:F:273:GLN:NE2	1:F:278:LYS:HE2	2.01	0.72
1:H:307:PHE:CE1	1:H:335:ASP:HB2	2.23	0.72
1:L:307:PHE:HA	1:L:311:TYR:OH	1.90	0.72
1:A:273:GLN:NE2	1:A:278:LYS:HE2	2.02	0.72
1:F:114:GLY:HA3	1:F:340:THR:HG23	1.71	0.72
1:A:368:VAL:HG11	1:B:169:TRP:CZ2	2.25	0.72
1:C:143:VAL:O	1:C:143:VAL:HG12	1.90	0.72
1:F:159:LEU:CD2	1:F:331:VAL:HG22	2.20	0.72
1:N:121:PRO:HG3	1:O:289:CYS:SG	2.29	0.72
1:N:247:PHE:CE2	1:N:322:GLY:HA2	2.24	0.72
1:C:70:TYR:OH	1:C:232:PRO:HD3	1.89	0.72
1:E:151:TYR:CG	1:E:203:THR:HB	2.24	0.72
1:G:24:THR:CG2	1:G:320:ASN:HA	2.20	0.72
1:H:138:ASN:HD22	1:H:140:SER:HB3	1.54	0.72
1:A:59:LYS:HD3	1:B:178:ARG:HG3	1.71	0.72
1:I:353:PRO:HG2	1:I:360:LYS:HZ3	1.54	0.71
1:A:293:PRO:HB3	1:E:117:LEU:HD11	1.71	0.71
1:F:233:ASP:CG	1:F:236:GLN:HB3	2.14	0.71
1:K:289:CYS:SG	1:O:121:PRO:HG3	2.30	0.71
1:C:329:LEU:HD23	1:C:329:LEU:C	2.15	0.71
1:N:344:ILE:HD11	1:O:188:LEU:HD11	1.73	0.71
1:H:313:LEU:HD23	1:H:313:LEU:H	1.55	0.71
1:H:111:GLN:HB3	1:H:112:PRO:HD2	1.72	0.71
1:H:138:ASN:ND2	1:H:140:SER:HB3	2.06	0.71
1:L:453:LYS:CD	1:L:453:LYS:NZ	2.54	0.71
1:D:72:VAL:HG23	1:D:197:ASP:HA	1.71	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:126:LEU:HB3	1:I:262:ASN:HB3	1.73	0.71
1:M:360:LYS:HE2	1:M:361:PHE:CE1	2.25	0.70
1:B:141:GLU:CB	1:B:141:GLU:CD	2.63	0.70
1:D:315:LYS:CD	1:D:315:LYS:CB	2.68	0.70
1:F:307:PHE:CE1	1:F:335:ASP:HB2	2.26	0.70
1:I:70:TYR:OH	1:I:232:PRO:HD3	1.91	0.70
1:J:385:THR:OG1	1:J:388:VAL:HG23	1.91	0.70
1:B:246:MET:HG3	1:B:246:MET:O	1.91	0.70
1:I:141:GLU:HG2	1:I:142:ASP:N	2.05	0.70
1:K:111:GLN:HB3	1:K:112:PRO:HD2	1.74	0.70
1:A:85:LEU:HB3	1:A:86:PRO:HD2	1.73	0.70
1:F:247:PHE:CE2	1:F:322:GLY:HA2	2.26	0.70
1:J:45:VAL:HG12	1:J:368:VAL:HG22	1.72	0.70
1:B:138:ASN:ND2	1:B:140:SER:CB	2.24	0.70
1:G:300:VAL:HG13	1:H:255:LEU:HD13	1.74	0.70
1:G:353:PRO:CG	1:G:360:LYS:HZ3	2.04	0.70
1:K:273:GLN:NE2	1:K:278:LYS:HE2	2.06	0.70
1:L:92:ASN:HD21	1:L:95:THR:HG23	1.57	0.70
1:L:114:GLY:HA3	1:L:340:THR:HG23	1.71	0.70
1:M:325:TRP:O	1:M:326:HIS:HB2	1.90	0.70
1:A:281:GLY:HA3	1:G:89:SER:O	1.92	0.70
1:H:96:GLN:HB3	1:H:383:THR:HA	1.72	0.70
1:K:353:PRO:CD	1:K:360:LYS:NZ	2.54	0.70
1:F:151:TYR:CG	1:F:203:THR:HB	2.27	0.70
1:H:141:GLU:HG2	1:H:142:ASP:CB	2.21	0.70
1:K:105:VAL:HG12	1:K:106:GLU:N	2.06	0.70
1:D:92:ASN:O	1:D:94:GLU:N	2.25	0.69
1:D:233:ASP:CG	1:D:236:GLN:HB3	2.16	0.69
1:H:156:LEU:HG	1:H:334:VAL:HB	1.74	0.69
1:J:475:LEU:HD23	1:J:475:LEU:H	1.55	0.69
1:M:384:LEU:HB3	1:M:389:MET:HE2	1.74	0.69
1:B:107:ILE:O	1:B:107:ILE:HG22	1.92	0.69
1:D:105:VAL:HG12	1:D:106:GLU:N	2.06	0.69
1:D:249:CYS:O	1:D:250:LEU:HD12	1.92	0.69
1:G:151:TYR:CG	1:G:203:THR:HB	2.27	0.69
1:H:87:ASP:O	1:H:90:ILE:HG12	1.92	0.69
1:I:353:PRO:CD	1:I:360:LYS:NZ	2.55	0.69
1:L:126:LEU:HB3	1:L:262:ASN:CB	2.22	0.69
1:O:87:ASP:O	1:O:90:ILE:HG12	1.93	0.69
1:B:350:SER:HB3	1:B:351:PRO:HD3	1.73	0.69
1:G:165:ILE:O	1:G:237:MET:HE2	1.91	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:369:GLU:HG3	1:F:371:TYR:HE1	1.57	0.69
1:H:24:THR:CG2	1:H:320:ASN:HA	2.22	0.69
1:F:214:GLN:OE1	1:F:219:GLU:HB2	1.92	0.69
1:I:368:VAL:HG12	1:I:369:GLU:N	2.07	0.69
1:O:273:GLN:HE22	1:O:278:LYS:HE2	1.57	0.69
1:A:282:MET:CG	1:G:89:SER:HB2	2.17	0.69
1:I:151:TYR:CG	1:I:203:THR:HB	2.28	0.69
1:I:307:PHE:HE1	1:I:335:ASP:HB2	1.57	0.69
1:M:368:VAL:HG11	1:N:169:TRP:CZ2	2.27	0.69
1:M:475:LEU:HD23	1:M:475:LEU:H	1.58	0.69
1:B:111:GLN:HB3	1:B:112:PRO:HD2	1.75	0.69
1:B:151:TYR:CG	1:B:203:THR:HB	2.27	0.69
1:F:233:ASP:OD2	1:J:41:ARG:NH2	2.25	0.69
1:F:253:GLU:HG3	1:J:113:LEU:HD22	1.73	0.69
1:I:121:PRO:HG3	1:J:289:CYS:SG	2.33	0.69
1:A:72:VAL:HG23	1:A:197:ASP:HA	1.75	0.69
1:D:99:VAL:HG21	1:D:382:ILE:HD11	1.74	0.69
1:F:36:HIS:ND1	1:F:37:ALA:N	2.40	0.69
1:L:233:ASP:CG	1:L:236:GLN:HB3	2.17	0.69
1:L:273:GLN:HE22	1:L:278:LYS:CE	1.96	0.69
1:M:151:TYR:CG	1:M:203:THR:HB	2.28	0.69
1:N:156:LEU:HA	1:N:250:LEU:O	1.92	0.69
1:B:99:VAL:HG21	1:B:382:ILE:HD11	1.75	0.68
1:J:85:LEU:HD12	1:J:88:THR:HA	1.73	0.68
1:A:59:LYS:O	1:A:59:LYS:HG2	1.91	0.68
1:G:141:GLU:O	1:G:141:GLU:HG2	1.93	0.68
1:M:126:LEU:HB3	1:M:262:ASN:CB	2.22	0.68
1:M:126:LEU:CB	1:M:262:ASN:HB3	2.21	0.68
1:O:388:VAL:O	1:O:392:ILE:HG13	1.92	0.68
1:I:349:GLN:HG2	1:I:360:LYS:HD2	1.74	0.68
1:G:126:LEU:HB3	1:G:262:ASN:HB3	1.75	0.68
1:J:233:ASP:CG	1:J:236:GLN:HB3	2.17	0.68
1:L:345:CYS:HB3	1:L:363:GLN:NE2	2.08	0.68
1:M:353:PRO:HG2	1:M:360:LYS:HZ3	1.58	0.68
1:N:306:LEU:O	1:N:311:TYR:OH	2.06	0.68
1:H:159:LEU:HD22	1:H:331:VAL:HG22	1.74	0.68
1:H:233:ASP:CG	1:H:236:GLN:HB3	2.19	0.68
1:J:114:GLY:HA3	1:J:340:THR:HG23	1.75	0.68
1:E:87:ASP:HB3	1:E:90:ILE:HD11	1.75	0.68
1:F:122:PHE:O	1:F:218:CYS:HB3	1.94	0.68
1:D:42:LEU:HB3	1:D:448:TRP:CZ2	2.27	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:353:PRO:CG	1:L:360:LYS:NZ	2.56	0.68
1:N:151:TYR:CG	1:N:203:THR:HB	2.28	0.68
1:G:196:GLU:N	1:G:199:ASP:OD2	2.23	0.68
1:H:475:LEU:HD23	1:H:475:LEU:H	1.58	0.68
1:E:159:LEU:HD22	1:E:331:VAL:HG22	1.77	0.67
1:H:258:ARG:NH1	1:I:130:GLU:OE1	2.26	0.67
1:G:233:ASP:CG	1:G:236:GLN:HB3	2.18	0.67
1:G:315:LYS:CD	1:G:315:LYS:NZ	2.56	0.67
1:O:91:TYR:HB2	1:O:96:GLN:HG3	1.76	0.67
1:J:200:MET:HE2	1:J:223:ASP:O	1.94	0.67
1:H:109:ARG:H	1:H:308:ASN:ND2	1.91	0.67
1:M:159:LEU:HD22	1:M:331:VAL:HG22	1.76	0.67
1:C:258:ARG:NH1	1:D:130:GLU:OE1	2.27	0.67
1:N:126:LEU:HB3	1:N:262:ASN:HB3	1.77	0.67
1:J:141:GLU:HG3	1:J:142:ASP:N	2.09	0.67
1:C:138:ASN:HD22	1:C:140:SER:HB3	1.60	0.67
1:L:36:HIS:ND1	1:L:37:ALA:N	2.43	0.67
1:B:345:CYS:HB3	1:B:363:GLN:NE2	2.10	0.67
1:C:105:VAL:HG12	1:C:106:GLU:N	2.10	0.67
1:D:159:LEU:CD2	1:D:331:VAL:HG22	2.25	0.67
1:H:22:VAL:HG12	1:H:23:ASN:N	2.10	0.67
1:H:24:THR:HG23	1:H:320:ASN:HA	1.75	0.67
1:K:310:PRO:HG2	1:K:310:PRO:O	1.93	0.67
1:M:313:LEU:HD23	1:M:313:LEU:N	2.09	0.67
1:E:87:ASP:O	1:E:90:ILE:HG12	1.95	0.66
1:G:220:VAL:HB	1:G:221:PRO:CD	2.25	0.66
1:F:384:LEU:HB3	1:F:389:MET:CE	2.11	0.66
1:J:122:PHE:O	1:J:218:CYS:HB3	1.96	0.66
1:K:233:ASP:CG	1:K:236:GLN:HB3	2.20	0.66
1:K:344:ILE:HD11	1:L:188:LEU:HD11	1.77	0.66
1:E:233:ASP:CG	1:E:236:GLN:HB3	2.20	0.66
1:K:384:LEU:CB	1:K:389:MET:HE2	2.22	0.66
1:N:475:LEU:HD23	1:N:475:LEU:N	2.01	0.66
1:E:143:VAL:HG12	1:E:143:VAL:O	1.95	0.66
1:A:216:THR:O	1:A:217:LYS:HB2	1.94	0.66
1:D:92:ASN:C	1:D:94:GLU:H	2.01	0.66
1:D:356:TYR:HE2	1:E:142:ASP:HA	1.60	0.66
1:J:384:LEU:CB	1:J:389:MET:HE2	2.18	0.66
1:L:85:LEU:HB3	1:L:86:PRO:HD2	1.76	0.66
1:L:105:VAL:HG21	1:L:159:LEU:HD11	1.78	0.66
1:M:345:CYS:HB3	1:M:363:GLN:NE2	2.09	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:369:GLU:HG3	1:N:371:TYR:HE1	1.59	0.66
1:G:249:CYS:O	1:G:250:LEU:HD12	1.96	0.66
1:G:247:PHE:CE2	1:G:322:GLY:HA2	2.30	0.65
1:H:59:LYS:HD3	1:I:178:ARG:HG3	1.76	0.65
1:N:475:LEU:H	1:N:475:LEU:CD2	1.94	0.65
1:A:151:TYR:CG	1:A:203:THR:HB	2.32	0.65
1:F:117:LEU:HD11	1:G:293:PRO:HB3	1.77	0.65
1:L:307:PHE:HE1	1:L:335:ASP:HB2	1.62	0.65
1:M:121:PRO:HG3	1:N:289:CYS:SG	2.37	0.65
1:B:200:MET:HE2	1:B:223:ASP:O	1.96	0.65
1:F:68:TYR:CE2	1:F:151:TYR:HB2	2.32	0.65
1:G:22:VAL:HG12	1:G:23:ASN:N	2.09	0.65
1:G:353:PRO:CG	1:G:360:LYS:NZ	2.60	0.65
1:O:475:LEU:H	1:O:475:LEU:CD2	2.09	0.65
1:A:307:PHE:HA	1:A:311:TYR:OH	1.95	0.65
1:C:355:GLN:HE22	1:H:386:ALA:HB2	1.59	0.65
1:E:45:VAL:CG1	1:E:368:VAL:HG22	2.25	0.65
1:F:200:MET:HE2	1:F:223:ASP:O	1.95	0.65
1:G:324:CYS:HB3	1:G:328:GLN:O	1.96	0.65
1:J:307:PHE:HA	1:J:311:TYR:OH	1.96	0.65
1:A:353:PRO:HG2	1:A:360:LYS:NZ	2.07	0.65
1:A:364:TYR:CD2	1:B:185:CYS:HB2	2.32	0.65
1:C:85:LEU:HB3	1:C:86:PRO:HD2	1.77	0.65
1:J:109:ARG:H	1:J:308:ASN:ND2	1.93	0.65
1:L:66:SER:HB3	1:L:69:GLN:HG2	1.77	0.65
1:B:188:LEU:HD22	1:B:188:LEU:N	2.12	0.65
1:B:307:PHE:HE1	1:B:335:ASP:HB2	1.62	0.65
1:J:151:TYR:CG	1:J:203:THR:HB	2.31	0.65
1:K:185:CYS:HB2	1:O:364:TYR:CD2	2.32	0.65
1:K:475:LEU:H	1:K:475:LEU:CD2	2.10	0.65
1:M:113:LEU:HD22	1:N:253:GLU:HG3	1.77	0.65
1:I:258:ARG:NH1	1:J:130:GLU:OE1	2.29	0.65
1:O:159:LEU:CD2	1:O:331:VAL:HG22	2.27	0.65
1:A:344:ILE:HD11	1:B:188:LEU:HD11	1.78	0.64
1:G:345:CYS:HB3	1:G:363:GLN:NE2	2.11	0.64
1:I:216:THR:CG2	1:I:218:CYS:HB2	2.28	0.64
1:E:46:GLY:HA3	1:E:65:VAL:HG23	1.77	0.64
1:I:313:LEU:HD23	1:I:313:LEU:H	1.62	0.64
1:L:246:MET:HG3	1:L:246:MET:O	1.95	0.64
1:E:114:GLY:HA3	1:E:340:THR:HG23	1.80	0.64
1:H:307:PHE:HA	1:H:311:TYR:OH	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:138:ASN:HD22	1:M:140:SER:HB3	1.62	0.64
1:F:105:VAL:HG12	1:F:106:GLU:N	2.12	0.64
1:N:87:ASP:O	1:N:90:ILE:HG12	1.97	0.64
1:H:72:VAL:HG23	1:H:197:ASP:HA	1.79	0.64
1:K:126:LEU:HB3	1:K:262:ASN:HB3	1.80	0.64
1:O:135:ALA:HB1	1:O:282:MET:HE1	1.79	0.64
1:N:214:GLN:OE1	1:N:219:GLU:HB2	1.97	0.64
1:G:143:VAL:O	1:G:143:VAL:HG12	1.98	0.64
1:K:114:GLY:HA3	1:K:340:THR:HG23	1.80	0.64
1:M:159:LEU:CD2	1:M:331:VAL:HG22	2.28	0.64
1:N:313:LEU:HD23	1:N:313:LEU:H	1.62	0.64
1:J:141:GLU:HG3	1:J:142:ASP:H	1.63	0.64
1:L:98:LEU:CD2	1:L:381:THR:HG22	2.27	0.64
1:F:36:HIS:ND1	1:F:36:HIS:C	2.56	0.64
1:J:109:ARG:H	1:J:308:ASN:HD21	1.44	0.64
1:K:364:TYR:CD2	1:L:185:CYS:HB2	2.33	0.64
1:A:368:VAL:HG12	1:A:369:GLU:N	2.12	0.63
1:B:324:CYS:HB3	1:B:328:GLN:O	1.98	0.63
1:C:24:THR:HG23	1:C:320:ASN:HA	1.80	0.63
1:F:24:THR:CG2	1:F:320:ASN:HA	2.27	0.63
1:K:369:GLU:HG3	1:K:371:TYR:CE1	2.32	0.63
1:B:126:LEU:HB3	1:B:262:ASN:CB	2.28	0.63
1:F:111:GLN:HB3	1:F:112:PRO:CD	2.29	0.63
1:N:22:VAL:HG12	1:N:23:ASN:N	2.13	0.63
1:O:22:VAL:HG12	1:O:23:ASN:N	2.12	0.63
1:O:193:THR:CG2	1:O:230:LYS:HD3	2.29	0.63
1:B:364:TYR:CG	1:C:185:CYS:HB2	2.34	0.63
1:G:114:GLY:HA3	1:G:340:THR:HG23	1.80	0.63
1:G:390:SER:O	1:G:393:GLN:HB3	1.98	0.63
1:I:127:ASP:OD2	1:I:136:THR:OG1	2.13	0.63
1:K:293:PRO:HD3	1:O:117:LEU:HG	1.81	0.63
1:L:353:PRO:HD2	1:L:360:LYS:CE	2.28	0.63
1:J:307:PHE:HE1	1:J:335:ASP:HB2	1.63	0.63
1:K:188:LEU:N	1:K:188:LEU:HD22	2.13	0.63
1:N:233:ASP:CG	1:N:236:GLN:HB3	2.23	0.63
1:E:353:PRO:CG	1:E:360:LYS:NZ	2.62	0.63
1:F:364:TYR:CD2	1:G:185:CYS:HB2	2.33	0.63
1:K:24:THR:CG2	1:K:320:ASN:HA	2.27	0.63
1:A:87:ASP:HB3	1:A:90:ILE:HD11	1.81	0.63
1:E:105:VAL:HG21	1:E:159:LEU:HD11	1.80	0.63
1:G:92:ASN:HD21	1:G:95:THR:HG23	1.63	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:99:VAL:HG21	1:L:382:ILE:HD11	1.79	0.63
1:O:109:ARG:H	1:O:308:ASN:ND2	1.96	0.63
1:H:384:LEU:HB3	1:H:389:MET:CE	2.26	0.63
1:K:151:TYR:CG	1:K:203:THR:HB	2.33	0.63
1:C:71:ARG:HA	1:C:197:ASP:OD1	1.99	0.62
1:E:353:PRO:CG	1:E:360:LYS:HZ3	2.11	0.62
1:I:244:ASP:OD1	1:I:320:ASN:ND2	2.28	0.62
1:L:109:ARG:H	1:L:308:ASN:ND2	1.97	0.62
1:L:71:ARG:HA	1:L:197:ASP:OD1	1.99	0.62
1:M:22:VAL:HG12	1:M:23:ASN:N	2.13	0.62
1:N:122:PHE:O	1:N:218:CYS:HB3	1.99	0.62
1:B:131:SER:O	1:B:132:SER:C	2.40	0.62
1:C:300:VAL:HG13	1:C:300:VAL:O	1.99	0.62
1:J:247:PHE:CD2	1:J:322:GLY:HA2	2.34	0.62
1:M:376:ILE:HG12	1:M:465:LEU:HD13	1.81	0.62
1:N:368:VAL:HG12	1:N:369:GLU:N	2.12	0.62
1:C:45:VAL:CG1	1:C:368:VAL:HG22	2.28	0.62
1:F:151:TYR:OH	1:F:221:PRO:HB2	1.99	0.62
1:H:390:SER:O	1:H:393:GLN:HB3	1.99	0.62
1:J:388:VAL:O	1:J:392:ILE:HG13	1.99	0.62
1:D:311:TYR:N	1:D:311:TYR:CD1	2.66	0.62
1:G:232:PRO:HB2	1:G:234:TYR:CE1	2.34	0.62
1:K:307:PHE:HA	1:K:311:TYR:OH	1.99	0.62
1:G:105:VAL:HG12	1:G:106:GLU:N	2.14	0.62
1:D:87:ASP:O	1:D:90:ILE:HG12	2.00	0.62
1:F:465:LEU:CD1	1:F:465:LEU:HG	2.16	0.62
1:G:325:TRP:O	1:G:326:HIS:HB2	1.99	0.62
1:L:188:LEU:HD22	1:L:188:LEU:N	2.13	0.62
1:M:191:LYS:CE	1:M:191:LYS:CG	2.76	0.62
1:C:24:THR:CG2	1:C:320:ASN:HA	2.29	0.62
1:H:69:GLN:NE2	1:H:71:ARG:HH22	1.97	0.62
1:I:233:ASP:CG	1:I:236:GLN:HB3	2.24	0.62
1:B:24:THR:HG23	1:B:319:HIS:O	2.00	0.62
1:C:70:TYR:CE1	1:C:201:VAL:HG12	2.35	0.62
1:D:475:LEU:H	1:D:475:LEU:CD2	2.00	0.62
1:E:74:ARG:HG3	1:E:330:PHE:CE2	2.34	0.62
1:F:98:LEU:CD2	1:F:381:THR:HG22	2.29	0.62
1:G:353:PRO:HG2	1:G:360:LYS:NZ	2.11	0.62
1:J:324:CYS:HB3	1:J:328:GLN:O	2.00	0.62
1:L:151:TYR:CG	1:L:203:THR:HB	2.34	0.61
1:L:390:SER:O	1:L:393:GLN:HB3	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:351:PRO:O	1:L:352:VAL:HB	2.00	0.61
1:F:246:MET:HG3	1:F:246:MET:O	2.00	0.61
1:G:444:LYS:HA	1:G:444:LYS:HE2	1.83	0.61
1:N:353:PRO:HD2	1:N:360:LYS:CE	2.30	0.61
1:C:273:GLN:HE22	1:C:278:LYS:CE	2.02	0.61
1:M:307:PHE:HE1	1:M:335:ASP:HB2	1.64	0.61
1:A:123:TYR:HD2	1:A:125:LYS:HB2	1.64	0.61
1:E:353:PRO:HG2	1:E:360:LYS:NZ	2.13	0.61
1:C:70:TYR:CZ	1:C:201:VAL:HG12	2.35	0.61
1:E:92:ASN:C	1:E:94:GLU:H	2.08	0.61
1:F:293:PRO:HB3	1:J:117:LEU:HD11	1.82	0.61
1:F:307:PHE:HA	1:F:311:TYR:OH	2.01	0.61
1:F:350:SER:HB3	1:F:351:PRO:HD3	1.82	0.61
1:H:92:ASN:HD21	1:H:95:THR:HG23	1.65	0.61
1:J:316:ALA:HB3	1:J:321:ASN:HA	1.81	0.61
1:L:364:TYR:CD2	1:M:185:CYS:HB2	2.36	0.61
1:M:454:GLU:C	1:M:455:LYS:HG2	2.26	0.61
1:O:390:SER:O	1:O:393:GLN:HB3	1.99	0.61
1:A:353:PRO:CG	1:A:360:LYS:NZ	2.63	0.61
1:B:364:TYR:CE2	1:C:185:CYS:HB2	2.36	0.61
1:C:200:MET:HE2	1:C:223:ASP:O	2.01	0.61
1:H:368:VAL:HG12	1:H:369:GLU:N	2.13	0.61
1:C:453:LYS:NZ	1:C:453:LYS:CD	2.61	0.61
1:I:113:LEU:HD22	1:J:253:GLU:HG3	1.83	0.61
1:C:368:VAL:HG11	1:D:169:TRP:CZ2	2.36	0.61
1:F:369:GLU:HG3	1:F:371:TYR:CE1	2.36	0.61
1:M:200:MET:HE2	1:M:223:ASP:O	2.01	0.61
1:N:384:LEU:CB	1:N:389:MET:HE2	2.18	0.61
1:B:214:GLN:OE1	1:B:219:GLU:HB2	2.01	0.60
1:C:36:HIS:ND1	1:C:37:ALA:N	2.49	0.60
1:D:117:LEU:HD11	1:E:293:PRO:HB3	1.83	0.60
1:E:369:GLU:HG3	1:E:371:TYR:HE1	1.66	0.60
1:F:368:VAL:HG12	1:F:369:GLU:N	2.13	0.60
1:G:315:LYS:CE	1:G:315:LYS:CG	2.75	0.60
1:H:151:TYR:CG	1:H:203:THR:HB	2.36	0.60
1:M:92:ASN:C	1:M:94:GLU:H	2.08	0.60
1:N:216:THR:O	1:N:217:LYS:HB2	2.01	0.60
1:N:307:PHE:HA	1:N:311:TYR:OH	2.01	0.60
1:O:143:VAL:O	1:O:143:VAL:CG1	2.45	0.60
1:O:233:ASP:CG	1:O:236:GLN:HB3	2.26	0.60
1:H:193:THR:HG21	1:H:230:LYS:HE2	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:88:THR:O	1:J:88:THR:HG22	2.00	0.60
1:D:138:ASN:HD22	1:D:140:SER:HB3	1.66	0.60
1:F:188:LEU:HD22	1:F:188:LEU:N	2.16	0.60
1:G:300:VAL:HG12	1:H:255:LEU:O	2.01	0.60
1:I:459:ASP:OD2	1:I:459:ASP:N	2.33	0.60
1:K:258:ARG:NH1	1:L:130:GLU:OE1	2.34	0.60
1:L:105:VAL:HG12	1:L:106:GLU:H	1.66	0.60
1:N:21:VAL:HG12	1:N:22:VAL:N	2.15	0.60
1:N:42:LEU:HB3	1:N:448:TRP:CZ2	2.37	0.60
1:C:91:TYR:HB2	1:C:96:GLN:HG3	1.84	0.60
1:D:216:THR:O	1:D:217:LYS:HB2	2.01	0.60
1:H:45:VAL:CG1	1:H:368:VAL:HG22	2.31	0.60
1:H:122:PHE:O	1:H:218:CYS:HB3	2.00	0.60
1:H:200:MET:HE2	1:H:223:ASP:O	2.02	0.60
1:O:353:PRO:CD	1:O:360:LYS:NZ	2.60	0.60
1:B:141:GLU:CG	1:B:141:GLU:C	2.75	0.60
1:B:233:ASP:CG	1:B:236:GLN:HB3	2.26	0.60
1:E:246:MET:O	1:E:246:MET:HG3	2.01	0.60
1:F:169:TRP:CZ2	1:J:368:VAL:HG11	2.36	0.60
1:J:138:ASN:C	1:J:140:SER:H	2.10	0.60
1:L:109:ARG:H	1:L:308:ASN:HD21	1.49	0.60
1:M:109:ARG:H	1:M:308:ASN:HD21	1.49	0.60
1:B:122:PHE:O	1:B:218:CYS:HB3	2.01	0.60
1:D:315:LYS:CG	1:D:315:LYS:CE	2.78	0.60
1:L:384:LEU:HB3	1:L:389:MET:HE2	1.82	0.60
1:O:151:TYR:CG	1:O:203:THR:HB	2.35	0.60
1:B:344:ILE:CD1	1:C:188:LEU:HD11	2.29	0.60
1:D:313:LEU:HD23	1:D:313:LEU:N	2.17	0.60
1:F:123:TYR:CB	1:F:147:VAL:HG22	2.31	0.60
1:G:92:ASN:ND2	1:G:95:THR:H	1.98	0.60
1:J:345:CYS:HB3	1:J:363:GLN:NE2	2.16	0.60
1:D:376:ILE:HG12	1:D:465:LEU:HD13	1.84	0.60
1:E:111:GLN:HB3	1:E:112:PRO:CD	2.31	0.60
1:F:313:LEU:HD23	1:F:313:LEU:N	2.15	0.60
1:G:369:GLU:HG3	1:G:371:TYR:HE1	1.66	0.60
1:M:114:GLY:HA3	1:M:340:THR:HG23	1.83	0.60
1:N:88:THR:HG22	1:N:88:THR:O	2.01	0.60
1:A:151:TYR:OH	1:A:221:PRO:HB2	2.02	0.60
1:A:247:PHE:CE2	1:A:322:GLY:HA2	2.36	0.60
1:A:385:THR:OG1	1:A:388:VAL:HG23	2.02	0.60
1:H:114:GLY:HA3	1:H:340:THR:HG23	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:465:LEU:CD1	1:F:465:LEU:CD2	2.74	0.60
1:G:87:ASP:O	1:G:90:ILE:HG12	2.00	0.60
1:K:246:MET:HG3	1:K:246:MET:O	2.02	0.60
1:L:45:VAL:HG12	1:L:368:VAL:HG22	1.83	0.60
1:O:111:GLN:HB3	1:O:112:PRO:HD2	1.82	0.60
1:C:344:ILE:HD11	1:D:188:LEU:HD11	1.83	0.59
1:G:81:ASN:C	1:G:83:PHE:H	2.10	0.59
1:K:76:GLN:HG3	1:K:453:LYS:HE3	1.84	0.59
1:A:87:ASP:O	1:A:90:ILE:HG12	2.01	0.59
1:F:34:PHE:CE2	1:F:378:GLN:HB2	2.36	0.59
1:K:69:GLN:NE2	1:K:71:ARG:HH22	1.99	0.59
1:L:372:ASP:OD2	1:L:372:ASP:C	2.44	0.59
1:B:293:PRO:O	1:B:293:PRO:HG2	2.01	0.59
1:H:36:HIS:C	1:H:36:HIS:ND1	2.60	0.59
1:L:344:ILE:HD11	1:M:188:LEU:HD11	1.83	0.59
1:A:216:THR:HG22	1:A:218:CYS:CB	2.27	0.59
1:D:444:LYS:HA	1:D:444:LYS:HE2	1.83	0.59
1:J:141:GLU:CG	1:J:142:ASP:N	2.65	0.59
1:M:342:LEU:HD22	1:N:208:MET:SD	2.43	0.59
1:O:98:LEU:HD21	1:O:381:THR:HG22	1.83	0.59
1:C:191:LYS:CE	1:C:191:LYS:CG	2.79	0.59
1:G:463:TYR:O	1:G:467:ARG:HG3	2.02	0.59
1:B:307:PHE:HA	1:B:311:TYR:OH	2.02	0.59
1:L:193:THR:HG21	1:L:230:LYS:HE2	1.85	0.59
1:M:368:VAL:HG12	1:M:369:GLU:N	2.16	0.59
1:O:105:VAL:HG21	1:O:159:LEU:HD11	1.83	0.59
1:O:156:LEU:HG	1:O:334:VAL:HB	1.84	0.59
1:E:307:PHE:HA	1:E:311:TYR:OH	2.03	0.59
1:H:109:ARG:H	1:H:308:ASN:HD21	1.49	0.59
1:M:98:LEU:CD2	1:M:381:THR:HG22	2.32	0.59
1:N:313:LEU:HD23	1:N:313:LEU:N	2.17	0.59
1:H:314:HIS:O	1:H:315:LYS:HG3	2.03	0.59
1:M:329:LEU:HD23	1:M:329:LEU:C	2.27	0.59
1:G:24:THR:HG23	1:G:320:ASN:HA	1.84	0.59
1:I:200:MET:HE2	1:I:223:ASP:O	2.02	0.59
1:I:307:PHE:CE1	1:I:335:ASP:HB2	2.37	0.59
1:K:231:TYR:CD1	1:O:112:PRO:HB3	2.38	0.59
1:K:345:CYS:HB3	1:K:363:GLN:NE2	2.18	0.59
1:N:81:ASN:OD1	1:N:98:LEU:HB2	2.03	0.59
1:A:165:ILE:HD12	1:A:165:ILE:N	2.17	0.59
1:D:439:LYS:NZ	1:D:439:LYS:CD	2.65	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:123:TYR:CB	1:I:147:VAL:HG22	2.33	0.59
1:A:300:VAL:HG13	1:A:300:VAL:O	2.03	0.58
1:D:111:GLN:HB3	1:D:112:PRO:HD2	1.85	0.58
1:E:360:LYS:HE2	1:E:361:PHE:CE1	2.38	0.58
1:G:475:LEU:HD23	1:G:475:LEU:H	1.67	0.58
1:J:357:ASP:O	1:J:358:ALA:C	2.46	0.58
1:M:138:ASN:ND2	1:M:140:SER:HB3	2.17	0.58
1:M:390:SER:O	1:M:393:GLN:HB3	2.03	0.58
1:N:385:THR:O	1:N:389:MET:HE3	2.02	0.58
1:O:307:PHE:HA	1:O:311:TYR:OH	2.02	0.58
1:A:390:SER:O	1:A:393:GLN:HB3	2.03	0.58
1:B:24:THR:CG2	1:B:320:ASN:HA	2.33	0.58
1:B:109:ARG:H	1:B:308:ASN:HD21	1.51	0.58
1:D:475:LEU:HD23	1:D:475:LEU:N	2.05	0.58
1:H:344:ILE:HD11	1:I:188:LEU:HD11	1.85	0.58
1:I:350:SER:HB3	1:I:351:PRO:HD3	1.85	0.58
1:B:226:GLN:OE1	1:B:226:GLN:HA	2.01	0.58
1:D:200:MET:HE2	1:D:223:ASP:O	2.02	0.58
1:G:98:LEU:CD2	1:G:381:THR:HG22	2.33	0.58
1:C:392:ILE:O	1:C:392:ILE:HG22	2.02	0.58
1:J:350:SER:HB3	1:J:351:PRO:HD3	1.84	0.58
1:K:329:LEU:HD23	1:K:329:LEU:C	2.28	0.58
1:M:350:SER:HB3	1:M:351:PRO:HD3	1.86	0.58
1:N:329:LEU:HD23	1:N:329:LEU:C	2.29	0.58
1:C:36:HIS:ND1	1:C:36:HIS:C	2.60	0.58
1:D:138:ASN:ND2	1:D:140:SER:HB3	2.18	0.58
1:F:98:LEU:HD13	1:F:379:LEU:HD11	1.85	0.58
1:F:324:CYS:HB3	1:F:328:GLN:O	2.02	0.58
1:H:239:ALA:O	1:H:240:ASP:C	2.46	0.58
1:L:325:TRP:O	1:L:326:HIS:HB2	2.03	0.58
1:M:24:THR:HG23	1:M:319:HIS:O	2.03	0.58
1:C:307:PHE:HE1	1:C:335:ASP:HB2	1.68	0.58
1:C:368:VAL:CG1	1:C:369:GLU:N	2.62	0.58
1:D:164:ALA:C	1:D:165:ILE:HD12	2.28	0.58
1:D:307:PHE:HE1	1:D:335:ASP:HB2	1.68	0.58
1:F:368:VAL:CG1	1:F:369:GLU:N	2.65	0.58
1:G:99:VAL:HG21	1:G:382:ILE:HD11	1.86	0.58
1:I:369:GLU:HG3	1:I:371:TYR:HE1	1.69	0.58
1:I:369:GLU:HG3	1:I:371:TYR:CE1	2.38	0.58
1:L:138:ASN:ND2	1:L:140:SER:HB3	2.19	0.58
1:M:368:VAL:HG11	1:N:169:TRP:HZ2	1.69	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:HG12	1:A:106:GLU:N	2.19	0.58
1:F:254:GLN:O	1:F:254:GLN:HG3	2.03	0.58
1:F:368:VAL:HG11	1:G:169:TRP:CZ2	2.38	0.58
1:G:313:LEU:HD23	1:G:313:LEU:H	1.68	0.58
1:H:74:ARG:NE	1:H:328:GLN:OE1	2.34	0.58
1:H:360:LYS:HE2	1:H:361:PHE:CE1	2.38	0.58
1:C:87:ASP:O	1:C:90:ILE:HG12	2.03	0.58
1:C:121:PRO:HG3	1:D:289:CYS:SG	2.44	0.58
1:D:45:VAL:CG1	1:D:368:VAL:HG22	2.28	0.58
1:J:246:MET:HG3	1:J:246:MET:O	2.04	0.58
1:A:389:MET:HG2	1:A:400:LEU:HD21	1.84	0.58
1:B:247:PHE:CD2	1:B:322:GLY:HA2	2.39	0.58
1:C:396:ASN:HB3	1:C:399:ILE:HG13	1.86	0.58
1:D:350:SER:HB3	1:D:351:PRO:HD3	1.86	0.58
1:G:85:LEU:HB3	1:G:86:PRO:HD2	1.85	0.58
1:H:156:LEU:C	1:H:156:LEU:HD12	2.29	0.58
1:K:117:LEU:CD1	1:L:260:PHE:HB3	2.34	0.58
1:M:201:VAL:HG11	1:M:334:VAL:HG11	1.84	0.58
1:G:364:TYR:CD2	1:H:185:CYS:HB2	2.39	0.58
1:J:446:LYS:CG	1:J:446:LYS:CE	2.81	0.58
1:K:234:TYR:HD2	1:K:246:MET:HE1	1.67	0.58
1:M:35:TYR:CE2	1:M:458:LEU:HG	2.39	0.58
1:A:214:GLN:OE1	1:A:219:GLU:HB2	2.03	0.57
1:F:71:ARG:HA	1:F:197:ASP:OD1	2.04	0.57
1:F:258:ARG:HG3	1:F:259:HIS:ND1	2.19	0.57
1:G:109:ARG:H	1:G:308:ASN:ND2	2.01	0.57
1:G:307:PHE:O	1:G:308:ASN:HB2	2.03	0.57
1:I:261:TRP:CZ3	1:I:294:SER:HB3	2.38	0.57
1:K:185:CYS:HB2	1:O:364:TYR:CE2	2.39	0.57
1:M:85:LEU:HB3	1:M:86:PRO:HD2	1.86	0.57
1:A:232:PRO:HB2	1:A:234:TYR:CE1	2.39	0.57
1:A:180:LEU:HD21	1:A:186:PRO:HA	1.84	0.57
1:E:390:SER:O	1:E:393:GLN:HB3	2.05	0.57
1:F:475:LEU:H	1:F:475:LEU:CD2	2.12	0.57
1:G:68:TYR:O	1:G:201:VAL:HG22	2.05	0.57
1:L:117:LEU:HD11	1:M:293:PRO:HB3	1.87	0.57
1:C:151:TYR:OH	1:C:221:PRO:HB2	2.04	0.57
1:I:353:PRO:CD	1:I:360:LYS:HZ2	2.12	0.57
1:A:126:LEU:HB3	1:A:262:ASN:HB3	1.87	0.57
1:A:267:MET:HE2	1:A:267:MET:HA	1.86	0.57
1:B:141:GLU:C	1:B:141:GLU:HG2	2.30	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:ASP:OD1	1:D:320:ASN:ND2	2.37	0.57
1:E:446:LYS:CD	1:E:446:LYS:NZ	2.67	0.57
1:H:85:LEU:HB3	1:H:86:PRO:HD2	1.85	0.57
1:M:344:ILE:HD11	1:N:188:LEU:HD11	1.86	0.57
1:N:364:TYR:CE2	1:O:185:CYS:HB2	2.40	0.57
1:O:385:THR:O	1:O:389:MET:HE3	2.04	0.57
1:E:109:ARG:H	1:E:308:ASN:HD21	1.53	0.57
1:H:36:HIS:ND1	1:H:37:ALA:N	2.51	0.57
1:J:46:GLY:HA3	1:J:65:VAL:HG23	1.87	0.57
1:M:191:LYS:CD	1:M:191:LYS:NZ	2.66	0.57
1:O:350:SER:HB3	1:O:351:PRO:HD3	1.87	0.57
1:O:376:ILE:HG12	1:O:465:LEU:HD13	1.87	0.57
1:D:390:SER:O	1:D:393:GLN:HB3	2.05	0.57
1:G:110:GLY:HA3	1:G:370:GLU:HB3	1.86	0.57
1:K:113:LEU:HD22	1:L:253:GLU:HG3	1.86	0.57
1:D:307:PHE:HA	1:D:311:TYR:OH	2.04	0.57
1:I:72:VAL:HG23	1:I:197:ASP:HA	1.87	0.57
1:N:45:VAL:HG12	1:N:368:VAL:HG22	1.86	0.57
1:N:246:MET:HG3	1:N:246:MET:O	2.05	0.57
1:O:261:TRP:CZ3	1:O:294:SER:HB3	2.39	0.57
1:A:246:MET:HG3	1:A:246:MET:O	2.04	0.57
1:B:85:LEU:HB3	1:B:86:PRO:HD2	1.87	0.57
1:E:85:LEU:HB3	1:E:86:PRO:HD2	1.87	0.57
1:G:113:LEU:HD22	1:H:253:GLU:HG3	1.86	0.57
1:K:42:LEU:HB3	1:K:448:TRP:CZ2	2.39	0.57
1:L:367:HIS:CE1	1:L:369:GLU:OE2	2.58	0.57
1:L:368:VAL:HG11	1:M:169:TRP:CZ2	2.40	0.57
1:M:117:LEU:HG	1:N:293:PRO:HD3	1.85	0.57
1:I:345:CYS:HB3	1:I:363:GLN:NE2	2.20	0.57
1:K:258:ARG:HG3	1:K:259:HIS:ND1	2.19	0.57
1:H:351:PRO:O	1:H:352:VAL:HB	2.05	0.56
1:I:107:ILE:HG22	1:I:107:ILE:O	2.05	0.56
1:I:313:LEU:HD23	1:I:313:LEU:N	2.20	0.56
1:O:159:LEU:HD22	1:O:331:VAL:HG22	1.87	0.56
1:O:193:THR:HG23	1:O:230:LYS:HD3	1.87	0.56
1:G:24:THR:HG21	1:G:320:ASN:HA	1.86	0.56
1:G:140:SER:O	1:G:141:GLU:CB	2.32	0.56
1:I:47:ASP:C	1:I:47:ASP:OD1	2.47	0.56
1:L:365:SER:HB2	1:M:290:VAL:HG13	1.86	0.56
1:B:353:PRO:CD	1:B:360:LYS:NZ	2.69	0.56
1:D:85:LEU:HB3	1:D:86:PRO:HD2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:VAL:CG2	1:D:159:LEU:HD11	2.34	0.56
1:E:105:VAL:HG12	1:E:106:GLU:H	1.69	0.56
1:G:45:VAL:HG12	1:G:368:VAL:HG22	1.87	0.56
1:G:300:VAL:HG13	1:G:300:VAL:O	2.04	0.56
1:I:92:ASN:HD21	1:I:95:THR:HG23	1.70	0.56
1:L:68:TYR:O	1:L:201:VAL:HG22	2.05	0.56
1:L:344:ILE:CD1	1:M:188:LEU:HD11	2.35	0.56
1:D:307:PHE:CE1	1:D:335:ASP:HB2	2.41	0.56
1:G:111:GLN:HB3	1:G:112:PRO:CD	2.35	0.56
1:I:159:LEU:CD2	1:I:331:VAL:HG22	2.35	0.56
1:N:71:ARG:HA	1:N:197:ASP:OD1	2.05	0.56
1:N:200:MET:HE2	1:N:223:ASP:O	2.05	0.56
1:N:258:ARG:NH1	1:O:130:GLU:OE1	2.38	0.56
1:C:69:GLN:NE2	1:C:71:ARG:HH22	2.03	0.56
1:G:261:TRP:CZ3	1:G:294:SER:HB3	2.41	0.56
1:G:273:GLN:HE22	1:G:278:LYS:HE2	1.69	0.56
1:J:324:CYS:SG	1:J:329:LEU:HD12	2.45	0.56
1:A:60:GLN:O	1:A:61:ASP:O	2.24	0.56
1:D:67:ALA:HB2	1:D:367:HIS:CE1	2.41	0.56
1:D:345:CYS:HB3	1:D:363:GLN:NE2	2.21	0.56
1:E:247:PHE:CD2	1:E:322:GLY:HA2	2.40	0.56
1:F:465:LEU:O	1:F:465:LEU:HD22	2.06	0.56
1:H:368:VAL:CG1	1:H:369:GLU:N	2.69	0.56
1:L:117:LEU:HD13	1:M:260:PHE:HB3	1.87	0.56
1:N:148:SER:HB3	1:O:291:TYR:CD2	2.41	0.56
1:B:68:TYR:O	1:B:201:VAL:HG22	2.06	0.56
1:B:396:ASN:HB3	1:B:399:ILE:HG13	1.88	0.56
1:D:92:ASN:HD21	1:D:95:THR:HG23	1.69	0.56
1:E:69:GLN:HE21	1:E:71:ARG:HH12	1.54	0.56
1:G:384:LEU:HB3	1:G:389:MET:HE2	1.86	0.56
1:M:24:THR:CG2	1:M:320:ASN:HA	2.35	0.56
1:N:72:VAL:HG23	1:N:197:ASP:HA	1.87	0.56
1:N:138:ASN:ND2	1:N:140:SER:HB3	2.21	0.56
1:N:316:ALA:CB	1:N:321:ASN:HA	2.36	0.56
1:B:140:SER:OG	1:B:141:GLU:N	2.38	0.56
1:D:385:THR:OG1	1:D:388:VAL:HG23	2.05	0.56
1:G:444:LYS:HA	1:G:444:LYS:CE	2.35	0.56
1:L:141:GLU:HG2	1:L:142:ASP:N	2.20	0.56
1:E:52:VAL:HB	1:E:62:ILE:HB	1.88	0.56
1:J:99:VAL:CG2	1:J:382:ILE:HD11	2.33	0.56
1:M:105:VAL:CG2	1:M:159:LEU:HD11	2.31	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:392:ILE:O	1:N:392:ILE:HG22	2.05	0.56
1:O:384:LEU:HB3	1:O:389:MET:HE2	1.87	0.56
1:A:167:GLU:OE1	1:E:111:GLN:NE2	2.39	0.56
1:C:151:TYR:CG	1:C:203:THR:HB	2.41	0.56
1:E:188:LEU:HD22	1:E:188:LEU:N	2.21	0.56
1:F:24:THR:HG23	1:F:320:ASN:HA	1.88	0.56
1:H:368:VAL:HG11	1:I:169:TRP:HZ2	1.71	0.56
1:M:87:ASP:O	1:M:90:ILE:HG12	2.06	0.56
1:M:112:PRO:HB3	1:N:231:TYR:CD1	2.41	0.56
1:N:120:HIS:ND1	1:N:121:PRO:HD2	2.21	0.56
1:D:384:LEU:CB	1:D:389:MET:HE2	2.28	0.55
1:F:464:PRO:HA	1:F:467:ARG:NH1	2.20	0.55
1:G:50:PHE:HA	1:G:64:LYS:HG3	1.86	0.55
1:K:122:PHE:O	1:K:218:CYS:HB3	2.06	0.55
1:L:475:LEU:HD23	1:L:475:LEU:H	1.71	0.55
1:C:358:ALA:HB2	1:D:141:GLU:O	2.07	0.55
1:D:111:GLN:NE2	1:D:370:GLU:OE1	2.39	0.55
1:E:388:VAL:O	1:E:392:ILE:HG13	2.06	0.55
1:I:368:VAL:HG11	1:J:169:TRP:CZ2	2.41	0.55
1:A:150:ASP:O	1:A:296:SER:HA	2.05	0.55
1:A:258:ARG:HG3	1:A:259:HIS:ND1	2.22	0.55
1:B:258:ARG:NH1	1:C:130:GLU:OE1	2.39	0.55
1:C:307:PHE:HA	1:C:311:TYR:OH	2.06	0.55
1:D:159:LEU:HD22	1:D:331:VAL:HG22	1.88	0.55
1:H:176:LYS:HG3	1:H:177:SER:H	1.69	0.55
1:I:31:THR:HG23	1:I:379:LEU:O	2.06	0.55
1:A:281:GLY:HA3	1:G:89:SER:C	2.30	0.55
1:B:369:GLU:HG3	1:B:371:TYR:HE1	1.70	0.55
1:C:22:VAL:HG12	1:C:23:ASN:N	2.21	0.55
1:C:113:LEU:HD22	1:D:253:GLU:HG3	1.89	0.55
1:F:107:ILE:O	1:F:107:ILE:HG22	2.05	0.55
1:G:109:ARG:H	1:G:308:ASN:HD21	1.55	0.55
1:G:389:MET:O	1:G:393:GLN:HB2	2.06	0.55
1:I:151:TYR:OH	1:I:221:PRO:HB2	2.06	0.55
1:K:293:PRO:O	1:K:293:PRO:HG2	2.04	0.55
1:O:372:ASP:C	1:O:372:ASP:OD2	2.49	0.55
1:C:70:TYR:CE1	1:C:201:VAL:CG1	2.88	0.55
1:C:239:ALA:O	1:C:240:ASP:C	2.49	0.55
1:D:247:PHE:CE2	1:D:322:GLY:HA2	2.42	0.55
1:G:70:TYR:HH	1:G:232:PRO:HD3	1.71	0.55
1:H:141:GLU:HG2	1:H:142:ASP:CA	2.34	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:123:TYR:HB2	1:I:147:VAL:HG22	1.89	0.55
1:J:307:PHE:CE1	1:J:335:ASP:HB2	2.41	0.55
1:M:232:PRO:HB2	1:M:234:TYR:CE1	2.41	0.55
1:M:307:PHE:HA	1:M:311:TYR:OH	2.06	0.55
1:N:109:ARG:H	1:N:308:ASN:HD21	1.55	0.55
1:N:364:TYR:CD2	1:O:185:CYS:HB2	2.42	0.55
1:A:24:THR:CG2	1:A:320:ASN:HA	2.37	0.55
1:A:43:LEU:HD13	1:A:370:GLU:HB2	1.89	0.55
1:A:165:ILE:O	1:A:237:MET:HE2	2.06	0.55
1:G:70:TYR:CE1	1:G:201:VAL:HG12	2.42	0.55
1:G:311:TYR:N	1:G:311:TYR:CD1	2.75	0.55
1:L:36:HIS:ND1	1:L:36:HIS:C	2.65	0.55
1:A:76:GLN:HG3	1:A:453:LYS:HE3	1.88	0.55
1:B:109:ARG:H	1:B:308:ASN:ND2	2.05	0.55
1:B:368:VAL:CG1	1:B:369:GLU:N	2.68	0.55
1:D:138:ASN:C	1:D:140:SER:H	2.15	0.55
1:E:309:LYS:NZ	1:E:309:LYS:CD	2.66	0.55
1:E:372:ASP:C	1:E:372:ASP:OD2	2.49	0.55
1:G:156:LEU:HG	1:G:334:VAL:HB	1.88	0.55
1:J:123:TYR:HD2	1:J:125:LYS:HB2	1.71	0.55
1:M:70:TYR:OH	1:M:232:PRO:HD3	2.05	0.55
1:N:33:ILE:HD13	1:N:33:ILE:N	2.22	0.55
1:N:92:ASN:C	1:N:94:GLU:H	2.15	0.55
1:N:159:LEU:CD2	1:N:331:VAL:HG22	2.37	0.55
1:C:122:PHE:O	1:C:218:CYS:HB3	2.06	0.55
1:H:108:GLY:HA2	1:H:308:ASN:ND2	2.21	0.55
1:I:136:THR:O	1:I:137:SER:C	2.49	0.55
1:N:85:LEU:HB3	1:N:86:PRO:HD2	1.89	0.55
1:C:307:PHE:CE1	1:C:335:ASP:HB2	2.42	0.55
1:K:169:TRP:CZ2	1:O:368:VAL:HG11	2.42	0.55
1:M:249:CYS:O	1:M:250:LEU:HD12	2.07	0.55
1:O:244:ASP:OD1	1:O:320:ASN:ND2	2.35	0.55
1:A:112:PRO:HB3	1:B:231:TYR:CD1	2.42	0.54
1:B:142:ASP:CG	1:C:283:ARG:HD2	2.32	0.54
1:F:112:PRO:HB3	1:G:231:TYR:CD1	2.42	0.54
1:G:159:LEU:CD2	1:G:331:VAL:HG22	2.38	0.54
1:I:156:LEU:HG	1:I:334:VAL:HB	1.88	0.54
1:K:117:LEU:HD13	1:L:260:PHE:HB3	1.90	0.54
1:L:92:ASN:ND2	1:L:95:THR:HG23	2.22	0.54
1:L:111:GLN:HB3	1:L:112:PRO:CD	2.29	0.54
1:A:36:HIS:C	1:A:36:HIS:ND1	2.65	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:ASP:CG	1:C:236:GLN:HB3	2.33	0.54
1:F:98:LEU:HD21	1:F:381:THR:HG22	1.89	0.54
1:F:154:THR:HG23	1:F:253:GLU:HB3	1.89	0.54
1:I:267:MET:HE2	1:I:267:MET:HA	1.89	0.54
1:N:142:ASP:CG	1:O:283:ARG:HD2	2.32	0.54
1:A:24:THR:HG23	1:A:319:HIS:O	2.07	0.54
1:B:69:GLN:NE2	1:B:71:ARG:HH22	2.06	0.54
1:E:35:TYR:CE2	1:E:458:LEU:HG	2.43	0.54
1:I:353:PRO:CG	1:I:360:LYS:HZ3	2.19	0.54
1:J:68:TYR:CE2	1:J:151:TYR:HB2	2.41	0.54
1:K:208:MET:HE2	1:K:210:PHE:CD2	2.43	0.54
1:M:122:PHE:O	1:M:218:CYS:HB3	2.07	0.54
1:N:70:TYR:OH	1:N:232:PRO:HD3	2.07	0.54
1:A:92:ASN:HD21	1:A:95:THR:HG23	1.71	0.54
1:A:159:LEU:HD22	1:A:331:VAL:HG22	1.90	0.54
1:F:390:SER:O	1:F:393:GLN:HB3	2.07	0.54
1:G:244:ASP:OD1	1:G:320:ASN:ND2	2.40	0.54
1:H:349:GLN:HG3	1:H:360:LYS:HD2	1.89	0.54
1:J:156:LEU:HA	1:J:250:LEU:O	2.07	0.54
1:J:446:LYS:CD	1:J:446:LYS:CB	2.76	0.54
1:K:109:ARG:NH2	1:K:369:GLU:OE1	2.41	0.54
1:K:350:SER:HB3	1:K:351:PRO:HD3	1.89	0.54
1:L:156:LEU:HA	1:L:250:LEU:O	2.07	0.54
1:M:233:ASP:CG	1:M:236:GLN:HB3	2.33	0.54
1:A:117:LEU:HD11	1:B:293:PRO:HB3	1.89	0.54
1:D:329:LEU:C	1:D:329:LEU:HD23	2.32	0.54
1:J:81:ASN:C	1:J:83:PHE:H	2.16	0.54
1:D:122:PHE:O	1:D:218:CYS:HB3	2.08	0.54
1:G:92:ASN:C	1:G:94:GLU:H	2.16	0.54
1:G:367:HIS:CE1	1:G:369:GLU:OE2	2.61	0.54
1:H:92:ASN:C	1:H:94:GLU:H	2.14	0.54
1:H:247:PHE:CE2	1:H:322:GLY:HA2	2.42	0.54
1:K:36:HIS:C	1:K:36:HIS:ND1	2.66	0.54
1:A:36:HIS:ND1	1:A:37:ALA:N	2.56	0.54
1:A:98:LEU:CD2	1:A:381:THR:HG22	2.38	0.54
1:A:233:ASP:CG	1:A:236:GLN:HB3	2.32	0.54
1:B:159:LEU:HD22	1:B:331:VAL:HG22	1.89	0.54
1:C:131:SER:O	1:C:132:SER:C	2.50	0.54
1:G:364:TYR:CE2	1:H:185:CYS:HB2	2.41	0.54
1:G:369:GLU:HG3	1:G:371:TYR:CE1	2.43	0.54
1:K:310:PRO:O	1:K:310:PRO:CG	2.55	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:396:ASN:ND2	1:K:398:SER:OG	2.41	0.54
1:M:169:TRP:CZ2	1:M:190:LEU:HD13	2.43	0.54
1:O:353:PRO:HG2	1:O:360:LYS:HZ3	1.73	0.54
1:A:389:MET:HG2	1:A:400:LEU:CD2	2.37	0.54
1:E:325:TRP:O	1:E:326:HIS:HB2	2.06	0.54
1:G:123:TYR:HD2	1:G:125:LYS:HB2	1.73	0.54
1:H:196:GLU:HB3	1:H:446:LYS:O	2.06	0.54
1:C:138:ASN:ND2	1:C:140:SER:HB3	2.22	0.54
1:F:87:ASP:O	1:F:90:ILE:HG12	2.08	0.54
1:F:123:TYR:CG	1:F:147:VAL:HG22	2.43	0.54
1:I:36:HIS:ND1	1:I:37:ALA:N	2.56	0.54
1:J:216:THR:O	1:J:217:LYS:HB2	2.07	0.54
1:K:87:ASP:O	1:K:90:ILE:CG1	2.55	0.54
1:D:22:VAL:HG12	1:D:23:ASN:N	2.23	0.53
1:F:345:CYS:HB3	1:F:363:GLN:HE22	1.72	0.53
1:G:79:ASP:O	1:G:83:PHE:HB2	2.08	0.53
1:M:109:ARG:H	1:M:308:ASN:ND2	2.04	0.53
1:N:342:LEU:HD22	1:O:208:MET:SD	2.48	0.53
1:N:369:GLU:HG3	1:N:371:TYR:CE1	2.41	0.53
1:C:351:PRO:O	1:C:352:VAL:HB	2.09	0.53
1:H:138:ASN:C	1:H:140:SER:H	2.16	0.53
1:N:35:TYR:CE2	1:N:458:LEU:HG	2.43	0.53
1:A:313:LEU:HD23	1:A:313:LEU:N	2.22	0.53
1:C:69:GLN:HE21	1:C:71:ARG:HH12	1.57	0.53
1:F:152:LYS:HE3	1:F:253:GLU:HB2	1.90	0.53
1:G:35:TYR:CE2	1:G:458:LEU:HG	2.43	0.53
1:H:71:ARG:HA	1:H:197:ASP:OD1	2.07	0.53
1:L:138:ASN:HD22	1:L:140:SER:HB3	1.72	0.53
1:L:142:ASP:CG	1:M:283:ARG:HD2	2.33	0.53
1:B:126:LEU:CB	1:B:262:ASN:HB3	2.37	0.53
1:D:92:ASN:ND2	1:D:95:THR:HG23	2.23	0.53
1:E:374:GLN:OE1	1:E:464:PRO:HG2	2.09	0.53
1:F:78:PRO:HG2	1:F:100:TRP:HE1	1.72	0.53
1:F:92:ASN:ND2	1:F:95:THR:HG23	2.23	0.53
1:H:92:ASN:OD1	1:H:94:GLU:HB2	2.08	0.53
1:J:258:ARG:HG3	1:J:259:HIS:ND1	2.24	0.53
1:O:140:SER:O	1:O:141:GLU:HB2	2.08	0.53
1:O:273:GLN:NE2	1:O:278:LYS:HE2	2.23	0.53
1:A:91:TYR:HB2	1:A:96:GLN:HG3	1.90	0.53
1:A:138:ASN:C	1:A:140:SER:H	2.16	0.53
1:A:368:VAL:CG1	1:A:369:GLU:N	2.71	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:PHE:O	1:C:308:ASN:HB2	2.09	0.53
1:K:24:THR:HG23	1:K:320:ASN:HA	1.89	0.53
1:K:110:GLY:HA3	1:K:370:GLU:CD	2.33	0.53
1:M:300:VAL:O	1:M:300:VAL:HG13	2.07	0.53
1:D:114:GLY:HA3	1:D:340:THR:HG23	1.91	0.53
1:F:109:ARG:NH1	1:F:371:TYR:CE1	2.77	0.53
1:F:188:LEU:HD11	1:J:344:ILE:HD11	1.90	0.53
1:H:305:GLN:HA	1:H:305:GLN:NE2	2.23	0.53
1:I:293:PRO:HG2	1:I:293:PRO:O	2.08	0.53
1:O:246:MET:HG3	1:O:246:MET:O	2.08	0.53
1:O:325:TRP:O	1:O:326:HIS:HB2	2.09	0.53
1:C:261:TRP:CZ3	1:C:294:SER:HB3	2.43	0.53
1:D:165:ILE:HD12	1:D:165:ILE:N	2.22	0.53
1:G:359:THR:HA	1:H:266:THR:HG23	1.91	0.53
1:J:105:VAL:HG21	1:J:159:LEU:HD11	1.90	0.53
1:L:360:LYS:CE	1:L:360:LYS:CG	2.80	0.53
1:N:368:VAL:HG11	1:O:169:TRP:HZ2	1.69	0.53
1:A:396:ASN:HD22	1:A:396:ASN:C	2.15	0.53
1:D:342:LEU:HD22	1:E:208:MET:SD	2.49	0.53
1:D:375:PHE:O	1:D:376:ILE:HD13	2.09	0.53
1:F:367:HIS:CE1	1:F:369:GLU:OE2	2.62	0.53
1:G:120:HIS:ND1	1:G:121:PRO:HD2	2.23	0.53
1:K:317:GLN:NE2	1:K:317:GLN:C	2.67	0.53
1:M:42:LEU:HB3	1:M:448:TRP:CZ2	2.42	0.53
1:A:306:LEU:O	1:A:311:TYR:OH	2.12	0.53
1:A:328:GLN:O	1:A:329:LEU:HB2	2.09	0.53
1:K:151:TYR:OH	1:K:221:PRO:HB2	2.09	0.53
1:O:387:ASP:OD1	1:O:388:VAL:N	2.42	0.53
1:H:313:LEU:HD23	1:H:313:LEU:N	2.22	0.53
1:K:255:LEU:HD13	1:O:300:VAL:HG13	1.89	0.53
1:M:364:TYR:CD2	1:N:185:CYS:HB2	2.44	0.53
1:N:368:VAL:CG1	1:N:369:GLU:N	2.72	0.53
1:A:350:SER:HB3	1:A:351:PRO:HD3	1.90	0.52
1:B:31:THR:HG23	1:B:379:LEU:O	2.08	0.52
1:D:36:HIS:ND1	1:D:37:ALA:N	2.57	0.52
1:D:258:ARG:NH1	1:E:130:GLU:OE1	2.42	0.52
1:E:475:LEU:H	1:E:475:LEU:CD2	2.19	0.52
1:G:70:TYR:CZ	1:G:201:VAL:HG12	2.44	0.52
1:G:246:MET:HG3	1:G:246:MET:O	2.08	0.52
1:H:117:LEU:HD11	1:I:293:PRO:HB3	1.91	0.52
1:I:300:VAL:HG13	1:J:255:LEU:HD13	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:247:PHE:CE2	1:L:322:GLY:HA2	2.44	0.52
1:L:385:THR:H	1:L:388:VAL:HB	1.74	0.52
1:M:111:GLN:NE2	1:M:370:GLU:OE1	2.42	0.52
1:F:255:LEU:HD13	1:J:300:VAL:HG13	1.91	0.52
1:I:76:GLN:HG3	1:I:453:LYS:HE3	1.91	0.52
1:K:231:TYR:CG	1:O:112:PRO:HB3	2.44	0.52
1:L:131:SER:O	1:L:132:SER:C	2.52	0.52
1:L:220:VAL:HB	1:L:224:ILE:HD11	1.91	0.52
1:A:188:LEU:HD11	1:E:344:ILE:HD11	1.92	0.52
1:F:45:VAL:HG12	1:F:368:VAL:HG22	1.91	0.52
1:F:79:ASP:O	1:F:83:PHE:HB2	2.09	0.52
1:G:258:ARG:HG3	1:G:259:HIS:ND1	2.25	0.52
1:I:105:VAL:CG1	1:I:106:GLU:N	2.71	0.52
1:I:267:MET:HE2	1:I:267:MET:CA	2.39	0.52
1:A:140:SER:OG	1:A:141:GLU:N	2.42	0.52
1:B:272:PRO:HD2	1:B:275:LEU:HD12	1.92	0.52
1:D:261:TRP:CZ3	1:D:294:SER:HB3	2.44	0.52
1:E:123:TYR:HD2	1:E:125:LYS:HB2	1.75	0.52
1:G:307:PHE:HE1	1:G:335:ASP:HB2	1.74	0.52
1:I:444:LYS:HE2	1:I:444:LYS:HA	1.90	0.52
1:J:169:TRP:CZ2	1:J:190:LEU:HD13	2.44	0.52
1:M:255:LEU:HD22	1:M:256:PHE:N	2.24	0.52
1:N:105:VAL:CG1	1:N:106:GLU:N	2.73	0.52
1:N:151:TYR:OH	1:N:221:PRO:HB2	2.09	0.52
1:O:98:LEU:CD2	1:O:381:THR:HG22	2.40	0.52
1:E:313:LEU:H	1:E:313:LEU:HD23	1.75	0.52
1:H:220:VAL:CG2	1:H:225:CYS:HA	2.40	0.52
1:M:72:VAL:HG23	1:M:197:ASP:HA	1.89	0.52
1:A:92:ASN:ND2	1:A:95:THR:HG23	2.23	0.52
1:A:113:LEU:HD22	1:B:253:GLU:HG3	1.92	0.52
1:C:126:LEU:HB3	1:C:262:ASN:CB	2.38	0.52
1:C:258:ARG:HG3	1:C:259:HIS:ND1	2.23	0.52
1:D:113:LEU:HD22	1:E:253:GLU:HG3	1.92	0.52
1:J:367:HIS:CE1	1:J:369:GLU:OE2	2.62	0.52
1:K:368:VAL:HG11	1:L:169:TRP:HZ2	1.73	0.52
1:L:119:GLY:HA2	1:L:148:SER:HA	1.91	0.52
1:L:300:VAL:HG13	1:L:300:VAL:O	2.09	0.52
1:N:247:PHE:CZ	1:N:322:GLY:HA2	2.43	0.52
1:O:156:LEU:HA	1:O:250:LEU:O	2.09	0.52
1:B:156:LEU:HG	1:B:334:VAL:HB	1.91	0.52
1:D:368:VAL:HG11	1:E:169:TRP:HZ2	1.71	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:310:PRO:HG3	1:F:468:LYS:HD3	1.91	0.52
1:K:353:PRO:CG	1:K:360:LYS:HZ2	2.18	0.52
1:A:164:ALA:C	1:A:165:ILE:HD12	2.33	0.52
1:D:344:ILE:HD11	1:E:188:LEU:HD11	1.92	0.52
1:F:389:MET:O	1:F:393:GLN:N	2.42	0.52
1:I:385:THR:OG1	1:I:388:VAL:HG23	2.09	0.52
1:J:231:TYR:O	1:J:232:PRO:C	2.50	0.52
1:K:188:LEU:HD11	1:O:344:ILE:HD11	1.92	0.52
1:K:260:PHE:HB3	1:O:117:LEU:HD13	1.92	0.52
1:L:307:PHE:CE1	1:L:335:ASP:HB2	2.42	0.52
1:L:350:SER:HB3	1:L:351:PRO:HD3	1.91	0.52
1:A:111:GLN:HB3	1:A:112:PRO:CD	2.39	0.52
1:A:231:TYR:CD1	1:E:112:PRO:HB3	2.45	0.52
1:E:151:TYR:OH	1:E:221:PRO:HB2	2.10	0.52
1:F:117:LEU:HD13	1:G:260:PHE:HB3	1.91	0.52
1:H:105:VAL:HG21	1:H:159:LEU:HD11	1.92	0.52
1:I:126:LEU:HB3	1:I:262:ASN:CB	2.40	0.52
1:I:249:CYS:O	1:I:250:LEU:HD12	2.10	0.52
1:I:364:TYR:CD2	1:J:185:CYS:HB2	2.44	0.52
1:B:220:VAL:HB	1:B:221:PRO:HD2	1.91	0.52
1:B:388:VAL:O	1:B:392:ILE:HG13	2.10	0.52
1:C:98:LEU:CD2	1:C:381:THR:HG22	2.40	0.52
1:F:329:LEU:HD23	1:F:329:LEU:C	2.35	0.52
1:F:387:ASP:O	1:F:388:VAL:C	2.53	0.52
1:G:368:VAL:HG12	1:G:369:GLU:N	2.25	0.52
1:J:92:ASN:HD21	1:J:94:GLU:HB2	1.75	0.52
1:K:293:PRO:HB3	1:O:117:LEU:HD11	1.91	0.52
1:M:156:LEU:HA	1:M:250:LEU:O	2.09	0.52
1:N:36:HIS:C	1:N:36:HIS:ND1	2.67	0.52
1:B:42:LEU:HB3	1:B:448:TRP:CZ2	2.44	0.51
1:B:159:LEU:CD2	1:B:331:VAL:HG22	2.40	0.51
1:B:307:PHE:CE1	1:B:335:ASP:HB2	2.43	0.51
1:C:159:LEU:CD2	1:C:331:VAL:HG22	2.40	0.51
1:F:46:GLY:HA3	1:F:65:VAL:HG23	1.91	0.51
1:F:70:TYR:OH	1:F:232:PRO:HD3	2.10	0.51
1:F:113:LEU:HD22	1:G:253:GLU:HG3	1.92	0.51
1:F:369:GLU:CG	1:F:371:TYR:HE1	2.22	0.51
1:G:313:LEU:HD23	1:G:313:LEU:N	2.24	0.51
1:J:24:THR:HG23	1:J:320:ASN:HA	1.91	0.51
1:J:152:LYS:HE3	1:J:253:GLU:HB2	1.91	0.51
1:J:316:ALA:CB	1:J:321:ASN:HA	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:368:VAL:HG12	1:J:369:GLU:N	2.22	0.51
1:L:112:PRO:HB3	1:M:231:TYR:CD1	2.46	0.51
1:D:368:VAL:HG12	1:D:369:GLU:N	2.24	0.51
1:F:42:LEU:HB3	1:F:448:TRP:CZ2	2.45	0.51
1:H:159:LEU:HD21	1:H:331:VAL:HG22	1.92	0.51
1:M:382:ILE:HD12	1:M:403:TRP:CH2	2.45	0.51
1:O:91:TYR:H	1:O:91:TYR:HD2	1.59	0.51
1:H:43:LEU:CD1	1:H:370:GLU:HB2	2.40	0.51
1:I:325:TRP:O	1:I:326:HIS:HB2	2.08	0.51
1:O:258:ARG:HG3	1:O:259:HIS:ND1	2.25	0.51
1:D:50:PHE:C	1:D:50:PHE:CD1	2.89	0.51
1:F:353:PRO:HD2	1:F:360:LYS:HZ1	1.76	0.51
1:O:87:ASP:HB3	1:O:90:ILE:HD11	1.92	0.51
1:B:138:ASN:C	1:B:140:SER:H	2.18	0.51
1:B:353:PRO:HD2	1:B:360:LYS:NZ	2.26	0.51
1:B:463:TYR:O	1:B:467:ARG:HG3	2.11	0.51
1:D:36:HIS:ND1	1:D:36:HIS:C	2.68	0.51
1:I:114:GLY:HA3	1:I:340:THR:HG23	1.92	0.51
1:I:392:ILE:O	1:I:392:ILE:HG22	2.10	0.51
1:M:311:TYR:N	1:M:311:TYR:CD1	2.78	0.51
1:N:159:LEU:HD21	1:N:331:VAL:HG22	1.93	0.51
1:J:69:GLN:NE2	1:J:71:ARG:HH22	2.09	0.51
1:N:87:ASP:HB3	1:N:90:ILE:HD11	1.93	0.51
1:O:42:LEU:HB3	1:O:448:TRP:CZ2	2.46	0.51
1:E:156:LEU:HA	1:E:250:LEU:O	2.11	0.51
1:E:307:PHE:HE1	1:E:335:ASP:HB2	1.75	0.51
1:F:185:CYS:HB2	1:J:364:TYR:CD2	2.46	0.51
1:K:99:VAL:HG21	1:K:382:ILE:HD11	1.92	0.51
1:K:130:GLU:OE1	1:O:258:ARG:NH1	2.44	0.51
1:K:232:PRO:HB2	1:K:234:TYR:CE1	2.45	0.51
1:L:98:LEU:HD13	1:L:379:LEU:HD11	1.93	0.51
1:N:367:HIS:CE1	1:N:369:GLU:OE2	2.64	0.51
1:A:180:LEU:O	1:A:181:SER:C	2.50	0.51
1:B:109:ARG:NH2	1:B:369:GLU:OE1	2.44	0.51
1:D:69:GLN:NE2	1:D:71:ARG:HH22	2.09	0.51
1:N:159:LEU:HB2	1:N:248:PHE:HB3	1.93	0.51
1:O:108:GLY:HA2	1:O:308:ASN:ND2	2.25	0.51
1:A:188:LEU:HD22	1:A:188:LEU:N	2.25	0.51
1:A:352:VAL:O	1:A:352:VAL:HG12	2.10	0.51
1:D:155:GLN:OE1	1:D:306:LEU:HB2	2.10	0.51
1:E:92:ASN:C	1:E:94:GLU:N	2.69	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:50:PHE:HA	1:F:64:LYS:HG3	1.93	0.51
1:I:155:GLN:OE1	1:I:306:LEU:HB2	2.10	0.51
1:K:92:ASN:C	1:K:94:GLU:H	2.17	0.51
1:B:353:PRO:CG	1:B:360:LYS:NZ	2.64	0.51
1:G:307:PHE:HA	1:G:311:TYR:OH	2.11	0.51
1:G:368:VAL:CG1	1:G:369:GLU:N	2.73	0.51
1:H:45:VAL:C	1:H:65:VAL:HG21	2.36	0.51
1:I:24:THR:HG23	1:I:320:ASN:HA	1.92	0.51
1:I:50:PHE:CD1	1:I:50:PHE:C	2.89	0.51
1:J:251:ARG:HH11	1:J:251:ARG:CG	2.24	0.50
1:K:311:TYR:CD1	1:K:311:TYR:N	2.78	0.50
1:L:71:ARG:HG3	1:L:371:TYR:CZ	2.46	0.50
1:M:314:HIS:O	1:M:315:LYS:HG3	2.11	0.50
1:A:43:LEU:CD1	1:A:370:GLU:HB2	2.41	0.50
1:B:35:TYR:CE2	1:B:458:LEU:HG	2.46	0.50
1:F:364:TYR:CE2	1:G:185:CYS:HB2	2.46	0.50
1:G:372:ASP:C	1:G:372:ASP:OD2	2.54	0.50
1:I:42:LEU:HB3	1:I:448:TRP:CZ2	2.46	0.50
1:J:329:LEU:HD23	1:J:329:LEU:C	2.35	0.50
1:K:85:LEU:HB3	1:K:86:PRO:HD2	1.93	0.50
1:N:157:CYS:HA	1:N:332:THR:O	2.11	0.50
1:A:99:VAL:O	1:A:380:CYS:HB2	2.11	0.50
1:B:365:SER:O	1:B:366:ARG:HD3	2.11	0.50
1:C:369:GLU:HG3	1:C:371:TYR:HE1	1.75	0.50
1:E:369:GLU:HG3	1:E:371:TYR:CE1	2.46	0.50
1:H:141:GLU:HG3	1:H:142:ASP:N	2.21	0.50
1:J:307:PHE:O	1:J:308:ASN:HB2	2.11	0.50
1:K:256:PHE:CD1	1:K:256:PHE:C	2.88	0.50
1:M:157:CYS:HA	1:M:332:THR:O	2.11	0.50
1:M:307:PHE:O	1:M:308:ASN:HB2	2.10	0.50
1:O:232:PRO:HB2	1:O:234:TYR:CE1	2.46	0.50
1:E:42:LEU:HB3	1:E:448:TRP:CZ2	2.47	0.50
1:I:156:LEU:HA	1:I:250:LEU:O	2.10	0.50
1:K:200:MET:HE2	1:K:223:ASP:O	2.10	0.50
1:N:353:PRO:HD2	1:N:360:LYS:HE3	1.93	0.50
1:C:188:LEU:HD12	1:C:213:LEU:HD21	1.91	0.50
1:C:369:GLU:HG3	1:C:371:TYR:CE1	2.47	0.50
1:D:92:ASN:C	1:D:94:GLU:N	2.64	0.50
1:E:79:ASP:C	1:E:79:ASP:OD1	2.53	0.50
1:F:396:ASN:HB3	1:F:399:ILE:HG13	1.94	0.50
1:G:58:ASN:HB2	1:H:178:ARG:HH12	0.68	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:141:GLU:O	1:J:142:ASP:C	2.54	0.50
1:K:307:PHE:HA	1:K:311:TYR:HH	1.76	0.50
1:K:344:ILE:CD1	1:L:188:LEU:HD11	2.40	0.50
1:N:196:GLU:HG2	1:N:445:LEU:HB3	1.93	0.50
1:O:59:LYS:O	1:O:60:GLN:HB3	2.12	0.50
1:E:444:LYS:HE2	1:E:444:LYS:HA	1.92	0.50
1:G:357:ASP:O	1:G:358:ALA:C	2.53	0.50
1:H:353:PRO:CD	1:H:360:LYS:HZ3	2.17	0.50
1:I:463:TYR:O	1:I:467:ARG:HG3	2.11	0.50
1:M:307:PHE:CE1	1:M:335:ASP:HB2	2.46	0.50
1:N:47:ASP:C	1:N:47:ASP:OD1	2.54	0.50
1:A:307:PHE:HE1	1:A:335:ASP:HB2	1.77	0.50
1:I:475:LEU:H	1:I:475:LEU:CD2	2.21	0.50
1:M:24:THR:HG21	1:M:320:ASN:HA	1.92	0.50
1:B:258:ARG:HG3	1:B:259:HIS:ND1	2.27	0.50
1:B:305:GLN:HA	1:B:305:GLN:NE2	2.27	0.50
1:C:110:GLY:HA3	1:C:370:GLU:CG	2.42	0.50
1:C:156:LEU:HG	1:C:334:VAL:HB	1.94	0.50
1:C:226:GLN:HA	1:C:226:GLN:OE1	2.11	0.50
1:E:109:ARG:H	1:E:308:ASN:ND2	2.10	0.50
1:F:123:TYR:HD2	1:F:125:LYS:HB2	1.76	0.50
1:G:41:ARG:NH2	1:H:233:ASP:OD2	2.44	0.50
1:K:156:LEU:HG	1:K:334:VAL:HB	1.93	0.50
1:K:196:GLU:N	1:K:199:ASP:OD2	2.39	0.50
1:M:216:THR:CG2	1:M:218:CYS:HB2	2.42	0.50
1:M:446:LYS:CD	1:M:446:LYS:CB	2.80	0.50
1:F:325:TRP:O	1:F:326:HIS:HB2	2.12	0.50
1:G:72:VAL:HG21	1:G:195:LEU:O	2.12	0.50
1:I:70:TYR:CZ	1:I:201:VAL:HG12	2.47	0.50
1:J:36:HIS:ND1	1:J:37:ALA:N	2.60	0.50
1:J:325:TRP:O	1:J:326:HIS:HB2	2.12	0.50
1:K:109:ARG:H	1:K:308:ASN:ND2	2.09	0.50
1:L:45:VAL:CG1	1:L:368:VAL:HG22	2.42	0.50
1:L:261:TRP:CZ3	1:L:294:SER:HB3	2.47	0.50
1:B:24:THR:HG23	1:B:320:ASN:HA	1.94	0.49
1:C:267:MET:SD	1:C:290:VAL:HG23	2.52	0.49
1:E:392:ILE:O	1:E:392:ILE:HG22	2.12	0.49
1:F:45:VAL:CG1	1:F:368:VAL:HG22	2.42	0.49
1:I:92:ASN:ND2	1:I:95:THR:H	2.10	0.49
1:I:260:PHE:CD2	1:I:260:PHE:N	2.78	0.49
1:M:66:SER:H	1:M:69:GLN:NE2	2.10	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:273:GLN:HE22	1:M:278:LYS:CE	1.98	0.49
1:N:126:LEU:HB3	1:N:262:ASN:CB	2.41	0.49
1:O:74:ARG:NH2	1:O:328:GLN:OE1	2.42	0.49
1:A:72:VAL:HG23	1:A:197:ASP:CA	2.41	0.49
1:A:165:ILE:CG2	1:A:166:GLY:N	2.72	0.49
1:A:253:GLU:HG3	1:E:113:LEU:HD22	1.94	0.49
1:B:79:ASP:C	1:B:79:ASP:OD1	2.54	0.49
1:C:114:GLY:HA3	1:C:340:THR:HG23	1.94	0.49
1:G:462:GLN:HE22	1:H:21:VAL:HB	1.77	0.49
1:K:120:HIS:CD2	1:K:222:LEU:CD1	2.94	0.49
1:L:122:PHE:O	1:L:218:CYS:HB3	2.12	0.49
1:L:216:THR:O	1:L:217:LYS:HB2	2.12	0.49
1:M:105:VAL:HG12	1:M:106:GLU:N	2.27	0.49
1:O:45:VAL:HG12	1:O:368:VAL:HG22	1.94	0.49
1:A:123:TYR:CD2	1:A:125:LYS:HB2	2.47	0.49
1:D:96:GLN:HB3	1:D:383:THR:HA	1.94	0.49
1:D:99:VAL:HG21	1:D:382:ILE:CD1	2.40	0.49
1:E:71:ARG:HA	1:E:197:ASP:OD1	2.12	0.49
1:E:74:ARG:NE	1:E:328:GLN:OE1	2.45	0.49
1:E:307:PHE:CE1	1:E:335:ASP:HB2	2.47	0.49
1:F:307:PHE:O	1:F:308:ASN:HB2	2.12	0.49
1:I:74:ARG:HH22	1:I:440:ASP:CG	2.20	0.49
1:I:111:GLN:HB3	1:I:112:PRO:CD	2.39	0.49
1:K:68:TYR:O	1:K:201:VAL:HG22	2.12	0.49
1:K:131:SER:O	1:K:132:SER:C	2.54	0.49
1:N:376:ILE:HG12	1:N:465:LEU:HD13	1.94	0.49
1:O:389:MET:O	1:O:393:GLN:HB2	2.12	0.49
1:C:475:LEU:H	1:C:475:LEU:CD2	2.21	0.49
1:D:70:TYR:CZ	1:D:201:VAL:HG12	2.47	0.49
1:E:135:ALA:HB1	1:E:282:MET:HE1	1.94	0.49
1:H:126:LEU:HB3	1:H:262:ASN:CB	2.42	0.49
1:H:326:HIS:CD2	1:H:402:ASP:OD1	2.65	0.49
1:J:52:VAL:HB	1:J:62:ILE:HB	1.92	0.49
1:N:328:GLN:O	1:N:329:LEU:HB2	2.12	0.49
1:O:122:PHE:O	1:O:218:CYS:HB3	2.12	0.49
1:A:349:GLN:HG3	1:A:360:LYS:HD2	1.93	0.49
1:C:79:ASP:C	1:C:79:ASP:OD1	2.56	0.49
1:C:208:MET:HE2	1:C:210:PHE:CE2	2.47	0.49
1:H:369:GLU:HG3	1:H:371:TYR:HE1	1.77	0.49
1:N:24:THR:HG23	1:N:320:ASN:HA	1.94	0.49
1:N:105:VAL:HG21	1:N:159:LEU:HD11	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:THR:HG23	1:A:320:ASN:HA	1.94	0.49
1:N:21:VAL:CG1	1:N:22:VAL:N	2.75	0.49
1:N:41:ARG:NH2	1:O:233:ASP:OD2	2.46	0.49
1:N:156:LEU:HG	1:N:334:VAL:HB	1.95	0.49
1:B:87:ASP:O	1:B:90:ILE:HG12	2.13	0.49
1:D:208:MET:HE2	1:D:210:PHE:CD2	2.48	0.49
1:D:232:PRO:HB2	1:D:234:TYR:CE1	2.47	0.49
1:E:107:ILE:O	1:E:107:ILE:HG22	2.13	0.49
1:G:368:VAL:HG21	1:H:169:TRP:CE2	2.48	0.49
1:I:123:TYR:HD2	1:I:125:LYS:HB2	1.77	0.49
1:J:368:VAL:CG1	1:J:369:GLU:N	2.75	0.49
1:L:105:VAL:CG1	1:L:106:GLU:N	2.72	0.49
1:M:366:ARG:HA	1:M:366:ARG:HD3	1.66	0.49
1:F:120:HIS:ND1	1:F:121:PRO:HD2	2.28	0.49
1:F:353:PRO:CG	1:F:360:LYS:NZ	2.71	0.49
1:K:35:TYR:CE2	1:K:458:LEU:HG	2.48	0.49
1:B:46:GLY:HA3	1:B:65:VAL:HG23	1.94	0.49
1:D:151:TYR:OH	1:D:221:PRO:HB2	2.13	0.49
1:F:247:PHE:CD2	1:F:322:GLY:HA2	2.47	0.49
1:G:117:LEU:HD11	1:H:293:PRO:HB3	1.94	0.49
1:H:172:GLY:C	1:H:173:THR:O	2.54	0.49
1:J:267:MET:HA	1:J:267:MET:HE2	1.94	0.49
1:K:324:CYS:SG	1:K:329:LEU:HD12	2.53	0.49
1:N:464:PRO:HA	1:N:467:ARG:NH1	2.27	0.49
1:A:111:GLN:NE2	1:A:370:GLU:OE1	2.44	0.49
1:B:70:TYR:OH	1:B:232:PRO:HD3	2.12	0.49
1:C:67:ALA:HB2	1:C:367:HIS:CE1	2.48	0.49
1:C:459:ASP:OD2	1:C:459:ASP:N	2.44	0.49
1:F:92:ASN:C	1:F:92:ASN:OD1	2.55	0.49
1:G:131:SER:O	1:G:132:SER:C	2.56	0.49
1:H:70:TYR:OH	1:H:232:PRO:HD3	2.12	0.49
1:J:242:TYR:CE2	1:J:395:MET:HG3	2.47	0.49
1:L:119:GLY:HA3	1:M:291:TYR:CE1	2.48	0.49
1:L:196:GLU:HG2	1:L:445:LEU:HB3	1.95	0.49
1:M:226:GLN:OE1	1:M:226:GLN:HA	2.11	0.49
1:N:92:ASN:O	1:N:94:GLU:N	2.46	0.49
1:B:72:VAL:HG23	1:B:197:ASP:HA	1.95	0.48
1:B:313:LEU:H	1:B:313:LEU:HD23	1.78	0.48
1:F:69:GLN:NE2	1:F:71:ARG:HH22	2.11	0.48
1:F:92:ASN:HD21	1:F:95:THR:HG23	1.78	0.48
1:F:99:VAL:HG21	1:F:382:ILE:HD11	1.93	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:123:TYR:HB2	1:F:147:VAL:HG22	1.95	0.48
1:G:92:ASN:OD1	1:G:94:GLU:HB2	2.13	0.48
1:H:141:GLU:CG	1:H:142:ASP:HB2	2.36	0.48
1:I:85:LEU:HB3	1:I:86:PRO:HD2	1.95	0.48
1:J:87:ASP:O	1:J:90:ILE:HG12	2.13	0.48
1:K:22:VAL:HG12	1:K:23:ASN:N	2.28	0.48
1:L:156:LEU:HG	1:L:334:VAL:HB	1.95	0.48
1:O:47:ASP:OD1	1:O:49:TYR:N	2.37	0.48
1:O:120:HIS:ND1	1:O:121:PRO:HD2	2.28	0.48
1:A:109:ARG:H	1:A:308:ASN:ND2	2.11	0.48
1:A:169:TRP:CE2	1:E:368:VAL:HG21	2.48	0.48
1:D:112:PRO:HB3	1:E:231:TYR:CD1	2.48	0.48
1:E:138:ASN:C	1:E:140:SER:H	2.21	0.48
1:G:92:ASN:ND2	1:G:95:THR:HG23	2.27	0.48
1:H:349:GLN:CG	1:H:360:LYS:HD2	2.43	0.48
1:I:239:ALA:O	1:I:240:ASP:C	2.55	0.48
1:J:70:TYR:OH	1:J:232:PRO:HD3	2.13	0.48
1:L:353:PRO:HG2	1:L:360:LYS:NZ	2.16	0.48
1:L:353:PRO:CG	1:L:360:LYS:HZ3	2.10	0.48
1:M:388:VAL:O	1:M:392:ILE:HG13	2.13	0.48
1:B:196:GLU:N	1:B:199:ASP:OD2	2.42	0.48
1:B:317:GLN:CD	1:B:318:GLY:N	2.71	0.48
1:C:92:ASN:O	1:C:94:GLU:N	2.45	0.48
1:C:188:LEU:CD1	1:C:213:LEU:HD21	2.44	0.48
1:F:444:LYS:HE2	1:F:444:LYS:HA	1.95	0.48
1:G:307:PHE:CE1	1:G:335:ASP:HB2	2.48	0.48
1:H:92:ASN:ND2	1:H:95:THR:HG23	2.28	0.48
1:I:141:GLU:HG2	1:I:142:ASP:H	1.75	0.48
1:I:351:PRO:C	1:I:352:VAL:HG23	2.38	0.48
1:I:397:SER:O	1:I:398:SER:C	2.56	0.48
1:J:110:GLY:HA3	1:J:370:GLU:HB3	1.95	0.48
1:A:216:THR:O	1:A:217:LYS:CB	2.61	0.48
1:B:353:PRO:HD2	1:B:360:LYS:HZ1	1.78	0.48
1:E:24:THR:HG23	1:E:320:ASN:HA	1.96	0.48
1:F:159:LEU:HD21	1:F:331:VAL:HG22	1.93	0.48
1:J:96:GLN:HB3	1:J:383:THR:HA	1.93	0.48
1:J:247:PHE:HB2	1:J:316:ALA:HB1	1.95	0.48
1:L:234:TYR:HD2	1:L:246:MET:HE1	1.77	0.48
1:N:91:TYR:HB2	1:N:96:GLN:HG3	1.95	0.48
1:O:142:ASP:OD2	1:O:144:ARG:NE	2.42	0.48
1:A:156:LEU:HG	1:A:334:VAL:HB	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:GLN:CG	1:A:360:LYS:HD2	2.43	0.48
1:G:247:PHE:CD2	1:G:322:GLY:HA2	2.48	0.48
1:H:68:TYR:O	1:H:201:VAL:HG22	2.13	0.48
1:K:96:GLN:HB3	1:K:383:THR:HA	1.96	0.48
1:K:254:GLN:HE21	1:K:298:SER:H	1.62	0.48
1:M:67:ALA:HB2	1:M:367:HIS:CE1	2.48	0.48
1:B:364:TYR:CD2	1:C:185:CYS:CB	2.93	0.48
1:D:72:VAL:HG23	1:D:197:ASP:CA	2.42	0.48
1:D:310:PRO:O	1:D:310:PRO:HG2	2.14	0.48
1:F:372:ASP:OD2	1:F:372:ASP:C	2.57	0.48
1:G:109:ARG:NH2	1:G:369:GLU:OE1	2.45	0.48
1:H:364:TYR:CG	1:I:185:CYS:HB2	2.48	0.48
1:L:140:SER:O	1:L:141:GLU:HB2	2.14	0.48
1:L:342:LEU:HD22	1:M:208:MET:SD	2.54	0.48
1:M:367:HIS:CE1	1:M:369:GLU:OE2	2.66	0.48
1:A:300:VAL:CG1	1:B:255:LEU:HD13	2.43	0.48
1:G:122:PHE:O	1:G:218:CYS:HB3	2.14	0.48
1:G:342:LEU:HD22	1:H:208:MET:SD	2.54	0.48
1:H:96:GLN:NE2	1:H:383:THR:OG1	2.47	0.48
1:K:219:GLU:C	1:K:220:VAL:HG13	2.38	0.48
1:L:111:GLN:CB	1:L:112:PRO:CD	2.91	0.48
1:A:384:LEU:HD22	1:A:389:MET:HG3	1.95	0.48
1:C:232:PRO:HB2	1:C:234:TYR:CE1	2.49	0.48
1:D:109:ARG:H	1:D:308:ASN:ND2	2.12	0.48
1:F:231:TYR:CD1	1:J:112:PRO:HB3	2.48	0.48
1:F:267:MET:SD	1:F:290:VAL:HG23	2.53	0.48
1:F:365:SER:O	1:F:366:ARG:HD3	2.14	0.48
1:K:316:ALA:CB	1:K:321:ASN:HA	2.44	0.48
1:O:151:TYR:CE2	1:O:221:PRO:HG2	2.49	0.48
1:B:41:ARG:HG2	1:B:41:ARG:O	2.13	0.48
1:F:261:TRP:CZ3	1:F:294:SER:HB3	2.48	0.48
1:G:45:VAL:CG1	1:G:368:VAL:HG22	2.44	0.48
1:I:77:LEU:HB3	1:I:78:PRO:HD2	1.96	0.48
1:I:368:VAL:CG1	1:I:369:GLU:N	2.76	0.48
1:L:368:VAL:HG12	1:L:369:GLU:N	2.23	0.48
1:C:92:ASN:C	1:C:94:GLU:H	2.22	0.48
1:C:110:GLY:HA3	1:C:370:GLU:CD	2.39	0.48
1:D:246:MET:HG3	1:D:246:MET:O	2.13	0.48
1:E:92:ASN:O	1:E:94:GLU:N	2.46	0.48
1:E:260:PHE:N	1:E:260:PHE:CD2	2.81	0.48
1:F:66:SER:H	1:F:69:GLN:NE2	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:385:THR:H	1:F:388:VAL:HB	1.79	0.48
1:I:36:HIS:ND1	1:I:36:HIS:C	2.71	0.48
1:B:311:TYR:N	1:B:311:TYR:CD1	2.82	0.47
1:C:367:HIS:CE1	1:C:369:GLU:OE2	2.67	0.47
1:L:125:LYS:HG3	1:L:261:TRP:CG	2.49	0.47
1:L:462:GLN:HE22	1:M:21:VAL:H	1.61	0.47
1:M:81:ASN:C	1:M:83:PHE:H	2.21	0.47
1:M:344:ILE:CD1	1:N:188:LEU:HD11	2.43	0.47
1:M:471:VAL:C	1:M:473:ALA:N	2.71	0.47
1:N:300:VAL:HG13	1:O:255:LEU:HD13	1.95	0.47
1:C:332:THR:O	1:C:333:VAL:HG23	2.14	0.47
1:E:59:LYS:O	1:E:60:GLN:HB3	2.13	0.47
1:F:72:VAL:HG23	1:F:197:ASP:HA	1.96	0.47
1:F:159:LEU:HD22	1:F:331:VAL:HG22	1.95	0.47
1:G:375:PHE:CD1	1:G:375:PHE:N	2.82	0.47
1:J:353:PRO:C	1:J:355:GLN:H	2.21	0.47
1:M:120:HIS:ND1	1:M:121:PRO:HD2	2.30	0.47
1:M:246:MET:O	1:M:246:MET:HG3	2.12	0.47
1:O:104:GLY:C	1:O:105:VAL:HG23	2.39	0.47
1:O:105:VAL:HG12	1:O:106:GLU:N	2.29	0.47
1:B:59:LYS:O	1:B:60:GLN:HB3	2.15	0.47
1:C:85:LEU:HD12	1:C:88:THR:HG23	1.96	0.47
1:C:98:LEU:HD21	1:C:381:THR:HG22	1.97	0.47
1:D:156:LEU:HA	1:D:250:LEU:O	2.14	0.47
1:D:300:VAL:HG13	1:E:255:LEU:HD13	1.96	0.47
1:E:151:TYR:CD2	1:E:203:THR:HB	2.48	0.47
1:E:353:PRO:HG3	1:E:360:LYS:HD2	1.95	0.47
1:I:92:ASN:C	1:I:94:GLU:H	2.22	0.47
1:K:364:TYR:CE2	1:L:185:CYS:HB2	2.48	0.47
1:M:369:GLU:HG3	1:M:371:TYR:HE1	1.78	0.47
1:A:396:ASN:C	1:A:396:ASN:ND2	2.72	0.47
1:B:105:VAL:CG1	1:B:106:GLU:N	2.75	0.47
1:B:300:VAL:HG13	1:C:255:LEU:HD13	1.97	0.47
1:C:123:TYR:HD2	1:C:125:LYS:HB2	1.80	0.47
1:C:188:LEU:N	1:C:188:LEU:HD22	2.29	0.47
1:G:24:THR:HG23	1:G:319:HIS:O	2.14	0.47
1:H:31:THR:HG23	1:H:379:LEU:O	2.15	0.47
1:H:125:LYS:HD2	1:H:261:TRP:NE1	2.30	0.47
1:I:99:VAL:HG12	1:I:100:TRP:N	2.29	0.47
1:K:353:PRO:HG2	1:K:360:LYS:NZ	2.24	0.47
1:L:159:LEU:CD2	1:L:331:VAL:HG22	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:138:ASN:HD22	1:N:140:SER:HB3	1.78	0.47
1:A:249:CYS:O	1:A:250:LEU:HD12	2.15	0.47
1:C:59:LYS:O	1:C:60:GLN:HB3	2.14	0.47
1:C:208:MET:HE2	1:C:210:PHE:CD2	2.49	0.47
1:E:396:ASN:C	1:E:396:ASN:HD22	2.21	0.47
1:G:22:VAL:CG1	1:G:23:ASN:N	2.77	0.47
1:G:138:ASN:C	1:G:140:SER:H	2.23	0.47
1:H:51:ARG:CZ	1:H:61:ASP:OD2	2.60	0.47
1:I:99:VAL:HG21	1:I:382:ILE:HD11	1.96	0.47
1:L:46:GLY:HA3	1:L:65:VAL:HG23	1.97	0.47
1:L:376:ILE:HG12	1:L:465:LEU:HD13	1.95	0.47
1:A:74:ARG:NH2	1:A:328:GLN:OE1	2.46	0.47
1:A:185:CYS:HB2	1:E:364:TYR:CG	2.49	0.47
1:A:256:PHE:CD1	1:A:256:PHE:C	2.93	0.47
1:F:396:ASN:C	1:F:396:ASN:HD22	2.22	0.47
1:G:98:LEU:HD21	1:G:381:THR:HG22	1.96	0.47
1:H:155:GLN:OE1	1:H:306:LEU:HB2	2.14	0.47
1:J:105:VAL:HG12	1:J:106:GLU:N	2.29	0.47
1:L:351:PRO:O	1:L:352:VAL:CB	2.63	0.47
1:M:446:LYS:HD3	1:M:446:LYS:HA	1.97	0.47
1:N:261:TRP:CZ3	1:N:294:SER:HB3	2.49	0.47
1:B:92:ASN:C	1:B:94:GLU:H	2.22	0.47
1:B:368:VAL:HG11	1:C:169:TRP:CZ2	2.50	0.47
1:C:372:ASP:OD2	1:C:372:ASP:C	2.57	0.47
1:E:146:ASN:C	1:E:146:ASN:OD1	2.57	0.47
1:H:52:VAL:HB	1:H:62:ILE:HB	1.96	0.47
1:H:66:SER:HB3	1:H:69:GLN:HG2	1.97	0.47
1:H:113:LEU:HD22	1:I:253:GLU:HG3	1.96	0.47
1:K:49:TYR:O	1:K:50:PHE:HB3	2.15	0.47
1:K:143:VAL:O	1:K:143:VAL:HG12	2.14	0.47
1:L:220:VAL:CG2	1:L:224:ILE:HG13	2.44	0.47
1:N:68:TYR:CE2	1:N:151:TYR:HB2	2.49	0.47
1:N:126:LEU:HG	1:N:127:ASP:OD2	2.15	0.47
1:O:111:GLN:NE2	1:O:370:GLU:OE1	2.48	0.47
1:O:125:LYS:HD2	1:O:261:TRP:CE2	2.50	0.47
1:O:140:SER:OG	1:O:141:GLU:N	2.47	0.47
1:O:196:GLU:HB3	1:O:446:LYS:O	2.15	0.47
1:A:130:GLU:OE1	1:E:258:ARG:NH1	2.48	0.47
1:B:131:SER:O	1:B:132:SER:O	2.33	0.47
1:B:391:TYR:C	1:B:393:GLN:N	2.70	0.47
1:C:159:LEU:HD22	1:C:331:VAL:HG22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:88:THR:HG22	1:I:88:THR:O	2.15	0.47
1:L:121:PRO:CG	1:M:289:CYS:SG	2.84	0.47
1:M:22:VAL:CG1	1:M:23:ASN:N	2.77	0.47
1:M:262:ASN:HD22	1:M:262:ASN:HA	1.28	0.47
1:M:300:VAL:HG13	1:N:255:LEU:HD13	1.96	0.47
1:N:109:ARG:H	1:N:308:ASN:ND2	2.12	0.47
1:N:131:SER:O	1:N:132:SER:C	2.56	0.47
1:O:267:MET:HA	1:O:267:MET:HE2	1.97	0.47
1:D:224:ILE:O	1:D:225:CYS:C	2.56	0.47
1:D:385:THR:H	1:D:388:VAL:HB	1.79	0.47
1:F:22:VAL:HG12	1:F:23:ASN:N	2.30	0.47
1:F:373:LEU:N	1:F:373:LEU:HD23	2.29	0.47
1:H:273:GLN:HE22	1:H:278:LYS:CE	1.95	0.47
1:I:24:THR:CG2	1:I:320:ASN:HA	2.45	0.47
1:I:232:PRO:HB2	1:I:234:TYR:CE1	2.50	0.47
1:K:120:HIS:CD2	1:K:222:LEU:HD13	2.50	0.47
1:K:369:GLU:CG	1:K:371:TYR:HE1	2.27	0.47
1:M:261:TRP:CZ3	1:M:294:SER:HB3	2.50	0.47
1:N:74:ARG:HH22	1:N:440:ASP:CG	2.23	0.47
1:A:126:LEU:HB3	1:A:262:ASN:CB	2.45	0.47
1:A:159:LEU:CD2	1:A:331:VAL:HG22	2.44	0.47
1:A:165:ILE:N	1:A:165:ILE:CD1	2.79	0.47
1:A:283:ARG:HD2	1:E:142:ASP:CG	2.40	0.47
1:B:390:SER:O	1:B:393:GLN:HB3	2.14	0.47
1:E:45:VAL:C	1:E:65:VAL:HG21	2.40	0.47
1:E:216:THR:O	1:E:217:LYS:CB	2.56	0.47
1:G:159:LEU:HD22	1:G:331:VAL:HG22	1.96	0.47
1:J:214:GLN:OE1	1:J:219:GLU:HB2	2.15	0.47
1:K:45:VAL:HG12	1:K:368:VAL:HG22	1.97	0.47
1:L:96:GLN:HB3	1:L:383:THR:HA	1.96	0.47
1:L:196:GLU:N	1:L:199:ASP:OD2	2.48	0.47
1:N:140:SER:O	1:N:141:GLU:HB2	2.14	0.47
1:N:316:ALA:HB2	1:N:321:ASN:HA	1.97	0.47
1:O:108:GLY:HA2	1:O:308:ASN:HD22	1.80	0.47
1:B:135:ALA:O	1:B:136:THR:HG23	2.15	0.46
1:C:254:GLN:O	1:C:255:LEU:HB3	2.15	0.46
1:D:369:GLU:HG3	1:D:371:TYR:CE1	2.50	0.46
1:G:366:ARG:HA	1:G:366:ARG:HD3	1.81	0.46
1:H:109:ARG:NH2	1:H:369:GLU:OE1	2.47	0.46
1:J:127:ASP:OD1	1:J:127:ASP:N	2.45	0.46
1:L:68:TYR:CZ	1:L:151:TYR:HB2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:108:GLY:HA2	1:L:308:ASN:ND2	2.31	0.46
1:O:316:ALA:CB	1:O:321:ASN:HA	2.45	0.46
1:D:324:CYS:HB3	1:D:328:GLN:O	2.15	0.46
1:D:372:ASP:C	1:D:372:ASP:OD2	2.58	0.46
1:F:283:ARG:HD2	1:J:142:ASP:CG	2.40	0.46
1:K:188:LEU:N	1:K:188:LEU:CD2	2.78	0.46
1:M:125:LYS:HD2	1:M:261:TRP:CE2	2.50	0.46
1:N:113:LEU:HD22	1:O:253:GLU:HG3	1.98	0.46
1:A:467:ARG:O	1:A:471:VAL:HG23	2.15	0.46
1:A:475:LEU:H	1:A:475:LEU:CD2	2.24	0.46
1:B:141:GLU:HG2	1:B:141:GLU:O	2.15	0.46
1:C:125:LYS:HG3	1:C:261:TRP:CG	2.50	0.46
1:C:366:ARG:HA	1:C:366:ARG:HD3	1.77	0.46
1:E:196:GLU:N	1:E:199:ASP:OD2	2.40	0.46
1:F:185:CYS:HB2	1:J:364:TYR:CE2	2.50	0.46
1:G:300:VAL:HG13	1:H:255:LEU:CD1	2.43	0.46
1:I:369:GLU:CG	1:I:371:TYR:HE1	2.28	0.46
1:J:86:PRO:HB3	1:J:458:LEU:HD11	1.98	0.46
1:M:216:THR:O	1:M:217:LYS:HB2	2.15	0.46
1:O:34:PHE:CE2	1:O:378:GLN:HB2	2.49	0.46
1:A:169:TRP:CZ2	1:E:368:VAL:HG11	2.50	0.46
1:B:367:HIS:CE1	1:B:369:GLU:OE2	2.68	0.46
1:B:385:THR:O	1:B:389:MET:HE3	2.15	0.46
1:C:364:TYR:CD2	1:D:185:CYS:HB2	2.51	0.46
1:D:332:THR:C	1:D:333:VAL:HG23	2.40	0.46
1:H:143:VAL:O	1:H:143:VAL:HG12	2.15	0.46
1:H:325:TRP:O	1:H:326:HIS:HB2	2.15	0.46
1:J:99:VAL:CG2	1:J:382:ILE:CD1	2.94	0.46
1:K:353:PRO:CG	1:K:360:LYS:NZ	2.77	0.46
1:K:366:ARG:HD3	1:K:366:ARG:HA	1.75	0.46
1:N:69:GLN:NE2	1:N:71:ARG:HH22	2.14	0.46
1:E:70:TYR:OH	1:E:232:PRO:HD3	2.16	0.46
1:G:123:TYR:CB	1:G:147:VAL:HG22	2.46	0.46
1:H:109:ARG:N	1:H:308:ASN:HD21	2.11	0.46
1:H:320:ASN:C	1:H:320:ASN:OD1	2.58	0.46
1:I:454:GLU:C	1:I:455:LYS:HG2	2.40	0.46
1:J:22:VAL:HG12	1:J:23:ASN:N	2.31	0.46
1:K:138:ASN:ND2	1:K:140:SER:HB3	2.31	0.46
1:L:22:VAL:HG12	1:L:23:ASN:N	2.30	0.46
1:L:200:MET:HE2	1:L:223:ASP:O	2.15	0.46
1:M:349:GLN:CG	1:M:360:LYS:HD2	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:356:TYR:CD2	1:O:142:ASP:OD2	2.69	0.46
1:A:109:ARG:H	1:A:308:ASN:HD21	1.62	0.46
1:A:367:HIS:CE1	1:A:369:GLU:OE2	2.69	0.46
1:B:369:GLU:HG3	1:B:371:TYR:CE1	2.48	0.46
1:C:138:ASN:C	1:C:140:SER:H	2.24	0.46
1:C:156:LEU:HA	1:C:250:LEU:O	2.15	0.46
1:E:36:HIS:ND1	1:E:36:HIS:C	2.74	0.46
1:G:211:SER:HA	1:G:226:GLN:OE1	2.15	0.46
1:H:332:THR:C	1:H:333:VAL:HG23	2.40	0.46
1:I:208:MET:HE3	1:I:213:LEU:HD23	1.98	0.46
1:N:216:THR:HG22	1:N:218:CYS:HB2	1.96	0.46
1:N:262:ASN:HD22	1:N:262:ASN:HA	1.33	0.46
1:D:92:ASN:HD21	1:D:94:GLU:HB2	1.81	0.46
1:E:368:VAL:HG12	1:E:369:GLU:N	2.27	0.46
1:E:459:ASP:OD2	1:E:459:ASP:N	2.48	0.46
1:F:109:ARG:H	1:F:308:ASN:ND2	2.14	0.46
1:G:138:ASN:ND2	1:G:140:SER:HB3	2.30	0.46
1:H:267:MET:SD	1:H:290:VAL:HG23	2.55	0.46
1:H:329:LEU:HD23	1:H:329:LEU:C	2.41	0.46
1:J:367:HIS:HE1	1:J:369:GLU:OE2	1.99	0.46
1:K:156:LEU:HA	1:K:250:LEU:O	2.16	0.46
1:L:267:MET:SD	1:L:290:VAL:HG23	2.56	0.46
1:O:36:HIS:ND1	1:O:37:ALA:N	2.64	0.46
1:O:71:ARG:HG3	1:O:371:TYR:OH	2.16	0.46
1:A:131:SER:O	1:A:132:SER:C	2.59	0.46
1:A:255:LEU:HD13	1:E:300:VAL:HG13	1.98	0.46
1:A:311:TYR:CD1	1:A:311:TYR:N	2.84	0.46
1:C:216:THR:HG22	1:C:218:CYS:HB2	1.96	0.46
1:D:143:VAL:O	1:D:143:VAL:HG12	2.16	0.46
1:E:159:LEU:CD2	1:E:331:VAL:HG22	2.44	0.46
1:E:395:MET:HE3	1:E:399:ILE:HD12	1.98	0.46
1:F:24:THR:HG21	1:F:320:ASN:HA	1.96	0.46
1:F:130:GLU:OE1	1:J:259:HIS:HE1	1.98	0.46
1:H:369:GLU:HG3	1:H:371:TYR:CE1	2.51	0.46
1:I:440:ASP:HB3	1:I:443:ASP:CG	2.41	0.46
1:J:107:ILE:N	1:J:107:ILE:HD12	2.31	0.46
1:K:71:ARG:HA	1:K:197:ASP:OD1	2.16	0.46
1:L:71:ARG:HG3	1:L:371:TYR:OH	2.16	0.46
1:L:244:ASP:OD1	1:L:320:ASN:ND2	2.46	0.46
1:L:258:ARG:HG3	1:L:259:HIS:ND1	2.31	0.46
1:M:43:LEU:HD12	1:M:369:GLU:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:382:ILE:HD12	1:M:403:TRP:HH2	1.80	0.46
1:A:117:LEU:HG	1:B:293:PRO:HD3	1.98	0.46
1:A:185:CYS:HB2	1:E:364:TYR:CD2	2.50	0.46
1:A:454:GLU:C	1:A:455:LYS:HG2	2.41	0.46
1:B:237:MET:HB3	1:B:246:MET:HG2	1.97	0.46
1:D:369:GLU:CG	1:D:371:TYR:HE1	2.29	0.46
1:E:96:GLN:HB3	1:E:383:THR:HA	1.97	0.46
1:F:42:LEU:H	1:F:42:LEU:HG	1.47	0.46
1:F:97:ARG:O	1:F:98:LEU:HD23	2.15	0.46
1:G:58:ASN:CA	1:H:178:ARG:NH1	2.77	0.46
1:H:385:THR:H	1:H:388:VAL:HB	1.81	0.46
1:I:79:ASP:O	1:I:83:PHE:HB2	2.16	0.46
1:I:92:ASN:ND2	1:I:95:THR:HG23	2.30	0.46
1:K:36:HIS:ND1	1:K:37:ALA:N	2.64	0.46
1:K:475:LEU:HD23	1:K:475:LEU:N	2.19	0.46
1:L:220:VAL:HG21	1:L:224:ILE:HG13	1.98	0.46
1:L:260:PHE:N	1:L:260:PHE:CD2	2.83	0.46
1:M:258:ARG:HG3	1:M:259:HIS:ND1	2.30	0.46
1:B:475:LEU:HD23	1:B:475:LEU:H	1.81	0.46
1:D:24:THR:HG23	1:D:320:ASN:HA	1.98	0.46
1:F:232:PRO:HB2	1:F:234:TYR:CE1	2.51	0.46
1:O:66:SER:H	1:O:69:GLN:NE2	2.14	0.46
1:A:360:LYS:HE2	1:A:361:PHE:CE1	2.51	0.45
1:A:368:VAL:CG1	1:B:169:TRP:CZ2	2.99	0.45
1:E:308:ASN:HD22	1:E:308:ASN:HA	1.51	0.45
1:F:47:ASP:OD1	1:F:49:TYR:N	2.36	0.45
1:F:112:PRO:HB3	1:G:231:TYR:CG	2.51	0.45
1:F:165:ILE:N	1:F:165:ILE:HD12	2.31	0.45
1:F:389:MET:HG2	1:F:400:LEU:HD21	1.98	0.45
1:F:396:ASN:O	1:F:399:ILE:HG13	2.15	0.45
1:G:148:SER:HB3	1:H:291:TYR:CD2	2.51	0.45
1:J:99:VAL:HG11	1:J:323:VAL:CG1	2.47	0.45
1:M:52:VAL:HB	1:M:62:ILE:HB	1.98	0.45
1:N:368:VAL:CG1	1:O:169:TRP:CZ2	2.95	0.45
1:O:375:PHE:O	1:O:376:ILE:HD13	2.16	0.45
1:A:185:CYS:HB2	1:E:364:TYR:CD1	2.51	0.45
1:A:314:HIS:ND1	1:A:314:HIS:N	2.63	0.45
1:B:163:PRO:HD3	1:B:330:PHE:CZ	2.51	0.45
1:D:262:ASN:HD22	1:D:262:ASN:HA	1.37	0.45
1:H:72:VAL:HG23	1:H:197:ASP:CA	2.43	0.45
1:I:159:LEU:HB2	1:I:248:PHE:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:333:VAL:HG11	1:J:371:TYR:HE2	1.81	0.45
1:N:111:GLN:CB	1:N:112:PRO:CD	2.90	0.45
1:N:120:HIS:CD2	1:N:222:LEU:HD13	2.51	0.45
1:O:99:VAL:HG21	1:O:382:ILE:HD11	1.98	0.45
1:A:135:ALA:HB1	1:A:282:MET:HE1	1.99	0.45
1:A:382:ILE:HD12	1:A:403:TRP:CH2	2.51	0.45
1:D:323:VAL:HG11	1:D:325:TRP:CZ2	2.51	0.45
1:H:165:ILE:O	1:H:237:MET:HE2	2.17	0.45
1:I:69:GLN:HE21	1:I:71:ARG:HH12	1.62	0.45
1:K:210:PHE:HE1	1:K:229:CYS:HG	1.64	0.45
1:L:111:GLN:CB	1:L:112:PRO:HD2	2.33	0.45
1:M:90:ILE:HD12	1:M:90:ILE:HG23	1.75	0.45
1:A:114:GLY:HA3	1:A:340:THR:HG23	1.99	0.45
1:B:464:PRO:HA	1:B:467:ARG:NH1	2.32	0.45
1:H:125:LYS:HG3	1:H:261:TRP:CD2	2.51	0.45
1:I:92:ASN:O	1:I:92:ASN:CG	2.58	0.45
1:I:349:GLN:CG	1:I:360:LYS:HD2	2.45	0.45
1:J:36:HIS:ND1	1:J:36:HIS:C	2.74	0.45
1:J:293:PRO:HG2	1:J:293:PRO:O	2.16	0.45
1:J:454:GLU:C	1:J:455:LYS:HG2	2.41	0.45
1:M:357:ASP:O	1:M:358:ALA:C	2.60	0.45
1:O:156:LEU:C	1:O:156:LEU:HD12	2.41	0.45
1:O:454:GLU:C	1:O:455:LYS:HG2	2.40	0.45
1:A:74:ARG:NE	1:A:328:GLN:OE1	2.45	0.45
1:A:188:LEU:HD11	1:E:344:ILE:CD1	2.46	0.45
1:A:364:TYR:CE2	1:B:185:CYS:HB2	2.51	0.45
1:C:109:ARG:H	1:C:308:ASN:ND2	2.15	0.45
1:D:308:ASN:HD22	1:D:308:ASN:HA	1.56	0.45
1:D:465:LEU:O	1:D:465:LEU:HD22	2.17	0.45
1:E:24:THR:CG2	1:E:320:ASN:HA	2.46	0.45
1:E:105:VAL:CG1	1:E:106:GLU:N	2.74	0.45
1:F:117:LEU:CD1	1:G:293:PRO:HB3	2.45	0.45
1:G:36:HIS:ND1	1:G:36:HIS:C	2.75	0.45
1:H:22:VAL:CG1	1:H:23:ASN:N	2.79	0.45
1:H:126:LEU:HB3	1:H:262:ASN:HB3	1.99	0.45
1:J:43:LEU:HA	1:J:43:LEU:HD12	1.77	0.45
1:L:74:ARG:NE	1:L:328:GLN:OE1	2.46	0.45
1:M:368:VAL:CG1	1:M:369:GLU:N	2.77	0.45
1:N:22:VAL:CG1	1:N:23:ASN:N	2.79	0.45
1:O:74:ARG:HG3	1:O:330:PHE:CE2	2.52	0.45
1:A:126:LEU:HD13	1:A:264:ALA:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:TYR:OH	1:B:221:PRO:HB2	2.16	0.45
1:E:43:LEU:CD1	1:E:370:GLU:HB2	2.47	0.45
1:I:81:ASN:C	1:I:83:PHE:H	2.24	0.45
1:I:396:ASN:HD22	1:I:396:ASN:C	2.25	0.45
1:J:140:SER:OG	1:J:141:GLU:N	2.43	0.45
1:K:372:ASP:C	1:K:372:ASP:OD2	2.59	0.45
1:N:62:ILE:HG23	1:N:62:ILE:HD12	1.67	0.45
1:N:152:LYS:HE3	1:N:253:GLU:HB2	1.99	0.45
1:C:52:VAL:HB	1:C:62:ILE:HB	1.98	0.45
1:D:366:ARG:HD3	1:D:366:ARG:HA	1.71	0.45
1:D:385:THR:O	1:D:389:MET:HE3	2.16	0.45
1:E:74:ARG:HH22	1:E:440:ASP:CG	2.25	0.45
1:F:21:VAL:HB	1:J:462:GLN:HE22	1.82	0.45
1:H:307:PHE:HE1	1:H:335:ASP:CB	2.25	0.45
1:J:247:PHE:CZ	1:J:322:GLY:HA2	2.51	0.45
1:J:249:CYS:O	1:J:250:LEU:HD12	2.17	0.45
1:J:451:ASP:OD2	1:J:453:LYS:HD2	2.16	0.45
1:M:308:ASN:HD22	1:M:308:ASN:HA	1.58	0.45
1:N:68:TYR:CZ	1:N:151:TYR:HB2	2.51	0.45
1:A:92:ASN:C	1:A:94:GLU:H	2.24	0.45
1:A:180:LEU:HD12	1:A:180:LEU:HA	1.83	0.45
1:C:213:LEU:HA	1:C:213:LEU:HD12	1.73	0.45
1:D:68:TYR:CE2	1:D:151:TYR:HB2	2.52	0.45
1:D:70:TYR:OH	1:D:232:PRO:HD3	2.17	0.45
1:D:306:LEU:O	1:D:311:TYR:OH	2.30	0.45
1:G:220:VAL:HG23	1:G:225:CYS:HA	1.98	0.45
1:G:300:VAL:CG1	1:H:255:LEU:CD1	2.92	0.45
1:G:464:PRO:HA	1:G:467:ARG:NH1	2.32	0.45
1:H:35:TYR:CE2	1:H:458:LEU:HG	2.52	0.45
1:H:464:PRO:O	1:H:465:LEU:C	2.58	0.45
1:I:78:PRO:HG2	1:I:100:TRP:HE1	1.81	0.45
1:I:267:MET:HE2	1:I:267:MET:N	2.31	0.45
1:I:349:GLN:HG2	1:I:360:LYS:CD	2.45	0.45
1:J:111:GLN:CB	1:J:112:PRO:HD2	2.41	0.45
1:J:165:ILE:HD12	1:J:165:ILE:N	2.32	0.45
1:K:123:TYR:HD2	1:K:125:LYS:HB2	1.82	0.45
1:L:113:LEU:HD22	1:M:253:GLU:HG3	1.98	0.45
1:L:126:LEU:CB	1:L:262:ASN:HB3	2.33	0.45
1:N:109:ARG:NH1	1:N:371:TYR:CE1	2.85	0.45
1:E:262:ASN:HD22	1:E:262:ASN:HA	1.38	0.45
1:E:267:MET:SD	1:E:290:VAL:HG23	2.57	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:LEU:HB3	1:F:78:PRO:HD2	1.99	0.45
1:F:216:THR:HG22	1:F:218:CYS:N	2.32	0.45
1:H:344:ILE:CD1	1:I:188:LEU:HD11	2.46	0.45
1:K:353:PRO:HD2	1:K:360:LYS:CE	2.47	0.45
1:B:151:TYR:CD2	1:B:203:THR:HB	2.52	0.45
1:D:216:THR:O	1:D:217:LYS:CB	2.65	0.45
1:D:364:TYR:CZ	1:E:268:GLY:HA3	2.51	0.45
1:E:239:ALA:O	1:E:240:ASP:C	2.60	0.45
1:F:384:LEU:C	1:F:389:MET:HE2	2.42	0.45
1:G:150:ASP:O	1:G:296:SER:HA	2.16	0.45
1:G:200:MET:HE2	1:G:223:ASP:O	2.16	0.45
1:J:71:ARG:HA	1:J:197:ASP:OD1	2.17	0.45
1:J:108:GLY:HA2	1:J:308:ASN:ND2	2.32	0.45
1:L:300:VAL:HG13	1:M:255:LEU:HD13	1.99	0.45
1:O:92:ASN:HA	1:O:93:PRO:HD2	1.63	0.45
1:O:96:GLN:HB3	1:O:383:THR:HA	1.99	0.45
1:B:148:SER:HB3	1:C:291:TYR:CD2	2.53	0.44
1:C:111:GLN:HB3	1:C:112:PRO:CD	2.43	0.44
1:F:226:GLN:HG3	1:G:275:LEU:HD23	1.99	0.44
1:F:235:LEU:HD12	1:J:370:GLU:OE2	2.16	0.44
1:H:262:ASN:HD22	1:H:262:ASN:HA	1.34	0.44
1:H:475:LEU:H	1:H:475:LEU:CD2	2.28	0.44
1:I:136:THR:C	1:I:137:SER:O	2.58	0.44
1:I:316:ALA:CB	1:I:321:ASN:HA	2.47	0.44
1:K:314:HIS:ND1	1:K:314:HIS:N	2.63	0.44
1:L:329:LEU:C	1:L:329:LEU:HD23	2.42	0.44
1:M:96:GLN:HB3	1:M:383:THR:HA	1.99	0.44
1:N:52:VAL:HB	1:N:62:ILE:HB	1.99	0.44
1:O:71:ARG:HA	1:O:197:ASP:OD1	2.17	0.44
1:O:314:HIS:C	1:O:315:LYS:HG3	2.42	0.44
1:A:122:PHE:HB3	1:A:144:ARG:HD2	2.00	0.44
1:D:135:ALA:O	1:D:136:THR:CG2	2.65	0.44
1:F:244:ASP:OD1	1:F:320:ASN:ND2	2.48	0.44
1:F:353:PRO:CD	1:F:360:LYS:HZ1	2.30	0.44
1:G:376:ILE:HG12	1:G:465:LEU:HD13	1.97	0.44
1:I:109:ARG:H	1:I:308:ASN:HD21	1.65	0.44
1:I:329:LEU:C	1:I:329:LEU:HD23	2.43	0.44
1:I:353:PRO:CD	1:I:360:LYS:HZ3	2.29	0.44
1:J:119:GLY:HA2	1:J:148:SER:HA	1.98	0.44
1:M:255:LEU:HA	1:M:297:GLY:HA2	2.00	0.44
1:O:22:VAL:CG1	1:O:23:ASN:N	2.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:193:THR:HG21	1:O:230:LYS:HD3	2.00	0.44
1:O:329:LEU:HD23	1:O:329:LEU:O	2.17	0.44
1:A:255:LEU:HD13	1:E:300:VAL:CG1	2.48	0.44
1:C:111:GLN:NE2	1:C:370:GLU:OE1	2.50	0.44
1:C:150:ASP:O	1:C:296:SER:HA	2.17	0.44
1:F:59:LYS:HD3	1:G:178:ARG:HG3	2.00	0.44
1:F:233:ASP:C	1:F:233:ASP:OD1	2.60	0.44
1:G:42:LEU:HB3	1:G:448:TRP:CZ2	2.52	0.44
1:G:66:SER:O	1:G:69:GLN:HG2	2.17	0.44
1:G:368:VAL:CG1	1:H:169:TRP:CZ2	2.95	0.44
1:H:163:PRO:HD3	1:H:330:PHE:CZ	2.52	0.44
1:H:300:VAL:CG1	1:I:255:LEU:HD13	2.47	0.44
1:I:341:ASN:HD22	1:I:341:ASN:HA	1.59	0.44
1:J:267:MET:SD	1:J:290:VAL:HG23	2.57	0.44
1:K:349:GLN:HG3	1:K:360:LYS:HD2	2.00	0.44
1:K:384:LEU:C	1:K:389:MET:HE2	2.42	0.44
1:M:205:TYR:CD2	1:M:220:VAL:HG12	2.53	0.44
1:A:376:ILE:HG12	1:A:465:LEU:HD13	1.99	0.44
1:C:313:LEU:N	1:C:313:LEU:HD23	2.33	0.44
1:D:307:PHE:O	1:D:309:LYS:HG3	2.18	0.44
1:E:98:LEU:HD13	1:E:379:LEU:HD11	1.99	0.44
1:E:368:VAL:CG1	1:E:369:GLU:N	2.78	0.44
1:F:216:THR:HG22	1:F:218:CYS:H	1.81	0.44
1:I:262:ASN:HD22	1:I:262:ASN:HA	1.45	0.44
1:J:314:HIS:O	1:J:315:LYS:HG3	2.17	0.44
1:K:385:THR:OG1	1:K:388:VAL:HG23	2.17	0.44
1:L:31:THR:HG23	1:L:379:LEU:O	2.18	0.44
1:M:71:ARG:HA	1:M:197:ASP:OD1	2.17	0.44
1:M:349:GLN:HG3	1:M:360:LYS:HD2	2.00	0.44
1:D:151:TYR:CD2	1:D:203:THR:HB	2.53	0.44
1:D:316:ALA:CB	1:D:321:ASN:HA	2.47	0.44
1:F:68:TYR:CZ	1:F:151:TYR:HB2	2.52	0.44
1:H:108:GLY:HA2	1:H:308:ASN:HD22	1.83	0.44
1:H:208:MET:HE2	1:H:210:PHE:CD2	2.51	0.44
1:I:70:TYR:CE1	1:I:201:VAL:HG12	2.51	0.44
1:I:148:SER:HB3	1:J:291:TYR:CD2	2.52	0.44
1:I:460:LEU:HB2	1:I:470:LEU:HD11	2.00	0.44
1:J:150:ASP:O	1:J:296:SER:HA	2.17	0.44
1:O:138:ASN:C	1:O:140:SER:H	2.25	0.44
1:O:200:MET:HE2	1:O:223:ASP:O	2.17	0.44
1:A:57:GLY:C	1:B:184:ASP:OD2	2.59	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:THR:HG23	1:C:319:HIS:O	2.17	0.44
1:C:96:GLN:HB3	1:C:383:THR:HA	1.99	0.44
1:C:375:PHE:O	1:C:376:ILE:HD13	2.17	0.44
1:D:66:SER:HB3	1:D:69:GLN:HG2	1.99	0.44
1:D:126:LEU:HB3	1:D:262:ASN:CB	2.43	0.44
1:F:52:VAL:O	1:F:53:PRO:C	2.61	0.44
1:F:178:ARG:HG3	1:J:59:LYS:HD2	1.99	0.44
1:I:115:VAL:HG13	1:J:255:LEU:HD21	1.99	0.44
1:K:87:ASP:HB3	1:K:90:ILE:HD11	1.99	0.44
1:L:68:TYR:CE2	1:L:151:TYR:HB2	2.52	0.44
1:O:68:TYR:CE2	1:O:151:TYR:HB2	2.53	0.44
1:O:72:VAL:H	1:O:197:ASP:HB2	1.82	0.44
1:O:214:GLN:OE1	1:O:219:GLU:HB2	2.17	0.44
1:O:279:GLY:O	1:O:284:ALA:HA	2.18	0.44
1:O:365:SER:O	1:O:366:ARG:HD3	2.18	0.44
1:A:317:GLN:CG	1:A:318:GLY:N	2.80	0.44
1:C:68:TYR:CZ	1:C:151:TYR:HB2	2.52	0.44
1:E:366:ARG:HD3	1:E:366:ARG:HA	1.64	0.44
1:F:311:TYR:CD1	1:F:311:TYR:N	2.86	0.44
1:G:112:PRO:HB3	1:H:231:TYR:CD1	2.52	0.44
1:K:372:ASP:C	1:K:373:LEU:HD23	2.43	0.44
1:L:306:LEU:O	1:L:311:TYR:OH	2.36	0.44
1:M:124:ASN:N	1:M:218:CYS:O	2.42	0.44
1:M:235:LEU:HA	1:M:235:LEU:HD23	1.81	0.44
1:N:60:GLN:HG3	1:N:61:ASP:N	2.33	0.44
1:O:399:ILE:HG21	1:O:399:ILE:HD13	1.67	0.44
1:A:57:GLY:HA3	1:B:184:ASP:CG	2.25	0.44
1:B:62:ILE:HA	1:B:63:PRO:HD3	1.80	0.44
1:D:120:HIS:CD2	1:D:222:LEU:CD1	3.01	0.44
1:E:50:PHE:CD1	1:E:50:PHE:C	2.96	0.44
1:G:81:ASN:O	1:G:83:PHE:N	2.49	0.44
1:G:92:ASN:HA	1:G:93:PRO:HD2	1.75	0.44
1:K:244:ASP:OD1	1:K:320:ASN:ND2	2.34	0.44
1:L:91:TYR:CD2	1:L:91:TYR:C	2.95	0.44
1:M:43:LEU:HD12	1:M:43:LEU:HA	1.80	0.44
1:N:105:VAL:HG12	1:N:106:GLU:H	1.80	0.44
1:N:220:VAL:HG23	1:N:225:CYS:HA	1.99	0.44
1:N:367:HIS:HE1	1:N:369:GLU:OE2	2.00	0.44
1:A:77:LEU:N	1:A:77:LEU:HD23	2.32	0.44
1:A:300:VAL:HG13	1:B:255:LEU:HD13	2.00	0.44
1:B:151:TYR:CE2	1:B:221:PRO:HG2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:LEU:CD1	1:C:370:GLU:HB2	2.47	0.44
1:C:72:VAL:HG23	1:C:197:ASP:HA	2.00	0.44
1:C:117:LEU:HD11	1:D:293:PRO:HB3	2.00	0.44
1:D:214:GLN:OE1	1:D:219:GLU:HB2	2.18	0.44
1:D:258:ARG:HG3	1:D:259:HIS:ND1	2.33	0.44
1:F:157:CYS:HA	1:F:332:THR:O	2.18	0.44
1:F:260:PHE:HB3	1:J:117:LEU:HD13	2.00	0.44
1:H:51:ARG:NH2	1:H:61:ASP:OD1	2.51	0.44
1:H:374:GLN:OE1	1:H:464:PRO:HG2	2.18	0.44
1:K:96:GLN:HB3	1:K:96:GLN:HE21	1.45	0.44
1:K:272:PRO:HB2	1:K:275:LEU:HG	1.98	0.44
1:L:92:ASN:HA	1:L:93:PRO:HD2	1.60	0.44
1:L:219:GLU:C	1:L:220:VAL:HG13	2.42	0.44
1:N:316:ALA:HB3	1:N:321:ASN:HA	1.98	0.44
1:O:48:PRO:HG2	1:O:49:TYR:CD2	2.53	0.44
1:O:316:ALA:HB3	1:O:321:ASN:HA	1.99	0.44
1:O:324:CYS:HB3	1:O:328:GLN:O	2.18	0.44
1:A:329:LEU:C	1:A:329:LEU:HD23	2.42	0.43
1:A:351:PRO:O	1:A:352:VAL:HB	2.18	0.43
1:A:382:ILE:HG21	1:A:382:ILE:HD13	1.70	0.43
1:D:344:ILE:CD1	1:E:188:LEU:HD11	2.48	0.43
1:E:104:GLY:C	1:E:105:VAL:HG23	2.43	0.43
1:F:213:LEU:HA	1:F:213:LEU:HD12	1.79	0.43
1:G:231:TYR:O	1:G:232:PRO:C	2.60	0.43
1:J:310:PRO:O	1:J:310:PRO:HG2	2.17	0.43
1:L:316:ALA:HB3	1:L:321:ASN:HA	2.00	0.43
1:O:347:SER:HA	1:O:361:PHE:HA	2.00	0.43
1:A:385:THR:H	1:A:388:VAL:HB	1.83	0.43
1:B:96:GLN:HE21	1:B:96:GLN:HB3	1.49	0.43
1:B:123:TYR:HD2	1:B:125:LYS:HB2	1.83	0.43
1:B:385:THR:H	1:B:388:VAL:HB	1.83	0.43
1:D:369:GLU:HG3	1:D:371:TYR:HE1	1.83	0.43
1:D:395:MET:HE3	1:D:399:ILE:HD12	1.98	0.43
1:G:467:ARG:HD2	1:H:317:GLN:O	2.18	0.43
1:I:47:ASP:OD1	1:I:48:PRO:N	2.51	0.43
1:I:67:ALA:HB2	1:I:367:HIS:CE1	2.52	0.43
1:J:104:GLY:C	1:J:105:VAL:HG23	2.42	0.43
1:J:254:GLN:HE21	1:J:298:SER:H	1.65	0.43
1:J:311:TYR:N	1:J:311:TYR:CD1	2.85	0.43
1:K:112:PRO:HB3	1:L:231:TYR:CD1	2.52	0.43
1:K:144:ARG:O	1:L:283:ARG:NH1	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:372:ASP:OD2	1:O:372:ASP:O	2.35	0.43
1:B:465:LEU:HA	1:B:465:LEU:HD23	1.70	0.43
1:G:117:LEU:HD13	1:H:260:PHE:HB3	1.99	0.43
1:G:384:LEU:C	1:G:389:MET:HE2	2.43	0.43
1:H:300:VAL:HG13	1:H:300:VAL:O	2.19	0.43
1:K:249:CYS:O	1:K:250:LEU:HD12	2.19	0.43
1:K:255:LEU:HD13	1:O:300:VAL:CG1	2.48	0.43
1:L:237:MET:HB3	1:L:246:MET:HG2	2.00	0.43
1:M:36:HIS:ND1	1:M:37:ALA:N	2.67	0.43
1:M:216:THR:HG22	1:M:218:CYS:HB2	2.01	0.43
1:N:165:ILE:O	1:N:237:MET:HE2	2.19	0.43
1:A:74:ARG:HH22	1:A:440:ASP:CG	2.26	0.43
1:A:261:TRP:CZ3	1:A:294:SER:HB3	2.53	0.43
1:A:310:PRO:O	1:A:310:PRO:HG2	2.18	0.43
1:B:111:GLN:HB3	1:B:112:PRO:CD	2.48	0.43
1:B:143:VAL:O	1:B:143:VAL:HG12	2.17	0.43
1:C:231:TYR:O	1:C:232:PRO:C	2.61	0.43
1:D:98:LEU:CD2	1:D:381:THR:HG22	2.48	0.43
1:E:92:ASN:OD1	1:E:94:GLU:HB2	2.18	0.43
1:E:350:SER:HB3	1:E:351:PRO:HD3	1.99	0.43
1:F:24:THR:HG23	1:F:319:HIS:O	2.18	0.43
1:F:134:ALA:C	1:F:135:ALA:O	2.61	0.43
1:F:169:TRP:HZ2	1:J:368:VAL:HG11	1.83	0.43
1:F:306:LEU:HA	1:F:306:LEU:HD12	1.58	0.43
1:G:176:LYS:HB2	1:G:176:LYS:NZ	2.33	0.43
1:I:224:ILE:HD13	1:I:224:ILE:HG21	1.82	0.43
1:I:360:LYS:HE2	1:I:361:PHE:CE1	2.54	0.43
1:J:110:GLY:O	1:J:111:GLN:O	2.37	0.43
1:J:325:TRP:CD2	1:J:399:ILE:HD13	2.53	0.43
1:K:68:TYR:CE2	1:K:151:TYR:HB2	2.52	0.43
1:K:126:LEU:HB3	1:K:262:ASN:CB	2.45	0.43
1:L:24:THR:HG23	1:L:320:ASN:HA	2.01	0.43
1:N:83:PHE:CG	1:N:84:GLY:N	2.87	0.43
1:N:324:CYS:SG	1:N:329:LEU:HD12	2.58	0.43
1:A:71:ARG:HA	1:A:197:ASP:OD1	2.17	0.43
1:C:262:ASN:HD22	1:C:262:ASN:HA	1.47	0.43
1:D:107:ILE:HD12	1:D:107:ILE:N	2.33	0.43
1:E:376:ILE:HG12	1:E:465:LEU:HD13	2.00	0.43
1:H:244:ASP:OD1	1:H:320:ASN:ND2	2.51	0.43
1:I:123:TYR:CG	1:I:147:VAL:CG2	3.01	0.43
1:I:311:TYR:CD1	1:I:311:TYR:N	2.86	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:316:ALA:HB3	1:I:321:ASN:HA	2.00	0.43
1:I:366:ARG:HD3	1:I:366:ARG:HA	1.55	0.43
1:J:261:TRP:CZ3	1:J:294:SER:HB3	2.54	0.43
1:K:351:PRO:O	1:K:352:VAL:HB	2.19	0.43
1:K:454:GLU:C	1:K:455:LYS:HG2	2.44	0.43
1:L:110:GLY:O	1:L:111:GLN:O	2.36	0.43
1:L:453:LYS:CD	1:L:453:LYS:HB2	2.44	0.43
1:M:92:ASN:HD21	1:M:95:THR:HG23	1.83	0.43
1:O:52:VAL:O	1:O:53:PRO:C	2.61	0.43
1:A:247:PHE:CD2	1:A:322:GLY:HA2	2.54	0.43
1:A:344:ILE:CD1	1:B:188:LEU:HD11	2.48	0.43
1:B:114:GLY:HA3	1:B:340:THR:HG23	2.00	0.43
1:C:48:PRO:HG2	1:C:49:TYR:CD2	2.53	0.43
1:C:220:VAL:HG23	1:C:225:CYS:HA	2.00	0.43
1:D:46:GLY:HA3	1:D:65:VAL:HG23	2.00	0.43
1:D:79:ASP:O	1:D:83:PHE:HB2	2.18	0.43
1:F:126:LEU:HB3	1:F:262:ASN:CB	2.39	0.43
1:F:379:LEU:HG	1:F:380:CYS:N	2.33	0.43
1:G:154:THR:HG23	1:G:253:GLU:HB3	2.00	0.43
1:J:213:LEU:HD12	1:J:213:LEU:HA	1.68	0.43
1:K:55:GLY:HA2	1:K:58:ASN:C	2.43	0.43
1:K:92:ASN:O	1:K:94:GLU:N	2.51	0.43
1:M:125:LYS:HD2	1:M:261:TRP:NE1	2.33	0.43
1:A:384:LEU:HB3	1:A:389:MET:HE2	2.00	0.43
1:C:75:VAL:CG1	1:C:452:LEU:HD12	2.48	0.43
1:C:324:CYS:HB3	1:C:328:GLN:O	2.18	0.43
1:D:224:ILE:HD13	1:D:224:ILE:HG21	1.71	0.43
1:E:216:THR:HG22	1:E:218:CYS:HB2	2.01	0.43
1:E:249:CYS:O	1:E:250:LEU:HD12	2.18	0.43
1:G:353:PRO:HG3	1:G:360:LYS:HD2	2.00	0.43
1:H:364:TYR:CD2	1:I:185:CYS:HB2	2.54	0.43
1:I:357:ASP:O	1:I:358:ALA:C	2.60	0.43
1:K:24:THR:HG23	1:K:319:HIS:O	2.19	0.43
1:K:261:TRP:CZ3	1:K:294:SER:HB3	2.53	0.43
1:K:317:GLN:C	1:K:317:GLN:HE21	2.26	0.43
1:N:196:GLU:N	1:N:199:ASP:OD2	2.48	0.43
1:N:324:CYS:HB3	1:N:328:GLN:O	2.19	0.43
1:O:188:LEU:HD22	1:O:188:LEU:N	2.33	0.43
1:A:78:PRO:HD2	1:A:456:PHE:CE1	2.53	0.43
1:F:231:TYR:CD1	1:F:232:PRO:HD2	2.54	0.43
1:G:167:GLU:HB3	1:G:233:ASP:HB2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:49:TYR:O	1:I:50:PHE:HB3	2.19	0.43
1:I:135:ALA:O	1:I:136:THR:CG2	2.67	0.43
1:K:316:ALA:HB2	1:K:321:ASN:HA	2.01	0.43
1:M:385:THR:OG1	1:M:388:VAL:HG23	2.19	0.43
1:M:448:TRP:CD1	1:M:448:TRP:C	2.95	0.43
1:N:49:TYR:O	1:N:64:LYS:HE3	2.19	0.43
1:N:96:GLN:HE21	1:N:96:GLN:HB3	1.57	0.43
1:N:115:VAL:HG21	1:O:257:ALA:HB2	2.01	0.43
1:O:216:THR:HG21	1:O:219:GLU:OE2	2.18	0.43
1:O:384:LEU:HD22	1:O:389:MET:HG3	2.01	0.43
1:A:70:TYR:OH	1:A:232:PRO:HD3	2.19	0.43
1:B:349:GLN:HG2	1:B:360:LYS:CG	2.49	0.43
1:E:150:ASP:O	1:E:296:SER:HA	2.18	0.43
1:E:367:HIS:CE1	1:E:369:GLU:OE2	2.72	0.43
1:F:50:PHE:CA	1:F:64:LYS:HG3	2.48	0.43
1:G:50:PHE:CA	1:G:64:LYS:HG3	2.48	0.43
1:I:117:LEU:HG	1:J:293:PRO:HD3	2.00	0.43
1:I:151:TYR:CD2	1:I:203:THR:HB	2.52	0.43
1:J:369:GLU:HG3	1:J:371:TYR:CE1	2.54	0.43
1:K:105:VAL:CG1	1:K:106:GLU:N	2.78	0.43
1:M:98:LEU:HD23	1:M:381:THR:HG22	2.01	0.43
1:M:369:GLU:HG3	1:M:371:TYR:CE1	2.54	0.43
1:N:117:LEU:HD13	1:O:260:PHE:HB3	2.01	0.43
1:N:373:LEU:N	1:N:373:LEU:HD23	2.30	0.43
1:A:104:GLY:C	1:A:105:VAL:HG23	2.43	0.43
1:B:235:LEU:HD23	1:B:235:LEU:HA	1.75	0.43
1:D:34:PHE:CE2	1:D:378:GLN:HB2	2.53	0.43
1:E:464:PRO:HA	1:E:467:ARG:NH1	2.34	0.43
1:F:240:ASP:HA	1:F:241:PRO:HD2	1.75	0.43
1:F:349:GLN:HG3	1:F:360:LYS:HD2	2.01	0.43
1:G:201:VAL:HG11	1:G:334:VAL:HG21	2.01	0.43
1:H:92:ASN:C	1:H:94:GLU:N	2.77	0.43
1:I:123:TYR:CG	1:I:147:VAL:HG22	2.54	0.43
1:I:171:LYS:HB2	1:I:213:LEU:CD1	2.49	0.43
1:J:156:LEU:HG	1:J:334:VAL:HB	2.01	0.43
1:L:69:GLN:NE2	1:L:71:ARG:HH22	2.17	0.43
1:L:69:GLN:HE21	1:L:71:ARG:HH12	1.67	0.43
1:L:109:ARG:HD3	1:L:335:ASP:OD2	2.18	0.43
1:N:46:GLY:HA3	1:N:65:VAL:HG23	2.01	0.43
1:A:235:LEU:HD23	1:A:235:LEU:HA	1.77	0.42
1:A:257:ALA:HB2	1:E:115:VAL:HG21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:LYS:CD	1:D:315:LYS:HB2	2.49	0.42
1:F:216:THR:CG2	1:F:218:CYS:HB2	2.48	0.42
1:F:256:PHE:CD1	1:F:256:PHE:C	2.97	0.42
1:F:366:ARG:HG3	1:F:366:ARG:HH11	1.84	0.42
1:G:58:ASN:CG	1:H:178:ARG:HH12	2.20	0.42
1:G:119:GLY:HA2	1:G:148:SER:HA	2.01	0.42
1:H:464:PRO:HG2	1:H:465:LEU:H	1.84	0.42
1:I:108:GLY:HA2	1:I:308:ASN:ND2	2.34	0.42
1:I:396:ASN:C	1:I:396:ASN:ND2	2.76	0.42
1:K:85:LEU:HD12	1:K:88:THR:HA	2.01	0.42
1:K:142:ASP:CG	1:L:283:ARG:HD2	2.43	0.42
1:K:226:GLN:OE1	1:K:226:GLN:HA	2.18	0.42
1:A:369:GLU:HG3	1:A:371:TYR:CE1	2.54	0.42
1:C:300:VAL:CG1	1:D:255:LEU:HD13	2.49	0.42
1:E:69:GLN:NE2	1:E:71:ARG:HH22	2.16	0.42
1:G:36:HIS:ND1	1:G:37:ALA:N	2.67	0.42
1:G:151:TYR:CD2	1:G:203:THR:HB	2.53	0.42
1:G:237:MET:HB3	1:G:246:MET:HG2	2.01	0.42
1:K:247:PHE:CE2	1:K:322:GLY:HA2	2.54	0.42
1:L:216:THR:O	1:L:217:LYS:CB	2.66	0.42
1:N:392:ILE:O	1:N:392:ILE:CG2	2.67	0.42
1:O:22:VAL:HG12	1:O:23:ASN:H	1.84	0.42
1:O:475:LEU:HD23	1:O:475:LEU:N	2.24	0.42
1:E:234:TYR:HD2	1:E:246:MET:HE1	1.85	0.42
1:F:465:LEU:CD2	1:F:465:LEU:O	2.68	0.42
1:G:126:LEU:HB3	1:G:262:ASN:CB	2.48	0.42
1:G:262:ASN:HD22	1:G:262:ASN:HA	1.30	0.42
1:G:333:VAL:HG11	1:G:371:TYR:HE2	1.84	0.42
1:H:74:ARG:HH22	1:H:440:ASP:CG	2.26	0.42
1:I:50:PHE:CD1	1:I:50:PHE:O	2.72	0.42
1:I:117:LEU:HD11	1:J:293:PRO:HB3	2.01	0.42
1:I:126:LEU:CB	1:I:262:ASN:HB3	2.44	0.42
1:K:76:GLN:CG	1:K:453:LYS:HE3	2.48	0.42
1:K:349:GLN:CG	1:K:360:LYS:HD2	2.49	0.42
1:L:42:LEU:HB3	1:L:448:TRP:CZ2	2.55	0.42
1:O:300:VAL:HG13	1:O:300:VAL:O	2.18	0.42
1:A:389:MET:O	1:A:393:GLN:HB2	2.20	0.42
1:B:105:VAL:HG21	1:B:159:LEU:CD1	2.45	0.42
1:B:366:ARG:HD3	1:B:366:ARG:HA	1.64	0.42
1:C:196:GLU:N	1:C:199:ASP:OD2	2.41	0.42
1:D:47:ASP:OD1	1:D:47:ASP:C	2.61	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:ARG:HA	1:D:197:ASP:OD1	2.20	0.42
1:D:117:LEU:HD13	1:E:260:PHE:HB3	2.00	0.42
1:E:22:VAL:HG12	1:E:23:ASN:N	2.33	0.42
1:H:150:ASP:O	1:H:296:SER:HA	2.20	0.42
1:H:357:ASP:O	1:H:358:ALA:C	2.62	0.42
1:I:92:ASN:O	1:I:94:GLU:N	2.52	0.42
1:I:307:PHE:HA	1:I:311:TYR:OH	2.19	0.42
1:K:460:LEU:H	1:K:460:LEU:HG	1.57	0.42
1:L:278:LYS:NZ	1:L:278:LYS:HG2	2.35	0.42
1:M:392:ILE:O	1:M:392:ILE:HG22	2.20	0.42
1:O:126:LEU:HB3	1:O:262:ASN:CB	2.43	0.42
1:O:216:THR:O	1:O:217:LYS:HB2	2.19	0.42
1:A:110:GLY:HA3	1:A:370:GLU:CG	2.49	0.42
1:B:314:HIS:O	1:B:315:LYS:HG3	2.20	0.42
1:D:74:ARG:HH22	1:D:440:ASP:CG	2.28	0.42
1:G:374:GLN:OE1	1:G:464:PRO:HG2	2.20	0.42
1:I:92:ASN:HA	1:I:93:PRO:HD2	1.82	0.42
1:K:159:LEU:CD2	1:K:331:VAL:HG22	2.50	0.42
1:A:91:TYR:H	1:A:91:TYR:HD2	1.67	0.42
1:A:143:VAL:O	1:A:143:VAL:HG12	2.20	0.42
1:B:22:VAL:HG12	1:B:23:ASN:N	2.34	0.42
1:C:385:THR:H	1:C:388:VAL:HB	1.84	0.42
1:F:239:ALA:O	1:F:240:ASP:C	2.61	0.42
1:G:98:LEU:CD2	1:G:380:CYS:O	2.67	0.42
1:G:138:ASN:C	1:G:140:SER:N	2.77	0.42
1:H:353:PRO:CG	1:H:360:LYS:NZ	2.70	0.42
1:I:72:VAL:HG23	1:I:197:ASP:CA	2.49	0.42
1:I:127:ASP:CG	1:I:136:THR:OG1	2.63	0.42
1:I:149:VAL:HG22	1:I:150:ASP:N	2.35	0.42
1:K:308:ASN:HD22	1:K:308:ASN:HA	1.64	0.42
1:L:67:ALA:HB2	1:L:367:HIS:CE1	2.55	0.42
1:M:324:CYS:HB3	1:M:328:GLN:O	2.19	0.42
1:N:353:PRO:HG3	1:N:360:LYS:HD2	2.00	0.42
1:O:308:ASN:HD22	1:O:308:ASN:HA	1.56	0.42
1:A:81:ASN:C	1:A:83:PHE:H	2.27	0.42
1:A:119:GLY:HA2	1:A:148:SER:HA	2.00	0.42
1:B:317:GLN:CG	1:B:318:GLY:N	2.83	0.42
1:C:256:PHE:CD1	1:C:256:PHE:C	2.97	0.42
1:C:260:PHE:CD2	1:C:260:PHE:N	2.83	0.42
1:F:220:VAL:CG2	1:F:225:CYS:HA	2.49	0.42
1:F:366:ARG:HD3	1:F:366:ARG:HA	1.64	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:201:VAL:O	1:G:202:ASP:C	2.62	0.42
1:H:351:PRO:O	1:H:352:VAL:CB	2.68	0.42
1:I:123:TYR:CD2	1:I:125:LYS:HB2	2.54	0.42
1:K:31:THR:HG23	1:K:379:LEU:O	2.19	0.42
1:K:209:ASP:O	1:K:213:LEU:HB2	2.19	0.42
1:O:124:ASN:OD1	1:O:264:ALA:HB3	2.20	0.42
1:A:369:GLU:HG3	1:A:371:TYR:HE1	1.85	0.42
1:E:78:PRO:HD2	1:E:456:PHE:CZ	2.55	0.42
1:F:316:ALA:CB	1:F:321:ASN:HA	2.50	0.42
1:G:98:LEU:HA	1:G:98:LEU:HD23	1.84	0.42
1:G:217:LYS:HE3	1:G:226:GLN:NE2	2.35	0.42
1:H:366:ARG:HD3	1:H:366:ARG:HA	1.74	0.42
1:J:45:VAL:C	1:J:65:VAL:HG21	2.45	0.42
1:K:108:GLY:HA2	1:K:308:ASN:ND2	2.35	0.42
1:K:117:LEU:CD1	1:L:260:PHE:CB	2.97	0.42
1:M:92:ASN:ND2	1:M:95:THR:H	2.17	0.42
1:N:98:LEU:CD2	1:N:381:THR:HG22	2.50	0.42
1:B:92:ASN:HD21	1:B:94:GLU:HB2	1.84	0.42
1:B:208:MET:HE2	1:B:210:PHE:CD2	2.55	0.42
1:D:201:VAL:H	1:D:201:VAL:HG22	1.60	0.42
1:E:99:VAL:HG21	1:E:382:ILE:HD11	2.01	0.42
1:E:151:TYR:CE2	1:E:221:PRO:HG2	2.54	0.42
1:G:235:LEU:HA	1:G:235:LEU:HD23	1.80	0.42
1:H:98:LEU:CD2	1:H:381:THR:HG22	2.50	0.42
1:H:160:GLY:HA2	1:H:247:PHE:CZ	2.55	0.42
1:H:258:ARG:HG3	1:H:259:HIS:ND1	2.34	0.42
1:I:216:THR:HG22	1:I:218:CYS:CB	2.46	0.42
1:K:98:LEU:CD2	1:K:381:THR:HG22	2.50	0.42
1:L:66:SER:H	1:L:69:GLN:NE2	2.18	0.42
1:N:92:ASN:C	1:N:94:GLU:N	2.78	0.42
1:O:368:VAL:HG12	1:O:369:GLU:N	2.27	0.42
1:A:271:VAL:HA	1:A:272:PRO:HD3	1.87	0.42
1:B:36:HIS:ND1	1:B:37:ALA:N	2.68	0.42
1:E:385:THR:O	1:E:389:MET:HE3	2.20	0.42
1:F:306:LEU:O	1:F:311:TYR:OH	2.30	0.42
1:G:306:LEU:HA	1:G:306:LEU:HD12	1.77	0.42
1:H:260:PHE:CD2	1:H:260:PHE:N	2.87	0.42
1:K:42:LEU:H	1:K:42:LEU:HG	1.57	0.42
1:K:74:ARG:HH22	1:K:440:ASP:CG	2.28	0.42
1:K:325:TRP:O	1:K:326:HIS:HB2	2.20	0.42
1:K:385:THR:O	1:K:389:MET:HE3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:256:PHE:CD1	1:L:256:PHE:C	2.97	0.42
1:A:35:TYR:CE2	1:A:458:LEU:HG	2.55	0.41
1:A:459:ASP:OD2	1:A:459:ASP:N	2.51	0.41
1:B:325:TRP:O	1:B:326:HIS:HB2	2.19	0.41
1:B:353:PRO:CD	1:B:360:LYS:HZ1	2.30	0.41
1:C:143:VAL:O	1:C:143:VAL:CG1	2.63	0.41
1:F:385:THR:OG1	1:F:388:VAL:HG23	2.21	0.41
1:G:98:LEU:HD22	1:G:380:CYS:O	2.19	0.41
1:G:232:PRO:HB2	1:G:234:TYR:CZ	2.54	0.41
1:G:317:GLN:NE2	1:G:317:GLN:C	2.78	0.41
1:H:451:ASP:C	1:H:451:ASP:OD1	2.63	0.41
1:J:99:VAL:HG12	1:J:100:TRP:N	2.34	0.41
1:L:92:ASN:OD1	1:L:94:GLU:HB2	2.20	0.41
1:L:364:TYR:CE2	1:M:185:CYS:HB2	2.55	0.41
1:N:317:GLN:NE2	1:N:317:GLN:C	2.78	0.41
1:N:366:ARG:HD3	1:N:366:ARG:HA	1.72	0.41
1:A:385:THR:O	1:A:386:ALA:C	2.60	0.41
1:B:71:ARG:HA	1:B:197:ASP:OD1	2.20	0.41
1:B:271:VAL:HA	1:B:272:PRO:HD3	1.86	0.41
1:C:105:VAL:CG1	1:C:106:GLU:N	2.81	0.41
1:H:42:LEU:HB3	1:H:448:TRP:CZ2	2.55	0.41
1:H:317:GLN:HG3	1:H:318:GLY:H	1.85	0.41
1:I:45:VAL:HG12	1:I:368:VAL:HG13	2.03	0.41
1:J:369:GLU:HG3	1:J:371:TYR:HE1	1.85	0.41
1:L:115:VAL:HG13	1:M:255:LEU:HD21	2.00	0.41
1:M:180:LEU:HD12	1:M:180:LEU:HA	1.89	0.41
1:M:216:THR:HG22	1:M:218:CYS:N	2.35	0.41
1:N:459:ASP:OD2	1:N:459:ASP:N	2.53	0.41
1:O:33:ILE:HD12	1:O:33:ILE:HG23	1.87	0.41
1:O:155:GLN:HA	1:O:334:VAL:O	2.21	0.41
1:O:201:VAL:HG11	1:O:334:VAL:HG11	2.02	0.41
1:O:391:TYR:C	1:O:393:GLN:N	2.77	0.41
1:B:90:ILE:O	1:B:90:ILE:HG22	2.20	0.41
1:B:464:PRO:O	1:B:465:LEU:C	2.60	0.41
1:C:33:ILE:HB	1:C:379:LEU:HB3	2.03	0.41
1:C:66:SER:O	1:C:69:GLN:HG2	2.20	0.41
1:C:160:GLY:HA2	1:C:247:PHE:CZ	2.56	0.41
1:C:467:ARG:O	1:C:471:VAL:HG23	2.20	0.41
1:D:464:PRO:HA	1:D:467:ARG:NH1	2.35	0.41
1:G:234:TYR:HD2	1:G:246:MET:HE1	1.85	0.41
1:G:326:HIS:O	1:G:327:ASN:C	2.61	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:VAL:HG12	1:H:106:GLU:N	2.35	0.41
1:H:214:GLN:OE1	1:H:219:GLU:HB2	2.20	0.41
1:H:353:PRO:HD2	1:H:360:LYS:CE	2.49	0.41
1:I:131:SER:O	1:I:132:SER:C	2.62	0.41
1:I:384:LEU:HB3	1:I:389:MET:HE2	2.02	0.41
1:K:364:TYR:CE2	1:L:268:GLY:HA3	2.55	0.41
1:L:119:GLY:HA3	1:M:291:TYR:CZ	2.55	0.41
1:L:313:LEU:HD23	1:L:313:LEU:H	1.85	0.41
1:L:460:LEU:H	1:L:460:LEU:HG	1.63	0.41
1:M:347:SER:HA	1:M:361:PHE:HA	2.02	0.41
1:N:36:HIS:ND1	1:N:37:ALA:N	2.68	0.41
1:N:123:TYR:CG	1:N:147:VAL:HG22	2.56	0.41
1:O:440:ASP:HB3	1:O:443:ASP:CG	2.46	0.41
1:A:65:VAL:O	1:A:367:HIS:HB3	2.21	0.41
1:A:260:PHE:HB3	1:E:117:LEU:HD13	2.02	0.41
1:A:324:CYS:SG	1:A:329:LEU:HD12	2.60	0.41
1:B:35:TYR:CZ	1:B:458:LEU:HD21	2.56	0.41
1:B:156:LEU:C	1:B:156:LEU:HD12	2.45	0.41
1:B:213:LEU:HA	1:B:213:LEU:HD12	1.81	0.41
1:B:391:TYR:C	1:B:393:GLN:H	2.27	0.41
1:C:460:LEU:H	1:C:460:LEU:HG	1.68	0.41
1:D:347:SER:HA	1:D:361:PHE:HA	2.02	0.41
1:E:258:ARG:HG3	1:E:259:HIS:ND1	2.36	0.41
1:F:138:ASN:ND2	1:F:140:SER:HB3	2.36	0.41
1:F:255:LEU:HD13	1:J:300:VAL:CG1	2.49	0.41
1:F:291:TYR:CD2	1:J:148:SER:HB3	2.55	0.41
1:F:374:GLN:OE1	1:F:465:LEU:HB2	2.20	0.41
1:G:316:ALA:CB	1:G:321:ASN:HA	2.50	0.41
1:G:351:PRO:O	1:G:352:VAL:HB	2.20	0.41
1:H:24:THR:HG21	1:H:320:ASN:HA	2.00	0.41
1:H:67:ALA:HB2	1:H:367:HIS:CE1	2.55	0.41
1:H:332:THR:O	1:H:333:VAL:HG23	2.20	0.41
1:J:85:LEU:HB3	1:J:86:PRO:HD2	2.01	0.41
1:N:217:LYS:HE3	1:O:274:SER:O	2.21	0.41
1:O:125:LYS:HD2	1:O:261:TRP:NE1	2.36	0.41
1:B:333:VAL:HG11	1:B:371:TYR:HE2	1.85	0.41
1:C:92:ASN:HA	1:C:93:PRO:HD2	1.87	0.41
1:C:247:PHE:CE2	1:C:322:GLY:HA2	2.56	0.41
1:F:140:SER:OG	1:F:141:GLU:N	2.53	0.41
1:G:105:VAL:CG1	1:G:106:GLU:N	2.83	0.41
1:G:329:LEU:HD23	1:G:329:LEU:C	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:384:LEU:HB3	1:G:389:MET:CE	2.51	0.41
1:H:51:ARG:O	1:H:53:PRO:CD	2.62	0.41
1:H:347:SER:HA	1:H:361:PHE:HA	2.03	0.41
1:J:151:TYR:OH	1:J:221:PRO:HB2	2.20	0.41
1:K:98:LEU:HD23	1:K:98:LEU:HA	1.88	0.41
1:L:249:CYS:O	1:L:250:LEU:HD12	2.21	0.41
1:L:262:ASN:HD22	1:L:262:ASN:HA	1.34	0.41
1:L:308:ASN:HD22	1:L:308:ASN:HA	1.65	0.41
1:M:36:HIS:ND1	1:M:36:HIS:C	2.78	0.41
1:N:42:LEU:H	1:N:42:LEU:HG	1.54	0.41
1:N:216:THR:CG2	1:N:218:CYS:HB2	2.51	0.41
1:N:247:PHE:CD2	1:N:322:GLY:HA2	2.53	0.41
1:O:42:LEU:HA	1:O:42:LEU:HD23	1.80	0.41
1:O:172:GLY:HA3	1:O:187:PRO:HG2	2.01	0.41
1:A:364:TYR:N	1:A:364:TYR:CD1	2.89	0.41
1:B:52:VAL:HB	1:B:62:ILE:HB	2.02	0.41
1:D:46:GLY:HA3	1:D:65:VAL:CG2	2.50	0.41
1:E:43:LEU:HD12	1:E:43:LEU:HA	1.84	0.41
1:F:141:GLU:O	1:F:141:GLU:CG	2.61	0.41
1:F:255:LEU:CD2	1:J:115:VAL:HG13	2.51	0.41
1:F:316:ALA:HB3	1:F:321:ASN:HA	2.03	0.41
1:H:224:ILE:HG21	1:H:224:ILE:HD13	1.77	0.41
1:I:163:PRO:HB2	1:I:194:VAL:HG13	2.02	0.41
1:I:216:THR:O	1:I:217:LYS:HB2	2.20	0.41
1:L:254:GLN:O	1:L:255:LEU:HB3	2.21	0.41
1:L:300:VAL:CG1	1:M:255:LEU:HD13	2.50	0.41
1:M:156:LEU:HG	1:M:334:VAL:HB	2.03	0.41
1:N:464:PRO:HG2	1:N:465:LEU:H	1.86	0.41
1:N:470:LEU:HD23	1:N:470:LEU:HA	1.86	0.41
1:B:262:ASN:HD22	1:B:262:ASN:HA	1.37	0.41
1:B:275:LEU:HA	1:B:275:LEU:HD23	1.87	0.41
1:C:46:GLY:HA3	1:C:65:VAL:HG23	2.02	0.41
1:C:142:ASP:CG	1:D:283:ARG:HD2	2.46	0.41
1:E:33:ILE:HG23	1:E:33:ILE:HD12	1.86	0.41
1:F:42:LEU:HA	1:F:42:LEU:HD23	1.71	0.41
1:F:308:ASN:HD22	1:F:308:ASN:HA	1.61	0.41
1:G:196:GLU:O	1:G:197:ASP:C	2.62	0.41
1:G:267:MET:HA	1:G:267:MET:HE2	2.02	0.41
1:H:247:PHE:CD2	1:H:322:GLY:HA2	2.56	0.41
1:J:460:LEU:HD12	1:J:470:LEU:HD21	2.02	0.41
1:N:92:ASN:HA	1:N:93:PRO:HD2	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:109:ARG:NH2	1:N:369:GLU:OE1	2.53	0.41
1:N:260:PHE:CD2	1:N:260:PHE:N	2.86	0.41
1:N:467:ARG:O	1:N:470:LEU:HB2	2.21	0.41
1:A:201:VAL:O	1:A:203:THR:HG23	2.20	0.41
1:A:233:ASP:OD2	1:E:41:ARG:NH2	2.53	0.41
1:A:260:PHE:CD2	1:A:260:PHE:N	2.84	0.41
1:A:281:GLY:HA2	1:G:90:ILE:C	2.45	0.41
1:A:317:GLN:HG3	1:A:318:GLY:H	1.85	0.41
1:B:36:HIS:ND1	1:B:36:HIS:C	2.79	0.41
1:D:109:ARG:HA	1:D:109:ARG:HD2	1.71	0.41
1:H:92:ASN:HD21	1:H:94:GLU:HB2	1.86	0.41
1:H:316:ALA:CB	1:H:321:ASN:HA	2.50	0.41
1:I:68:TYR:CZ	1:I:151:TYR:HB2	2.55	0.41
1:I:258:ARG:HG3	1:I:259:HIS:ND1	2.35	0.41
1:J:59:LYS:O	1:J:60:GLN:HB3	2.21	0.41
1:J:308:ASN:HD22	1:J:308:ASN:HA	1.63	0.41
1:K:45:VAL:C	1:K:65:VAL:HG21	2.45	0.41
1:K:139:VAL:HG12	1:K:139:VAL:O	2.20	0.41
1:L:24:THR:CG2	1:L:320:ASN:HA	2.50	0.41
1:N:150:ASP:O	1:N:296:SER:HA	2.21	0.41
1:N:389:MET:O	1:N:393:GLN:HB2	2.20	0.41
1:O:59:LYS:O	1:O:60:GLN:CB	2.69	0.41
1:O:307:PHE:O	1:O:308:ASN:HB2	2.20	0.41
1:A:47:ASP:OD1	1:A:47:ASP:C	2.64	0.41
1:A:463:TYR:O	1:A:467:ARG:HG3	2.20	0.41
1:B:51:ARG:O	1:B:53:PRO:HD3	2.21	0.41
1:B:156:LEU:HA	1:B:250:LEU:O	2.21	0.41
1:C:22:VAL:CG1	1:C:23:ASN:N	2.83	0.41
1:C:35:TYR:CE2	1:C:458:LEU:HG	2.55	0.41
1:C:96:GLN:NE2	1:C:383:THR:OG1	2.54	0.41
1:C:123:TYR:CB	1:C:147:VAL:HG22	2.50	0.41
1:D:76:GLN:HG3	1:D:453:LYS:HE3	2.03	0.41
1:D:233:ASP:O	1:D:234:TYR:C	2.64	0.41
1:E:131:SER:O	1:E:132:SER:C	2.64	0.41
1:F:46:GLY:HA3	1:F:65:VAL:CG2	2.51	0.41
1:F:52:VAL:HB	1:F:62:ILE:HB	2.03	0.41
1:F:59:LYS:O	1:F:60:GLN:HB3	2.19	0.41
1:F:120:HIS:HA	1:F:121:PRO:HD3	1.95	0.41
1:F:251:ARG:HH11	1:F:251:ARG:CG	2.34	0.41
1:G:62:ILE:HA	1:G:63:PRO:HD3	1.80	0.41
1:G:299:ILE:HA	1:H:256:PHE:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:85:LEU:C	1:H:87:ASP:H	2.29	0.41
1:H:125:LYS:HD2	1:H:261:TRP:CE2	2.56	0.41
1:H:126:LEU:HB3	1:H:262:ASN:HB2	2.03	0.41
1:H:163:PRO:HB2	1:H:194:VAL:HG13	2.03	0.41
1:H:311:TYR:CD1	1:H:311:TYR:N	2.89	0.41
1:H:376:ILE:HD12	1:H:376:ILE:HG23	1.66	0.41
1:I:87:ASP:O	1:I:90:ILE:HG12	2.21	0.41
1:I:109:ARG:NH2	1:I:369:GLU:OE1	2.54	0.41
1:J:42:LEU:HB3	1:J:448:TRP:CZ2	2.56	0.41
1:J:110:GLY:O	1:J:111:GLN:C	2.63	0.41
1:J:156:LEU:HD21	1:J:334:VAL:HG21	2.02	0.41
1:K:72:VAL:HG23	1:K:197:ASP:HA	2.03	0.41
1:K:79:ASP:O	1:K:83:PHE:HB2	2.20	0.41
1:L:98:LEU:HD21	1:L:381:THR:HG22	2.00	0.41
1:L:324:CYS:HB3	1:L:328:GLN:O	2.21	0.41
1:M:92:ASN:O	1:M:92:ASN:CG	2.61	0.41
1:M:247:PHE:CE2	1:M:322:GLY:HA2	2.56	0.41
1:M:353:PRO:HG2	1:M:360:LYS:NZ	2.32	0.41
1:N:156:LEU:HD21	1:N:334:VAL:HG21	2.02	0.41
1:N:165:ILE:HD12	1:N:165:ILE:N	2.36	0.41
1:N:463:TYR:O	1:N:467:ARG:HG3	2.21	0.41
1:O:71:ARG:HG3	1:O:371:TYR:CZ	2.55	0.41
1:O:157:CYS:HA	1:O:332:THR:O	2.21	0.41
1:O:367:HIS:CE1	1:O:369:GLU:OE2	2.74	0.41
1:O:459:ASP:OD2	1:O:459:ASP:N	2.53	0.41
1:A:112:PRO:HB3	1:B:231:TYR:CG	2.55	0.41
1:A:293:PRO:HB3	1:E:117:LEU:CD1	2.44	0.41
1:B:113:LEU:HD22	1:C:253:GLU:HG3	2.03	0.41
1:D:119:GLY:HA2	1:D:148:SER:HA	2.03	0.41
1:D:395:MET:HE3	1:D:399:ILE:CD1	2.52	0.41
1:E:128:ASP:O	1:E:132:SER:HB3	2.21	0.41
1:E:254:GLN:HE21	1:E:298:SER:H	1.69	0.41
1:F:130:GLU:OE1	1:J:258:ARG:NH1	2.54	0.41
1:G:45:VAL:C	1:G:65:VAL:HG21	2.46	0.41
1:G:127:ASP:HB2	1:G:136:THR:HG21	2.03	0.41
1:H:180:LEU:HD12	1:H:180:LEU:HA	1.90	0.41
1:I:460:LEU:O	1:I:461:ASP:C	2.63	0.41
1:J:99:VAL:HG11	1:J:323:VAL:HG13	2.03	0.41
1:J:392:ILE:O	1:J:392:ILE:HG22	2.20	0.41
1:K:79:ASP:OD1	1:K:79:ASP:C	2.64	0.41
1:L:151:TYR:OH	1:L:221:PRO:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:465:LEU:HA	1:L:465:LEU:HD23	1.91	0.41
1:M:140:SER:O	1:M:141:GLU:HB2	2.21	0.41
1:N:333:VAL:HG11	1:N:371:TYR:HE2	1.86	0.41
1:A:96:GLN:O	1:A:97:ARG:NH1	2.52	0.40
1:B:50:PHE:CD1	1:B:50:PHE:C	2.99	0.40
1:B:91:TYR:CD2	1:B:91:TYR:C	2.96	0.40
1:B:104:GLY:C	1:B:105:VAL:HG23	2.46	0.40
1:B:273:GLN:HE22	1:B:278:LYS:CE	2.02	0.40
1:D:159:LEU:HD21	1:D:331:VAL:HG22	2.01	0.40
1:E:43:LEU:HD12	1:E:369:GLU:O	2.21	0.40
1:E:47:ASP:OD1	1:E:47:ASP:C	2.64	0.40
1:E:143:VAL:O	1:E:143:VAL:CG1	2.66	0.40
1:E:448:TRP:C	1:E:448:TRP:CD1	2.99	0.40
1:F:41:ARG:O	1:F:41:ARG:HG2	2.19	0.40
1:F:391:TYR:C	1:F:393:GLN:N	2.79	0.40
1:G:67:ALA:HB2	1:G:367:HIS:CE1	2.56	0.40
1:H:77:LEU:HB3	1:H:78:PRO:HD2	2.04	0.40
1:K:176:LYS:HB2	1:K:176:LYS:NZ	2.37	0.40
1:K:232:PRO:HB2	1:K:234:TYR:CZ	2.56	0.40
1:L:219:GLU:C	1:L:220:VAL:CG1	2.94	0.40
1:L:369:GLU:HG3	1:L:371:TYR:CE1	2.56	0.40
1:M:45:VAL:HG12	1:M:368:VAL:HG22	2.03	0.40
1:M:148:SER:HB3	1:N:291:TYR:CD2	2.56	0.40
1:O:237:MET:HB3	1:O:246:MET:HG2	2.03	0.40
1:O:391:TYR:O	1:O:392:ILE:C	2.61	0.40
1:A:196:GLU:N	1:A:199:ASP:OD2	2.32	0.40
1:A:470:LEU:HD23	1:A:470:LEU:HA	1.83	0.40
1:B:259:HIS:HE1	1:C:130:GLU:OE1	2.03	0.40
1:B:261:TRP:CZ3	1:B:294:SER:HB3	2.57	0.40
1:B:317:GLN:HG3	1:B:318:GLY:H	1.86	0.40
1:C:376:ILE:HG12	1:C:465:LEU:HD13	2.02	0.40
1:E:111:GLN:H	1:E:111:GLN:HG2	1.63	0.40
1:F:22:VAL:CG1	1:F:23:ASN:N	2.84	0.40
1:F:70:TYR:CE1	1:F:201:VAL:HG12	2.56	0.40
1:F:333:VAL:HG11	1:F:371:TYR:HE2	1.86	0.40
1:G:49:TYR:HA	1:G:223:ASP:HB3	2.04	0.40
1:G:396:ASN:HB3	1:G:399:ILE:HG13	2.02	0.40
1:H:22:VAL:HG12	1:H:23:ASN:H	1.86	0.40
1:I:24:THR:HG23	1:I:319:HIS:O	2.21	0.40
1:I:115:VAL:HG13	1:J:255:LEU:CD2	2.52	0.40
1:I:135:ALA:C	1:I:136:THR:HG23	2.46	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:135:ALA:HB1	1:J:282:MET:HE1	2.03	0.40
1:K:126:LEU:HG	1:K:127:ASP:OD2	2.22	0.40
1:K:171:LYS:HB2	1:K:213:LEU:CD1	2.51	0.40
1:K:368:VAL:CG1	1:L:169:TRP:CZ2	2.98	0.40
1:L:249:CYS:O	1:L:250:LEU:CD1	2.70	0.40
1:M:146:ASN:OD1	1:M:146:ASN:C	2.64	0.40
1:N:35:TYR:OH	1:N:86:PRO:HD3	2.21	0.40
1:N:158:ILE:HG21	1:N:158:ILE:HD13	1.83	0.40
1:N:242:TYR:CE2	1:N:395:MET:HG3	2.57	0.40
1:O:465:LEU:HA	1:O:465:LEU:HD23	1.69	0.40
1:A:156:LEU:HA	1:A:250:LEU:O	2.20	0.40
1:B:444:LYS:HA	1:B:444:LYS:HE2	2.03	0.40
1:D:21:VAL:HG12	1:D:22:VAL:N	2.35	0.40
1:E:110:GLY:O	1:E:111:GLN:O	2.40	0.40
1:E:123:TYR:CD2	1:E:125:LYS:HB2	2.56	0.40
1:E:314:HIS:ND1	1:E:314:HIS:N	2.68	0.40
1:F:96:GLN:HB3	1:F:383:THR:HA	2.01	0.40
1:F:142:ASP:CG	1:G:283:ARG:HD2	2.45	0.40
1:F:353:PRO:CD	1:F:360:LYS:NZ	2.84	0.40
1:G:396:ASN:O	1:G:399:ILE:HG13	2.22	0.40
1:H:254:GLN:O	1:H:255:LEU:HB3	2.21	0.40
1:H:376:ILE:HA	1:H:376:ILE:HD13	1.78	0.40
1:I:234:TYR:HD2	1:I:246:MET:HE1	1.85	0.40
1:J:216:THR:O	1:J:217:LYS:CB	2.70	0.40
1:J:366:ARG:HA	1:J:366:ARG:HD3	1.78	0.40
1:K:237:MET:HB3	1:K:246:MET:HG2	2.01	0.40
1:L:34:PHE:CE2	1:L:378:GLN:HB2	2.57	0.40
1:L:146:ASN:OD1	1:L:146:ASN:C	2.65	0.40
1:M:99:VAL:HG21	1:M:382:ILE:HD11	2.02	0.40
1:M:111:GLN:HB3	1:M:112:PRO:CD	2.42	0.40
1:M:471:VAL:O	1:M:472:GLN:C	2.63	0.40
1:N:216:THR:O	1:N:217:LYS:CB	2.69	0.40
1:A:70:TYR:CZ	1:A:201:VAL:HG12	2.56	0.40
1:B:42:LEU:H	1:B:42:LEU:HG	1.58	0.40
1:B:157:CYS:HA	1:B:332:THR:O	2.22	0.40
1:B:165:ILE:O	1:B:237:MET:HE2	2.22	0.40
1:E:242:TYR:CE2	1:E:395:MET:HG3	2.57	0.40
1:E:353:PRO:CG	1:E:360:LYS:HD2	2.52	0.40
1:F:118:SER:O	1:F:149:VAL:N	2.54	0.40
1:F:123:TYR:CG	1:F:147:VAL:CG2	3.05	0.40
1:F:220:VAL:HG23	1:F:225:CYS:HA	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:353:PRO:HG3	1:F:360:LYS:HD2	2.03	0.40
1:G:35:TYR:CZ	1:G:458:LEU:HD21	2.57	0.40
1:H:364:TYR:CD1	1:I:185:CYS:HB2	2.56	0.40
1:J:114:GLY:CA	1:J:340:THR:HG23	2.50	0.40
1:J:444:LYS:HE2	1:J:444:LYS:HA	2.02	0.40
1:M:31:THR:HG23	1:M:379:LEU:O	2.21	0.40
1:M:216:THR:O	1:M:217:LYS:CB	2.69	0.40
1:N:213:LEU:HD12	1:N:213:LEU:HA	1.57	0.40
1:B:163:PRO:HB2	1:B:194:VAL:HG13	2.03	0.40
1:B:349:GLN:HG3	1:B:360:LYS:HD2	2.03	0.40
1:C:159:LEU:HB2	1:C:248:PHE:HB3	2.03	0.40
1:C:275:LEU:HD23	1:C:275:LEU:HA	1.79	0.40
1:D:440:ASP:OD1	1:D:442:TYR:HB2	2.20	0.40
1:E:52:VAL:O	1:E:53:PRO:C	2.64	0.40
1:E:201:VAL:HG11	1:E:334:VAL:HG11	2.03	0.40
1:F:35:TYR:OH	1:F:86:PRO:HD3	2.22	0.40
1:F:156:LEU:HA	1:F:250:LEU:O	2.21	0.40
1:G:81:ASN:C	1:G:83:PHE:N	2.75	0.40
1:H:52:VAL:HA	1:H:53:PRO:HD2	1.81	0.40
1:H:171:LYS:HB2	1:H:213:LEU:CD1	2.52	0.40
1:I:143:VAL:HG12	1:I:143:VAL:O	2.20	0.40
1:I:180:LEU:HD12	1:I:180:LEU:HA	1.74	0.40
1:I:370:GLU:OE2	1:J:235:LEU:HD12	2.22	0.40
1:I:400:LEU:HD23	1:I:400:LEU:HA	1.92	0.40
1:J:88:THR:O	1:J:88:THR:CG2	2.69	0.40
1:J:157:CYS:HA	1:J:332:THR:O	2.21	0.40
1:J:375:PHE:O	1:J:376:ILE:HD13	2.21	0.40
1:J:448:TRP:CD1	1:J:448:TRP:C	2.99	0.40
1:L:107:ILE:HD12	1:L:107:ILE:N	2.37	0.40
1:L:300:VAL:H	1:L:300:VAL:HG12	1.63	0.40
1:M:126:LEU:HD12	1:M:126:LEU:HA	1.60	0.40
1:O:72:VAL:HG23	1:O:197:ASP:HA	2.04	0.40
1:O:109:ARG:N	1:O:308:ASN:HD21	2.12	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ASP:OD2	1:C:360:LYS:NZ[1_565]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

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	419/428 (98%)	372 (89%)	34 (8%)	13 (3%)	3	18
1	B	419/428 (98%)	370 (88%)	34 (8%)	15 (4%)	2	16
1	C	419/428 (98%)	372 (89%)	36 (9%)	11 (3%)	4	21
1	D	419/428 (98%)	373 (89%)	38 (9%)	8 (2%)	6	26
1	E	419/428 (98%)	373 (89%)	34 (8%)	12 (3%)	3	19
1	F	419/428 (98%)	367 (88%)	43 (10%)	9 (2%)	5	24
1	G	419/428 (98%)	366 (87%)	42 (10%)	11 (3%)	4	21
1	H	419/428 (98%)	362 (86%)	46 (11%)	11 (3%)	4	21
1	I	419/428 (98%)	373 (89%)	32 (8%)	14 (3%)	3	17
1	J	419/428 (98%)	369 (88%)	39 (9%)	11 (3%)	4	21
1	K	419/428 (98%)	370 (88%)	39 (9%)	10 (2%)	4	22
1	L	419/428 (98%)	369 (88%)	36 (9%)	14 (3%)	3	17
1	M	419/428 (98%)	367 (88%)	37 (9%)	15 (4%)	2	16
1	N	419/428 (98%)	376 (90%)	30 (7%)	13 (3%)	3	18
1	O	419/428 (98%)	372 (89%)	38 (9%)	9 (2%)	5	24
All	All	6285/6420 (98%)	5551 (88%)	558 (9%)	176 (3%)	4	19

All (176) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	ASP
1	A	131	SER
1	A	135	ALA
1	B	59	LYS
1	B	131	SER
1	B	135	ALA
1	B	298	SER
1	C	40	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	137	SER
1	D	59	LYS
1	D	139	VAL
1	E	55	GLY
1	E	135	ALA
1	F	59	LYS
1	F	131	SER
1	G	59	LYS
1	H	135	ALA
1	H	173	THR
1	I	55	GLY
1	I	59	LYS
1	I	137	SER
1	I	142	ASP
1	J	59	LYS
1	K	40	SER
1	K	131	SER
1	K	137	SER
1	K	139	VAL
1	L	54	ALA
1	L	55	GLY
1	L	59	LYS
1	L	131	SER
1	L	142	ASP
1	M	55	GLY
1	M	59	LYS
1	O	137	SER
1	A	40	SER
1	A	56	GLY
1	A	139	VAL
1	A	296	SER
1	B	40	SER
1	B	132	SER
1	B	137	SER
1	B	461	ASP
1	C	55	GLY
1	C	82	LYS
1	C	139	VAL
1	C	142	ASP
1	D	135	ALA
1	D	137	SER
1	E	131	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	55	GLY
1	F	135	ALA
1	F	139	VAL
1	F	140	SER
1	G	40	SER
1	G	55	GLY
1	H	40	SER
1	H	54	ALA
1	H	139	VAL
1	I	93	PRO
1	I	131	SER
1	J	139	VAL
1	J	140	SER
1	J	142	ASP
1	K	54	ALA
1	K	55	GLY
1	K	142	ASP
1	L	137	SER
1	M	54	ALA
1	M	137	SER
1	M	142	ASP
1	M	461	ASP
1	N	55	GLY
1	N	137	SER
1	N	142	ASP
1	O	55	GLY
1	O	59	LYS
1	O	139	VAL
1	O	142	ASP
1	O	298	SER
1	A	54	ALA
1	A	60	GLN
1	A	141	GLU
1	C	59	LYS
1	C	93	PRO
1	C	140	SER
1	C	298	SER
1	D	93	PRO
1	E	40	SER
1	E	59	LYS
1	F	222	LEU
1	G	131	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	141	GLU
1	G	298	SER
1	H	140	SER
1	H	296	SER
1	H	298	SER
1	I	139	VAL
1	I	298	SER
1	J	40	SER
1	J	131	SER
1	J	464	PRO
1	K	59	LYS
1	K	135	ALA
1	L	40	SER
1	M	40	SER
1	M	93	PRO
1	M	131	SER
1	M	139	VAL
1	N	59	LYS
1	N	93	PRO
1	N	135	ALA
1	N	298	SER
1	A	57	GLY
1	A	82	LYS
1	B	55	GLY
1	C	131	SER
1	D	55	GLY
1	D	298	SER
1	E	111	GLN
1	E	137	SER
1	E	139	VAL
1	E	217	LYS
1	E	298	SER
1	G	82	LYS
1	G	93	PRO
1	I	40	SER
1	I	464	PRO
1	J	134	ALA
1	K	140	SER
1	L	132	SER
1	L	134	ALA
1	M	126	LEU
1	M	141	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	40	SER
1	N	134	ALA
1	B	54	ALA
1	B	82	LYS
1	B	139	VAL
1	B	386	ALA
1	D	131	SER
1	E	54	ALA
1	E	93	PRO
1	G	386	ALA
1	I	54	ALA
1	I	140	SER
1	I	461	ASP
1	J	386	ALA
1	L	139	VAL
1	L	141	GLU
1	L	298	SER
1	M	60	GLN
1	M	135	ALA
1	M	464	PRO
1	N	54	ALA
1	N	139	VAL
1	N	386	ALA
1	O	40	SER
1	F	60	GLN
1	F	386	ALA
1	G	139	VAL
1	G	461	ASP
1	H	93	PRO
1	H	179	PRO
1	I	134	ALA
1	J	296	SER
1	L	60	GLN
1	O	82	LYS
1	O	296	SER
1	B	464	PRO
1	J	111	GLN
1	N	464	PRO
1	A	464	PRO
1	B	111	GLN
1	H	464	PRO
1	L	93	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/371 (100%)	330 (89%)	40 (11%)	6	22
1	B	370/371 (100%)	336 (91%)	34 (9%)	8	29
1	C	370/371 (100%)	337 (91%)	33 (9%)	9	31
1	D	370/371 (100%)	334 (90%)	36 (10%)	8	28
1	E	370/371 (100%)	328 (89%)	42 (11%)	5	21
1	F	370/371 (100%)	334 (90%)	36 (10%)	8	28
1	G	370/371 (100%)	325 (88%)	45 (12%)	5	19
1	H	370/371 (100%)	334 (90%)	36 (10%)	8	28
1	I	370/371 (100%)	333 (90%)	37 (10%)	7	26
1	J	370/371 (100%)	333 (90%)	37 (10%)	7	26
1	K	370/371 (100%)	329 (89%)	41 (11%)	6	21
1	L	370/371 (100%)	329 (89%)	41 (11%)	6	21
1	M	370/371 (100%)	334 (90%)	36 (10%)	8	28
1	N	370/371 (100%)	333 (90%)	37 (10%)	7	26
1	O	370/371 (100%)	331 (90%)	39 (10%)	6	23
All	All	5550/5565 (100%)	4980 (90%)	570 (10%)	7	24

All (570) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	29	THR
1	A	36	HIS
1	A	40	SER
1	A	48	PRO
1	A	60	GLN
1	A	61	ASP
1	A	72	VAL
1	A	91	TYR
1	A	96	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	99	VAL
1	A	127	ASP
1	A	139	VAL
1	A	147	VAL
1	A	173	THR
1	A	176	LYS
1	A	188	LEU
1	A	193	THR
1	A	213	LEU
1	A	222	LEU
1	A	227	SER
1	A	247	PHE
1	A	250	LEU
1	A	251	ARG
1	A	255	LEU
1	A	262	ASN
1	A	272	PRO
1	A	293	PRO
1	A	300	VAL
1	A	301	THR
1	A	311	TYR
1	A	313	LEU
1	A	317	GLN
1	A	328	GLN
1	A	340	THR
1	A	372	ASP
1	A	387	ASP
1	A	459	ASP
1	A	465	LEU
1	A	475	LEU
1	B	23	ASN
1	B	29	THR
1	B	48	PRO
1	B	91	TYR
1	B	92	ASN
1	B	96	GLN
1	B	99	VAL
1	B	113	LEU
1	B	136	THR
1	B	138	ASN
1	B	176	LYS
1	B	193	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	213	LEU
1	B	222	LEU
1	B	227	SER
1	B	236	GLN
1	B	247	PHE
1	B	249	CYS
1	B	250	LEU
1	B	251	ARG
1	B	255	LEU
1	B	262	ASN
1	B	293	PRO
1	B	300	VAL
1	B	301	THR
1	B	311	TYR
1	B	313	LEU
1	B	317	GLN
1	B	340	THR
1	B	372	ASP
1	B	444	LYS
1	B	459	ASP
1	B	465	LEU
1	B	475	LEU
1	C	23	ASN
1	C	36	HIS
1	C	91	TYR
1	C	99	VAL
1	C	107	ILE
1	C	127	ASP
1	C	139	VAL
1	C	165	ILE
1	C	176	LYS
1	C	193	THR
1	C	213	LEU
1	C	222	LEU
1	C	236	GLN
1	C	247	PHE
1	C	249	CYS
1	C	250	LEU
1	C	251	ARG
1	C	255	LEU
1	C	262	ASN
1	C	300	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	301	THR
1	C	308	ASN
1	C	310	PRO
1	C	311	TYR
1	C	313	LEU
1	C	317	GLN
1	C	328	GLN
1	C	340	THR
1	C	372	ASP
1	C	387	ASP
1	C	459	ASP
1	C	465	LEU
1	C	475	LEU
1	D	23	ASN
1	D	29	THR
1	D	36	HIS
1	D	48	PRO
1	D	69	GLN
1	D	91	TYR
1	D	99	VAL
1	D	127	ASP
1	D	139	VAL
1	D	173	THR
1	D	176	LYS
1	D	193	THR
1	D	213	LEU
1	D	222	LEU
1	D	227	SER
1	D	247	PHE
1	D	249	CYS
1	D	250	LEU
1	D	251	ARG
1	D	255	LEU
1	D	262	ASN
1	D	300	VAL
1	D	301	THR
1	D	308	ASN
1	D	311	TYR
1	D	313	LEU
1	D	317	GLN
1	D	328	GLN
1	D	340	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	352	VAL
1	D	360	LYS
1	D	366	ARG
1	D	372	ASP
1	D	459	ASP
1	D	465	LEU
1	D	475	LEU
1	E	22	VAL
1	E	23	ASN
1	E	29	THR
1	E	53	PRO
1	E	60	GLN
1	E	91	TYR
1	E	96	GLN
1	E	99	VAL
1	E	107	ILE
1	E	127	ASP
1	E	139	VAL
1	E	147	VAL
1	E	152	LYS
1	E	156	LEU
1	E	165	ILE
1	E	176	LYS
1	E	187	PRO
1	E	193	THR
1	E	213	LEU
1	E	222	LEU
1	E	236	GLN
1	E	247	PHE
1	E	249	CYS
1	E	250	LEU
1	E	251	ARG
1	E	255	LEU
1	E	262	ASN
1	E	272	PRO
1	E	277	ILE
1	E	300	VAL
1	E	301	THR
1	E	308	ASN
1	E	311	TYR
1	E	317	GLN
1	E	327	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	328	GLN
1	E	340	THR
1	E	372	ASP
1	E	387	ASP
1	E	459	ASP
1	E	465	LEU
1	E	475	LEU
1	F	23	ASN
1	F	29	THR
1	F	36	HIS
1	F	44	THR
1	F	60	GLN
1	F	91	TYR
1	F	96	GLN
1	F	99	VAL
1	F	112	PRO
1	F	133	HIS
1	F	147	VAL
1	F	154	THR
1	F	158	ILE
1	F	173	THR
1	F	176	LYS
1	F	193	THR
1	F	213	LEU
1	F	222	LEU
1	F	227	SER
1	F	247	PHE
1	F	251	ARG
1	F	255	LEU
1	F	262	ASN
1	F	301	THR
1	F	308	ASN
1	F	311	TYR
1	F	313	LEU
1	F	317	GLN
1	F	327	ASN
1	F	328	GLN
1	F	340	THR
1	F	372	ASP
1	F	444	LYS
1	F	459	ASP
1	F	465	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	475	LEU
1	G	23	ASN
1	G	29	THR
1	G	40	SER
1	G	47	ASP
1	G	88	THR
1	G	92	ASN
1	G	96	GLN
1	G	99	VAL
1	G	118	SER
1	G	127	ASP
1	G	147	VAL
1	G	154	THR
1	G	156	LEU
1	G	157	CYS
1	G	158	ILE
1	G	176	LYS
1	G	188	LEU
1	G	193	THR
1	G	213	LEU
1	G	222	LEU
1	G	227	SER
1	G	232	PRO
1	G	249	CYS
1	G	250	LEU
1	G	251	ARG
1	G	255	LEU
1	G	262	ASN
1	G	270	THR
1	G	295	PRO
1	G	300	VAL
1	G	301	THR
1	G	308	ASN
1	G	311	TYR
1	G	313	LEU
1	G	317	GLN
1	G	327	ASN
1	G	340	THR
1	G	372	ASP
1	G	382	ILE
1	G	387	ASP
1	G	392	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	444	LYS
1	G	459	ASP
1	G	465	LEU
1	G	475	LEU
1	H	23	ASN
1	H	36	HIS
1	H	53	PRO
1	H	91	TYR
1	H	99	VAL
1	H	107	ILE
1	H	127	ASP
1	H	139	VAL
1	H	147	VAL
1	H	165	ILE
1	H	173	THR
1	H	176	LYS
1	H	178	ARG
1	H	188	LEU
1	H	193	THR
1	H	213	LEU
1	H	222	LEU
1	H	225	CYS
1	H	227	SER
1	H	247	PHE
1	H	250	LEU
1	H	251	ARG
1	H	255	LEU
1	H	262	ASN
1	H	301	THR
1	H	311	TYR
1	H	313	LEU
1	H	317	GLN
1	H	340	THR
1	H	365	SER
1	H	366	ARG
1	H	372	ASP
1	H	387	ASP
1	H	459	ASP
1	H	465	LEU
1	H	475	LEU
1	I	23	ASN
1	I	36	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	40	SER
1	I	60	GLN
1	I	92	ASN
1	I	96	GLN
1	I	99	VAL
1	I	107	ILE
1	I	156	LEU
1	I	159	LEU
1	I	173	THR
1	I	176	LYS
1	I	193	THR
1	I	213	LEU
1	I	222	LEU
1	I	227	SER
1	I	232	PRO
1	I	236	GLN
1	I	247	PHE
1	I	249	CYS
1	I	251	ARG
1	I	255	LEU
1	I	262	ASN
1	I	272	PRO
1	I	293	PRO
1	I	300	VAL
1	I	301	THR
1	I	311	TYR
1	I	313	LEU
1	I	317	GLN
1	I	340	THR
1	I	372	ASP
1	I	398	SER
1	I	401	GLU
1	I	459	ASP
1	I	465	LEU
1	I	475	LEU
1	J	23	ASN
1	J	36	HIS
1	J	52	VAL
1	J	92	ASN
1	J	96	GLN
1	J	112	PRO
1	J	127	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	143	VAL
1	J	147	VAL
1	J	157	CYS
1	J	173	THR
1	J	176	LYS
1	J	187	PRO
1	J	213	LEU
1	J	222	LEU
1	J	236	GLN
1	J	245	SER
1	J	247	PHE
1	J	249	CYS
1	J	251	ARG
1	J	255	LEU
1	J	262	ASN
1	J	293	PRO
1	J	300	VAL
1	J	301	THR
1	J	308	ASN
1	J	311	TYR
1	J	313	LEU
1	J	317	GLN
1	J	328	GLN
1	J	340	THR
1	J	372	ASP
1	J	387	ASP
1	J	401	GLU
1	J	459	ASP
1	J	465	LEU
1	J	475	LEU
1	K	22	VAL
1	K	23	ASN
1	K	29	THR
1	K	36	HIS
1	K	60	GLN
1	K	91	TYR
1	K	92	ASN
1	K	96	GLN
1	K	99	VAL
1	K	107	ILE
1	K	112	PRO
1	K	127	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	157	CYS
1	K	176	LYS
1	K	193	THR
1	K	213	LEU
1	K	222	LEU
1	K	236	GLN
1	K	247	PHE
1	K	249	CYS
1	K	250	LEU
1	K	251	ARG
1	K	255	LEU
1	K	262	ASN
1	K	272	PRO
1	K	293	PRO
1	K	301	THR
1	K	308	ASN
1	K	311	TYR
1	K	313	LEU
1	K	317	GLN
1	K	327	ASN
1	K	328	GLN
1	K	340	THR
1	K	366	ARG
1	K	372	ASP
1	K	389	MET
1	K	401	GLU
1	K	459	ASP
1	K	465	LEU
1	K	475	LEU
1	L	23	ASN
1	L	36	HIS
1	L	91	TYR
1	L	92	ASN
1	L	96	GLN
1	L	99	VAL
1	L	127	ASP
1	L	139	VAL
1	L	147	VAL
1	L	156	LEU
1	L	159	LEU
1	L	173	THR
1	L	176	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	187	PRO
1	L	188	LEU
1	L	193	THR
1	L	201	VAL
1	L	222	LEU
1	L	227	SER
1	L	236	GLN
1	L	247	PHE
1	L	249	CYS
1	L	250	LEU
1	L	251	ARG
1	L	255	LEU
1	L	262	ASN
1	L	270	THR
1	L	272	PRO
1	L	293	PRO
1	L	300	VAL
1	L	301	THR
1	L	311	TYR
1	L	317	GLN
1	L	328	GLN
1	L	340	THR
1	L	372	ASP
1	L	387	ASP
1	L	398	SER
1	L	459	ASP
1	L	465	LEU
1	L	475	LEU
1	M	23	ASN
1	M	29	THR
1	M	80	PRO
1	M	91	TYR
1	M	92	ASN
1	M	96	GLN
1	M	99	VAL
1	M	107	ILE
1	M	127	ASP
1	M	139	VAL
1	M	156	LEU
1	M	173	THR
1	M	176	LYS
1	M	188	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	193	THR
1	M	213	LEU
1	M	222	LEU
1	M	227	SER
1	M	247	PHE
1	M	250	LEU
1	M	251	ARG
1	M	255	LEU
1	M	262	ASN
1	M	270	THR
1	M	300	VAL
1	M	301	THR
1	M	311	TYR
1	M	313	LEU
1	M	317	GLN
1	M	327	ASN
1	M	340	THR
1	M	372	ASP
1	M	387	ASP
1	M	459	ASP
1	M	465	LEU
1	M	475	LEU
1	N	23	ASN
1	N	60	GLN
1	N	92	ASN
1	N	96	GLN
1	N	99	VAL
1	N	127	ASP
1	N	147	VAL
1	N	157	CYS
1	N	159	LEU
1	N	165	ILE
1	N	173	THR
1	N	176	LYS
1	N	201	VAL
1	N	213	LEU
1	N	222	LEU
1	N	225	CYS
1	N	247	PHE
1	N	249	CYS
1	N	250	LEU
1	N	251	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	255	LEU
1	N	262	ASN
1	N	272	PRO
1	N	277	ILE
1	N	300	VAL
1	N	301	THR
1	N	311	TYR
1	N	313	LEU
1	N	317	GLN
1	N	327	ASN
1	N	328	GLN
1	N	340	THR
1	N	355	GLN
1	N	372	ASP
1	N	459	ASP
1	N	465	LEU
1	N	475	LEU
1	O	23	ASN
1	O	36	HIS
1	O	47	ASP
1	O	91	TYR
1	O	92	ASN
1	O	96	GLN
1	O	99	VAL
1	O	107	ILE
1	O	127	ASP
1	O	139	VAL
1	O	147	VAL
1	O	157	CYS
1	O	165	ILE
1	O	176	LYS
1	O	187	PRO
1	O	201	VAL
1	O	213	LEU
1	O	222	LEU
1	O	225	CYS
1	O	227	SER
1	O	247	PHE
1	O	249	CYS
1	O	251	ARG
1	O	255	LEU
1	O	262	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	293	PRO
1	O	300	VAL
1	O	301	THR
1	O	311	TYR
1	O	313	LEU
1	O	317	GLN
1	O	328	GLN
1	O	340	THR
1	O	365	SER
1	O	372	ASP
1	O	392	ILE
1	O	459	ASP
1	O	465	LEU
1	O	475	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (230) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	153	GLN
1	A	182	GLN
1	A	254	GLN
1	A	262	ASN
1	A	273	GLN
1	A	308	ASN
1	A	317	GLN
1	A	341	ASN
1	A	367	HIS
1	A	396	ASN
1	A	404	ASN
1	A	462	GLN
1	A	472	GLN
1	B	23	ASN
1	B	69	GLN
1	B	96	GLN
1	B	138	ASN
1	B	168	HIS
1	B	182	GLN
1	B	259	HIS
1	B	262	ASN
1	B	273	GLN
1	B	305	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	308	ASN
1	B	317	GLN
1	B	341	ASN
1	B	367	HIS
1	B	396	ASN
1	B	462	GLN
1	B	472	GLN
1	C	69	GLN
1	C	96	GLN
1	C	138	ASN
1	C	153	GLN
1	C	182	GLN
1	C	262	ASN
1	C	273	GLN
1	C	308	ASN
1	C	317	GLN
1	C	326	HIS
1	C	341	ASN
1	C	355	GLN
1	C	367	HIS
1	C	396	ASN
1	C	462	GLN
1	D	60	GLN
1	D	69	GLN
1	D	138	ASN
1	D	153	GLN
1	D	182	GLN
1	D	262	ASN
1	D	273	GLN
1	D	305	GLN
1	D	308	ASN
1	D	317	GLN
1	D	327	ASN
1	D	355	GLN
1	D	367	HIS
1	D	396	ASN
1	D	449	ASN
1	D	472	GLN
1	E	23	ASN
1	E	69	GLN
1	E	138	ASN
1	E	153	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	182	GLN
1	E	254	GLN
1	E	262	ASN
1	E	273	GLN
1	E	308	ASN
1	E	317	GLN
1	E	341	ASN
1	E	363	GLN
1	E	367	HIS
1	E	396	ASN
1	E	449	ASN
1	E	462	GLN
1	F	58	ASN
1	F	69	GLN
1	F	96	GLN
1	F	138	ASN
1	F	153	GLN
1	F	182	GLN
1	F	254	GLN
1	F	262	ASN
1	F	273	GLN
1	F	305	GLN
1	F	308	ASN
1	F	317	GLN
1	F	321	ASN
1	F	326	HIS
1	F	341	ASN
1	F	367	HIS
1	F	396	ASN
1	F	449	ASN
1	G	69	GLN
1	G	138	ASN
1	G	168	HIS
1	G	182	GLN
1	G	262	ASN
1	G	308	ASN
1	G	317	GLN
1	G	341	ASN
1	G	367	HIS
1	G	396	ASN
1	G	449	ASN
1	G	462	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	472	GLN
1	H	23	ASN
1	H	69	GLN
1	H	96	GLN
1	H	138	ASN
1	H	153	GLN
1	H	182	GLN
1	H	254	GLN
1	H	262	ASN
1	H	273	GLN
1	H	308	ASN
1	H	317	GLN
1	H	321	ASN
1	H	326	HIS
1	H	327	ASN
1	H	341	ASN
1	H	367	HIS
1	H	396	ASN
1	H	462	GLN
1	H	472	GLN
1	I	23	ASN
1	I	69	GLN
1	I	76	GLN
1	I	96	GLN
1	I	168	HIS
1	I	182	GLN
1	I	262	ASN
1	I	273	GLN
1	I	308	ASN
1	I	317	GLN
1	I	341	ASN
1	I	355	GLN
1	I	367	HIS
1	I	396	ASN
1	I	462	GLN
1	J	23	ASN
1	J	69	GLN
1	J	96	GLN
1	J	138	ASN
1	J	182	GLN
1	J	254	GLN
1	J	259	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	262	ASN
1	J	273	GLN
1	J	308	ASN
1	J	317	GLN
1	J	327	ASN
1	J	341	ASN
1	J	363	GLN
1	J	367	HIS
1	J	396	ASN
1	J	462	GLN
1	K	69	GLN
1	K	96	GLN
1	K	138	ASN
1	K	153	GLN
1	K	182	GLN
1	K	254	GLN
1	K	262	ASN
1	K	273	GLN
1	K	308	ASN
1	K	317	GLN
1	K	341	ASN
1	K	367	HIS
1	K	396	ASN
1	K	462	GLN
1	L	69	GLN
1	L	96	GLN
1	L	138	ASN
1	L	182	GLN
1	L	262	ASN
1	L	273	GLN
1	L	305	GLN
1	L	308	ASN
1	L	317	GLN
1	L	321	ASN
1	L	341	ASN
1	L	363	GLN
1	L	367	HIS
1	L	396	ASN
1	L	462	GLN
1	M	69	GLN
1	M	138	ASN
1	M	182	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	254	GLN
1	M	262	ASN
1	M	273	GLN
1	M	308	ASN
1	M	317	GLN
1	M	326	HIS
1	M	327	ASN
1	M	341	ASN
1	M	355	GLN
1	M	367	HIS
1	M	396	ASN
1	N	69	GLN
1	N	96	GLN
1	N	138	ASN
1	N	153	GLN
1	N	262	ASN
1	N	273	GLN
1	N	308	ASN
1	N	317	GLN
1	N	341	ASN
1	N	355	GLN
1	N	367	HIS
1	N	396	ASN
1	N	462	GLN
1	O	60	GLN
1	O	69	GLN
1	O	96	GLN
1	O	138	ASN
1	O	182	GLN
1	O	262	ASN
1	O	273	GLN
1	O	308	ASN
1	O	317	GLN
1	O	326	HIS
1	O	341	ASN
1	O	363	GLN
1	O	367	HIS
1	O	396	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	423/428 (98%)	-0.17	6 (1%) 73 59	16, 46, 103, 121	0
1	B	423/428 (98%)	-0.13	6 (1%) 73 59	19, 45, 101, 127	0
1	C	423/428 (98%)	-0.16	4 (0%) 81 68	15, 45, 103, 123	0
1	D	423/428 (98%)	-0.13	5 (1%) 76 63	14, 44, 102, 126	0
1	E	423/428 (98%)	-0.18	8 (1%) 66 51	15, 45, 104, 123	0
1	F	423/428 (98%)	-0.10	3 (0%) 84 73	19, 50, 105, 123	0
1	G	423/428 (98%)	0.02	7 (1%) 69 54	22, 50, 103, 127	0
1	H	423/428 (98%)	-0.14	6 (1%) 73 59	19, 46, 103, 124	0
1	I	423/428 (98%)	-0.15	8 (1%) 66 51	17, 45, 101, 123	0
1	J	423/428 (98%)	-0.06	10 (2%) 59 45	18, 46, 103, 123	0
1	K	423/428 (98%)	-0.15	7 (1%) 69 54	18, 44, 103, 122	0
1	L	423/428 (98%)	-0.13	5 (1%) 76 63	16, 46, 103, 122	0
1	M	423/428 (98%)	-0.08	9 (2%) 63 48	18, 46, 102, 126	0
1	N	423/428 (98%)	-0.12	7 (1%) 69 54	19, 45, 103, 125	0
1	O	423/428 (98%)	-0.11	10 (2%) 59 45	17, 46, 103, 126	0
All	All	6345/6420 (98%)	-0.12	101 (1%) 70 56	14, 46, 104, 127	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	86	PRO	5.4
1	O	139	VAL	5.4
1	D	135	ALA	4.8
1	J	84	GLY	4.7
1	F	139	VAL	4.5
1	E	86	PRO	4.2
1	G	139	VAL	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	58	ASN	3.8
1	A	139	VAL	3.8
1	N	85	LEU	3.7
1	C	139	VAL	3.6
1	O	134	ALA	3.5
1	I	135	ALA	3.5
1	A	442	TYR	3.4
1	M	139	VAL	3.3
1	I	139	VAL	3.3
1	L	139	VAL	3.3
1	N	88	THR	3.3
1	M	282	MET	3.2
1	C	138	ASN	3.2
1	K	139	VAL	3.2
1	N	86	PRO	3.2
1	J	139	VAL	3.2
1	H	88	THR	3.2
1	O	138	ASN	3.1
1	I	133	HIS	3.1
1	J	137	SER	3.1
1	C	86	PRO	3.1
1	E	172	GLY	3.0
1	M	135	ALA	3.0
1	O	140	SER	3.0
1	I	134	ALA	3.0
1	L	354	GLY	3.0
1	I	84	GLY	3.0
1	B	139	VAL	3.0
1	B	401	GLU	3.0
1	N	84	GLY	2.9
1	M	133	HIS	2.9
1	J	135	ALA	2.9
1	O	137	SER	2.8
1	L	136	THR	2.8
1	J	85	LEU	2.8
1	M	56	GLY	2.8
1	H	134	ALA	2.8
1	K	85	LEU	2.8
1	F	285	SER	2.8
1	G	56	GLY	2.7
1	C	174	ALA	2.6
1	O	135	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	139	VAL	2.6
1	G	86	PRO	2.6
1	H	139	VAL	2.5
1	K	87	ASP	2.5
1	B	135	ALA	2.5
1	J	133	HIS	2.5
1	E	84	GLY	2.4
1	D	393	GLN	2.4
1	H	89	SER	2.4
1	M	454	GLU	2.4
1	D	133	HIS	2.4
1	J	311	TYR	2.4
1	J	282	MET	2.4
1	G	439	LYS	2.4
1	M	57	GLY	2.3
1	J	134	ALA	2.3
1	G	84	GLY	2.3
1	K	135	ALA	2.3
1	I	138	ASN	2.3
1	L	134	ALA	2.3
1	E	131	SER	2.3
1	D	139	VAL	2.3
1	A	20	ALA	2.3
1	J	91	TYR	2.3
1	A	174	ALA	2.2
1	F	89	SER	2.2
1	B	282	MET	2.2
1	A	88	THR	2.2
1	L	133	HIS	2.2
1	E	394	SER	2.2
1	E	85	LEU	2.2
1	H	145	ASP	2.2
1	O	174	ALA	2.2
1	E	83	PHE	2.2
1	B	133	HIS	2.2
1	O	136	THR	2.1
1	O	389	MET	2.1
1	D	134	ALA	2.1
1	I	454	GLU	2.1
1	G	88	THR	2.1
1	K	84	GLY	2.1
1	A	138	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	58	ASN	2.1
1	O	133	HIS	2.1
1	H	135	ALA	2.1
1	B	131	SER	2.1
1	N	140	SER	2.1
1	N	400	LEU	2.1
1	M	88	THR	2.1
1	M	95	THR	2.1
1	E	135	ALA	2.0
1	G	386	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.