wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:54 PM BST

PDB ID	:	3ZX9
EMDB ID:	:	EMD-1864
Title	:	Cryo-EM reconstruction of native and expanded Turnip Crinkle virus
Authors	:	Bakker, S.E.; Robottom, J.; Pearson, A.R.; Stockley, P.G.; Ranson, N.A.
Deposited on	:	2011-08-08
Resolution	:	17.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

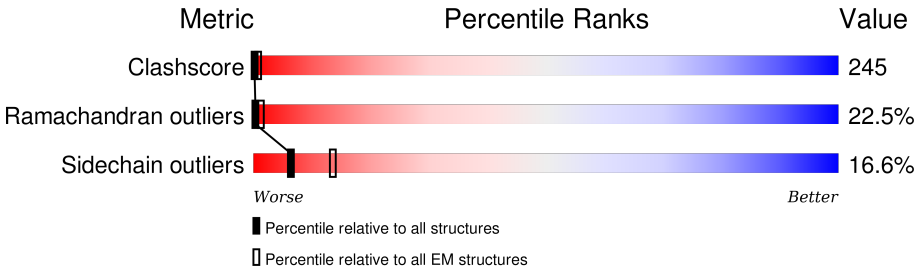
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 17.00 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	347	6% 35% 24% 12% 23%
1	B	347	6% 35% 25% 11% 23%
1	C	347	• 40% 28% 13% 15%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6284 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 CAPSID PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	267	Total	C	N	O	S	0	0
			2024	1280	343	396	5		
1	B	267	Total	C	N	O	S	0	0
			2024	1280	343	396	5		
1	C	295	Total	C	N	O	S	0	0
			2236	1409	386	436	5		

There are 15 discrepancies between the modelled and reference sequences:

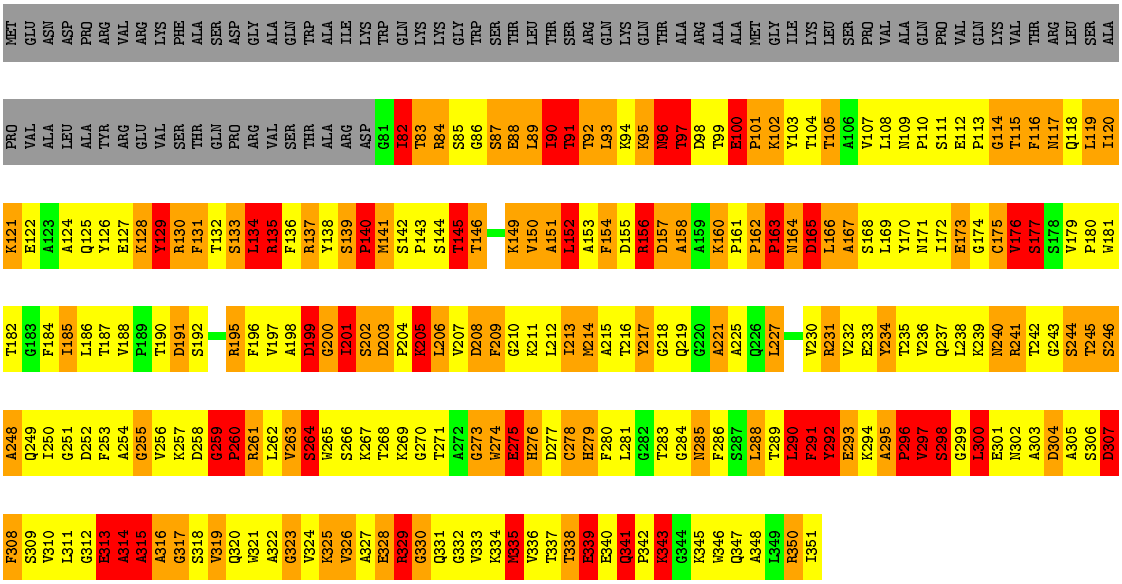
Chain	Residue	Modelled	Actual	Comment	Reference
A	.	-	ASN	DELETION	UNP P06663
A	.	-	ASP	DELETION	UNP P06663
A	.	-	ALA	DELETION	UNP P06663
A	.	-	ASP	DELETION	UNP P06663
A	346	TRP	LEU	VARIANT	UNP P06663
B	.	-	ASN	DELETION	UNP P06663
B	.	-	ASP	DELETION	UNP P06663
B	.	-	ALA	DELETION	UNP P06663
B	.	-	ASP	DELETION	UNP P06663
B	346	TRP	LEU	VARIANT	UNP P06663
C	.	-	ASN	DELETION	UNP P06663
C	.	-	ASP	DELETION	UNP P06663
C	.	-	ALA	DELETION	UNP P06663
C	.	-	ASP	DELETION	UNP P06663
C	346	TRP	LEU	VARIANT	UNP P06663

3 Residue-property plots (i)

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

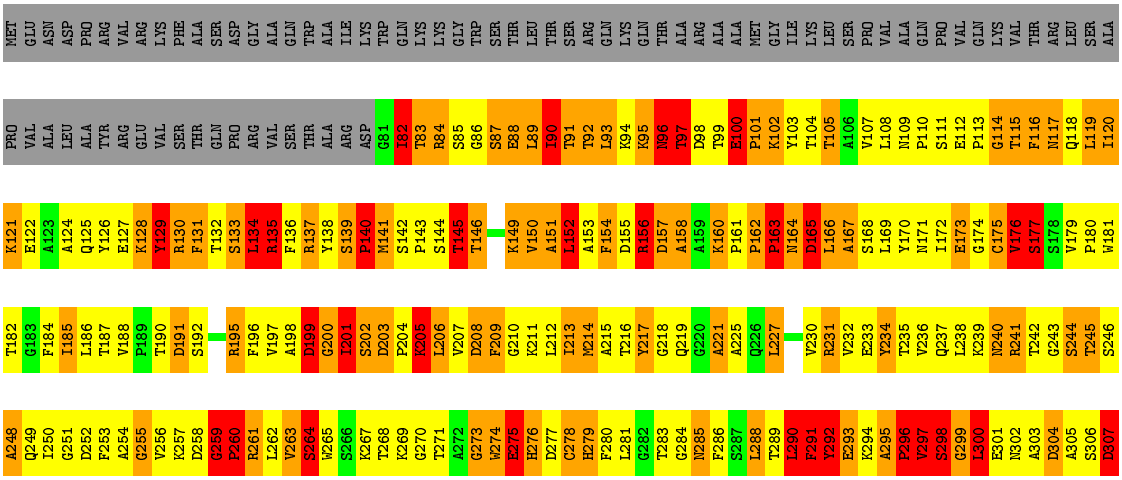
- Molecule 1: CAPSID PROTEIN

Chain A:



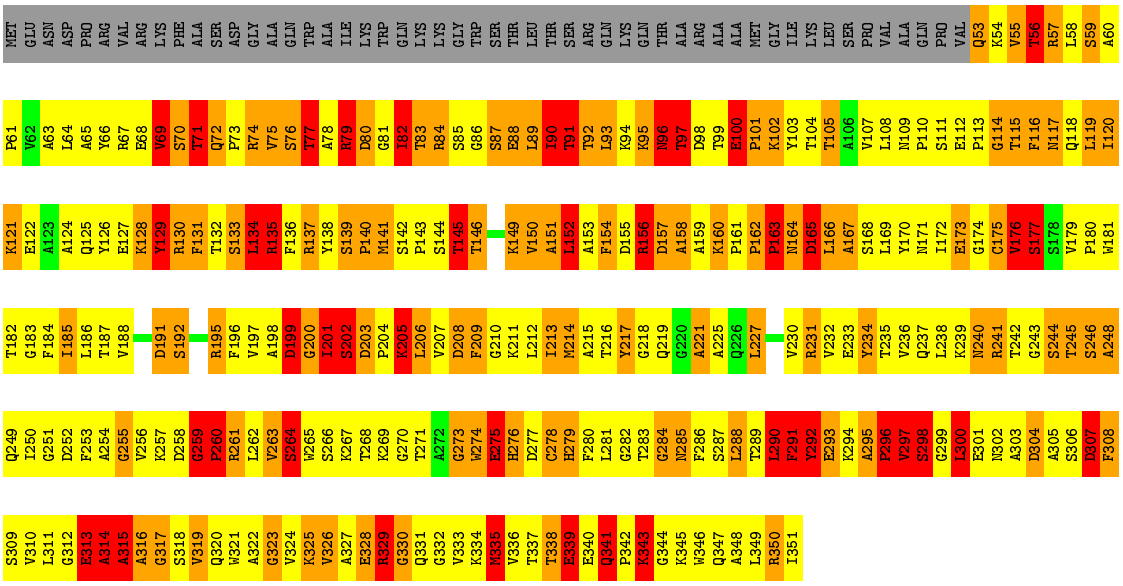
- Molecule 1: CAPSID PROTEIN

Chain B:



- Molecule 1: CAPSID PROTEIN

Chain C:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE-FLIPPING EACH PARTICLE	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO163 FILM	Depositor

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	#$\|Z\|$ >2	RMSZ	#$\|Z\|$ >2
1	A	2.49	42/2068 (2.0%)	2.48	130/2804 (4.6%)
1	B	2.49	42/2068 (2.0%)	2.48	130/2804 (4.6%)
1	C	2.51	56/2282 (2.5%)	2.46	145/3096 (4.7%)
All	All	2.50	140/6418 (2.2%)	2.47	405/8704 (4.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	8
1	C	0	10
All	All	0	26

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	201	ILE	C-N	-42.35	0.36	1.34
1	C	201	ILE	C-N	-42.34	0.36	1.34
1	A	201	ILE	C-N	-42.34	0.36	1.34
1	B	93	LEU	N-CA	-41.10	0.64	1.46
1	C	93	LEU	N-CA	-41.09	0.64	1.46
1	A	93	LEU	N-CA	-41.09	0.64	1.46
1	A	259	GLY	C-N	33.07	1.97	1.34
1	C	259	GLY	C-N	33.04	1.97	1.34
1	B	259	GLY	C-N	33.02	1.97	1.34
1	C	133	SER	CB-OG	29.87	1.81	1.42
1	B	133	SER	CB-OG	29.86	1.81	1.42
1	A	133	SER	CB-OG	29.78	1.80	1.42
1	B	82	ILE	C-N	20.46	1.81	1.34
1	A	82	ILE	C-N	20.44	1.81	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	82	ILE	C-N	20.43	1.81	1.34
1	B	149	LYS	CD-CE	19.49	2.00	1.51
1	C	149	LYS	CD-CE	19.45	1.99	1.51
1	A	149	LYS	CD-CE	19.41	1.99	1.51
1	A	279	HIS	C-N	17.63	1.74	1.34
1	B	279	HIS	C-N	17.59	1.74	1.34
1	C	279	HIS	C-N	17.56	1.74	1.34
1	A	288	LEU	C-N	-17.33	0.94	1.34
1	B	288	LEU	C-N	-17.28	0.94	1.34
1	C	288	LEU	C-N	-17.26	0.94	1.34
1	A	291	PHE	C-N	16.19	1.71	1.34
1	C	291	PHE	C-N	16.18	1.71	1.34
1	B	291	PHE	C-N	16.15	1.71	1.34
1	A	264	SER	C-N	15.13	1.68	1.34
1	C	264	SER	C-N	15.12	1.68	1.34
1	B	264	SER	C-N	15.11	1.68	1.34
1	B	339	GLU	C-N	14.95	1.68	1.34
1	A	339	GLU	C-N	14.94	1.68	1.34
1	C	339	GLU	C-N	14.94	1.68	1.34
1	C	76	SER	N-CA	14.84	1.76	1.46
1	C	297	VAL	C-N	-14.48	1.00	1.34
1	B	297	VAL	C-N	-14.45	1.00	1.34
1	A	297	VAL	C-N	-14.44	1.00	1.34
1	C	53	GLN	C-N	14.32	1.67	1.34
1	C	177	SER	C-N	-12.83	1.04	1.34
1	B	177	SER	C-N	-12.83	1.04	1.34
1	A	177	SER	C-N	-12.76	1.04	1.34
1	A	121	LYS	CE-NZ	12.07	1.79	1.49
1	B	121	LYS	CE-NZ	12.07	1.79	1.49
1	C	121	LYS	CE-NZ	12.05	1.79	1.49
1	A	319	VAL	C-N	11.99	1.61	1.34
1	B	319	VAL	C-N	11.99	1.61	1.34
1	C	319	VAL	C-N	11.98	1.61	1.34
1	B	139	SER	C-N	-11.58	1.12	1.34
1	A	139	SER	C-N	-11.53	1.12	1.34
1	C	139	SER	C-N	-11.47	1.12	1.34
1	C	75	VAL	C-N	11.45	1.60	1.34
1	C	140	PRO	N-CD	-10.99	1.32	1.47
1	A	140	PRO	N-CD	-10.95	1.32	1.47
1	C	75	VAL	N-CA	10.87	1.68	1.46
1	B	140	PRO	N-CD	-10.86	1.32	1.47
1	C	308	PHE	C-N	-9.60	1.11	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	308	PHE	C-N	-9.59	1.11	1.34
1	A	308	PHE	C-N	-9.59	1.11	1.34
1	A	200	GLY	C-N	-9.39	1.12	1.34
1	C	200	GLY	C-N	-9.38	1.12	1.34
1	B	200	GLY	C-N	-9.36	1.12	1.34
1	B	91	THR	N-CA	9.31	1.65	1.46
1	C	91	THR	N-CA	9.27	1.64	1.46
1	A	91	THR	N-CA	9.25	1.64	1.46
1	B	298	SER	C-N	-9.15	1.16	1.33
1	C	298	SER	C-N	-9.12	1.16	1.33
1	A	298	SER	C-N	-9.10	1.16	1.33
1	B	299	GLY	N-CA	-9.04	1.32	1.46
1	C	299	GLY	N-CA	-9.01	1.32	1.46
1	A	299	GLY	N-CA	-9.01	1.32	1.46
1	C	75	VAL	CA-C	8.92	1.76	1.52
1	C	77	THR	N-CA	8.68	1.63	1.46
1	A	315	ALA	C-N	-8.64	1.14	1.34
1	C	315	ALA	C-N	-8.63	1.14	1.34
1	B	315	ALA	C-N	-8.63	1.14	1.34
1	C	76	SER	CA-C	8.62	1.75	1.52
1	A	299	GLY	CA-C	-8.51	1.38	1.51
1	C	299	GLY	CA-C	-8.48	1.38	1.51
1	B	299	GLY	CA-C	-8.44	1.38	1.51
1	A	260	PRO	C-N	-8.04	1.15	1.34
1	C	260	PRO	C-N	-8.03	1.15	1.34
1	C	74	ARG	C-N	8.02	1.52	1.34
1	B	260	PRO	C-N	-8.01	1.15	1.34
1	C	323	GLY	C-N	-7.71	1.16	1.34
1	B	323	GLY	C-N	-7.70	1.16	1.34
1	A	323	GLY	C-N	-7.66	1.16	1.34
1	C	290	LEU	C-N	7.61	1.51	1.34
1	B	290	LEU	C-N	7.60	1.51	1.34
1	A	290	LEU	C-N	7.57	1.51	1.34
1	C	300	LEU	N-CA	-7.56	1.31	1.46
1	B	300	LEU	N-CA	-7.54	1.31	1.46
1	A	300	LEU	N-CA	-7.53	1.31	1.46
1	B	330	GLY	C-N	7.13	1.50	1.34
1	A	330	GLY	C-N	7.10	1.50	1.34
1	C	330	GLY	C-N	7.09	1.50	1.34
1	B	303	ALA	C-N	7.07	1.50	1.34
1	C	303	ALA	C-N	7.04	1.50	1.34
1	A	303	ALA	C-N	7.00	1.50	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	299	GLY	C-N	-6.99	1.18	1.34
1	B	299	GLY	C-N	-6.96	1.18	1.34
1	C	299	GLY	C-N	-6.95	1.18	1.34
1	C	72	GLN	C-N	6.88	1.47	1.34
1	C	74	ARG	N-CA	6.68	1.59	1.46
1	C	76	SER	C-N	6.64	1.49	1.34
1	B	259	GLY	CA-C	6.51	1.62	1.51
1	C	74	ARG	CA-C	6.49	1.69	1.52
1	C	259	GLY	CA-C	6.44	1.62	1.51
1	A	259	GLY	CA-C	6.39	1.62	1.51
1	A	175	CYS	C-N	-6.38	1.19	1.34
1	C	175	CYS	C-N	-6.37	1.19	1.34
1	B	175	CYS	C-N	-6.34	1.19	1.34
1	B	90	ILE	CA-C	6.26	1.69	1.52
1	A	90	ILE	CA-C	6.25	1.69	1.52
1	C	90	ILE	CA-C	6.23	1.69	1.52
1	A	140	PRO	CA-CB	-6.14	1.41	1.53
1	B	140	PRO	CA-CB	-6.13	1.41	1.53
1	C	140	PRO	CA-CB	-6.11	1.41	1.53
1	C	163	PRO	N-CA	-6.06	1.36	1.47
1	B	163	PRO	N-CA	-6.05	1.36	1.47
1	A	163	PRO	N-CA	-6.01	1.37	1.47
1	B	221	ALA	C-N	5.84	1.47	1.34
1	A	221	ALA	C-N	5.84	1.47	1.34
1	C	221	ALA	C-N	5.82	1.47	1.34
1	B	175	CYS	CA-C	-5.74	1.38	1.52
1	C	175	CYS	CA-C	-5.73	1.38	1.52
1	A	175	CYS	CA-C	-5.70	1.38	1.52
1	A	88	GLU	C-N	-5.51	1.21	1.34
1	C	70	SER	C-N	-5.50	1.21	1.34
1	B	88	GLU	C-N	-5.46	1.21	1.34
1	C	88	GLU	C-N	-5.45	1.21	1.34
1	A	284	GLY	N-CA	5.32	1.54	1.46
1	B	284	GLY	N-CA	5.29	1.53	1.46
1	C	284	GLY	N-CA	5.26	1.53	1.46
1	C	176	VAL	N-CA	-5.26	1.35	1.46
1	A	176	VAL	N-CA	-5.23	1.35	1.46
1	B	176	VAL	N-CA	-5.22	1.35	1.46
1	C	203	ASP	C-N	5.21	1.44	1.34
1	B	203	ASP	C-N	5.20	1.44	1.34
1	A	203	ASP	C-N	5.19	1.44	1.34
1	C	274	TRP	NE1-CE2	-5.03	1.31	1.37

All (405) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	201	ILE	O-C-N	-59.03	28.25	122.70
1	A	201	ILE	O-C-N	-59.02	28.27	122.70
1	C	201	ILE	O-C-N	-58.96	28.37	122.70
1	A	82	ILE	O-C-N	-16.84	95.75	122.70
1	C	82	ILE	O-C-N	-16.83	95.78	122.70
1	B	82	ILE	O-C-N	-16.82	95.78	122.70
1	C	338	THR	O-C-N	15.64	147.72	122.70
1	B	338	THR	O-C-N	15.63	147.72	122.70
1	A	338	THR	O-C-N	15.57	147.62	122.70
1	B	300	LEU	O-C-N	14.54	145.97	122.70
1	A	300	LEU	O-C-N	14.50	145.90	122.70
1	C	300	LEU	O-C-N	14.49	145.89	122.70
1	C	307	ASP	C-N-CA	14.02	156.76	121.70
1	B	307	ASP	C-N-CA	14.00	156.70	121.70
1	A	307	ASP	C-N-CA	14.00	156.69	121.70
1	C	129	TYR	O-C-N	12.92	143.38	122.70
1	A	129	TYR	O-C-N	12.87	143.29	122.70
1	B	129	TYR	O-C-N	12.87	143.29	122.70
1	C	307	ASP	O-C-N	-12.85	102.14	122.70
1	A	307	ASP	O-C-N	-12.82	102.19	122.70
1	B	307	ASP	O-C-N	-12.81	102.20	122.70
1	C	93	LEU	N-CA-C	-12.67	76.80	111.00
1	A	93	LEU	N-CA-C	-12.62	76.93	111.00
1	B	93	LEU	N-CA-C	-12.61	76.97	111.00
1	C	201	ILE	CA-C-N	12.54	144.79	117.20
1	B	200	GLY	O-C-N	12.48	142.66	122.70
1	B	201	ILE	CA-C-N	12.44	144.57	117.20
1	B	290	LEU	O-C-N	12.44	142.60	122.70
1	C	200	GLY	O-C-N	12.44	142.60	122.70
1	B	264	SER	O-C-N	12.43	142.59	122.70
1	A	200	GLY	O-C-N	12.42	142.57	122.70
1	C	264	SER	O-C-N	12.39	142.53	122.70
1	A	290	LEU	O-C-N	12.39	142.52	122.70
1	A	201	ILE	CA-C-N	12.39	144.45	117.20
1	C	290	LEU	O-C-N	12.38	142.51	122.70
1	A	264	SER	O-C-N	12.35	142.47	122.70
1	B	339	GLU	C-N-CA	-12.35	90.83	121.70
1	C	339	GLU	C-N-CA	-12.34	90.86	121.70
1	A	339	GLU	C-N-CA	-12.34	90.86	121.70
1	B	330	GLY	O-C-N	-12.14	103.28	122.70
1	C	330	GLY	O-C-N	-12.11	103.33	122.70
1	A	330	GLY	O-C-N	-12.09	103.35	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	299	GLY	O-C-N	11.96	141.83	122.70
1	C	299	GLY	O-C-N	11.96	141.83	122.70
1	A	299	GLY	O-C-N	11.94	141.81	122.70
1	A	297	VAL	C-N-CA	-11.77	92.28	121.70
1	B	297	VAL	C-N-CA	-11.77	92.29	121.70
1	C	297	VAL	C-N-CA	-11.74	92.34	121.70
1	C	338	THR	CA-C-N	-11.54	91.81	117.20
1	B	338	THR	CA-C-N	-11.53	91.84	117.20
1	A	338	THR	CA-C-N	-11.52	91.86	117.20
1	C	264	SER	CA-C-N	-10.45	94.22	117.20
1	B	264	SER	CA-C-N	-10.45	94.22	117.20
1	A	264	SER	CA-C-N	-10.43	94.26	117.20
1	B	300	LEU	CA-C-N	-10.21	94.75	117.20
1	C	300	LEU	CA-C-N	-10.20	94.75	117.20
1	A	300	LEU	CA-C-N	-10.17	94.83	117.20
1	B	200	GLY	CA-C-N	-9.83	95.58	117.20
1	C	200	GLY	CA-C-N	-9.80	95.65	117.20
1	A	200	GLY	CA-C-N	-9.78	95.68	117.20
1	C	313	GLU	O-C-N	9.71	138.23	122.70
1	C	200	GLY	C-N-CA	9.70	145.95	121.70
1	B	313	GLU	O-C-N	9.70	138.22	122.70
1	B	200	GLY	C-N-CA	9.69	145.94	121.70
1	A	200	GLY	C-N-CA	9.69	145.93	121.70
1	A	313	GLU	O-C-N	9.69	138.21	122.70
1	C	129	TYR	CA-C-N	-9.60	96.07	117.20
1	A	279	HIS	O-C-N	-9.60	107.34	122.70
1	B	279	HIS	O-C-N	-9.60	107.34	122.70
1	C	279	HIS	O-C-N	-9.60	107.34	122.70
1	A	129	TYR	CA-C-N	-9.57	96.15	117.20
1	B	129	TYR	CA-C-N	-9.56	96.17	117.20
1	B	140	PRO	N-CD-CG	-9.39	89.11	103.20
1	C	140	PRO	N-CD-CG	-9.38	89.13	103.20
1	A	140	PRO	N-CD-CG	-9.37	89.15	103.20
1	B	100	GLU	O-C-N	-9.36	103.32	121.10
1	C	100	GLU	O-C-N	-9.35	103.34	121.10
1	A	299	GLY	CA-C-N	-9.35	96.64	117.20
1	C	299	GLY	CA-C-N	-9.34	96.64	117.20
1	B	299	GLY	CA-C-N	-9.34	96.65	117.20
1	A	100	GLU	O-C-N	-9.33	103.38	121.10
1	A	335	MET	CA-C-N	-9.31	96.71	117.20
1	C	140	PRO	CA-N-CD	9.31	124.73	111.70
1	C	335	MET	CA-C-N	-9.30	96.73	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	335	MET	CA-C-N	-9.29	96.75	117.20
1	C	202	SER	CB-CA-C	-9.26	92.51	110.10
1	A	202	SER	CB-CA-C	-9.25	92.53	110.10
1	B	202	SER	CB-CA-C	-9.24	92.54	110.10
1	A	140	PRO	CA-N-CD	9.23	124.62	111.70
1	B	140	PRO	CA-N-CD	9.20	124.58	111.70
1	C	264	SER	C-N-CA	-9.13	98.88	121.70
1	B	264	SER	C-N-CA	-9.12	98.89	121.70
1	A	264	SER	C-N-CA	-9.12	98.90	121.70
1	B	278	CYS	CA-CB-SG	-8.81	98.15	114.00
1	A	278	CYS	CA-CB-SG	-8.79	98.17	114.00
1	C	278	CYS	CA-CB-SG	-8.77	98.21	114.00
1	C	328	GLU	O-C-N	8.68	136.59	122.70
1	B	328	GLU	O-C-N	8.68	136.58	122.70
1	A	328	GLU	O-C-N	8.66	136.56	122.70
1	A	279	HIS	CA-C-N	-8.58	98.32	117.20
1	B	279	HIS	CA-C-N	-8.57	98.34	117.20
1	C	279	HIS	CA-C-N	-8.56	98.36	117.20
1	A	275	GLU	N-CA-C	-8.51	88.03	111.00
1	C	275	GLU	N-CA-C	-8.48	88.10	111.00
1	C	325	LYS	C-N-CA	-8.48	100.50	121.70
1	B	275	GLU	N-CA-C	-8.47	88.14	111.00
1	A	325	LYS	C-N-CA	-8.46	100.56	121.70
1	B	90	ILE	O-C-N	-8.46	109.17	122.70
1	A	90	ILE	O-C-N	-8.45	109.18	122.70
1	B	325	LYS	C-N-CA	-8.45	100.57	121.70
1	C	90	ILE	O-C-N	-8.44	109.19	122.70
1	C	314	ALA	N-CA-C	-8.43	88.25	111.00
1	A	314	ALA	N-CA-C	-8.41	88.28	111.00
1	B	314	ALA	N-CA-C	-8.41	88.29	111.00
1	A	175	CYS	CA-CB-SG	-8.29	99.07	114.00
1	C	175	CYS	CA-CB-SG	-8.29	99.08	114.00
1	B	175	CYS	CA-CB-SG	-8.28	99.11	114.00
1	A	175	CYS	C-N-CA	-8.27	101.03	121.70
1	B	175	CYS	C-N-CA	-8.27	101.03	121.70
1	C	175	CYS	C-N-CA	-8.26	101.06	121.70
1	A	307	ASP	CA-C-N	8.15	135.13	117.20
1	B	163	PRO	O-C-N	8.15	135.74	122.70
1	B	307	ASP	CA-C-N	8.15	135.12	117.20
1	C	307	ASP	CA-C-N	8.15	135.12	117.20
1	B	296	PRO	O-C-N	8.14	135.73	122.70
1	A	296	PRO	O-C-N	8.11	135.68	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	163	PRO	O-C-N	8.11	135.68	122.70
1	C	296	PRO	O-C-N	8.11	135.68	122.70
1	A	163	PRO	O-C-N	8.11	135.67	122.70
1	C	350	ARG	NE-CZ-NH2	8.04	124.32	120.30
1	B	350	ARG	NE-CZ-NH2	8.01	124.31	120.30
1	A	350	ARG	NE-CZ-NH2	8.00	124.30	120.30
1	B	291	PHE	CB-CG-CD2	-7.99	115.21	120.80
1	C	291	PHE	CB-CG-CD2	-7.97	115.22	120.80
1	C	76	SER	CB-CA-C	-7.96	94.98	110.10
1	B	203	ASP	O-C-N	-7.95	106.00	121.10
1	A	203	ASP	O-C-N	-7.94	106.02	121.10
1	C	74	ARG	NE-CZ-NH2	7.93	124.26	120.30
1	C	291	PHE	N-CA-CB	-7.91	96.36	110.60
1	C	203	ASP	O-C-N	-7.90	106.09	121.10
1	B	291	PHE	N-CA-CB	-7.90	96.39	110.60
1	A	291	PHE	N-CA-CB	-7.88	96.41	110.60
1	B	330	GLY	CA-C-N	7.83	134.43	117.20
1	C	330	GLY	CA-C-N	7.83	134.43	117.20
1	A	330	GLY	CA-C-N	7.83	134.42	117.20
1	A	291	PHE	CB-CG-CD2	-7.78	115.35	120.80
1	C	140	PRO	N-CA-CB	-7.78	93.96	103.30
1	C	273	GLY	O-C-N	7.71	135.03	122.70
1	A	140	PRO	N-CA-CB	-7.70	94.06	103.30
1	A	273	GLY	O-C-N	7.70	135.03	122.70
1	B	140	PRO	N-CA-CB	-7.70	94.06	103.30
1	B	273	GLY	O-C-N	7.67	134.97	122.70
1	A	273	GLY	C-N-CA	-7.54	102.85	121.70
1	B	273	GLY	C-N-CA	-7.53	102.88	121.70
1	A	84	ARG	NE-CZ-NH2	7.53	124.06	120.30
1	C	273	GLY	C-N-CA	-7.52	102.89	121.70
1	A	261	ARG	NE-CZ-NH2	7.51	124.05	120.30
1	C	57	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	A	135	ARG	NE-CZ-NH2	7.49	124.04	120.30
1	C	135	ARG	NE-CZ-NH2	7.49	124.04	120.30
1	B	84	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	C	241	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	B	135	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	A	241	ARG	NE-CZ-NH2	7.45	124.03	120.30
1	B	261	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	C	63	ALA	O-C-N	7.44	134.61	122.70
1	A	195	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	B	130	ARG	NE-CZ-NH2	7.43	124.01	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	329	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	C	195	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	C	261	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	C	84	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	C	130	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	A	156	ARG	NE-CZ-NH2	7.37	123.99	120.30
1	C	329	ARG	NE-CZ-NH2	7.37	123.99	120.30
1	B	241	ARG	NE-CZ-NH2	7.37	123.98	120.30
1	B	195	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	C	57	ARG	O-C-N	7.34	134.45	122.70
1	A	130	ARG	NE-CZ-NH2	7.34	123.97	120.30
1	A	290	LEU	CA-C-N	-7.32	101.10	117.20
1	B	290	LEU	CA-C-N	-7.31	101.11	117.20
1	C	290	LEU	CA-C-N	-7.31	101.12	117.20
1	A	313	GLU	CA-C-N	-7.30	101.13	117.20
1	B	313	GLU	CA-C-N	-7.30	101.14	117.20
1	B	156	ARG	NE-CZ-NH2	7.29	123.94	120.30
1	B	329	ARG	NE-CZ-NH2	7.27	123.93	120.30
1	C	313	GLU	CA-C-N	-7.27	101.21	117.20
1	C	156	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	C	79	ARG	NE-CZ-NH2	7.25	123.93	120.30
1	A	274	TRP	O-C-N	7.24	134.28	122.70
1	C	274	TRP	O-C-N	7.23	134.27	122.70
1	C	176	VAL	O-C-N	7.22	134.26	122.70
1	B	274	TRP	O-C-N	7.19	134.21	122.70
1	A	176	VAL	O-C-N	7.18	134.20	122.70
1	B	290	LEU	CB-CA-C	-7.15	96.61	110.20
1	B	191	ASP	O-C-N	7.14	134.12	122.70
1	A	290	LEU	CB-CA-C	-7.13	96.66	110.20
1	C	290	LEU	CB-CA-C	-7.12	96.67	110.20
1	B	176	VAL	O-C-N	7.12	134.09	122.70
1	A	191	ASP	O-C-N	7.11	134.07	122.70
1	C	191	ASP	O-C-N	7.03	133.95	122.70
1	B	328	GLU	CA-C-N	-7.03	101.74	117.20
1	A	91	THR	N-CA-CB	7.01	123.63	110.30
1	C	328	GLU	CA-C-N	-7.01	101.78	117.20
1	A	328	GLU	CA-C-N	-7.00	101.80	117.20
1	C	91	THR	N-CA-CB	6.98	123.56	110.30
1	B	91	THR	N-CA-CB	6.97	123.54	110.30
1	C	202	SER	O-C-N	6.95	133.82	122.70
1	A	202	SER	O-C-N	6.94	133.81	122.70
1	B	202	SER	O-C-N	6.94	133.80	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	165	ASP	O-C-N	6.92	133.78	122.70
1	A	165	ASP	O-C-N	6.92	133.77	122.70
1	C	165	ASP	O-C-N	6.91	133.76	122.70
1	A	341	GLN	O-C-N	-6.88	108.03	121.10
1	B	341	GLN	O-C-N	-6.88	108.03	121.10
1	C	341	GLN	O-C-N	-6.85	108.09	121.10
1	A	137	ARG	NE-CZ-NH2	6.84	123.72	120.30
1	C	137	ARG	NE-CZ-NH2	6.84	123.72	120.30
1	A	338	THR	C-N-CA	6.83	138.78	121.70
1	B	137	ARG	NE-CZ-NH2	6.83	123.71	120.30
1	C	338	THR	C-N-CA	6.80	138.71	121.70
1	B	338	THR	C-N-CA	6.80	138.71	121.70
1	A	82	ILE	C-N-CA	6.78	138.66	121.70
1	B	82	ILE	C-N-CA	6.78	138.65	121.70
1	C	82	ILE	C-N-CA	6.77	138.63	121.70
1	C	69	VAL	O-C-N	-6.76	111.89	122.70
1	B	273	GLY	CA-C-N	-6.62	102.64	117.20
1	C	273	GLY	CA-C-N	-6.62	102.64	117.20
1	A	273	GLY	CA-C-N	-6.60	102.68	117.20
1	B	274	TRP	C-N-CA	6.58	138.15	121.70
1	C	313	GLU	C-N-CA	6.56	138.09	121.70
1	A	313	GLU	C-N-CA	6.55	138.08	121.70
1	C	274	TRP	C-N-CA	6.55	138.07	121.70
1	A	274	TRP	C-N-CA	6.54	138.05	121.70
1	B	313	GLU	C-N-CA	6.54	138.06	121.70
1	A	202	SER	N-CA-C	6.52	128.61	111.00
1	B	202	SER	N-CA-C	6.50	128.55	111.00
1	C	202	SER	N-CA-C	6.49	128.53	111.00
1	A	102	LYS	CB-CA-C	6.47	123.35	110.40
1	C	102	LYS	CB-CA-C	6.45	123.31	110.40
1	B	102	LYS	CB-CA-C	6.44	123.28	110.40
1	B	329	ARG	O-C-N	6.42	134.12	123.20
1	A	329	ARG	O-C-N	6.42	134.11	123.20
1	C	199	ASP	O-C-N	6.41	134.09	123.20
1	A	199	ASP	O-C-N	6.41	134.09	123.20
1	B	199	ASP	O-C-N	6.40	134.07	123.20
1	C	329	ARG	O-C-N	6.38	134.04	123.20
1	C	175	CYS	CB-CA-C	-6.34	97.72	110.40
1	A	175	CYS	CB-CA-C	-6.33	97.75	110.40
1	A	326	VAL	O-C-N	6.31	132.79	122.70
1	B	175	CYS	CB-CA-C	-6.29	97.82	110.40
1	B	326	VAL	O-C-N	6.28	132.75	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	326	VAL	O-C-N	6.27	132.74	122.70
1	B	288	LEU	O-C-N	6.26	132.72	122.70
1	C	288	LEU	O-C-N	6.25	132.71	122.70
1	A	288	LEU	O-C-N	6.21	132.64	122.70
1	C	67	ARG	NE-CZ-NH2	6.21	123.40	120.30
1	A	335	MET	CG-SD-CE	6.15	110.04	100.20
1	C	71	THR	N-CA-CB	-6.15	98.61	110.30
1	C	335	MET	CG-SD-CE	6.13	110.00	100.20
1	B	335	MET	CG-SD-CE	6.12	109.99	100.20
1	A	141	MET	CG-SD-CE	6.08	109.94	100.20
1	C	141	MET	CG-SD-CE	6.08	109.92	100.20
1	B	141	MET	CG-SD-CE	6.07	109.92	100.20
1	C	214	MET	CG-SD-CE	6.06	109.89	100.20
1	B	214	MET	CG-SD-CE	6.05	109.88	100.20
1	A	214	MET	CG-SD-CE	6.04	109.86	100.20
1	A	339	GLU	O-C-N	6.01	132.31	122.70
1	A	298	SER	C-N-CA	-6.00	109.69	122.30
1	C	298	SER	C-N-CA	-6.00	109.70	122.30
1	B	288	LEU	CA-C-N	-6.00	104.01	117.20
1	B	298	SER	C-N-CA	-5.99	109.72	122.30
1	C	288	LEU	CA-C-N	-5.98	104.04	117.20
1	B	339	GLU	O-C-N	5.98	132.27	122.70
1	C	339	GLU	O-C-N	5.98	132.26	122.70
1	C	53	GLN	O-C-N	-5.95	113.19	122.70
1	C	274	TRP	CA-C-N	-5.93	104.16	117.20
1	C	76	SER	N-CA-C	5.93	127.00	111.00
1	A	288	LEU	CA-C-N	-5.92	104.17	117.20
1	A	274	TRP	CA-C-N	-5.89	104.23	117.20
1	B	274	TRP	CA-C-N	-5.88	104.26	117.20
1	C	325	LYS	O-C-N	5.87	132.09	122.70
1	B	317	GLY	O-C-N	-5.86	113.32	122.70
1	C	317	GLY	O-C-N	-5.86	113.32	122.70
1	B	314	ALA	CB-CA-C	5.86	118.89	110.10
1	A	314	ALA	CB-CA-C	5.85	118.87	110.10
1	C	162	PRO	O-C-N	-5.85	109.99	121.10
1	A	315	ALA	O-C-N	-5.84	113.35	122.70
1	C	202	SER	CA-C-N	-5.84	104.35	117.20
1	A	325	LYS	O-C-N	5.84	132.04	122.70
1	B	202	SER	CA-C-N	-5.84	104.36	117.20
1	A	317	GLY	O-C-N	-5.83	113.36	122.70
1	A	162	PRO	O-C-N	-5.82	110.03	121.10
1	A	202	SER	CA-C-N	-5.82	104.39	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	63	ALA	CA-C-N	-5.82	104.39	117.20
1	B	315	ALA	O-C-N	-5.82	113.39	122.70
1	C	314	ALA	CB-CA-C	5.82	118.82	110.10
1	B	162	PRO	O-C-N	-5.81	110.06	121.10
1	B	325	LYS	O-C-N	5.81	132.00	122.70
1	C	315	ALA	O-C-N	-5.81	113.41	122.70
1	A	130	ARG	CB-CA-C	-5.76	98.88	110.40
1	B	231	ARG	NE-CZ-NH2	5.76	123.18	120.30
1	C	130	ARG	CB-CA-C	-5.75	98.90	110.40
1	C	231	ARG	NE-CZ-NH2	5.73	123.16	120.30
1	B	130	ARG	CB-CA-C	-5.72	98.95	110.40
1	A	231	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	A	177	SER	CA-C-N	-5.71	104.64	117.20
1	B	177	SER	CA-C-N	-5.71	104.65	117.20
1	C	177	SER	CA-C-N	-5.67	104.73	117.20
1	C	56	THR	CB-CA-C	-5.65	96.35	111.60
1	B	305	ALA	O-C-N	5.63	131.71	122.70
1	C	305	ALA	O-C-N	5.60	131.66	122.70
1	A	305	ALA	O-C-N	5.58	131.64	122.70
1	A	191	ASP	CA-C-N	-5.56	104.97	117.20
1	B	191	ASP	CA-C-N	-5.54	105.00	117.20
1	A	300	LEU	CA-CB-CG	-5.54	102.56	115.30
1	B	300	LEU	CA-CB-CG	-5.53	102.58	115.30
1	C	300	LEU	CA-CB-CG	-5.53	102.58	115.30
1	C	57	ARG	CA-C-N	-5.53	105.04	117.20
1	C	191	ASP	CA-C-N	-5.51	105.09	117.20
1	A	199	ASP	CA-C-N	-5.50	105.20	116.20
1	B	199	ASP	CA-C-N	-5.50	105.20	116.20
1	B	93	LEU	N-CA-CB	-5.48	99.44	110.40
1	A	93	LEU	N-CA-CB	-5.47	99.45	110.40
1	B	163	PRO	CA-C-N	-5.47	105.16	117.20
1	C	199	ASP	CA-C-N	-5.47	105.25	116.20
1	C	176	VAL	CA-C-N	-5.47	105.17	117.20
1	C	163	PRO	CA-C-N	-5.46	105.19	117.20
1	C	93	LEU	N-CA-CB	-5.46	99.48	110.40
1	A	163	PRO	CA-C-N	-5.45	105.21	117.20
1	B	273	GLY	N-CA-C	-5.45	99.48	113.10
1	C	273	GLY	N-CA-C	-5.45	99.48	113.10
1	A	273	GLY	N-CA-C	-5.43	99.53	113.10
1	A	176	VAL	CA-C-N	-5.43	105.26	117.20
1	B	176	VAL	CA-C-N	-5.42	105.27	117.20
1	C	90	ILE	CA-C-N	5.39	129.06	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	90	ILE	CA-C-N	5.39	129.05	117.20
1	C	72	GLN	C-N-CD	-5.38	108.77	120.60
1	B	90	ILE	CA-C-N	5.37	129.00	117.20
1	B	264	SER	CB-CA-C	-5.35	99.94	110.10
1	A	264	SER	CB-CA-C	-5.34	99.95	110.10
1	B	296	PRO	CA-C-N	-5.34	105.45	117.20
1	B	203	ASP	CA-C-N	5.33	132.04	117.10
1	A	296	PRO	CA-C-N	-5.33	105.47	117.20
1	A	203	ASP	CA-C-N	5.33	132.01	117.10
1	C	296	PRO	CA-C-N	-5.32	105.49	117.20
1	A	165	ASP	CA-C-N	-5.32	105.49	117.20
1	C	203	ASP	CA-C-N	5.32	131.98	117.10
1	B	165	ASP	CA-C-N	-5.31	105.52	117.20
1	C	264	SER	CB-CA-C	-5.31	100.02	110.10
1	B	248	ALA	CB-CA-C	-5.30	102.16	110.10
1	C	165	ASP	CA-C-N	-5.29	105.56	117.20
1	B	176	VAL	N-CA-CB	-5.29	99.87	111.50
1	A	248	ALA	CB-CA-C	-5.27	102.20	110.10
1	C	176	VAL	N-CA-CB	-5.27	99.91	111.50
1	A	176	VAL	N-CA-CB	-5.26	99.92	111.50
1	C	248	ALA	CB-CA-C	-5.26	102.21	110.10
1	B	291	PHE	CB-CA-C	5.24	120.89	110.40
1	B	338	THR	CB-CA-C	-5.24	97.45	111.60
1	B	100	GLU	CA-C-N	5.24	131.77	117.10
1	C	338	THR	CB-CA-C	-5.24	97.45	111.60
1	C	291	PHE	CB-CA-C	5.24	120.87	110.40
1	A	338	THR	CB-CA-C	-5.23	97.48	111.60
1	C	175	CYS	O-C-N	-5.22	114.34	122.70
1	B	304	ASP	O-C-N	5.21	131.04	122.70
1	A	291	PHE	CB-CA-C	5.21	120.83	110.40
1	B	175	CYS	O-C-N	-5.21	114.36	122.70
1	C	100	GLU	CA-C-N	5.21	131.69	117.10
1	A	100	GLU	CA-C-N	5.20	131.66	117.10
1	B	129	TYR	C-N-CA	5.19	134.68	121.70
1	A	175	CYS	O-C-N	-5.19	114.40	122.70
1	C	129	TYR	C-N-CA	5.18	134.65	121.70
1	A	129	TYR	C-N-CA	5.17	134.64	121.70
1	A	304	ASP	O-C-N	5.17	130.97	122.70
1	C	304	ASP	O-C-N	5.15	130.94	122.70
1	C	323	GLY	C-N-CA	5.15	134.58	121.70
1	A	176	VAL	CB-CA-C	5.15	121.19	111.40
1	A	290	LEU	C-N-CA	5.15	134.57	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	323	GLY	C-N-CA	5.15	134.56	121.70
1	C	290	LEU	C-N-CA	5.14	134.56	121.70
1	B	176	VAL	CB-CA-C	5.14	121.16	111.40
1	A	329	ARG	CA-C-N	-5.13	105.94	116.20
1	B	323	GLY	C-N-CA	5.12	134.51	121.70
1	B	290	LEU	C-N-CA	5.12	134.49	121.70
1	B	329	ARG	CA-C-N	-5.12	105.97	116.20
1	C	329	ARG	CA-C-N	-5.11	105.97	116.20
1	C	176	VAL	CB-CA-C	5.09	121.08	111.40
1	A	343	LYS	CB-CA-C	-5.08	100.24	110.40
1	B	343	LYS	CB-CA-C	-5.06	100.28	110.40
1	C	343	LYS	CB-CA-C	-5.05	100.29	110.40
1	A	326	VAL	CA-C-N	-5.05	106.09	117.20
1	C	326	VAL	CA-C-N	-5.05	106.09	117.20
1	A	339	GLU	CA-C-N	-5.05	106.10	117.20
1	C	325	LYS	CA-C-N	-5.05	106.10	117.20
1	B	326	VAL	CA-C-N	-5.04	106.11	117.20
1	C	339	GLU	CA-C-N	-5.04	106.12	117.20
1	A	130	ARG	N-CA-C	5.03	124.59	111.00
1	B	290	LEU	N-CA-C	5.02	124.56	111.00
1	B	339	GLU	CA-C-N	-5.02	106.16	117.20
1	C	290	LEU	N-CA-C	5.02	124.55	111.00
1	A	325	LYS	CA-C-N	-5.01	106.17	117.20
1	B	130	ARG	N-CA-C	5.01	124.54	111.00
1	C	130	ARG	N-CA-C	5.01	124.53	111.00
1	B	325	LYS	CA-C-N	-5.01	106.19	117.20
1	A	290	LEU	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	GLU	Mainchain
1	A	177	SER	Mainchain
1	A	201	ILE	Mainchain
1	A	260	PRO	Mainchain
1	A	307	ASP	Mainchain
1	A	330	GLY	Mainchain
1	A	335	MET	Mainchain
1	A	92	THR	Peptide
1	B	100	GLU	Mainchain
1	B	177	SER	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	201	ILE	Mainchain
1	B	260	PRO	Mainchain
1	B	307	ASP	Mainchain
1	B	330	GLY	Mainchain
1	B	335	MET	Mainchain
1	B	92	THR	Peptide
1	C	100	GLU	Mainchain
1	C	177	SER	Mainchain
1	C	201	ILE	Mainchain
1	C	260	PRO	Mainchain
1	C	307	ASP	Mainchain
1	C	330	GLY	Mainchain
1	C	335	MET	Mainchain
1	C	59	SER	Mainchain
1	C	69	VAL	Mainchain
1	C	92	THR	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	2024	0	1964	947	0
1	B	2024	0	1963	941	0
1	C	2236	0	2181	1146	0
All	All	6284	0	6108	3034	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 245.

All (3034) 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:A:138:TYR:CB	1:A:184:PHE:CE1	1.75	1.66
1:C:138:TYR:CB	1:C:184:PHE:CE1	1.75	1.65
1:C:138:TYR:HB2	1:C:184:PHE:CZ	1.15	1.64
1:A:138:TYR:HB2	1:A:184:PHE:CZ	1.15	1.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:PRO:CD	1:B:166:LEU:CD1	1.75	1.64
1:B:138:TYR:CB	1:B:184:PHE:CE1	1.75	1.64
1:C:101:PRO:CD	1:C:166:LEU:HD11	1.21	1.63
1:A:101:PRO:CD	1:A:166:LEU:CD1	1.75	1.63
1:B:138:TYR:HB2	1:B:184:PHE:CZ	1.15	1.62
1:B:101:PRO:CD	1:B:166:LEU:HD11	1.22	1.57
1:A:101:PRO:CD	1:A:166:LEU:HD11	1.21	1.56
1:B:130:ARG:CD	1:B:237:GLN:CB	1.82	1.56
1:A:130:ARG:CD	1:A:237:GLN:CB	1.81	1.54
1:C:101:PRO:CD	1:C:166:LEU:CD1	1.75	1.53
1:C:130:ARG:CD	1:C:237:GLN:CB	1.82	1.53
1:C:75:VAL:CA	1:C:75:VAL:C	1.76	1.53
1:A:248:ALA:CB	1:A:264:SER:C	1.75	1.53
1:A:278:CYS:H	1:A:334:LYS:CD	1.21	1.53
1:C:278:CYS:H	1:C:334:LYS:CD	1.21	1.52
1:C:159:ALA:HB1	1:C:328:GLU:CB	1.32	1.52
1:C:76:SER:CA	1:C:76:SER:C	1.75	1.52
1:B:278:CYS:H	1:B:334:LYS:CD	1.21	1.51
1:A:101:PRO:HD3	1:A:166:LEU:CD1	1.34	1.51
1:C:75:VAL:CA	1:C:75:VAL:N	1.68	1.51
1:C:101:PRO:HD3	1:C:166:LEU:CD1	1.34	1.50
1:C:76:SER:N	1:C:76:SER:CA	1.76	1.49
1:C:185:ILE:HD12	1:C:186:LEU:N	1.18	1.49
1:C:153:ALA:CB	1:C:174:GLY:HA3	1.43	1.48
1:A:153:ALA:CB	1:A:174:GLY:HA3	1.43	1.47
1:C:200:GLY:N	1:C:265:TRP:CD1	1.82	1.47
1:A:130:ARG:CD	1:A:237:GLN:HB2	0.98	1.46
1:C:80:ASP:HA	1:C:241:ARG:NH2	1.24	1.46
1:B:153:ALA:CB	1:B:174:GLY:HA3	1.43	1.45
1:A:121:LYS:NZ	1:A:121:LYS:CE	1.79	1.45
1:C:130:ARG:CD	1:C:237:GLN:HB2	0.98	1.45
1:C:207:VAL:CG1	1:C:329:ARG:CZ	1.93	1.45
1:B:130:ARG:CD	1:B:237:GLN:HB2	0.98	1.45
1:B:264:SER:C	1:B:265:TRP:N	1.68	1.45
1:C:291:PHE:C	1:C:292:TYR:N	1.71	1.44
1:C:339:GLU:C	1:C:340:GLU:N	1.68	1.44
1:B:101:PRO:HD3	1:B:166:LEU:CD1	1.34	1.43
1:C:134:LEU:CA	1:C:233:GLU:O	1.66	1.43
1:C:207:VAL:N	1:C:329:ARG:HH22	0.96	1.43
1:B:121:LYS:NZ	1:B:121:LYS:CE	1.79	1.43
1:A:264:SER:C	1:A:265:TRP:N	1.68	1.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LYS:O	1:A:277:ASP:CB	1.67	1.43
1:A:296:PRO:CG	1:A:337:THR:HG22	0.96	1.43
1:C:264:SER:C	1:C:265:TRP:N	1.68	1.43
1:C:207:VAL:HG12	1:C:329:ARG:NH2	1.27	1.43
1:C:296:PRO:CG	1:C:337:THR:HG22	0.96	1.43
1:A:339:GLU:C	1:A:340:GLU:N	1.68	1.42
1:C:207:VAL:H	1:C:329:ARG:NH2	1.11	1.42
1:C:121:LYS:NZ	1:C:121:LYS:CE	1.79	1.42
1:C:207:VAL:HG12	1:C:329:ARG:CZ	0.96	1.42
1:B:185:ILE:HD12	1:B:186:LEU:N	1.18	1.42
1:B:269:LYS:O	1:B:277:ASP:CB	1.67	1.42
1:C:197:VAL:CG2	1:C:350:ARG:HH22	1.30	1.42
1:B:296:PRO:CG	1:B:337:THR:HG22	0.96	1.42
1:C:269:LYS:O	1:C:277:ASP:CB	1.67	1.41
1:B:185:ILE:CD1	1:B:186:LEU:H	1.32	1.41
1:C:203:ASP:OD1	1:C:205:LYS:CD	1.68	1.41
1:B:339:GLU:C	1:B:340:GLU:N	1.68	1.41
1:A:134:LEU:CA	1:A:233:GLU:O	1.66	1.41
1:A:203:ASP:OD1	1:A:205:LYS:CD	1.68	1.40
1:C:207:VAL:CG1	1:C:329:ARG:NH2	1.81	1.40
1:B:279:HIS:C	1:B:280:PHE:N	1.74	1.40
1:A:291:PHE:C	1:A:292:TYR:N	1.71	1.40
1:B:149:LYS:CE	1:B:149:LYS:CD	2.00	1.39
1:B:291:PHE:C	1:B:292:TYR:N	1.71	1.39
1:A:185:ILE:HD12	1:A:186:LEU:N	1.18	1.39
1:C:185:ILE:CD1	1:C:186:LEU:H	1.32	1.39
1:A:130:ARG:HD2	1:A:237:GLN:CB	1.47	1.39
1:A:149:LYS:CE	1:A:149:LYS:CD	1.99	1.39
1:C:279:HIS:C	1:C:280:PHE:N	1.74	1.39
1:B:115:THR:O	1:B:116:PHE:CD1	1.75	1.39
1:B:350:ARG:O	1:B:351:ILE:CG2	1.71	1.39
1:A:185:ILE:CD1	1:A:186:LEU:H	1.32	1.39
1:C:149:LYS:CE	1:C:149:LYS:CD	1.99	1.39
1:A:115:THR:O	1:A:116:PHE:CD1	1.76	1.38
1:B:138:TYR:CB	1:B:184:PHE:CZ	1.96	1.38
1:B:203:ASP:OD1	1:B:205:LYS:CD	1.68	1.38
1:B:134:LEU:CA	1:B:233:GLU:O	1.66	1.38
1:C:350:ARG:O	1:C:351:ILE:CG2	1.71	1.38
1:A:248:ALA:HB3	1:A:264:SER:C	1.01	1.37
1:B:149:LYS:CD	1:B:170:TYR:OH	1.72	1.37
1:A:149:LYS:CD	1:A:170:TYR:OH	1.72	1.37

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:PRO:HG2	1:C:328:GLU:CG	1.54	1.37
1:C:115:THR:O	1:C:116:PHE:CD1	1.75	1.37
1:C:149:LYS:CD	1:C:170:TYR:OH	1.72	1.36
1:A:138:TYR:CG	1:A:184:PHE:CE1	2.12	1.36
1:B:130:ARG:HD3	1:B:237:GLN:CB	1.46	1.36
1:A:279:HIS:C	1:A:280:PHE:N	1.74	1.36
1:C:138:TYR:CG	1:C:184:PHE:CE1	2.12	1.36
1:A:350:ARG:O	1:A:351:ILE:CG2	1.71	1.36
1:C:165:ASP:O	1:C:168:SER:HB2	1.25	1.35
1:C:138:TYR:CB	1:C:184:PHE:CZ	1.96	1.35
1:C:159:ALA:CB	1:C:328:GLU:HB2	1.54	1.35
1:C:296:PRO:HG2	1:C:337:THR:CG2	0.89	1.34
1:B:138:TYR:CG	1:B:184:PHE:CE1	2.12	1.34
1:B:278:CYS:N	1:B:334:LYS:CD	1.87	1.34
1:A:296:PRO:HG2	1:A:337:THR:CG2	0.89	1.34
1:B:296:PRO:HG2	1:B:337:THR:CG2	0.88	1.34
1:A:82:ILE:C	1:A:83:THR:N	1.81	1.34
1:C:278:CYS:N	1:C:334:LYS:CD	1.87	1.34
1:C:82:ILE:C	1:C:83:THR:N	1.81	1.34
1:B:82:ILE:C	1:B:83:THR:N	1.81	1.34
1:B:291:PHE:HA	1:B:345:LYS:O	1.23	1.34
1:A:309:SER:O	1:A:322:ALA:HA	1.19	1.34
1:C:153:ALA:HB1	1:C:174:GLY:CA	1.57	1.34
1:B:153:ALA:HB1	1:B:174:GLY:CA	1.57	1.34
1:B:278:CYS:H	1:B:334:LYS:CE	1.41	1.34
1:A:153:ALA:HB1	1:A:174:GLY:CA	1.57	1.33
1:C:138:TYR:CD2	1:C:184:PHE:HE1	1.46	1.33
1:A:278:CYS:N	1:A:334:LYS:CD	1.87	1.33
1:C:278:CYS:H	1:C:334:LYS:CE	1.41	1.33
1:A:278:CYS:H	1:A:334:LYS:CE	1.41	1.33
1:C:130:ARG:HD3	1:C:237:GLN:CB	1.46	1.33
1:B:138:TYR:CD2	1:B:184:PHE:HE1	1.46	1.32
1:B:130:ARG:HD2	1:B:237:GLN:CB	1.47	1.32
1:A:138:TYR:CD2	1:A:184:PHE:HE1	1.46	1.32
1:A:130:ARG:HD3	1:A:237:GLN:CB	1.46	1.32
1:C:265:TRP:CZ3	1:C:348:ALA:O	1.82	1.32
1:A:133:SER:O	1:A:234:TYR:HA	1.28	1.32
1:A:198:ALA:HB1	1:A:200:GLY:O	1.17	1.32
1:A:304:ASP:O	1:A:331:GLN:HB3	1.14	1.32
1:C:130:ARG:HD2	1:C:237:GLN:CB	1.47	1.32
1:A:265:TRP:CZ3	1:A:348:ALA:O	1.82	1.32

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ASP:O	1:B:168:SER:HB2	1.26	1.31
1:C:149:LYS:HG2	1:C:177:SER:OG	1.22	1.31
1:B:265:TRP:CZ3	1:B:348:ALA:O	1.82	1.31
1:A:165:ASP:O	1:A:168:SER:HB2	1.26	1.30
1:C:291:PHE:CA	1:C:345:LYS:O	1.78	1.30
1:C:71:THR:CG2	1:C:87:SER:OG	1.78	1.30
1:A:138:TYR:CB	1:A:184:PHE:CZ	1.96	1.30
1:C:159:ALA:HB1	1:C:328:GLU:CG	1.60	1.30
1:A:291:PHE:HA	1:A:345:LYS:O	1.22	1.30
1:C:204:PRO:CG	1:C:328:GLU:HG2	1.59	1.29
1:A:248:ALA:CB	1:A:264:SER:OG	1.81	1.29
1:B:291:PHE:CA	1:B:345:LYS:O	1.79	1.29
1:C:154:PHE:CD1	1:C:155:ASP:N	2.01	1.29
1:A:313:GLU:HG3	1:A:318:SER:CB	1.63	1.29
1:C:309:SER:O	1:C:322:ALA:HA	1.19	1.29
1:B:88:GLU:O	1:B:231:ARG:HB2	1.19	1.29
1:A:291:PHE:CA	1:A:345:LYS:O	1.78	1.29
1:B:327:ALA:HB3	1:B:331:GLN:CD	1.53	1.29
1:A:333:VAL:O	1:A:334:LYS:HD3	1.30	1.29
1:C:313:GLU:HG3	1:C:318:SER:CB	1.63	1.28
1:A:119:LEU:CD2	1:A:234:TYR:OH	1.82	1.28
1:A:154:PHE:CD1	1:A:155:ASP:N	2.01	1.28
1:C:88:GLU:O	1:C:231:ARG:HB2	1.19	1.28
1:B:154:PHE:CD1	1:B:155:ASP:N	2.01	1.28
1:B:133:SER:OG	1:B:133:SER:CB	1.81	1.28
1:B:149:LYS:HG2	1:B:177:SER:OG	1.23	1.28
1:B:105:THR:OG1	1:B:211:LYS:CD	1.82	1.28
1:A:154:PHE:HD1	1:A:155:ASP:N	1.32	1.28
1:C:291:PHE:HA	1:C:345:LYS:O	1.23	1.27
1:B:119:LEU:CD2	1:B:234:TYR:OH	1.82	1.27
1:C:78:ALA:O	1:C:80:ASP:N	1.63	1.27
1:C:133:SER:O	1:C:234:TYR:HA	1.28	1.27
1:C:304:ASP:O	1:C:331:GLN:HB3	1.15	1.27
1:B:198:ALA:HB1	1:B:200:GLY:O	1.17	1.27
1:C:105:THR:OG1	1:C:211:LYS:CD	1.82	1.27
1:A:133:SER:CB	1:A:133:SER:OG	1.81	1.27
1:C:159:ALA:CB	1:C:328:GLU:CB	2.08	1.27
1:C:198:ALA:HB1	1:C:200:GLY:O	1.16	1.27
1:A:105:THR:OG1	1:A:211:LYS:CD	1.82	1.26
1:C:133:SER:CB	1:C:133:SER:OG	1.81	1.26
1:A:149:LYS:HG2	1:A:177:SER:OG	1.23	1.26

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:LEU:CD2	1:C:234:TYR:OH	1.82	1.26
1:B:313:GLU:HG3	1:B:318:SER:CB	1.63	1.26
1:B:309:SER:O	1:B:322:ALA:HA	1.19	1.26
1:A:156:ARG:O	1:A:210:GLY:HA3	1.36	1.25
1:C:327:ALA:HB3	1:C:331:GLN:CD	1.53	1.25
1:C:138:TYR:HB3	1:C:184:PHE:CE1	1.51	1.25
1:B:133:SER:O	1:B:234:TYR:HA	1.28	1.25
1:C:80:ASP:CA	1:C:241:ARG:HH22	1.49	1.25
1:A:327:ALA:HB3	1:A:331:GLN:CD	1.53	1.25
1:C:179:VAL:HG11	1:C:181:TRP:CD1	1.71	1.25
1:A:138:TYR:HB3	1:A:184:PHE:CE1	1.51	1.25
1:A:88:GLU:O	1:A:231:ARG:HB2	1.18	1.25
1:C:201:ILE:HB	1:C:265:TRP:O	1.12	1.25
1:B:154:PHE:HD1	1:B:155:ASP:N	1.32	1.25
1:B:288:LEU:HD11	1:B:290:LEU:CD2	1.67	1.25
1:C:156:ARG:O	1:C:210:GLY:HA3	1.37	1.24
1:B:328:GLU:O	1:B:329:ARG:O	1.55	1.24
1:A:248:ALA:HB1	1:A:264:SER:OG	1.20	1.24
1:A:179:VAL:HG11	1:A:181:TRP:CD1	1.71	1.24
1:A:96:ASN:O	1:A:98:ASP:N	1.70	1.24
1:C:159:ALA:CB	1:C:328:GLU:CG	2.15	1.24
1:C:333:VAL:O	1:C:334:LYS:HD3	1.30	1.24
1:C:138:TYR:OH	1:C:227:LEU:HB3	1.38	1.24
1:B:304:ASP:O	1:B:331:GLN:HB3	1.15	1.23
1:B:138:TYR:HB3	1:B:184:PHE:CE1	1.51	1.23
1:B:179:VAL:HG11	1:B:181:TRP:CD1	1.71	1.23
1:B:156:ARG:O	1:B:210:GLY:HA3	1.36	1.23
1:B:293:GLU:O	1:B:317:GLY:N	1.72	1.23
1:B:333:VAL:O	1:B:334:LYS:HD3	1.30	1.23
1:A:248:ALA:CB	1:A:264:SER:O	1.87	1.23
1:A:288:LEU:HD11	1:A:290:LEU:CD2	1.66	1.23
1:C:96:ASN:O	1:C:98:ASP:N	1.70	1.22
1:C:154:PHE:HD1	1:C:155:ASP:N	1.32	1.22
1:C:197:VAL:CG2	1:C:350:ARG:NH2	2.01	1.22
1:C:90:ILE:HD11	1:C:232:VAL:CG2	1.69	1.22
1:B:96:ASN:O	1:B:98:ASP:N	1.70	1.22
1:C:288:LEU:HD11	1:C:290:LEU:CD2	1.66	1.22
1:C:293:GLU:O	1:C:317:GLY:N	1.72	1.22
1:C:101:PRO:O	1:C:102:LYS:CG	1.88	1.22
1:A:293:GLU:O	1:A:317:GLY:N	1.72	1.22
1:C:200:GLY:C	1:C:282:GLY:CA	2.08	1.22

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:GLU:O	1:C:329:ARG:O	1.55	1.21
1:C:149:LYS:HB3	1:C:217:TYR:CE1	1.75	1.21
1:A:328:GLU:O	1:A:329:ARG:O	1.55	1.21
1:C:201:ILE:CB	1:C:265:TRP:O	1.87	1.21
1:C:207:VAL:HG12	1:C:329:ARG:NE	1.52	1.21
1:A:327:ALA:CB	1:A:331:GLN:OE1	1.88	1.21
1:A:90:ILE:HD11	1:A:232:VAL:CG2	1.69	1.20
1:B:294:LYS:O	1:B:296:PRO:HD3	1.04	1.20
1:C:327:ALA:CB	1:C:331:GLN:OE1	1.88	1.20
1:B:327:ALA:CB	1:B:331:GLN:OE1	1.88	1.20
1:A:294:LYS:O	1:A:296:PRO:HD3	1.04	1.20
1:B:90:ILE:HD11	1:B:232:VAL:CG2	1.69	1.20
1:C:200:GLY:HA2	1:C:265:TRP:CB	1.70	1.20
1:C:200:GLY:CA	1:C:265:TRP:CD1	2.25	1.19
1:A:149:LYS:HB3	1:A:217:TYR:CE1	1.75	1.19
1:C:204:PRO:HG3	1:C:328:GLU:C	1.61	1.19
1:B:149:LYS:HB3	1:B:217:TYR:CE1	1.75	1.19
1:B:101:PRO:O	1:B:102:LYS:CG	1.88	1.19
1:C:294:LYS:O	1:C:296:PRO:HD3	1.04	1.19
1:A:101:PRO:O	1:A:102:LYS:CG	1.88	1.19
1:A:101:PRO:C	1:A:102:LYS:HG3	1.57	1.18
1:C:204:PRO:CG	1:C:329:ARG:N	2.06	1.18
1:B:164:ASN:HD22	1:B:164:ASN:N	1.19	1.18
1:C:138:TYR:HB3	1:C:184:PHE:CD1	1.78	1.18
1:B:259:GLY:C	1:B:260:PRO:N	1.97	1.18
1:B:101:PRO:C	1:B:102:LYS:HG3	1.57	1.18
1:B:326:VAL:CG1	1:B:327:ALA:H	1.54	1.18
1:A:295:ALA:N	1:A:316:ALA:HA	1.51	1.18
1:C:138:TYR:CG	1:C:184:PHE:HE1	1.56	1.17
1:C:259:GLY:C	1:C:260:PRO:N	1.97	1.17
1:B:138:TYR:OH	1:B:227:LEU:HB3	1.38	1.17
1:A:138:TYR:OH	1:A:227:LEU:HB3	1.38	1.17
1:A:326:VAL:CG1	1:A:327:ALA:H	1.54	1.17
1:C:295:ALA:N	1:C:316:ALA:HA	1.51	1.17
1:B:138:TYR:HB3	1:B:184:PHE:CD1	1.78	1.17
1:A:101:PRO:HD2	1:A:166:LEU:CD1	1.68	1.17
1:A:138:TYR:HB3	1:A:184:PHE:CD1	1.78	1.17
1:A:149:LYS:HD3	1:A:170:TYR:HH	1.05	1.17
1:A:248:ALA:CB	1:A:265:TRP:HA	1.73	1.17
1:A:259:GLY:C	1:A:260:PRO:N	1.97	1.16
1:A:326:VAL:HG12	1:A:327:ALA:N	1.60	1.16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:GLU:O	1:C:231:ARG:CB	1.93	1.15
1:B:309:SER:O	1:B:322:ALA:CA	1.94	1.15
1:B:88:GLU:O	1:B:231:ARG:CB	1.93	1.15
1:C:204:PRO:HG3	1:C:329:ARG:N	1.13	1.15
1:A:179:VAL:HG11	1:A:181:TRP:NE1	1.61	1.15
1:A:88:GLU:O	1:A:231:ARG:CB	1.93	1.15
1:C:179:VAL:HG11	1:C:181:TRP:NE1	1.61	1.15
1:C:105:THR:OG1	1:C:211:LYS:HD3	0.98	1.15
1:C:138:TYR:CD2	1:C:184:PHE:CE1	2.34	1.15
1:B:138:TYR:CD2	1:B:184:PHE:CE1	2.34	1.15
1:A:313:GLU:HG3	1:A:318:SER:HB2	1.28	1.15
1:B:116:PHE:O	1:B:120:ILE:HG21	1.46	1.14
1:B:151:ALA:HA	1:B:177:SER:HB2	1.28	1.14
1:A:116:PHE:O	1:A:120:ILE:HG21	1.46	1.14
1:A:277:ASP:CA	1:A:334:LYS:HD2	1.77	1.14
1:A:294:LYS:O	1:A:296:PRO:CD	1.96	1.14
1:C:101:PRO:CD	1:C:166:LEU:HD12	1.73	1.14
1:C:204:PRO:CG	1:C:328:GLU:CG	2.20	1.14
1:C:204:PRO:CB	1:C:328:GLU:HG3	1.77	1.14
1:B:277:ASP:CA	1:B:334:LYS:HD2	1.77	1.14
1:B:294:LYS:O	1:B:296:PRO:CD	1.96	1.14
1:A:105:THR:OG1	1:A:211:LYS:HD3	0.98	1.14
1:A:309:SER:O	1:A:322:ALA:CA	1.94	1.14
1:A:101:PRO:HG3	1:A:217:TYR:CE2	1.83	1.14
1:C:86:GLY:HA2	1:C:234:TYR:CD1	1.83	1.14
1:B:112:GLU:HG3	1:B:329:ARG:NH2	1.61	1.14
1:B:86:GLY:HA2	1:B:234:TYR:CD1	1.83	1.14
1:C:294:LYS:O	1:C:296:PRO:CD	1.96	1.14
1:C:297:VAL:HB	1:C:336:VAL:O	1.47	1.14
1:C:277:ASP:CA	1:C:334:LYS:HD2	1.77	1.13
1:B:179:VAL:HG11	1:B:181:TRP:NE1	1.61	1.13
1:B:105:THR:OG1	1:B:211:LYS:HD3	0.98	1.13
1:A:297:VAL:HB	1:A:336:VAL:HG13	1.26	1.13
1:C:116:PHE:O	1:C:120:ILE:HG21	1.46	1.13
1:A:265:TRP:HZ3	1:A:348:ALA:O	1.20	1.13
1:C:101:PRO:HG3	1:C:217:TYR:CE2	1.83	1.12
1:A:126:TYR:CA	1:A:242:THR:HG22	1.80	1.12
1:C:309:SER:O	1:C:322:ALA:CA	1.94	1.12
1:C:101:PRO:C	1:C:102:LYS:HG3	1.57	1.12
1:C:249:GLN:NE2	1:C:265:TRP:CE3	2.15	1.12
1:A:248:ALA:HB2	1:A:265:TRP:HA	1.31	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:VAL:HB	1:B:336:VAL:HG13	1.27	1.12
1:A:119:LEU:HD22	1:A:234:TYR:CZ	1.85	1.12
1:A:86:GLY:HA2	1:A:234:TYR:CD1	1.83	1.12
1:C:164:ASN:N	1:C:164:ASN:HD22	1.19	1.12
1:B:101:PRO:O	1:B:102:LYS:HG3	0.95	1.12
1:B:101:PRO:HG3	1:B:217:TYR:CE2	1.83	1.12
1:B:326:VAL:HG12	1:B:327:ALA:N	1.60	1.12
1:B:301:GLU:O	1:B:333:VAL:HG13	1.50	1.12
1:C:120:ILE:HD11	1:C:351:ILE:C	1.69	1.12
1:B:126:TYR:CA	1:B:242:THR:HG22	1.80	1.12
1:A:248:ALA:HB3	1:A:264:SER:CA	1.79	1.12
1:B:297:VAL:HB	1:B:336:VAL:O	1.47	1.12
1:C:326:VAL:HG12	1:C:327:ALA:N	1.60	1.12
1:C:301:GLU:O	1:C:333:VAL:HG13	1.50	1.12
1:C:265:TRP:HZ3	1:C:348:ALA:O	1.20	1.12
1:B:295:ALA:H	1:B:316:ALA:CA	1.63	1.11
1:B:295:ALA:N	1:B:316:ALA:HA	1.51	1.11
1:C:198:ALA:CB	1:C:200:GLY:O	1.96	1.11
1:A:101:PRO:O	1:A:102:LYS:HG3	0.95	1.11
1:C:126:TYR:CA	1:C:242:THR:HG22	1.80	1.11
1:B:119:LEU:HD22	1:B:234:TYR:CZ	1.85	1.11
1:B:149:LYS:HD2	1:B:170:TYR:OH	1.44	1.11
1:C:248:ALA:HB1	1:C:287:SER:O	1.48	1.11
1:A:198:ALA:CB	1:A:200:GLY:O	1.97	1.11
1:C:295:ALA:H	1:C:316:ALA:CA	1.63	1.11
1:A:151:ALA:HA	1:A:177:SER:HB2	1.28	1.11
1:C:151:ALA:HA	1:C:177:SER:HB2	1.28	1.11
1:B:164:ASN:ND2	1:B:164:ASN:N	1.88	1.11
1:A:295:ALA:H	1:A:316:ALA:CA	1.63	1.11
1:C:313:GLU:HG3	1:C:318:SER:HB2	1.28	1.10
1:C:80:ASP:CA	1:C:241:ARG:NH2	2.10	1.10
1:A:297:VAL:HB	1:A:336:VAL:O	1.47	1.10
1:C:101:PRO:O	1:C:102:LYS:HG3	0.95	1.10
1:B:198:ALA:CB	1:B:200:GLY:O	1.97	1.10
1:A:301:GLU:O	1:A:333:VAL:HG13	1.50	1.10
1:C:119:LEU:HD22	1:C:234:TYR:CZ	1.85	1.10
1:C:116:PHE:O	1:C:120:ILE:CG2	2.00	1.10
1:C:326:VAL:CG1	1:C:327:ALA:H	1.54	1.10
1:A:164:ASN:N	1:A:164:ASN:ND2	1.88	1.10
1:C:101:PRO:HD2	1:C:166:LEU:CD1	1.68	1.10
1:A:248:ALA:HB3	1:A:264:SER:O	1.45	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ALA:CB	1:A:318:SER:HB3	1.82	1.10
1:A:116:PHE:O	1:A:120:ILE:CG2	2.00	1.10
1:C:164:ASN:N	1:C:164:ASN:ND2	1.88	1.10
1:C:199:ASP:C	1:C:265:TRP:CD1	2.25	1.10
1:C:315:ALA:CB	1:C:318:SER:HB3	1.82	1.10
1:B:313:GLU:HG3	1:B:318:SER:HB2	1.28	1.10
1:B:116:PHE:O	1:B:120:ILE:CG2	2.00	1.09
1:A:288:LEU:HD11	1:A:290:LEU:HD21	1.31	1.09
1:B:138:TYR:CG	1:B:184:PHE:HE1	1.56	1.09
1:A:86:GLY:CA	1:A:234:TYR:CD1	2.34	1.09
1:C:249:GLN:HB3	1:C:265:TRP:HZ3	1.17	1.09
1:B:101:PRO:CD	1:B:166:LEU:HD12	1.73	1.09
1:B:86:GLY:CA	1:B:234:TYR:CD1	2.34	1.09
1:A:101:PRO:CD	1:A:166:LEU:HD12	1.73	1.09
1:A:138:TYR:CG	1:A:184:PHE:HE1	1.56	1.09
1:C:160:LYS:HG3	1:C:161:PRO:HD2	1.11	1.09
1:C:86:GLY:CA	1:C:234:TYR:CD1	2.34	1.09
1:C:204:PRO:HB2	1:C:328:GLU:HG3	1.15	1.09
1:A:149:LYS:CG	1:A:177:SER:OG	2.01	1.09
1:C:179:VAL:CG2	1:C:180:PRO:HD2	1.83	1.09
1:B:149:LYS:CG	1:B:177:SER:OG	2.01	1.09
1:B:315:ALA:HB1	1:B:318:SER:N	1.67	1.09
1:B:101:PRO:HD2	1:B:166:LEU:CD1	1.68	1.09
1:A:149:LYS:HD2	1:A:170:TYR:OH	1.44	1.08
1:A:138:TYR:CD2	1:A:184:PHE:CE1	2.34	1.08
1:A:315:ALA:HB1	1:A:318:SER:N	1.67	1.08
1:C:134:LEU:HD21	1:C:188:VAL:HG21	1.08	1.08
1:C:315:ALA:HB1	1:C:318:SER:N	1.67	1.08
1:B:179:VAL:CG2	1:B:180:PRO:HD2	1.83	1.08
1:B:315:ALA:CB	1:B:318:SER:HB3	1.82	1.08
1:B:248:ALA:O	1:B:263:VAL:HB	1.54	1.08
1:C:297:VAL:HB	1:C:336:VAL:HG13	1.27	1.08
1:A:179:VAL:CG2	1:A:180:PRO:HD2	1.83	1.08
1:C:130:ARG:HD3	1:C:237:GLN:CA	1.83	1.08
1:C:71:THR:HG21	1:C:87:SER:OG	0.92	1.08
1:B:278:CYS:HB3	1:B:333:VAL:O	1.52	1.08
1:C:244:SER:O	1:C:245:THR:HG22	1.54	1.08
1:C:197:VAL:HG23	1:C:350:ARG:HH22	1.17	1.08
1:B:278:CYS:N	1:B:334:LYS:HD2	1.68	1.08
1:B:255:GLY:HA2	1:B:342:PRO:HB3	1.33	1.08
1:A:130:ARG:HD3	1:A:237:GLN:CA	1.84	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:GLY:HA2	1:C:265:TRP:CG	1.88	1.07
1:C:327:ALA:N	1:C:331:GLN:OE1	1.87	1.07
1:A:125:GLN:HA	1:A:243:GLY:HA2	1.37	1.07
1:C:149:LYS:CG	1:C:177:SER:OG	2.01	1.07
1:C:130:ARG:HB2	1:C:237:GLN:HB3	1.07	1.07
1:B:249:GLN:HB3	1:B:265:TRP:HZ3	1.17	1.07
1:C:69:VAL:HG12	1:C:70:SER:H	1.09	1.07
1:A:244:SER:O	1:A:245:THR:HG22	1.54	1.07
1:C:149:LYS:HD3	1:C:170:TYR:OH	1.43	1.07
1:C:200:GLY:C	1:C:282:GLY:HA3	1.51	1.07
1:C:172:ILE:O	1:C:173:GLU:O	1.72	1.07
1:A:288:LEU:HD11	1:A:290:LEU:CG	1.84	1.07
1:C:296:PRO:CG	1:C:337:THR:CG2	1.76	1.07
1:B:297:VAL:CB	1:B:336:VAL:HG13	1.41	1.07
1:A:166:LEU:O	1:A:169:LEU:N	1.88	1.07
1:A:86:GLY:HA2	1:A:234:TYR:CE1	1.90	1.07
1:B:277:ASP:HA	1:B:334:LYS:HD2	1.34	1.07
1:B:166:LEU:O	1:B:169:LEU:N	1.88	1.07
1:B:149:LYS:HD3	1:B:170:TYR:HH	0.94	1.07
1:B:125:GLN:HA	1:B:243:GLY:HA2	1.37	1.07
1:B:327:ALA:N	1:B:331:GLN:OE1	1.87	1.07
1:C:149:LYS:HD2	1:C:170:TYR:OH	1.44	1.06
1:C:152:LEU:HD22	1:C:186:LEU:CD1	1.85	1.06
1:B:156:ARG:O	1:B:210:GLY:CA	2.03	1.06
1:B:244:SER:O	1:B:245:THR:HG22	1.54	1.06
1:A:327:ALA:N	1:A:331:GLN:OE1	1.87	1.06
1:A:156:ARG:O	1:A:210:GLY:CA	2.03	1.06
1:C:149:LYS:HD3	1:C:170:TYR:HH	1.07	1.06
1:C:288:LEU:HD11	1:C:290:LEU:CG	1.84	1.06
1:B:86:GLY:HA2	1:B:234:TYR:CE1	1.90	1.06
1:B:288:LEU:HD11	1:B:290:LEU:CG	1.84	1.06
1:B:288:LEU:HD11	1:B:290:LEU:HD21	1.31	1.06
1:C:278:CYS:HB3	1:C:333:VAL:O	1.53	1.06
1:C:120:ILE:CD1	1:C:351:ILE:C	2.24	1.06
1:C:201:ILE:HG22	1:C:265:TRP:HA	1.38	1.06
1:B:252:ASP:OD2	1:B:345:LYS:HE2	1.55	1.06
1:B:291:PHE:CB	1:B:345:LYS:O	2.03	1.06
1:A:315:ALA:HB1	1:A:318:SER:H	1.16	1.06
1:A:252:ASP:OD2	1:A:345:LYS:HE2	1.55	1.06
1:A:339:GLU:C	1:A:340:GLU:CA	2.24	1.06
1:C:156:ARG:O	1:C:210:GLY:CA	2.03	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:CYS:N	1:C:334:LYS:HD2	1.68	1.06
1:B:86:GLY:CA	1:B:234:TYR:HD1	1.68	1.06
1:A:304:ASP:O	1:A:331:GLN:CB	2.04	1.06
1:B:339:GLU:C	1:B:340:GLU:CA	2.24	1.06
1:C:69:VAL:HG12	1:C:70:SER:N	1.66	1.06
1:A:160:LYS:HG3	1:A:161:PRO:HD2	1.11	1.06
1:A:134:LEU:HD21	1:A:188:VAL:HG21	1.08	1.06
1:C:288:LEU:HD11	1:C:290:LEU:HD21	1.31	1.06
1:C:207:VAL:N	1:C:329:ARG:NH2	1.78	1.06
1:B:248:ALA:O	1:B:263:VAL:CB	2.03	1.06
1:B:160:LYS:HG3	1:B:161:PRO:HD2	1.11	1.06
1:A:172:ILE:O	1:A:173:GLU:O	1.72	1.05
1:A:152:LEU:HD22	1:A:186:LEU:CD1	1.85	1.05
1:B:152:LEU:HD22	1:B:186:LEU:CD1	1.85	1.05
1:B:265:TRP:HZ3	1:B:348:ALA:O	1.20	1.05
1:C:277:ASP:HA	1:C:334:LYS:HD2	1.35	1.05
1:B:130:ARG:HD3	1:B:237:GLN:CA	1.84	1.05
1:A:278:CYS:N	1:A:334:LYS:HD2	1.68	1.05
1:A:278:CYS:HB3	1:A:333:VAL:O	1.53	1.05
1:C:255:GLY:HA2	1:C:342:PRO:HB3	1.33	1.05
1:A:96:ASN:OD1	1:A:216:THR:O	1.74	1.05
1:A:255:GLY:HA2	1:A:342:PRO:HB3	1.33	1.05
1:C:166:LEU:O	1:C:169:LEU:N	1.88	1.05
1:C:327:ALA:HB3	1:C:331:GLN:OE1	1.48	1.05
1:C:291:PHE:CB	1:C:345:LYS:O	2.03	1.05
1:C:86:GLY:HA2	1:C:234:TYR:CE1	1.90	1.05
1:B:304:ASP:O	1:B:331:GLN:CB	2.04	1.05
1:B:172:ILE:O	1:B:173:GLU:O	1.72	1.05
1:B:327:ALA:HB3	1:B:331:GLN:OE1	1.48	1.05
1:C:339:GLU:C	1:C:340:GLU:CA	2.24	1.05
1:A:130:ARG:HB2	1:A:237:GLN:HB3	1.07	1.04
1:B:134:LEU:HD21	1:B:188:VAL:HG21	1.08	1.04
1:A:249:GLN:HB3	1:A:265:TRP:HZ3	1.17	1.04
1:A:291:PHE:CB	1:A:345:LYS:O	2.03	1.04
1:A:179:VAL:CG1	1:A:181:TRP:CD1	2.40	1.04
1:A:89:LEU:C	1:A:89:LEU:HD23	1.78	1.04
1:C:96:ASN:OD1	1:C:216:THR:O	1.74	1.04
1:B:89:LEU:HD23	1:B:89:LEU:C	1.77	1.04
1:B:96:ASN:OD1	1:B:216:THR:O	1.74	1.04
1:A:164:ASN:HD22	1:A:164:ASN:N	1.19	1.04
1:C:159:ALA:HB2	1:C:328:GLU:HB2	1.35	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:ALA:HB2	1:C:318:SER:HB3	1.36	1.04
1:B:179:VAL:CG1	1:B:181:TRP:CD1	2.40	1.04
1:B:315:ALA:HB2	1:B:318:SER:HB3	1.36	1.04
1:B:278:CYS:N	1:B:334:LYS:HD3	1.71	1.04
1:C:252:ASP:OD2	1:C:345:LYS:HE2	1.55	1.04
1:C:304:ASP:O	1:C:331:GLN:CB	2.04	1.04
1:A:315:ALA:HB2	1:A:318:SER:HB3	1.36	1.04
1:A:277:ASP:HA	1:A:334:LYS:HD2	1.35	1.04
1:C:179:VAL:CG1	1:C:181:TRP:CD1	2.40	1.03
1:B:296:PRO:CG	1:B:337:THR:CG2	1.76	1.03
1:B:130:ARG:HB2	1:B:237:GLN:CB	1.88	1.03
1:C:207:VAL:CA	1:C:329:ARG:NH2	2.21	1.03
1:C:315:ALA:HB1	1:C:318:SER:H	1.16	1.03
1:B:130:ARG:HB2	1:B:237:GLN:HB3	1.07	1.03
1:C:297:VAL:HB	1:C:336:VAL:C	1.78	1.03
1:A:119:LEU:HD22	1:A:234:TYR:OH	0.86	1.03
1:C:119:LEU:HD22	1:C:234:TYR:OH	0.86	1.03
1:C:130:ARG:HB2	1:C:237:GLN:CB	1.88	1.03
1:A:297:VAL:HB	1:A:336:VAL:C	1.78	1.03
1:A:86:GLY:CA	1:A:234:TYR:HD1	1.68	1.03
1:C:290:LEU:HD22	1:C:346:TRP:HB2	1.41	1.03
1:C:89:LEU:HD23	1:C:89:LEU:C	1.78	1.03
1:B:290:LEU:HD22	1:B:346:TRP:HB2	1.41	1.03
1:B:119:LEU:HD22	1:B:234:TYR:OH	0.86	1.03
1:A:254:ALA:O	1:A:256:VAL:N	1.91	1.03
1:A:308:PHE:CE2	1:A:310:VAL:CG2	2.42	1.02
1:A:327:ALA:HB3	1:A:331:GLN:OE1	1.48	1.02
1:C:254:ALA:O	1:C:256:VAL:N	1.91	1.02
1:B:297:VAL:HB	1:B:336:VAL:C	1.78	1.02
1:A:286:PHE:HA	1:A:351:ILE:CG2	1.89	1.02
1:C:308:PHE:CE2	1:C:310:VAL:CG2	2.42	1.02
1:B:248:ALA:O	1:B:263:VAL:CG1	2.08	1.02
1:C:326:VAL:HG12	1:C:327:ALA:H	1.18	1.02
1:B:308:PHE:CE2	1:B:310:VAL:CG2	2.42	1.02
1:C:286:PHE:HA	1:C:351:ILE:CG2	1.89	1.01
1:C:338:THR:OG1	1:C:339:GLU:HB2	1.60	1.01
1:A:338:THR:OG1	1:A:339:GLU:HB2	1.60	1.01
1:B:338:THR:OG1	1:B:339:GLU:HB2	1.60	1.01
1:B:254:ALA:O	1:B:256:VAL:N	1.91	1.01
1:A:85:SER:HA	1:A:234:TYR:O	1.60	1.01
1:A:130:ARG:HB2	1:A:237:GLN:CB	1.88	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:GLY:CA	1:C:234:TYR:HD1	1.68	1.01
1:B:165:ASP:O	1:B:168:SER:CB	2.07	1.01
1:A:165:ASP:O	1:A:168:SER:CB	2.07	1.01
1:A:86:GLY:N	1:A:234:TYR:CD1	2.29	1.01
1:C:68:GLU:OE2	1:C:137:ARG:NH2	1.94	1.01
1:C:200:GLY:HA2	1:C:265:TRP:CD1	1.90	1.01
1:C:165:ASP:O	1:C:168:SER:CB	2.07	1.01
1:B:134:LEU:HD21	1:B:188:VAL:CG2	1.91	1.01
1:B:86:GLY:N	1:B:234:TYR:CD1	2.29	1.01
1:B:286:PHE:HA	1:B:351:ILE:CG2	1.89	1.01
1:C:135:ARG:HG3	1:C:233:GLU:HB3	1.43	1.01
1:C:200:GLY:HA2	1:C:265:TRP:HB3	1.42	1.01
1:B:315:ALA:HB1	1:B:318:SER:H	1.16	1.01
1:A:134:LEU:CD2	1:A:188:VAL:HG21	1.91	1.01
1:C:86:GLY:N	1:C:234:TYR:CD1	2.29	1.01
1:C:85:SER:HA	1:C:234:TYR:O	1.60	1.01
1:A:203:ASP:CG	1:A:205:LYS:HD3	1.81	1.01
1:C:278:CYS:N	1:C:334:LYS:HD3	1.71	1.00
1:A:278:CYS:H	1:A:334:LYS:HD3	1.25	1.00
1:C:133:SER:O	1:C:234:TYR:CA	2.09	1.00
1:C:253:PHE:HA	1:C:258:ASP:HA	1.44	1.00
1:B:253:PHE:HA	1:B:258:ASP:HA	1.44	1.00
1:C:278:CYS:H	1:C:334:LYS:HE2	1.27	1.00
1:B:134:LEU:CD2	1:B:188:VAL:HG21	1.91	1.00
1:B:85:SER:HA	1:B:234:TYR:O	1.60	1.00
1:A:253:PHE:HA	1:A:258:ASP:HA	1.44	1.00
1:C:125:GLN:HA	1:C:243:GLY:HA2	1.36	1.00
1:A:249:GLN:HB3	1:A:265:TRP:CZ3	1.97	1.00
1:C:197:VAL:HG21	1:C:350:ARG:HH22	1.20	1.00
1:A:297:VAL:CB	1:A:336:VAL:HG13	1.41	1.00
1:B:133:SER:O	1:B:234:TYR:CA	2.09	1.00
1:A:135:ARG:HG3	1:A:233:GLU:HB3	1.43	0.99
1:A:133:SER:O	1:A:234:TYR:CA	2.09	0.99
1:A:134:LEU:HD21	1:A:188:VAL:CG2	1.91	0.99
1:C:308:PHE:CE2	1:C:310:VAL:HG23	1.97	0.99
1:A:326:VAL:HG12	1:A:327:ALA:H	1.18	0.99
1:C:159:ALA:HB1	1:C:328:GLU:CD	1.80	0.99
1:B:269:LYS:C	1:B:277:ASP:HB3	1.82	0.99
1:B:203:ASP:CG	1:B:205:LYS:HD3	1.82	0.99
1:A:185:ILE:CD1	1:A:186:LEU:N	2.05	0.99
1:A:269:LYS:C	1:A:277:ASP:HB3	1.82	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:GLN:HB3	1:B:265:TRP:CZ3	1.97	0.99
1:C:79:ARG:O	1:C:80:ASP:HB2	1.61	0.99
1:C:297:VAL:CB	1:C:336:VAL:HG13	1.41	0.99
1:B:278:CYS:H	1:B:334:LYS:HE2	1.27	0.99
1:C:134:LEU:CD2	1:C:188:VAL:HG21	1.91	0.99
1:A:160:LYS:HG3	1:A:161:PRO:CD	1.93	0.99
1:A:290:LEU:HD22	1:A:346:TRP:HB2	1.41	0.98
1:B:160:LYS:HG3	1:B:161:PRO:CD	1.93	0.98
1:C:249:GLN:HB3	1:C:265:TRP:CZ3	1.97	0.98
1:C:152:LEU:HD22	1:C:186:LEU:HD13	1.45	0.98
1:B:179:VAL:HG23	1:B:180:PRO:HD2	1.46	0.98
1:B:152:LEU:HD22	1:B:186:LEU:HD13	1.45	0.98
1:B:252:ASP:CG	1:B:345:LYS:HG2	1.84	0.98
1:A:252:ASP:CG	1:A:345:LYS:HG2	1.84	0.98
1:C:134:LEU:HD21	1:C:188:VAL:CG2	1.91	0.98
1:B:135:ARG:HG3	1:B:233:GLU:HB3	1.43	0.98
1:A:308:PHE:CE2	1:A:310:VAL:HG23	1.97	0.98
1:C:203:ASP:CG	1:C:205:LYS:HD3	1.81	0.98
1:A:296:PRO:CG	1:A:337:THR:CG2	1.76	0.98
1:B:308:PHE:CE2	1:B:310:VAL:HG23	1.97	0.98
1:A:278:CYS:N	1:A:334:LYS:HE2	1.78	0.98
1:C:160:LYS:HG3	1:C:161:PRO:CD	1.93	0.98
1:C:77:THR:HG22	1:C:78:ALA:N	1.78	0.98
1:C:200:GLY:HA3	1:C:265:TRP:HA	1.43	0.98
1:C:269:LYS:C	1:C:277:ASP:HB3	1.82	0.98
1:B:174:GLY:C	1:B:175:CYS:SG	2.42	0.98
1:A:338:THR:OG1	1:A:339:GLU:N	1.94	0.98
1:C:277:ASP:C	1:C:334:LYS:HD2	1.84	0.98
1:C:278:CYS:CB	1:C:333:VAL:O	2.12	0.98
1:C:252:ASP:CG	1:C:345:LYS:HG2	1.84	0.97
1:B:290:LEU:CD2	1:B:346:TRP:HB2	1.94	0.97
1:C:143:PRO:O	1:C:146:THR:CG2	2.13	0.97
1:C:269:LYS:HG2	1:C:270:GLY:N	1.75	0.97
1:C:278:CYS:N	1:C:334:LYS:HE2	1.78	0.97
1:B:185:ILE:CD1	1:B:186:LEU:N	2.05	0.97
1:B:269:LYS:HG2	1:B:270:GLY:N	1.75	0.97
1:A:138:TYR:HB2	1:A:184:PHE:CE2	1.99	0.97
1:B:101:PRO:HG3	1:B:217:TYR:HE2	1.28	0.97
1:A:155:ASP:HB2	1:A:172:ILE:HD11	1.47	0.97
1:C:101:PRO:HD2	1:C:166:LEU:HD12	1.37	0.97
1:B:315:ALA:O	1:B:316:ALA:C	2.00	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:CYS:N	1:A:334:LYS:HD3	1.72	0.97
1:C:290:LEU:CD2	1:C:346:TRP:HB2	1.94	0.97
1:A:278:CYS:H	1:A:334:LYS:HE2	1.26	0.97
1:C:174:GLY:C	1:C:175:CYS:SG	2.42	0.97
1:B:278:CYS:CB	1:B:333:VAL:O	2.12	0.97
1:B:277:ASP:C	1:B:334:LYS:HD2	1.84	0.97
1:A:278:CYS:CB	1:A:333:VAL:O	2.12	0.97
1:A:174:GLY:C	1:A:175:CYS:SG	2.42	0.97
1:C:95:LYS:NZ	1:C:221:ALA:HA	1.80	0.97
1:B:138:TYR:HB2	1:B:184:PHE:CE2	1.99	0.97
1:B:155:ASP:HB2	1:B:172:ILE:HD11	1.47	0.97
1:A:269:LYS:HG2	1:A:270:GLY:N	1.75	0.97
1:C:150:VAL:HG12	1:C:150:VAL:O	1.65	0.96
1:C:185:ILE:CD1	1:C:186:LEU:N	2.05	0.96
1:A:277:ASP:C	1:A:334:LYS:HD2	1.84	0.96
1:C:274:TRP:NE1	1:C:339:GLU:O	1.98	0.96
1:A:154:PHE:CE1	1:A:155:ASP:C	2.39	0.96
1:A:179:VAL:HG23	1:A:180:PRO:HD2	1.45	0.96
1:C:113:PRO:O	1:C:115:THR:N	1.99	0.96
1:C:278:CYS:H	1:C:334:LYS:HD3	1.25	0.96
1:A:290:LEU:CD2	1:A:346:TRP:HB2	1.94	0.96
1:A:101:PRO:HG3	1:A:217:TYR:HE2	1.28	0.96
1:A:86:GLY:N	1:A:234:TYR:HD1	1.62	0.96
1:C:154:PHE:CE1	1:C:155:ASP:C	2.39	0.96
1:B:154:PHE:CE1	1:B:155:ASP:C	2.39	0.96
1:A:350:ARG:C	1:A:351:ILE:HG22	1.86	0.96
1:C:138:TYR:HB2	1:C:184:PHE:CE2	2.00	0.96
1:A:326:VAL:HG12	1:A:327:ALA:O	1.65	0.96
1:B:350:ARG:O	1:B:351:ILE:HG22	0.78	0.96
1:C:206:LEU:O	1:C:206:LEU:HD12	1.66	0.96
1:C:159:ALA:CB	1:C:328:GLU:CD	2.33	0.96
1:B:105:THR:HG1	1:B:211:LYS:CD	1.70	0.96
1:A:95:LYS:NZ	1:A:221:ALA:HA	1.80	0.96
1:B:119:LEU:HD22	1:B:234:TYR:HH	1.21	0.96
1:A:350:ARG:O	1:A:351:ILE:HG22	0.78	0.96
1:A:285:ASN:O	1:A:351:ILE:HG23	1.66	0.96
1:C:296:PRO:HG2	1:C:337:THR:CB	1.95	0.96
1:C:315:ALA:O	1:C:316:ALA:C	2.00	0.95
1:C:326:VAL:HG12	1:C:327:ALA:O	1.65	0.95
1:C:285:ASN:O	1:C:351:ILE:HG23	1.66	0.95
1:B:149:LYS:CB	1:B:217:TYR:HE1	1.79	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LYS:NZ	1:B:221:ALA:HA	1.80	0.95
1:A:248:ALA:HB3	1:A:264:SER:CB	1.96	0.95
1:B:274:TRP:NE1	1:B:339:GLU:O	1.98	0.95
1:A:143:PRO:O	1:A:146:THR:CG2	2.13	0.95
1:A:149:LYS:CB	1:A:217:TYR:HE1	1.79	0.95
1:B:143:PRO:O	1:B:146:THR:CG2	2.13	0.95
1:A:206:LEU:O	1:A:206:LEU:HD12	1.66	0.95
1:A:149:LYS:HB3	1:A:217:TYR:HE1	1.11	0.95
1:C:207:VAL:CA	1:C:329:ARG:HH22	1.79	0.95
1:B:130:ARG:NH1	1:B:236:VAL:O	2.00	0.95
1:B:149:LYS:HB3	1:B:217:TYR:HE1	1.11	0.95
1:C:149:LYS:CB	1:C:217:TYR:HE1	1.79	0.95
1:C:130:ARG:CB	1:C:237:GLN:HB3	1.97	0.95
1:B:206:LEU:O	1:B:206:LEU:HD12	1.66	0.95
1:A:152:LEU:HD22	1:A:186:LEU:HD13	1.45	0.95
1:A:274:TRP:NE1	1:A:339:GLU:O	1.98	0.95
1:C:350:ARG:O	1:C:351:ILE:HG22	0.78	0.95
1:B:326:VAL:HG12	1:B:327:ALA:O	1.65	0.95
1:C:291:PHE:HB2	1:C:346:TRP:HB3	1.48	0.95
1:B:291:PHE:HB2	1:B:346:TRP:HB3	1.48	0.95
1:A:130:ARG:NH1	1:A:236:VAL:O	2.00	0.95
1:B:150:VAL:HG12	1:B:150:VAL:O	1.65	0.95
1:A:150:VAL:HG12	1:A:150:VAL:O	1.65	0.95
1:C:155:ASP:HB2	1:C:172:ILE:HD11	1.47	0.95
1:B:278:CYS:N	1:B:334:LYS:HE2	1.78	0.95
1:A:277:ASP:OD1	1:A:334:LYS:HE2	1.67	0.95
1:A:130:ARG:CB	1:A:237:GLN:HB3	1.96	0.94
1:B:277:ASP:OD1	1:B:334:LYS:HE2	1.67	0.94
1:A:113:PRO:O	1:A:115:THR:N	1.99	0.94
1:A:296:PRO:HG2	1:A:337:THR:CB	1.95	0.94
1:C:205:LYS:H	1:C:329:ARG:CZ	1.79	0.94
1:B:248:ALA:C	1:B:263:VAL:HG12	1.88	0.94
1:C:101:PRO:HG3	1:C:217:TYR:HE2	1.28	0.94
1:B:113:PRO:O	1:B:115:THR:N	1.99	0.94
1:B:350:ARG:C	1:B:351:ILE:HG22	1.86	0.94
1:B:296:PRO:HG2	1:B:337:THR:CB	1.95	0.94
1:B:141:MET:HG3	1:B:141:MET:O	1.66	0.94
1:C:130:ARG:NH1	1:C:236:VAL:O	2.00	0.94
1:A:119:LEU:HD22	1:A:234:TYR:HH	1.21	0.94
1:C:179:VAL:HG23	1:C:180:PRO:HD2	1.46	0.94
1:B:285:ASN:O	1:B:351:ILE:HG23	1.66	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LYS:O	1:A:277:ASP:HB3	0.76	0.94
1:C:350:ARG:C	1:C:351:ILE:HG22	1.86	0.94
1:A:101:PRO:CG	1:A:166:LEU:CD1	2.45	0.94
1:C:277:ASP:OD1	1:C:334:LYS:HE2	1.67	0.94
1:B:101:PRO:CG	1:B:166:LEU:CD1	2.46	0.94
1:B:130:ARG:CB	1:B:237:GLN:HB3	1.96	0.94
1:B:86:GLY:N	1:B:234:TYR:HD1	1.63	0.94
1:A:291:PHE:HB2	1:A:346:TRP:HB3	1.48	0.94
1:C:204:PRO:HB3	1:C:329:ARG:HG3	1.47	0.94
1:A:315:ALA:CB	1:A:318:SER:CB	2.46	0.94
1:A:289:THR:HG23	1:A:321:TRP:CE3	2.03	0.94
1:C:101:PRO:CG	1:C:166:LEU:CD1	2.45	0.93
1:B:326:VAL:CG1	1:B:327:ALA:N	2.19	0.93
1:B:163:PRO:CA	1:B:164:ASN:HD22	1.82	0.93
1:B:269:LYS:O	1:B:277:ASP:HB3	0.76	0.93
1:B:289:THR:HG23	1:B:321:TRP:CE3	2.03	0.93
1:A:265:TRP:O	1:A:281:LEU:N	2.02	0.93
1:C:112:GLU:HA	1:C:284:GLY:HA3	1.50	0.93
1:C:269:LYS:O	1:C:277:ASP:HB3	0.76	0.93
1:B:89:LEU:CD2	1:B:89:LEU:C	2.37	0.93
1:C:141:MET:O	1:C:141:MET:HG3	1.66	0.93
1:C:89:LEU:CD2	1:C:89:LEU:C	2.37	0.93
1:B:315:ALA:CB	1:B:318:SER:CB	2.46	0.93
1:A:141:MET:HG3	1:A:141:MET:O	1.66	0.93
1:C:207:VAL:CG1	1:C:329:ARG:HH21	1.75	0.93
1:B:124:ALA:HB1	1:B:245:THR:HG22	1.51	0.93
1:C:265:TRP:O	1:C:281:LEU:N	2.02	0.93
1:C:149:LYS:HB3	1:C:217:TYR:HE1	1.11	0.93
1:C:289:THR:HG23	1:C:321:TRP:CE3	2.03	0.93
1:C:86:GLY:N	1:C:234:TYR:HD1	1.63	0.93
1:B:154:PHE:HB2	1:B:212:LEU:CD1	1.99	0.93
1:B:82:ILE:HD11	1:B:122:GLU:OE2	1.69	0.93
1:A:124:ALA:HB1	1:A:245:THR:HG22	1.51	0.92
1:A:154:PHE:HB2	1:A:212:LEU:CD1	1.99	0.92
1:C:154:PHE:HB2	1:C:212:LEU:CD1	1.99	0.92
1:C:333:VAL:O	1:C:334:LYS:CD	2.18	0.92
1:A:130:ARG:HD3	1:A:237:GLN:N	1.84	0.92
1:C:159:ALA:HB1	1:C:328:GLU:HB3	1.50	0.92
1:C:315:ALA:CB	1:C:318:SER:CB	2.46	0.92
1:B:285:ASN:O	1:B:351:ILE:CG2	2.17	0.92
1:A:333:VAL:O	1:A:334:LYS:CD	2.18	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LYS:C	1:A:296:PRO:HD3	1.90	0.92
1:A:82:ILE:HD11	1:A:122:GLU:OE2	1.69	0.92
1:C:204:PRO:CB	1:C:329:ARG:HG3	1.60	0.92
1:B:333:VAL:O	1:B:334:LYS:CD	2.18	0.92
1:B:338:THR:OG1	1:B:339:GLU:N	1.94	0.92
1:A:163:PRO:CA	1:A:164:ASN:HD22	1.82	0.92
1:C:294:LYS:C	1:C:296:PRO:HD3	1.90	0.92
1:C:342:PRO:O	1:C:343:LYS:HD3	1.70	0.92
1:C:82:ILE:HD11	1:C:122:GLU:OE2	1.69	0.92
1:A:278:CYS:N	1:A:334:LYS:CE	2.20	0.92
1:B:294:LYS:C	1:B:296:PRO:HD3	1.90	0.92
1:B:265:TRP:O	1:B:281:LEU:N	2.02	0.92
1:C:163:PRO:C	1:C:164:ASN:HD22	1.73	0.91
1:C:83:THR:HG22	1:C:84:ARG:H	1.34	0.91
1:B:308:PHE:HE2	1:B:310:VAL:HG21	1.34	0.91
1:A:248:ALA:HB2	1:A:264:SER:C	1.89	0.91
1:C:126:TYR:HA	1:C:242:THR:HG22	1.50	0.91
1:A:286:PHE:HA	1:A:351:ILE:HG22	1.52	0.91
1:A:342:PRO:O	1:A:343:LYS:HD3	1.70	0.91
1:A:83:THR:HG22	1:A:84:ARG:H	1.34	0.91
1:C:163:PRO:CA	1:C:164:ASN:HD22	1.82	0.91
1:B:150:VAL:O	1:B:150:VAL:CG1	2.18	0.91
1:B:163:PRO:C	1:B:164:ASN:HD22	1.73	0.91
1:B:248:ALA:O	1:B:263:VAL:HG12	1.70	0.91
1:A:143:PRO:O	1:A:146:THR:HG23	1.71	0.91
1:C:296:PRO:CB	1:C:337:THR:HG22	2.00	0.91
1:A:296:PRO:CB	1:A:337:THR:HG22	2.00	0.91
1:A:313:GLU:CG	1:A:318:SER:CB	2.49	0.91
1:B:296:PRO:CB	1:B:337:THR:HG22	2.00	0.91
1:A:130:ARG:HD3	1:A:237:GLN:HB2	0.97	0.91
1:C:124:ALA:HB1	1:C:245:THR:HG22	1.51	0.91
1:C:338:THR:OG1	1:C:339:GLU:N	1.94	0.91
1:A:296:PRO:CD	1:A:337:THR:HG22	2.01	0.91
1:C:113:PRO:C	1:C:115:THR:H	1.74	0.91
1:C:159:ALA:CB	1:C:328:GLU:HG3	2.01	0.91
1:C:207:VAL:CB	1:C:329:ARG:NH2	2.34	0.91
1:B:164:ASN:ND2	1:B:164:ASN:H	1.47	0.91
1:B:342:PRO:O	1:B:343:LYS:HD3	1.70	0.91
1:C:313:GLU:CG	1:C:318:SER:CB	2.49	0.91
1:B:130:ARG:HD3	1:B:237:GLN:N	1.84	0.91
1:B:83:THR:HG22	1:B:84:ARG:H	1.34	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ASN:O	1:A:351:ILE:CG2	2.17	0.91
1:C:134:LEU:HA	1:C:233:GLU:O	0.73	0.91
1:C:285:ASN:O	1:C:351:ILE:CG2	2.17	0.91
1:C:130:ARG:HH11	1:C:237:GLN:HA	1.36	0.90
1:B:286:PHE:HA	1:B:351:ILE:HG22	1.52	0.90
1:B:300:LEU:HG	1:B:308:PHE:CZ	2.06	0.90
1:A:126:TYR:N	1:A:242:THR:HG22	1.86	0.90
1:A:134:LEU:HA	1:A:233:GLU:O	0.73	0.90
1:A:150:VAL:O	1:A:150:VAL:CG1	2.18	0.90
1:C:130:ARG:HD3	1:C:237:GLN:N	1.84	0.90
1:A:296:PRO:HG2	1:A:337:THR:HG21	1.51	0.90
1:B:296:PRO:CD	1:B:337:THR:HG22	2.01	0.90
1:A:163:PRO:C	1:A:164:ASN:HD22	1.73	0.90
1:B:134:LEU:CD2	1:B:188:VAL:CG2	2.49	0.90
1:C:126:TYR:N	1:C:242:THR:HG22	1.86	0.90
1:C:150:VAL:CG1	1:C:150:VAL:O	2.18	0.90
1:C:264:SER:C	1:C:265:TRP:CA	2.40	0.90
1:A:277:ASP:HA	1:A:334:LYS:CD	2.02	0.90
1:A:186:LEU:HD23	1:A:187:THR:N	1.87	0.90
1:B:134:LEU:HA	1:B:233:GLU:O	0.73	0.90
1:B:130:ARG:HH11	1:B:237:GLN:HA	1.36	0.90
1:A:164:ASN:ND2	1:A:164:ASN:H	1.47	0.90
1:A:90:ILE:HD11	1:A:232:VAL:HG23	1.53	0.90
1:C:207:VAL:CG1	1:C:329:ARG:NE	2.17	0.90
1:B:277:ASP:HA	1:B:334:LYS:CD	2.02	0.90
1:B:89:LEU:CD2	1:B:89:LEU:O	2.20	0.90
1:A:126:TYR:HA	1:A:242:THR:HG22	1.50	0.90
1:B:186:LEU:HD23	1:B:187:THR:N	1.87	0.90
1:B:126:TYR:HA	1:B:242:THR:HG22	1.50	0.90
1:C:300:LEU:HG	1:C:308:PHE:CZ	2.06	0.90
1:C:308:PHE:HE2	1:C:310:VAL:HG21	1.34	0.90
1:C:246:SER:O	1:C:350:ARG:N	2.05	0.90
1:C:274:TRP:CD1	1:C:339:GLU:O	2.25	0.89
1:C:115:THR:O	1:C:116:PHE:HD1	1.48	0.89
1:C:143:PRO:O	1:C:146:THR:HG23	1.71	0.89
1:C:134:LEU:CD2	1:C:188:VAL:CG2	2.49	0.89
1:A:89:LEU:C	1:A:89:LEU:CD2	2.37	0.89
1:A:89:LEU:CD2	1:A:89:LEU:O	2.20	0.89
1:A:95:LYS:NZ	1:A:221:ALA:CA	2.35	0.89
1:C:204:PRO:CB	1:C:328:GLU:CG	2.48	0.89
1:A:308:PHE:HE2	1:A:310:VAL:HG21	1.34	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:ASP:OD1	1:B:205:LYS:HD3	0.71	0.89
1:C:200:GLY:CA	1:C:265:TRP:HD1	1.76	0.89
1:C:304:ASP:OD2	1:C:331:GLN:HA	1.72	0.89
1:C:164:ASN:H	1:C:164:ASN:ND2	1.47	0.89
1:C:203:ASP:OD1	1:C:205:LYS:HD3	0.71	0.89
1:C:277:ASP:HA	1:C:334:LYS:CD	2.02	0.89
1:B:143:PRO:O	1:B:146:THR:HG23	1.71	0.89
1:B:304:ASP:OD2	1:B:331:GLN:HA	1.73	0.89
1:B:90:ILE:HD11	1:B:232:VAL:HG23	1.53	0.89
1:A:300:LEU:HG	1:A:308:PHE:CZ	2.07	0.89
1:C:244:SER:O	1:C:245:THR:CG2	2.21	0.89
1:C:286:PHE:HA	1:C:351:ILE:HG22	1.52	0.89
1:C:89:LEU:O	1:C:89:LEU:CD2	2.20	0.89
1:A:134:LEU:CD2	1:A:188:VAL:CG2	2.49	0.89
1:B:115:THR:O	1:B:116:PHE:HD1	1.48	0.89
1:B:126:TYR:N	1:B:242:THR:HG22	1.86	0.89
1:A:203:ASP:OD1	1:A:205:LYS:HD3	0.71	0.89
1:B:114:GLY:HA3	1:B:329:ARG:HE	1.38	0.89
1:B:264:SER:C	1:B:265:TRP:CA	2.40	0.89
1:C:95:LYS:NZ	1:C:221:ALA:CA	2.35	0.89
1:C:130:ARG:HD3	1:C:237:GLN:HB2	0.97	0.88
1:B:154:PHE:HB2	1:B:212:LEU:HD12	1.56	0.88
1:A:264:SER:C	1:A:265:TRP:CA	2.40	0.88
1:A:274:TRP:CD1	1:A:339:GLU:O	2.25	0.88
1:B:274:TRP:CD1	1:B:339:GLU:O	2.26	0.88
1:C:119:LEU:HD22	1:C:234:TYR:HH	1.29	0.88
1:B:308:PHE:CE2	1:B:310:VAL:HG21	2.07	0.88
1:B:249:GLN:CB	1:B:265:TRP:CZ3	2.56	0.88
1:C:249:GLN:CB	1:C:265:TRP:CZ3	2.56	0.88
1:A:304:ASP:OD2	1:A:331:GLN:HA	1.73	0.88
1:C:296:PRO:CD	1:C:337:THR:HG22	2.01	0.88
1:A:130:ARG:HH11	1:A:237:GLN:HA	1.36	0.88
1:B:95:LYS:NZ	1:B:221:ALA:CA	2.35	0.88
1:B:326:VAL:HG12	1:B:327:ALA:H	1.18	0.88
1:A:315:ALA:O	1:A:316:ALA:C	2.00	0.88
1:A:105:THR:HG1	1:A:211:LYS:CD	1.74	0.88
1:A:138:TYR:HH	1:A:227:LEU:HB3	1.37	0.88
1:B:313:GLU:CG	1:B:318:SER:CB	2.49	0.88
1:A:249:GLN:CB	1:A:265:TRP:CZ3	2.56	0.88
1:A:113:PRO:C	1:A:115:THR:H	1.74	0.88
1:C:231:ARG:HG3	1:C:232:VAL:N	1.87	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:PHE:HB2	1:C:212:LEU:HD12	1.56	0.88
1:C:186:LEU:HD23	1:C:187:THR:N	1.87	0.88
1:A:154:PHE:HB2	1:A:212:LEU:HD12	1.56	0.88
1:A:244:SER:O	1:A:245:THR:CG2	2.21	0.88
1:B:244:SER:O	1:B:245:THR:CG2	2.21	0.88
1:C:296:PRO:HG2	1:C:337:THR:HG21	1.51	0.88
1:A:120:ILE:HD12	1:A:329:ARG:NH2	1.88	0.87
1:C:152:LEU:O	1:C:186:LEU:HD12	1.74	0.87
1:C:90:ILE:HD11	1:C:232:VAL:HG23	1.53	0.87
1:A:149:LYS:HD3	1:A:170:TYR:OH	1.43	0.87
1:C:308:PHE:CE2	1:C:310:VAL:HG21	2.07	0.87
1:B:109:ASN:OD1	1:B:110:PRO:HD2	1.74	0.87
1:C:56:THR:HG23	1:C:57:ARG:N	1.89	0.87
1:A:82:ILE:HG21	1:A:238:LEU:HB2	1.56	0.87
1:C:134:LEU:HA	1:C:233:GLU:C	1.94	0.87
1:C:251:GLY:O	1:C:346:TRP:CD2	2.28	0.87
1:C:71:THR:HG21	1:C:87:SER:CB	2.04	0.87
1:B:113:PRO:C	1:B:115:THR:H	1.74	0.87
1:C:76:SER:CB	1:C:76:SER:C	2.43	0.87
1:C:130:ARG:HH11	1:C:237:GLN:CA	1.88	0.87
1:B:130:ARG:HD3	1:B:237:GLN:HB2	0.97	0.87
1:B:251:GLY:O	1:B:346:TRP:CD2	2.28	0.87
1:C:109:ASN:OD1	1:C:110:PRO:HD2	1.74	0.87
1:B:231:ARG:HG3	1:B:232:VAL:N	1.87	0.87
1:A:130:ARG:HH11	1:A:237:GLN:CA	1.88	0.87
1:C:278:CYS:N	1:C:334:LYS:CE	2.20	0.87
1:B:82:ILE:HG21	1:B:238:LEU:HB2	1.56	0.87
1:A:101:PRO:HD2	1:A:166:LEU:HD12	1.37	0.86
1:C:264:SER:CA	1:C:265:TRP:N	2.38	0.86
1:B:296:PRO:CG	1:B:337:THR:CB	2.52	0.86
1:C:130:ARG:NE	1:C:237:GLN:HB2	1.90	0.86
1:B:134:LEU:HA	1:B:233:GLU:C	1.94	0.86
1:B:152:LEU:O	1:B:186:LEU:HD12	1.74	0.86
1:C:105:THR:HG1	1:C:211:LYS:CD	1.75	0.86
1:C:59:SER:O	1:C:61:PRO:HD3	1.74	0.86
1:C:198:ALA:C	1:C:200:GLY:H	1.78	0.86
1:C:288:LEU:CD1	1:C:290:LEU:CD2	2.53	0.86
1:C:68:GLU:HG2	1:C:137:ARG:HH22	1.38	0.86
1:A:248:ALA:CB	1:A:265:TRP:CA	2.53	0.86
1:B:264:SER:CA	1:B:265:TRP:N	2.38	0.86
1:A:130:ARG:NE	1:A:237:GLN:HB2	1.90	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LEU:HD11	1:A:290:LEU:HG	1.58	0.86
1:A:251:GLY:O	1:A:346:TRP:CD2	2.28	0.86
1:C:89:LEU:HD22	1:C:89:LEU:O	1.75	0.86
1:B:130:ARG:HH11	1:B:237:GLN:CA	1.88	0.86
1:A:109:ASN:OD1	1:A:110:PRO:HD2	1.74	0.86
1:A:115:THR:O	1:A:116:PHE:HD1	1.48	0.86
1:A:231:ARG:HG3	1:A:232:VAL:N	1.87	0.86
1:C:72:GLN:HE21	1:C:72:GLN:HA	1.39	0.86
1:C:318:SER:OG	1:C:319:VAL:N	2.07	0.86
1:B:101:PRO:CG	1:B:166:LEU:HD11	2.06	0.86
1:A:101:PRO:CG	1:A:166:LEU:HD11	2.06	0.86
1:C:154:PHE:HE1	1:C:155:ASP:O	1.59	0.85
1:C:77:THR:HG22	1:C:78:ALA:H	1.37	0.85
1:C:125:GLN:HA	1:C:243:GLY:CA	2.06	0.85
1:B:112:GLU:CG	1:B:329:ARG:NH2	2.39	0.85
1:B:154:PHE:HE1	1:B:155:ASP:O	1.59	0.85
1:B:130:ARG:NE	1:B:237:GLN:HB2	1.90	0.85
1:A:264:SER:CA	1:A:265:TRP:N	2.38	0.85
1:B:296:PRO:HG2	1:B:337:THR:HG21	1.51	0.85
1:C:200:GLY:N	1:C:265:TRP:HD1	1.36	0.85
1:C:90:ILE:HD11	1:C:232:VAL:HG21	1.58	0.85
1:B:296:PRO:CG	1:B:337:THR:HG21	2.06	0.85
1:A:136:PHE:CE1	1:A:232:VAL:HG22	2.12	0.85
1:A:89:LEU:HD22	1:A:89:LEU:O	1.75	0.85
1:B:89:LEU:O	1:B:89:LEU:HD22	1.75	0.85
1:A:90:ILE:HD11	1:A:232:VAL:HG21	1.58	0.85
1:C:277:ASP:OD1	1:C:279:HIS:ND1	2.10	0.85
1:C:101:PRO:CG	1:C:166:LEU:HD11	2.06	0.85
1:A:308:PHE:CE2	1:A:310:VAL:HG21	2.07	0.85
1:A:296:PRO:CG	1:A:337:THR:CB	2.52	0.85
1:A:125:GLN:HA	1:A:243:GLY:CA	2.06	0.85
1:A:152:LEU:O	1:A:186:LEU:HD12	1.74	0.85
1:A:130:ARG:HD2	1:A:237:GLN:HB2	0.85	0.85
1:B:149:LYS:HD3	1:B:170:TYR:OH	1.43	0.85
1:C:136:PHE:CE1	1:C:232:VAL:HG22	2.12	0.85
1:C:179:VAL:HG22	1:C:180:PRO:HD2	1.58	0.85
1:C:82:ILE:HG21	1:C:238:LEU:HB2	1.56	0.85
1:B:149:LYS:HG2	1:B:177:SER:HG	1.37	0.85
1:B:315:ALA:HB1	1:B:318:SER:CB	2.07	0.85
1:A:277:ASP:OD1	1:A:279:HIS:ND1	2.10	0.85
1:A:149:LYS:HG2	1:A:177:SER:HG	1.37	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:SER:OG	1:B:319:VAL:N	2.07	0.84
1:A:119:LEU:CD2	1:A:234:TYR:CZ	2.54	0.84
1:C:149:LYS:HG2	1:C:177:SER:HG	1.40	0.84
1:C:197:VAL:HG23	1:C:350:ARG:NH2	1.79	0.84
1:C:80:ASP:HA	1:C:241:ARG:CZ	2.07	0.84
1:A:154:PHE:HE1	1:A:155:ASP:O	1.59	0.84
1:B:119:LEU:CD2	1:B:234:TYR:CE2	2.60	0.84
1:C:204:PRO:CG	1:C:328:GLU:C	2.43	0.84
1:C:288:LEU:HD11	1:C:290:LEU:HG	1.57	0.84
1:B:288:LEU:CD1	1:B:290:LEU:CD2	2.53	0.84
1:B:136:PHE:CE1	1:B:232:VAL:HG22	2.12	0.84
1:B:130:ARG:HD2	1:B:237:GLN:HB2	0.85	0.84
1:B:90:ILE:HD11	1:B:232:VAL:HG21	1.58	0.84
1:A:288:LEU:HD21	1:A:290:LEU:HD11	1.60	0.84
1:B:277:ASP:OD1	1:B:279:HIS:ND1	2.10	0.84
1:A:315:ALA:HB1	1:A:318:SER:CA	2.08	0.84
1:C:119:LEU:CD2	1:C:234:TYR:CE2	2.60	0.84
1:C:133:SER:C	1:C:234:TYR:HA	1.99	0.84
1:C:207:VAL:H	1:C:329:ARG:CZ	1.90	0.84
1:C:149:LYS:HD3	1:C:217:TYR:OH	1.78	0.84
1:C:95:LYS:HZ2	1:C:221:ALA:HA	1.41	0.84
1:C:315:ALA:HB1	1:C:318:SER:CA	2.08	0.84
1:C:327:ALA:CA	1:C:331:GLN:OE1	2.26	0.84
1:B:125:GLN:HA	1:B:243:GLY:CA	2.06	0.84
1:B:179:VAL:HG22	1:B:180:PRO:HD2	1.58	0.84
1:B:149:LYS:HD3	1:B:217:TYR:OH	1.78	0.84
1:B:291:PHE:O	1:B:292:TYR:HB3	1.78	0.84
1:A:291:PHE:O	1:A:292:TYR:HB3	1.78	0.84
1:A:119:LEU:CD2	1:A:234:TYR:CE2	2.60	0.83
1:C:130:ARG:HD2	1:C:237:GLN:HB2	0.85	0.83
1:C:288:LEU:CD1	1:C:290:LEU:HD21	2.08	0.83
1:C:328:GLU:C	1:C:329:ARG:O	2.14	0.83
1:B:328:GLU:C	1:B:329:ARG:O	2.14	0.83
1:C:296:PRO:CG	1:C:337:THR:CB	2.52	0.83
1:A:152:LEU:HD22	1:A:186:LEU:HD12	1.61	0.83
1:A:315:ALA:HB1	1:A:318:SER:CB	2.07	0.83
1:C:338:THR:HG1	1:C:339:GLU:HB2	1.43	0.83
1:B:288:LEU:HD11	1:B:290:LEU:HG	1.58	0.83
1:C:295:ALA:HB1	1:C:315:ALA:N	1.93	0.83
1:C:315:ALA:HB1	1:C:318:SER:CB	2.08	0.83
1:B:327:ALA:CA	1:B:331:GLN:OE1	2.26	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ALA:HB1	1:A:315:ALA:N	1.93	0.83
1:A:134:LEU:HA	1:A:233:GLU:C	1.95	0.83
1:C:251:GLY:O	1:C:346:TRP:CE3	2.31	0.83
1:A:296:PRO:CG	1:A:337:THR:HG21	2.06	0.83
1:A:90:ILE:O	1:A:90:ILE:HG22	1.78	0.83
1:C:288:LEU:HG	1:C:289:THR:N	1.94	0.83
1:B:251:GLY:O	1:B:346:TRP:CE3	2.31	0.83
1:A:288:LEU:CD1	1:A:290:LEU:HD21	2.08	0.83
1:A:153:ALA:CB	1:A:174:GLY:CA	2.35	0.83
1:A:149:LYS:HD3	1:A:217:TYR:OH	1.78	0.83
1:A:198:ALA:C	1:A:200:GLY:H	1.77	0.83
1:C:249:GLN:HE22	1:C:265:TRP:N	1.77	0.83
1:C:291:PHE:O	1:C:292:TYR:HB3	1.78	0.83
1:B:278:CYS:H	1:B:334:LYS:HD3	1.25	0.83
1:C:55:VAL:HG22	1:C:56:THR:N	1.93	0.83
1:A:133:SER:C	1:A:234:TYR:HA	1.99	0.83
1:A:179:VAL:HG22	1:A:180:PRO:HD2	1.58	0.83
1:C:201:ILE:HG22	1:C:265:TRP:CA	2.09	0.83
1:C:207:VAL:HG13	1:C:329:ARG:HH21	1.44	0.83
1:B:288:LEU:HG	1:B:289:THR:N	1.94	0.83
1:C:79:ARG:O	1:C:80:ASP:CB	2.27	0.83
1:A:269:LYS:HG2	1:A:270:GLY:H	1.42	0.83
1:B:295:ALA:HB1	1:B:315:ALA:N	1.93	0.82
1:C:78:ALA:C	1:C:80:ASP:H	1.82	0.82
1:A:288:LEU:HG	1:A:289:THR:N	1.94	0.82
1:B:153:ALA:CB	1:B:174:GLY:CA	2.35	0.82
1:A:327:ALA:CB	1:A:331:GLN:CD	2.39	0.82
1:C:200:GLY:CA	1:C:265:TRP:HA	2.09	0.82
1:C:277:ASP:OD1	1:C:334:LYS:CE	2.27	0.82
1:B:152:LEU:HD22	1:B:186:LEU:HD12	1.60	0.82
1:C:69:VAL:CG1	1:C:70:SER:N	2.38	0.82
1:A:277:ASP:OD1	1:A:334:LYS:CE	2.27	0.82
1:A:138:TYR:C	1:A:139:SER:O	2.16	0.82
1:C:249:GLN:NE2	1:C:265:TRP:HE3	1.78	0.82
1:C:90:ILE:O	1:C:90:ILE:HG22	1.78	0.82
1:B:198:ALA:C	1:B:200:GLY:H	1.77	0.82
1:C:69:VAL:CG1	1:C:70:SER:H	1.81	0.82
1:B:288:LEU:HD21	1:B:290:LEU:HD11	1.60	0.82
1:A:251:GLY:O	1:A:346:TRP:CE3	2.31	0.82
1:A:327:ALA:CA	1:A:331:GLN:OE1	2.26	0.82
1:C:66:TYR:CE2	1:C:183:GLY:HA3	2.15	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LEU:O	1:A:172:ILE:HG22	1.80	0.82
1:B:169:LEU:O	1:B:172:ILE:HG22	1.80	0.82
1:B:300:LEU:HD11	1:B:333:VAL:CG1	2.09	0.82
1:B:90:ILE:O	1:B:90:ILE:HG22	1.78	0.82
1:A:340:GLU:O	1:A:342:PRO:HD2	1.79	0.82
1:C:170:TYR:CE1	1:C:217:TYR:OH	2.32	0.82
1:B:315:ALA:HB1	1:B:318:SER:CA	2.08	0.82
1:A:300:LEU:HD11	1:A:333:VAL:CG1	2.09	0.82
1:A:126:TYR:N	1:A:242:THR:CG2	2.43	0.82
1:C:288:LEU:HD21	1:C:290:LEU:HD11	1.60	0.82
1:C:300:LEU:HD11	1:C:333:VAL:CG1	2.09	0.82
1:B:277:ASP:OD1	1:B:334:LYS:CE	2.27	0.82
1:A:318:SER:OG	1:A:319:VAL:N	2.07	0.82
1:A:128:LYS:HA	1:A:195:ARG:O	1.80	0.81
1:C:269:LYS:HG2	1:C:270:GLY:H	1.42	0.81
1:B:138:TYR:C	1:B:139:SER:O	2.16	0.81
1:B:128:LYS:HA	1:B:195:ARG:O	1.80	0.81
1:B:285:ASN:ND2	1:B:324:VAL:O	2.13	0.81
1:A:328:GLU:C	1:A:329:ARG:O	2.14	0.81
1:C:101:PRO:CG	1:C:166:LEU:HD12	2.10	0.81
1:C:169:LEU:O	1:C:172:ILE:HG22	1.80	0.81
1:B:126:TYR:N	1:B:242:THR:CG2	2.43	0.81
1:B:95:LYS:NZ	1:B:225:ALA:N	2.28	0.81
1:B:251:GLY:O	1:B:346:TRP:CE2	2.34	0.81
1:C:296:PRO:CG	1:C:337:THR:HG21	2.06	0.81
1:B:164:ASN:HD22	1:B:164:ASN:H	0.82	0.81
1:B:340:GLU:O	1:B:342:PRO:HD2	1.80	0.81
1:A:112:GLU:O	1:A:115:THR:HG22	1.81	0.81
1:A:95:LYS:NZ	1:A:225:ALA:N	2.28	0.81
1:C:130:ARG:HD2	1:C:237:GLN:HE21	1.46	0.81
1:B:133:SER:C	1:B:234:TYR:HA	1.99	0.81
1:B:315:ALA:CB	1:B:318:SER:H	1.94	0.81
1:C:206:LEU:H	1:C:329:ARG:NH1	1.79	0.81
1:A:288:LEU:CD1	1:A:290:LEU:CD2	2.53	0.81
1:A:170:TYR:CE1	1:A:217:TYR:OH	2.32	0.81
1:C:249:GLN:HE22	1:C:265:TRP:H	1.29	0.81
1:C:285:ASN:ND2	1:C:324:VAL:O	2.13	0.81
1:A:296:PRO:HG3	1:A:337:THR:CG2	2.07	0.81
1:B:288:LEU:CD1	1:B:290:LEU:HD21	2.08	0.81
1:A:251:GLY:O	1:A:346:TRP:CE2	2.34	0.81
1:B:296:PRO:HG3	1:B:337:THR:CG2	2.07	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:VAL:O	1:C:115:THR:HG21	1.81	0.81
1:B:107:VAL:O	1:B:115:THR:HG21	1.81	0.81
1:B:170:TYR:CE1	1:B:217:TYR:OH	2.32	0.81
1:B:327:ALA:CB	1:B:331:GLN:CD	2.39	0.81
1:B:278:CYS:N	1:B:334:LYS:CE	2.20	0.81
1:B:119:LEU:CD2	1:B:234:TYR:CZ	2.55	0.81
1:B:95:LYS:HZ2	1:B:221:ALA:HA	1.42	0.81
1:B:90:ILE:CD1	1:B:232:VAL:CG2	2.58	0.81
1:B:286:PHE:HA	1:B:351:ILE:HG21	1.61	0.80
1:A:285:ASN:ND2	1:A:324:VAL:O	2.13	0.80
1:C:340:GLU:O	1:C:342:PRO:HD2	1.80	0.80
1:C:152:LEU:HD22	1:C:186:LEU:HD12	1.60	0.80
1:C:300:LEU:HD11	1:C:333:VAL:HG12	1.63	0.80
1:C:251:GLY:O	1:C:346:TRP:CE2	2.34	0.80
1:B:101:PRO:CG	1:B:166:LEU:HD12	2.10	0.80
1:B:96:ASN:HD21	1:B:102:LYS:HD3	1.45	0.80
1:A:101:PRO:HG3	1:A:217:TYR:CD2	2.17	0.80
1:A:96:ASN:HD21	1:A:102:LYS:HD3	1.45	0.80
1:C:96:ASN:HD21	1:C:102:LYS:HD3	1.45	0.80
1:C:315:ALA:CB	1:C:318:SER:H	1.94	0.80
1:A:300:LEU:HD11	1:A:333:VAL:HG12	1.63	0.80
1:A:90:ILE:CD1	1:A:232:VAL:CG2	2.58	0.80
1:C:95:LYS:NZ	1:C:225:ALA:N	2.28	0.80
1:A:248:ALA:HB1	1:A:265:TRP:HA	1.60	0.80
1:C:128:LYS:HA	1:C:195:ARG:O	1.80	0.80
1:C:138:TYR:C	1:C:139:SER:O	2.16	0.80
1:C:201:ILE:CG2	1:C:265:TRP:O	2.29	0.80
1:C:227:LEU:H	1:C:227:LEU:HD12	1.47	0.80
1:A:164:ASN:HD22	1:A:164:ASN:H	0.82	0.80
1:C:126:TYR:N	1:C:242:THR:CG2	2.43	0.80
1:B:112:GLU:O	1:B:115:THR:HG22	1.81	0.80
1:B:174:GLY:C	1:B:175:CYS:HG	1.82	0.80
1:B:130:ARG:HD2	1:B:237:GLN:HE21	1.46	0.80
1:A:248:ALA:CB	1:A:264:SER:CB	2.54	0.80
1:A:95:LYS:HZ1	1:A:225:ALA:N	1.79	0.80
1:B:300:LEU:HD11	1:B:333:VAL:HG12	1.63	0.80
1:B:291:PHE:HB2	1:B:345:LYS:O	1.82	0.80
1:B:326:VAL:HG12	1:B:327:ALA:C	2.02	0.80
1:C:101:PRO:HG3	1:C:217:TYR:CD2	2.17	0.80
1:B:101:PRO:HD2	1:B:166:LEU:HD12	1.37	0.80
1:A:286:PHE:HA	1:A:351:ILE:HG21	1.61	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LYS:NZ	1:B:225:ALA:H	1.80	0.79
1:C:296:PRO:HG3	1:C:337:THR:CG2	2.07	0.79
1:C:53:GLN:C	1:C:53:GLN:N	2.35	0.79
1:C:164:ASN:H	1:C:164:ASN:HD22	0.82	0.79
1:A:249:GLN:HB3	1:A:348:ALA:O	1.83	0.79
1:A:121:LYS:NZ	1:A:350:ARG:HH12	1.80	0.79
1:C:112:GLU:O	1:C:115:THR:HG22	1.81	0.79
1:C:153:ALA:CB	1:C:174:GLY:CA	2.35	0.79
1:C:199:ASP:HA	1:C:265:TRP:HE1	1.47	0.79
1:C:201:ILE:CG2	1:C:265:TRP:C	2.51	0.79
1:A:291:PHE:HB2	1:A:345:LYS:O	1.82	0.79
1:A:95:LYS:NZ	1:A:225:ALA:H	1.80	0.79
1:A:227:LEU:HD12	1:A:227:LEU:H	1.47	0.79
1:C:119:LEU:CD2	1:C:234:TYR:CZ	2.55	0.79
1:C:249:GLN:HB3	1:C:348:ALA:O	1.83	0.79
1:A:95:LYS:HZ2	1:A:221:ALA:HA	1.42	0.79
1:C:201:ILE:CD1	1:C:280:PHE:O	2.10	0.79
1:C:95:LYS:NZ	1:C:225:ALA:H	1.80	0.79
1:B:101:PRO:HG3	1:B:217:TYR:CD2	2.17	0.79
1:B:133:SER:HB3	1:B:235:THR:HG22	1.64	0.79
1:B:95:LYS:HZ1	1:B:225:ALA:N	1.80	0.79
1:A:315:ALA:CB	1:A:318:SER:H	1.94	0.79
1:A:133:SER:HB3	1:A:235:THR:HG22	1.64	0.79
1:C:293:GLU:O	1:C:317:GLY:CA	2.31	0.79
1:C:300:LEU:CD1	1:C:333:VAL:HG12	2.13	0.79
1:C:326:VAL:HG12	1:C:327:ALA:C	2.02	0.79
1:B:175:CYS:HB2	1:B:176:VAL:HB	1.65	0.79
1:A:248:ALA:HB2	1:A:264:SER:O	1.77	0.79
1:A:101:PRO:CG	1:A:166:LEU:HD12	2.10	0.79
1:C:133:SER:HB3	1:C:235:THR:HG22	1.64	0.79
1:C:95:LYS:HZ3	1:C:225:ALA:H	1.29	0.79
1:B:300:LEU:CD1	1:B:333:VAL:HG12	2.13	0.79
1:B:339:GLU:C	1:B:340:GLU:HA	2.04	0.79
1:A:107:VAL:O	1:A:115:THR:HG21	1.81	0.78
1:C:291:PHE:HB2	1:C:345:LYS:O	1.82	0.78
1:B:269:LYS:HG2	1:B:270:GLY:H	1.42	0.78
1:C:296:PRO:CD	1:C:337:THR:CG2	2.60	0.78
1:C:90:ILE:CD1	1:C:232:VAL:CG2	2.58	0.78
1:A:326:VAL:HG12	1:A:327:ALA:C	2.02	0.78
1:A:121:LYS:HZ2	1:A:350:ARG:HH12	1.30	0.78
1:A:134:LEU:O	1:A:134:LEU:HG	1.83	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:THR:HG21	1:C:87:SER:HG	0.95	0.78
1:C:179:VAL:HG11	1:C:181:TRP:HE1	1.49	0.78
1:C:286:PHE:HA	1:C:351:ILE:HG21	1.61	0.78
1:B:134:LEU:O	1:B:134:LEU:HG	1.83	0.78
1:B:169:LEU:HD23	1:B:169:LEU:C	2.04	0.78
1:B:227:LEU:H	1:B:227:LEU:HD12	1.47	0.78
1:A:293:GLU:O	1:A:317:GLY:CA	2.31	0.78
1:A:169:LEU:C	1:A:169:LEU:HD23	2.04	0.78
1:C:289:THR:O	1:C:290:LEU:HB3	1.83	0.78
1:C:249:GLN:O	1:C:348:ALA:N	2.17	0.78
1:B:289:THR:O	1:B:290:LEU:HB3	1.83	0.78
1:B:249:GLN:HB3	1:B:348:ALA:O	1.83	0.78
1:C:133:SER:N	1:C:235:THR:HG22	1.99	0.78
1:B:249:GLN:O	1:B:348:ALA:N	2.17	0.78
1:C:339:GLU:C	1:C:340:GLU:HA	2.04	0.78
1:C:204:PRO:HG2	1:C:328:GLU:HG2	0.80	0.78
1:B:236:VAL:HG12	1:B:238:LEU:HD12	1.66	0.78
1:A:130:ARG:HD2	1:A:237:GLN:HE21	1.46	0.78
1:B:293:GLU:O	1:B:317:GLY:CA	2.31	0.78
1:A:249:GLN:O	1:A:348:ALA:N	2.17	0.78
1:C:97:THR:HA	1:C:219:GLN:CA	2.14	0.78
1:C:179:VAL:CG2	1:C:180:PRO:CD	2.62	0.78
1:B:117:ASN:ND2	1:B:117:ASN:O	2.17	0.78
1:B:248:ALA:C	1:B:249:GLN:HB2	2.04	0.77
1:B:276:HIS:CG	1:B:277:ASP:H	2.03	0.77
1:A:117:ASN:ND2	1:A:117:ASN:O	2.17	0.77
1:B:135:ARG:HB2	1:B:185:ILE:HD11	1.67	0.77
1:A:300:LEU:CD1	1:A:333:VAL:HG12	2.13	0.77
1:A:109:ASN:HD21	1:A:197:VAL:HG23	1.50	0.77
1:A:149:LYS:HE2	1:A:151:ALA:HA	1.66	0.77
1:C:205:LYS:H	1:C:329:ARG:NH1	1.82	0.77
1:B:133:SER:N	1:B:235:THR:HG22	1.99	0.77
1:A:133:SER:N	1:A:235:THR:HG22	1.99	0.77
1:A:149:LYS:CB	1:A:217:TYR:CE1	2.60	0.77
1:A:296:PRO:CD	1:A:337:THR:CG2	2.60	0.77
1:B:204:PRO:C	1:B:205:LYS:HD2	2.05	0.77
1:C:124:ALA:O	1:C:244:SER:N	2.18	0.77
1:C:159:ALA:HB3	1:C:328:GLU:CG	2.11	0.77
1:C:204:PRO:C	1:C:205:LYS:HD2	2.05	0.77
1:C:86:GLY:CA	1:C:234:TYR:CE1	2.66	0.77
1:C:200:GLY:CA	1:C:265:TRP:CB	2.58	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:VAL:HG12	1:A:238:LEU:HD12	1.66	0.77
1:C:327:ALA:CB	1:C:331:GLN:CD	2.39	0.77
1:B:296:PRO:CD	1:B:337:THR:CG2	2.60	0.77
1:A:135:ARG:HB2	1:A:185:ILE:HD11	1.67	0.77
1:A:179:VAL:CG2	1:A:180:PRO:CD	2.62	0.77
1:A:339:GLU:C	1:A:340:GLU:HA	2.04	0.77
1:A:175:CYS:HB2	1:A:176:VAL:HB	1.65	0.77
1:C:169:LEU:C	1:C:169:LEU:HD23	2.04	0.77
1:B:95:LYS:HZ3	1:B:225:ALA:H	1.33	0.77
1:C:134:LEU:HG	1:C:134:LEU:O	1.83	0.76
1:C:163:PRO:CA	1:C:164:ASN:ND2	2.47	0.76
1:C:251:GLY:O	1:C:346:TRP:CZ3	2.38	0.76
1:B:185:ILE:HD12	1:B:186:LEU:CA	2.16	0.76
1:B:315:ALA:O	1:B:317:GLY:N	2.18	0.76
1:A:204:PRO:C	1:A:205:LYS:HD2	2.05	0.76
1:C:207:VAL:HG13	1:C:329:ARG:NH2	1.94	0.76
1:A:251:GLY:O	1:A:346:TRP:CZ3	2.38	0.76
1:C:97:THR:HA	1:C:218:GLY:O	1.85	0.76
1:B:97:THR:HA	1:B:219:GLN:CA	2.15	0.76
1:C:236:VAL:HG12	1:C:238:LEU:HD12	1.66	0.76
1:C:313:GLU:HB2	1:C:315:ALA:N	2.00	0.76
1:C:149:LYS:HE2	1:C:151:ALA:HA	1.66	0.76
1:B:156:ARG:O	1:B:158:ALA:N	2.18	0.76
1:A:156:ARG:O	1:A:158:ALA:N	2.18	0.76
1:A:179:VAL:HG11	1:A:181:TRP:HE1	1.49	0.76
1:A:289:THR:O	1:A:290:LEU:HB3	1.83	0.76
1:B:248:ALA:HB3	1:B:348:ALA:O	1.86	0.76
1:C:144:SER:C	1:C:146:THR:H	1.89	0.76
1:B:149:LYS:CB	1:B:217:TYR:CE1	2.60	0.76
1:B:109:ASN:HD21	1:B:197:VAL:HG23	1.50	0.76
1:A:313:GLU:HB2	1:A:315:ALA:N	2.00	0.76
1:C:156:ARG:O	1:C:158:ALA:N	2.18	0.76
1:C:175:CYS:HB2	1:C:176:VAL:HB	1.65	0.76
1:B:163:PRO:CA	1:B:164:ASN:ND2	2.47	0.76
1:A:97:THR:HA	1:A:218:GLY:O	1.85	0.76
1:C:117:ASN:O	1:C:117:ASN:ND2	2.17	0.76
1:A:163:PRO:CA	1:A:164:ASN:ND2	2.47	0.76
1:B:149:LYS:HE2	1:B:151:ALA:HA	1.66	0.76
1:A:276:HIS:CG	1:A:277:ASP:H	2.03	0.76
1:A:300:LEU:CD1	1:A:333:VAL:CG1	2.64	0.76
1:A:97:THR:HA	1:A:219:GLN:CA	2.14	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:ARG:HB2	1:C:185:ILE:HD11	1.67	0.76
1:A:315:ALA:O	1:A:317:GLY:N	2.18	0.76
1:C:248:ALA:CB	1:C:287:SER:O	2.32	0.76
1:A:185:ILE:HD12	1:A:186:LEU:CA	2.16	0.76
1:C:138:TYR:O	1:C:139:SER:C	2.25	0.76
1:C:149:LYS:HB3	1:C:217:TYR:CD1	2.20	0.76
1:C:314:ALA:O	1:C:315:ALA:CB	2.34	0.76
1:C:59:SER:C	1:C:61:PRO:HD3	2.06	0.76
1:C:95:LYS:HZ1	1:C:225:ALA:N	1.83	0.76
1:B:310:VAL:HA	1:B:321:TRP:O	1.86	0.76
1:A:314:ALA:O	1:A:315:ALA:CB	2.34	0.76
1:A:95:LYS:HZ3	1:A:225:ALA:H	1.34	0.75
1:C:276:HIS:CG	1:C:277:ASP:H	2.03	0.75
1:C:109:ASN:HD21	1:C:197:VAL:HG23	1.50	0.75
1:C:279:HIS:CA	1:C:280:PHE:N	2.50	0.75
1:C:301:GLU:O	1:C:333:VAL:CG1	2.34	0.75
1:C:83:THR:HG22	1:C:84:ARG:N	2.01	0.75
1:B:179:VAL:HG11	1:B:181:TRP:HE1	1.49	0.75
1:B:251:GLY:O	1:B:346:TRP:CZ3	2.39	0.75
1:B:313:GLU:HB2	1:B:315:ALA:N	2.00	0.75
1:A:83:THR:HG22	1:A:84:ARG:N	2.01	0.75
1:B:179:VAL:CG2	1:B:180:PRO:CD	2.62	0.75
1:B:300:LEU:CD1	1:B:333:VAL:CG1	2.64	0.75
1:C:306:SER:HB3	1:C:325:LYS:HB3	1.69	0.75
1:B:306:SER:HB3	1:B:325:LYS:HB3	1.69	0.75
1:C:115:THR:O	1:C:116:PHE:CG	2.40	0.75
1:C:136:PHE:CZ	1:C:212:LEU:HD22	2.22	0.75
1:C:300:LEU:CD1	1:C:333:VAL:CG1	2.64	0.75
1:A:136:PHE:CZ	1:A:212:LEU:HD22	2.22	0.75
1:C:199:ASP:C	1:C:265:TRP:NE1	2.40	0.75
1:C:288:LEU:CD1	1:C:290:LEU:HG	2.17	0.75
1:C:277:ASP:OD1	1:C:334:LYS:NZ	2.20	0.75
1:B:326:VAL:CG1	1:B:331:GLN:HG3	2.17	0.75
1:A:292:TYR:HB2	1:A:318:SER:O	1.86	0.75
1:C:315:ALA:O	1:C:317:GLY:N	2.18	0.75
1:B:138:TYR:CG	1:B:184:PHE:CZ	2.62	0.75
1:B:277:ASP:OD1	1:B:334:LYS:NZ	2.20	0.75
1:B:279:HIS:CA	1:B:280:PHE:N	2.50	0.74
1:A:279:HIS:CA	1:A:280:PHE:N	2.50	0.74
1:C:68:GLU:HG2	1:C:137:ARG:NH2	2.02	0.74
1:B:289:THR:O	1:B:290:LEU:CB	2.35	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:GLU:O	1:B:333:VAL:CG1	2.34	0.74
1:A:241:ARG:HD2	1:A:241:ARG:N	2.03	0.74
1:C:310:VAL:HA	1:C:321:TRP:O	1.86	0.74
1:A:277:ASP:OD1	1:A:334:LYS:NZ	2.20	0.74
1:B:271:THR:HG21	1:B:275:GLU:OE2	1.87	0.74
1:B:97:THR:HA	1:B:218:GLY:O	1.85	0.74
1:B:241:ARG:HD2	1:B:241:ARG:N	2.03	0.74
1:A:133:SER:CB	1:A:235:THR:HG22	2.17	0.74
1:C:136:PHE:CD1	1:C:232:VAL:HG22	2.23	0.74
1:C:271:THR:HG21	1:C:275:GLU:OE2	1.87	0.74
1:A:126:TYR:CA	1:A:242:THR:CG2	2.64	0.74
1:B:136:PHE:CZ	1:B:212:LEU:HD22	2.22	0.74
1:B:292:TYR:HB2	1:B:318:SER:O	1.86	0.74
1:B:314:ALA:O	1:B:315:ALA:CB	2.34	0.74
1:C:292:TYR:HB2	1:C:318:SER:O	1.86	0.74
1:B:138:TYR:O	1:B:139:SER:C	2.24	0.74
1:A:310:VAL:C	1:A:311:LEU:HD12	2.08	0.74
1:C:174:GLY:O	1:C:175:CYS:SG	2.45	0.74
1:C:75:VAL:CB	1:C:75:VAL:N	2.51	0.74
1:A:310:VAL:HA	1:A:321:TRP:O	1.86	0.74
1:A:313:GLU:HG3	1:A:318:SER:HB3	1.69	0.74
1:A:326:VAL:CG1	1:A:331:GLN:HG3	2.17	0.74
1:A:154:PHE:HD1	1:A:155:ASP:H	0.75	0.74
1:C:85:SER:CA	1:C:234:TYR:O	2.36	0.74
1:B:133:SER:CB	1:B:235:THR:HG22	2.17	0.74
1:B:83:THR:HG22	1:B:84:ARG:N	2.01	0.74
1:A:124:ALA:O	1:A:244:SER:N	2.18	0.74
1:A:135:ARG:HB3	1:A:186:LEU:O	1.88	0.74
1:C:109:ASN:HA	1:C:129:TYR:OH	1.88	0.74
1:C:197:VAL:HG22	1:C:350:ARG:NH2	2.01	0.74
1:B:130:ARG:HD2	1:B:237:GLN:HB3	1.64	0.74
1:B:149:LYS:HB3	1:B:217:TYR:CD1	2.20	0.74
1:B:174:GLY:O	1:B:175:CYS:SG	2.45	0.74
1:C:76:SER:N	1:C:76:SER:HA	2.01	0.74
1:A:248:ALA:HB2	1:A:265:TRP:CA	2.13	0.74
1:A:130:ARG:HD2	1:A:237:GLN:HB3	1.63	0.73
1:A:138:TYR:O	1:A:139:SER:C	2.24	0.73
1:A:174:GLY:O	1:A:175:CYS:SG	2.45	0.73
1:A:149:LYS:HB3	1:A:217:TYR:CD1	2.20	0.73
1:A:94:LYS:O	1:A:95:LYS:O	2.06	0.73
1:C:71:THR:OG1	1:C:87:SER:HB2	1.87	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:LEU:CD1	1:B:290:LEU:HG	2.18	0.73
1:C:78:ALA:C	1:C:80:ASP:N	2.32	0.73
1:A:288:LEU:CD1	1:A:290:LEU:HG	2.17	0.73
1:A:136:PHE:CD1	1:A:232:VAL:HG22	2.23	0.73
1:B:126:TYR:CA	1:B:242:THR:CG2	2.64	0.73
1:C:76:SER:OG	1:C:76:SER:C	2.26	0.73
1:A:271:THR:HG21	1:A:275:GLU:OE2	1.87	0.73
1:A:86:GLY:CA	1:A:234:TYR:CE1	2.66	0.73
1:B:154:PHE:HD1	1:B:155:ASP:H	0.75	0.73
1:C:326:VAL:CG1	1:C:331:GLN:HG3	2.17	0.73
1:B:149:LYS:HD3	1:B:217:TYR:CE1	2.23	0.73
1:B:136:PHE:CD1	1:B:232:VAL:HG22	2.23	0.73
1:B:94:LYS:O	1:B:95:LYS:O	2.06	0.73
1:C:149:LYS:HE2	1:C:151:ALA:CA	2.19	0.73
1:C:154:PHE:CE1	1:C:155:ASP:O	2.41	0.73
1:C:283:THR:OG1	1:C:329:ARG:HG2	1.89	0.73
1:C:94:LYS:O	1:C:95:LYS:O	2.06	0.73
1:B:115:THR:O	1:B:116:PHE:CG	2.40	0.73
1:C:133:SER:CB	1:C:235:THR:HG22	2.17	0.73
1:C:185:ILE:HD12	1:C:186:LEU:CA	2.16	0.73
1:A:253:PHE:CD2	1:A:346:TRP:HZ3	2.07	0.73
1:C:297:VAL:O	1:C:298:SER:OG	2.07	0.73
1:A:149:LYS:HD3	1:A:217:TYR:CE1	2.24	0.73
1:B:283:THR:OG1	1:B:329:ARG:HG2	1.89	0.73
1:C:241:ARG:HD2	1:C:241:ARG:N	2.03	0.73
1:A:306:SER:HB3	1:A:325:LYS:HB3	1.69	0.73
1:C:208:ASP:N	1:C:329:ARG:HH21	1.85	0.73
1:C:310:VAL:C	1:C:311:LEU:HD12	2.08	0.73
1:C:90:ILE:CD1	1:C:232:VAL:HG23	2.19	0.73
1:B:135:ARG:HB3	1:B:186:LEU:O	1.88	0.73
1:A:109:ASN:HA	1:A:129:TYR:OH	1.88	0.73
1:C:135:ARG:HB3	1:C:186:LEU:O	1.88	0.73
1:B:138:TYR:HH	1:B:227:LEU:HB3	1.52	0.73
1:A:101:PRO:C	1:A:102:LYS:CG	2.42	0.73
1:A:127:GLU:O	1:A:128:LYS:HB2	1.89	0.73
1:C:205:LYS:N	1:C:329:ARG:CZ	2.51	0.73
1:B:144:SER:C	1:B:146:THR:H	1.89	0.73
1:A:90:ILE:CD1	1:A:232:VAL:HG23	2.19	0.72
1:C:149:LYS:HD3	1:C:217:TYR:CE1	2.24	0.72
1:A:288:LEU:CG	1:A:289:THR:N	2.50	0.72
1:B:241:ARG:H	1:B:241:ARG:HD2	1.54	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:GLU:HG3	1:C:318:SER:HB3	1.69	0.72
1:B:127:GLU:O	1:B:128:LYS:HB2	1.89	0.72
1:A:252:ASP:OD2	1:A:345:LYS:CE	2.37	0.72
1:A:120:ILE:CD1	1:A:329:ARG:NH2	2.53	0.72
1:A:149:LYS:HE2	1:A:151:ALA:CA	2.19	0.72
1:B:109:ASN:HA	1:B:129:TYR:OH	1.88	0.72
1:B:85:SER:CA	1:B:234:TYR:O	2.36	0.72
1:B:310:VAL:C	1:B:311:LEU:HD12	2.08	0.72
1:A:115:THR:O	1:A:116:PHE:CG	2.40	0.72
1:B:90:ILE:CD1	1:B:232:VAL:HG23	2.19	0.72
1:A:301:GLU:O	1:A:333:VAL:CG1	2.34	0.72
1:A:241:ARG:H	1:A:241:ARG:HD2	1.54	0.72
1:A:144:SER:C	1:A:146:THR:H	1.89	0.72
1:B:113:PRO:HB2	1:B:283:THR:O	1.88	0.72
1:B:124:ALA:O	1:B:244:SER:N	2.18	0.72
1:B:253:PHE:CD2	1:B:346:TRP:HZ3	2.07	0.72
1:B:308:PHE:HE2	1:B:310:VAL:CG2	1.92	0.72
1:A:326:VAL:HG13	1:A:331:GLN:CG	2.20	0.72
1:A:283:THR:OG1	1:A:329:ARG:HG2	1.89	0.72
1:C:126:TYR:CA	1:C:242:THR:CG2	2.64	0.72
1:C:201:ILE:HD11	1:C:280:PHE:O	1.88	0.72
1:C:200:GLY:O	1:C:282:GLY:CA	2.38	0.72
1:B:132:THR:HG22	1:B:235:THR:O	1.89	0.72
1:C:241:ARG:HD2	1:C:241:ARG:H	1.54	0.72
1:B:179:VAL:HG22	1:B:180:PRO:CD	2.19	0.72
1:B:267:LYS:O	1:B:279:HIS:HB2	1.90	0.72
1:A:339:GLU:CA	1:A:340:GLU:N	2.53	0.72
1:B:339:GLU:CA	1:B:340:GLU:N	2.53	0.72
1:A:95:LYS:HZ2	1:A:221:ALA:CA	2.01	0.72
1:C:200:GLY:O	1:C:282:GLY:HA3	1.89	0.72
1:C:339:GLU:CA	1:C:340:GLU:N	2.53	0.72
1:A:169:LEU:O	1:A:169:LEU:HD23	1.89	0.72
1:C:253:PHE:CD2	1:C:346:TRP:HZ3	2.07	0.72
1:B:149:LYS:HE2	1:B:151:ALA:CA	2.19	0.72
1:A:179:VAL:HG22	1:A:180:PRO:CD	2.19	0.72
1:A:132:THR:HG22	1:A:235:THR:O	1.89	0.72
1:C:206:LEU:H	1:C:329:ARG:HH12	1.37	0.72
1:C:288:LEU:CG	1:C:289:THR:N	2.50	0.72
1:C:295:ALA:CB	1:C:315:ALA:N	2.53	0.72
1:C:326:VAL:HG13	1:C:331:GLN:CG	2.20	0.72
1:C:208:ASP:N	1:C:329:ARG:NH2	2.38	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:TYR:CG	1:C:184:PHE:CZ	2.62	0.71
1:C:149:LYS:CB	1:C:217:TYR:CE1	2.60	0.71
1:C:308:PHE:CD2	1:C:310:VAL:HG23	2.25	0.71
1:B:112:GLU:HG3	1:B:329:ARG:HH22	1.53	0.71
1:C:55:VAL:CG2	1:C:56:THR:H	2.03	0.71
1:C:132:THR:HG22	1:C:235:THR:O	1.89	0.71
1:C:208:ASP:H	1:C:329:ARG:NH2	1.87	0.71
1:C:290:LEU:HD22	1:C:346:TRP:CB	2.20	0.71
1:B:308:PHE:CD2	1:B:310:VAL:HG23	2.25	0.71
1:B:326:VAL:HG13	1:B:327:ALA:H	1.54	0.71
1:B:179:VAL:HG21	1:B:181:TRP:HD1	1.55	0.71
1:B:326:VAL:HG13	1:B:331:GLN:CG	2.20	0.71
1:A:308:PHE:CD2	1:A:310:VAL:HG23	2.25	0.71
1:A:297:VAL:O	1:A:298:SER:OG	2.07	0.71
1:A:242:THR:HG23	1:A:243:GLY:N	2.05	0.71
1:C:112:GLU:HA	1:C:284:GLY:CA	2.19	0.71
1:C:267:LYS:O	1:C:279:HIS:HB2	1.90	0.71
1:B:242:THR:HG23	1:B:243:GLY:N	2.05	0.71
1:B:252:ASP:OD2	1:B:345:LYS:CE	2.37	0.71
1:C:127:GLU:O	1:C:128:LYS:HB2	1.89	0.71
1:B:297:VAL:O	1:B:298:SER:OG	2.07	0.71
1:C:252:ASP:OD2	1:C:345:LYS:CE	2.37	0.71
1:B:179:VAL:CG2	1:B:181:TRP:HD1	2.03	0.71
1:B:242:THR:HG23	1:B:243:GLY:H	1.56	0.71
1:B:276:HIS:ND1	1:B:277:ASP:N	2.38	0.71
1:A:238:LEU:HD12	1:A:238:LEU:N	2.05	0.71
1:C:238:LEU:N	1:C:238:LEU:HD12	2.05	0.71
1:C:276:HIS:ND1	1:C:277:ASP:N	2.38	0.71
1:B:169:LEU:HD23	1:B:169:LEU:O	1.90	0.71
1:B:295:ALA:CB	1:B:315:ALA:N	2.53	0.71
1:C:56:THR:HG23	1:C:57:ARG:H	1.56	0.71
1:C:179:VAL:CG2	1:C:181:TRP:HD1	2.03	0.71
1:C:286:PHE:HA	1:C:350:ARG:O	1.91	0.71
1:B:238:LEU:HD12	1:B:238:LEU:N	2.05	0.71
1:A:295:ALA:CB	1:A:315:ALA:N	2.53	0.71
1:A:179:VAL:CG2	1:A:181:TRP:HD1	2.03	0.71
1:C:169:LEU:HD23	1:C:169:LEU:O	1.90	0.71
1:A:267:LYS:O	1:A:279:HIS:HB2	1.90	0.71
1:C:236:VAL:HG12	1:C:237:GLN:N	2.05	0.71
1:C:200:GLY:CA	1:C:265:TRP:CG	2.58	0.71
1:B:124:ALA:HB1	1:B:245:THR:CG2	2.20	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ALA:HB1	1:A:245:THR:CG2	2.20	0.70
1:C:116:PHE:O	1:C:120:ILE:HG22	1.90	0.70
1:C:179:VAL:HG22	1:C:180:PRO:CD	2.19	0.70
1:C:242:THR:HG23	1:C:243:GLY:N	2.05	0.70
1:B:236:VAL:HG12	1:B:237:GLN:N	2.05	0.70
1:A:252:ASP:OD1	1:A:253:PHE:N	2.24	0.70
1:B:130:ARG:HD2	1:B:237:GLN:NE2	2.06	0.70
1:A:167:ALA:O	1:A:171:ASN:CG	2.30	0.70
1:C:130:ARG:HD2	1:C:237:GLN:NE2	2.06	0.70
1:B:101:PRO:CG	1:B:217:TYR:CD2	2.75	0.70
1:B:86:GLY:CA	1:B:234:TYR:CE1	2.66	0.70
1:C:137:ARG:O	1:C:230:VAL:HG13	1.91	0.70
1:B:286:PHE:HA	1:B:350:ARG:O	1.91	0.70
1:B:288:LEU:CG	1:B:289:THR:N	2.50	0.70
1:A:130:ARG:HD2	1:A:237:GLN:NE2	2.06	0.70
1:C:242:THR:HG23	1:C:243:GLY:H	1.56	0.70
1:A:85:SER:CA	1:A:234:TYR:O	2.36	0.70
1:A:236:VAL:HG12	1:A:237:GLN:N	2.05	0.70
1:C:149:LYS:NZ	1:C:170:TYR:CE1	2.52	0.70
1:A:242:THR:HG23	1:A:243:GLY:H	1.56	0.70
1:C:124:ALA:HB1	1:C:245:THR:CG2	2.20	0.70
1:C:313:GLU:CG	1:C:318:SER:OG	2.40	0.70
1:A:138:TYR:CG	1:A:184:PHE:CZ	2.62	0.70
1:A:149:LYS:NZ	1:A:170:TYR:CE1	2.52	0.70
1:C:167:ALA:O	1:C:171:ASN:CG	2.30	0.70
1:C:156:ARG:O	1:C:210:GLY:N	2.25	0.70
1:C:101:PRO:CG	1:C:217:TYR:CD2	2.75	0.70
1:B:154:PHE:CE1	1:B:155:ASP:O	2.41	0.70
1:B:167:ALA:O	1:B:171:ASN:CG	2.30	0.70
1:B:313:GLU:CG	1:B:318:SER:OG	2.40	0.70
1:B:326:VAL:HG13	1:B:331:GLN:HG3	1.74	0.70
1:A:338:THR:OG1	1:A:339:GLU:CB	2.37	0.70
1:A:129:TYR:HA	1:A:237:GLN:O	1.92	0.70
1:A:103:TYR:HE1	1:A:169:LEU:HD12	1.56	0.70
1:C:55:VAL:CG2	1:C:56:THR:N	2.52	0.70
1:C:159:ALA:HB1	1:C:328:GLU:OE1	1.90	0.69
1:C:200:GLY:H	1:C:265:TRP:HD1	1.36	0.69
1:A:170:TYR:OH	1:A:217:TYR:OH	2.10	0.69
1:B:156:ARG:O	1:B:210:GLY:N	2.25	0.69
1:A:276:HIS:ND1	1:A:277:ASP:N	2.38	0.69
1:A:295:ALA:H	1:A:316:ALA:HA	0.69	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ARG:O	1:A:210:GLY:N	2.25	0.69
1:A:101:PRO:CG	1:A:217:TYR:CD2	2.75	0.69
1:C:244:SER:O	1:C:245:THR:CB	2.41	0.69
1:B:122:GLU:O	1:B:122:GLU:HG2	1.93	0.69
1:B:137:ARG:O	1:B:230:VAL:HG13	1.92	0.69
1:A:313:GLU:CG	1:A:318:SER:OG	2.40	0.69
1:A:154:PHE:C	1:A:154:PHE:CD1	2.62	0.69
1:A:179:VAL:HG21	1:A:181:TRP:HD1	1.56	0.69
1:A:137:ARG:O	1:A:230:VAL:HG13	1.91	0.69
1:C:103:TYR:HE1	1:C:169:LEU:HD12	1.56	0.69
1:C:179:VAL:HG21	1:C:181:TRP:HD1	1.55	0.69
1:B:101:PRO:C	1:B:102:LYS:CG	2.42	0.69
1:B:129:TYR:HA	1:B:237:GLN:O	1.92	0.69
1:B:252:ASP:OD1	1:B:253:PHE:N	2.24	0.69
1:C:66:TYR:CZ	1:C:183:GLY:HA3	2.27	0.69
1:A:244:SER:O	1:A:245:THR:CB	2.41	0.69
1:C:173:GLU:HG3	1:C:174:GLY:N	2.08	0.69
1:C:252:ASP:OD1	1:C:253:PHE:N	2.24	0.69
1:C:326:VAL:HG13	1:C:331:GLN:HG3	1.74	0.69
1:B:170:TYR:OH	1:B:217:TYR:OH	2.11	0.69
1:C:72:GLN:NE2	1:C:72:GLN:HA	2.04	0.69
1:C:101:PRO:C	1:C:102:LYS:CG	2.42	0.69
1:C:129:TYR:HA	1:C:237:GLN:O	1.92	0.69
1:C:326:VAL:HG13	1:C:327:ALA:H	1.54	0.69
1:C:333:VAL:C	1:C:334:LYS:HD3	2.12	0.69
1:B:95:LYS:HZ2	1:B:221:ALA:CA	2.01	0.69
1:A:290:LEU:HD22	1:A:346:TRP:CB	2.20	0.69
1:A:286:PHE:HA	1:A:350:ARG:O	1.91	0.69
1:B:103:TYR:HE1	1:B:169:LEU:HD12	1.56	0.69
1:B:244:SER:O	1:B:245:THR:CB	2.41	0.69
1:C:75:VAL:C	1:C:75:VAL:CB	2.59	0.69
1:A:289:THR:O	1:A:290:LEU:CB	2.35	0.69
1:C:327:ALA:HB3	1:C:331:GLN:NE2	2.07	0.69
1:C:278:CYS:CA	1:C:333:VAL:O	2.41	0.69
1:B:155:ASP:CB	1:B:172:ILE:HD11	2.23	0.69
1:B:290:LEU:HD12	1:B:290:LEU:O	1.93	0.69
1:B:112:GLU:CG	1:B:329:ARG:HH22	2.05	0.69
1:C:80:ASP:HA	1:C:241:ARG:HH22	0.70	0.69
1:C:338:THR:OG1	1:C:339:GLU:CB	2.37	0.69
1:C:200:GLY:CA	1:C:265:TRP:CA	2.70	0.69
1:C:289:THR:O	1:C:290:LEU:CB	2.35	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:VAL:C	1:B:334:LYS:HD3	2.12	0.69
1:A:290:LEU:O	1:A:290:LEU:HD12	1.93	0.69
1:C:122:GLU:O	1:C:122:GLU:HG2	1.93	0.69
1:B:169:LEU:HD22	1:B:170:TYR:HD1	1.58	0.69
1:B:173:GLU:HG3	1:B:174:GLY:N	2.08	0.69
1:B:338:THR:OG1	1:B:339:GLU:CB	2.37	0.69
1:C:143:PRO:O	1:C:146:THR:HG22	1.93	0.68
1:C:154:PHE:HD1	1:C:155:ASP:H	0.75	0.68
1:C:155:ASP:CB	1:C:172:ILE:HD11	2.23	0.68
1:C:159:ALA:C	1:C:328:GLU:OE1	2.31	0.68
1:A:154:PHE:CE1	1:A:155:ASP:O	2.41	0.68
1:C:151:ALA:CA	1:C:177:SER:HB2	2.17	0.68
1:B:327:ALA:HB3	1:B:331:GLN:NE2	2.08	0.68
1:A:258:ASP:CG	1:A:259:GLY:H	1.95	0.68
1:A:173:GLU:HG3	1:A:174:GLY:N	2.08	0.68
1:B:170:TYR:CZ	1:B:217:TYR:OH	2.45	0.68
1:A:122:GLU:HG2	1:A:122:GLU:O	1.92	0.68
1:C:170:TYR:OH	1:C:217:TYR:OH	2.11	0.68
1:B:124:ALA:O	1:B:243:GLY:HA2	1.93	0.68
1:C:251:GLY:O	1:C:346:TRP:CH2	2.47	0.68
1:A:124:ALA:O	1:A:243:GLY:HA2	1.93	0.68
1:A:170:TYR:CZ	1:A:217:TYR:OH	2.45	0.68
1:C:127:GLU:O	1:C:128:LYS:CB	2.41	0.68
1:C:154:PHE:CD1	1:C:154:PHE:C	2.62	0.68
1:A:251:GLY:O	1:A:346:TRP:CH2	2.47	0.68
1:A:230:VAL:HG12	1:A:231:ARG:N	2.09	0.68
1:C:230:VAL:HG12	1:C:231:ARG:N	2.09	0.68
1:B:258:ASP:CG	1:B:259:GLY:H	1.95	0.68
1:C:83:THR:O	1:C:84:ARG:HG2	1.94	0.68
1:B:313:GLU:HG3	1:B:318:SER:HB3	1.69	0.68
1:A:278:CYS:CA	1:A:333:VAL:O	2.41	0.68
1:A:254:ALA:N	1:A:257:LYS:O	2.27	0.68
1:C:149:LYS:HD3	1:C:217:TYR:CZ	2.29	0.68
1:C:159:ALA:HB3	1:C:328:GLU:CD	2.11	0.68
1:C:124:ALA:O	1:C:243:GLY:HA2	1.93	0.68
1:B:143:PRO:O	1:B:146:THR:HG22	1.92	0.68
1:C:295:ALA:H	1:C:316:ALA:HA	0.69	0.68
1:B:230:VAL:HG12	1:B:231:ARG:N	2.09	0.68
1:B:251:GLY:O	1:B:346:TRP:CH2	2.47	0.68
1:A:261:ARG:HG3	1:A:261:ARG:O	1.94	0.68
1:A:127:GLU:O	1:A:128:LYS:CB	2.42	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:LEU:O	1:C:290:LEU:HD12	1.93	0.67
1:B:251:GLY:O	1:B:346:TRP:CZ2	2.48	0.67
1:A:333:VAL:C	1:A:334:LYS:HD3	2.12	0.67
1:A:169:LEU:HD22	1:A:170:TYR:HD1	1.58	0.67
1:C:95:LYS:HZ2	1:C:221:ALA:CA	2.03	0.67
1:B:127:GLU:O	1:B:128:LYS:CB	2.42	0.67
1:B:289:THR:C	1:B:290:LEU:HG	2.14	0.67
1:A:269:LYS:HE2	1:A:270:GLY:O	1.94	0.67
1:C:169:LEU:HD22	1:C:170:TYR:HD1	1.58	0.67
1:C:258:ASP:CG	1:C:259:GLY:H	1.95	0.67
1:C:251:GLY:O	1:C:346:TRP:CZ2	2.47	0.67
1:A:289:THR:C	1:A:290:LEU:HG	2.14	0.67
1:B:340:GLU:O	1:B:342:PRO:CD	2.43	0.67
1:B:104:THR:O	1:B:105:THR:C	2.33	0.67
1:B:107:VAL:HB	1:B:329:ARG:HH12	1.58	0.67
1:B:253:PHE:CE2	1:B:346:TRP:CZ3	2.83	0.67
1:B:278:CYS:CA	1:B:333:VAL:O	2.41	0.67
1:C:340:GLU:O	1:C:342:PRO:CD	2.43	0.67
1:A:83:THR:O	1:A:84:ARG:HG2	1.94	0.67
1:C:104:THR:O	1:C:105:THR:C	2.33	0.67
1:B:149:LYS:HD3	1:B:217:TYR:CZ	2.29	0.67
1:B:286:PHE:CA	1:B:351:ILE:HG21	2.25	0.67
1:A:327:ALA:HB3	1:A:331:GLN:NE2	2.08	0.67
1:A:326:VAL:HG13	1:A:331:GLN:HG3	1.74	0.67
1:A:143:PRO:O	1:A:146:THR:HG22	1.93	0.67
1:C:135:ARG:HG3	1:C:233:GLU:CB	2.23	0.67
1:C:269:LYS:HE2	1:C:270:GLY:O	1.94	0.67
1:C:95:LYS:O	1:C:96:ASN:HB2	1.95	0.67
1:A:340:GLU:O	1:A:342:PRO:CD	2.43	0.67
1:B:254:ALA:N	1:B:257:LYS:O	2.27	0.67
1:A:96:ASN:ND2	1:A:102:LYS:HD3	2.10	0.67
1:A:126:TYR:O	1:A:242:THR:HG21	1.95	0.67
1:C:163:PRO:HA	1:C:164:ASN:ND2	2.10	0.67
1:B:269:LYS:HE2	1:B:270:GLY:O	1.94	0.67
1:B:83:THR:O	1:B:84:ARG:HG2	1.94	0.67
1:A:149:LYS:HD3	1:A:217:TYR:CZ	2.29	0.66
1:C:185:ILE:HD13	1:C:186:LEU:H	1.53	0.66
1:C:253:PHE:CE2	1:C:346:TRP:CZ3	2.83	0.66
1:A:121:LYS:HD3	1:A:350:ARG:HH22	1.61	0.66
1:A:104:THR:O	1:A:105:THR:C	2.33	0.66
1:A:136:PHE:HE1	1:A:232:VAL:HG22	1.59	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:PHE:CE2	1:A:346:TRP:CZ3	2.83	0.66
1:A:136:PHE:CE1	1:A:212:LEU:HD22	2.31	0.66
1:B:96:ASN:ND2	1:B:102:LYS:HD3	2.10	0.66
1:C:254:ALA:N	1:C:257:LYS:O	2.27	0.66
1:B:109:ASN:HB2	1:B:208:ASP:HB3	1.77	0.66
1:B:136:PHE:CE1	1:B:212:LEU:HD22	2.31	0.66
1:B:290:LEU:HD22	1:B:346:TRP:CB	2.20	0.66
1:A:300:LEU:CG	1:A:308:PHE:CZ	2.78	0.66
1:C:126:TYR:O	1:C:242:THR:HG21	1.95	0.66
1:C:130:ARG:HD2	1:C:237:GLN:HB3	1.64	0.66
1:C:170:TYR:CZ	1:C:217:TYR:OH	2.45	0.66
1:B:116:PHE:O	1:B:120:ILE:HG22	1.89	0.66
1:A:268:THR:O	1:A:268:THR:HG23	1.96	0.66
1:C:64:LEU:HD12	1:C:65:ALA:H	1.60	0.66
1:C:113:PRO:C	1:C:115:THR:N	2.43	0.66
1:C:199:ASP:HA	1:C:265:TRP:NE1	2.09	0.66
1:C:136:PHE:CE1	1:C:212:LEU:HD22	2.31	0.66
1:C:286:PHE:CA	1:C:351:ILE:HG21	2.25	0.66
1:C:308:PHE:HE2	1:C:310:VAL:CG2	1.92	0.66
1:B:163:PRO:HA	1:B:164:ASN:ND2	2.10	0.66
1:C:261:ARG:O	1:C:261:ARG:HG3	1.94	0.66
1:A:109:ASN:HB2	1:A:208:ASP:HB3	1.77	0.66
1:C:289:THR:C	1:C:290:LEU:HG	2.14	0.66
1:B:261:ARG:HG3	1:B:261:ARG:O	1.94	0.66
1:B:236:VAL:HG12	1:B:238:LEU:CD1	2.26	0.66
1:B:124:ALA:CB	1:B:245:THR:CG2	2.74	0.66
1:A:326:VAL:HG13	1:A:327:ALA:H	1.54	0.66
1:A:297:VAL:CB	1:A:336:VAL:O	2.36	0.66
1:A:116:PHE:O	1:A:120:ILE:HG22	1.90	0.66
1:A:124:ALA:CB	1:A:245:THR:CG2	2.74	0.66
1:C:236:VAL:HG12	1:C:238:LEU:CD1	2.26	0.66
1:C:268:THR:HG23	1:C:268:THR:O	1.96	0.66
1:B:126:TYR:O	1:B:242:THR:HG21	1.95	0.66
1:A:251:GLY:O	1:A:346:TRP:CZ2	2.47	0.66
1:A:95:LYS:O	1:A:96:ASN:HB2	1.95	0.65
1:C:124:ALA:CB	1:C:245:THR:CG2	2.74	0.65
1:A:249:GLN:HB2	1:A:265:TRP:CZ3	2.30	0.65
1:B:312:GLY:HA3	1:B:320:GLN:HG2	1.78	0.65
1:C:297:VAL:CB	1:C:336:VAL:O	2.36	0.65
1:A:163:PRO:HA	1:A:164:ASN:ND2	2.10	0.65
1:C:68:GLU:CG	1:C:137:ARG:NH2	2.59	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:ALA:H	1:B:316:ALA:HA	0.69	0.65
1:B:82:ILE:O	1:B:83:THR:N	2.29	0.65
1:C:326:VAL:HG12	1:C:327:ALA:CA	2.27	0.65
1:A:286:PHE:CA	1:A:351:ILE:HG21	2.25	0.65
1:C:118:GLN:O	1:C:119:LEU:HB2	1.97	0.65
1:C:138:TYR:HH	1:C:227:LEU:HB3	1.61	0.65
1:B:113:PRO:C	1:B:115:THR:N	2.43	0.65
1:B:119:LEU:CD2	1:B:234:TYR:HE2	2.10	0.65
1:A:300:LEU:C	1:A:308:PHE:HZ	2.00	0.65
1:B:249:GLN:HB2	1:B:265:TRP:CZ3	2.31	0.65
1:C:66:TYR:OH	1:C:183:GLY:HA3	1.97	0.65
1:C:120:ILE:HD12	1:C:351:ILE:C	2.17	0.65
1:B:149:LYS:NZ	1:B:170:TYR:CE1	2.52	0.65
1:B:130:ARG:NH1	1:B:237:GLN:HA	2.10	0.65
1:A:121:LYS:NZ	1:A:350:ARG:NH1	2.44	0.65
1:A:205:LYS:HD2	1:A:205:LYS:N	2.12	0.65
1:B:205:LYS:HD2	1:B:205:LYS:N	2.12	0.65
1:A:236:VAL:HG12	1:A:238:LEU:CD1	2.26	0.65
1:C:306:SER:O	1:C:307:ASP:O	2.14	0.65
1:A:119:LEU:CD2	1:A:234:TYR:HE2	2.10	0.65
1:A:130:ARG:HD2	1:A:237:GLN:CG	2.27	0.65
1:C:200:GLY:HA2	1:C:265:TRP:CA	2.26	0.65
1:C:96:ASN:ND2	1:C:102:LYS:HD3	2.10	0.65
1:B:268:THR:HG23	1:B:268:THR:O	1.96	0.65
1:C:309:SER:O	1:C:321:TRP:O	2.15	0.65
1:C:109:ASN:HB2	1:C:208:ASP:HB3	1.77	0.65
1:C:153:ALA:HA	1:C:186:LEU:HD11	1.78	0.65
1:B:300:LEU:CG	1:B:308:PHE:CZ	2.78	0.65
1:B:309:SER:O	1:B:321:TRP:O	2.15	0.65
1:B:296:PRO:HG3	1:B:337:THR:CB	2.27	0.65
1:A:312:GLY:HA3	1:A:320:GLN:HG2	1.78	0.65
1:C:207:VAL:HG13	1:C:208:ASP:CG	2.18	0.64
1:C:300:LEU:C	1:C:308:PHE:HZ	2.00	0.64
1:B:196:PHE:O	1:B:207:VAL:HG23	1.97	0.64
1:A:326:VAL:HG12	1:A:327:ALA:CA	2.27	0.64
1:B:306:SER:O	1:B:307:ASP:O	2.14	0.64
1:A:306:SER:O	1:A:307:ASP:O	2.14	0.64
1:C:166:LEU:O	1:C:167:ALA:C	2.36	0.64
1:C:300:LEU:CG	1:C:308:PHE:CZ	2.78	0.64
1:C:306:SER:HB3	1:C:325:LYS:CB	2.27	0.64
1:C:125:GLN:C	1:C:242:THR:CG2	2.66	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:GLU:OE2	1:C:139:SER:OG	2.14	0.64
1:B:95:LYS:O	1:B:96:ASN:HB2	1.95	0.64
1:A:253:PHE:CD2	1:A:346:TRP:CZ3	2.85	0.64
1:A:274:TRP:NE1	1:A:340:GLU:OE1	2.31	0.64
1:A:118:GLN:O	1:A:119:LEU:HB2	1.97	0.64
1:A:125:GLN:C	1:A:242:THR:CG2	2.66	0.64
1:B:118:GLN:O	1:B:119:LEU:HB2	1.96	0.64
1:B:125:GLN:C	1:B:242:THR:CG2	2.66	0.64
1:B:166:LEU:O	1:B:167:ALA:C	2.35	0.64
1:B:153:ALA:HA	1:B:186:LEU:HD11	1.78	0.64
1:B:253:PHE:CD2	1:B:346:TRP:CZ3	2.85	0.64
1:B:297:VAL:CB	1:B:336:VAL:O	2.36	0.64
1:A:153:ALA:HA	1:A:186:LEU:HD11	1.78	0.64
1:C:196:PHE:O	1:C:207:VAL:HG23	1.97	0.64
1:B:154:PHE:CD1	1:B:154:PHE:C	2.62	0.64
1:B:172:ILE:O	1:B:173:GLU:C	2.36	0.64
1:B:300:LEU:C	1:B:308:PHE:HZ	2.00	0.64
1:A:196:PHE:O	1:A:207:VAL:HG23	1.97	0.64
1:A:135:ARG:HG3	1:A:233:GLU:CB	2.23	0.64
1:A:166:LEU:O	1:A:167:ALA:C	2.36	0.64
1:A:172:ILE:O	1:A:173:GLU:C	2.36	0.64
1:C:112:GLU:OE2	1:C:283:THR:HG22	1.97	0.64
1:B:136:PHE:HE1	1:B:232:VAL:HG22	1.59	0.64
1:B:309:SER:O	1:B:322:ALA:CB	2.46	0.64
1:A:82:ILE:O	1:A:83:THR:N	2.29	0.64
1:C:154:PHE:CZ	1:C:156:ARG:HA	2.33	0.64
1:C:152:LEU:CD2	1:C:186:LEU:HD13	2.25	0.64
1:C:309:SER:O	1:C:322:ALA:CB	2.46	0.64
1:B:306:SER:HB3	1:B:325:LYS:CB	2.27	0.64
1:A:152:LEU:CD2	1:A:186:LEU:HD13	2.25	0.64
1:C:138:TYR:O	1:C:139:SER:O	2.15	0.64
1:C:172:ILE:O	1:C:173:GLU:C	2.36	0.64
1:C:327:ALA:HB2	1:C:331:GLN:OE1	1.96	0.64
1:C:253:PHE:CD2	1:C:346:TRP:CZ3	2.85	0.64
1:B:207:VAL:HG13	1:B:208:ASP:CG	2.18	0.64
1:C:163:PRO:HG3	1:C:168:SER:HB3	1.80	0.64
1:C:249:GLN:O	1:C:347:GLN:HA	1.98	0.64
1:B:248:ALA:HB3	1:B:249:GLN:CB	2.28	0.64
1:A:138:TYR:O	1:A:139:SER:O	2.15	0.63
1:A:155:ASP:CB	1:A:172:ILE:HD11	2.23	0.63
1:C:61:PRO:HD2	1:C:181:TRP:CZ3	2.33	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:ASP:CA	1:C:265:TRP:NE1	2.61	0.63
1:C:205:LYS:HD2	1:C:205:LYS:N	2.12	0.63
1:C:206:LEU:O	1:C:206:LEU:CD1	2.45	0.63
1:C:249:GLN:HB2	1:C:265:TRP:CZ3	2.30	0.63
1:A:151:ALA:CA	1:A:177:SER:HB2	2.17	0.63
1:C:136:PHE:HE1	1:C:232:VAL:HG22	1.59	0.63
1:C:246:SER:O	1:C:349:LEU:CA	2.42	0.63
1:B:138:TYR:O	1:B:139:SER:O	2.15	0.63
1:B:155:ASP:O	1:B:156:ARG:C	2.36	0.63
1:C:312:GLY:HA3	1:C:320:GLN:HG2	1.78	0.63
1:A:154:PHE:CE1	1:A:156:ARG:N	2.66	0.63
1:B:152:LEU:CD2	1:B:186:LEU:HD13	2.25	0.63
1:A:309:SER:O	1:A:321:TRP:O	2.15	0.63
1:A:306:SER:HB3	1:A:325:LYS:CB	2.27	0.63
1:A:137:ARG:O	1:A:230:VAL:HG22	1.98	0.63
1:C:125:GLN:C	1:C:242:THR:HG22	2.19	0.63
1:B:154:PHE:CE1	1:B:156:ARG:N	2.66	0.63
1:B:156:ARG:O	1:B:209:PHE:C	2.37	0.63
1:A:249:GLN:O	1:A:347:GLN:HA	1.98	0.63
1:B:249:GLN:O	1:B:347:GLN:HA	1.98	0.63
1:A:135:ARG:CB	1:A:186:LEU:O	2.47	0.63
1:A:154:PHE:CZ	1:A:156:ARG:HA	2.33	0.63
1:A:155:ASP:O	1:A:156:ARG:C	2.36	0.63
1:C:83:THR:CG2	1:C:84:ARG:H	2.08	0.63
1:C:86:GLY:N	1:C:234:TYR:O	2.31	0.63
1:B:135:ARG:CB	1:B:186:LEU:O	2.47	0.63
1:B:109:ASN:ND2	1:B:197:VAL:HG23	2.14	0.63
1:B:292:TYR:CB	1:B:318:SER:O	2.47	0.63
1:A:248:ALA:C	1:A:264:SER:HB3	2.19	0.63
1:B:206:LEU:CD1	1:B:206:LEU:O	2.45	0.63
1:A:207:VAL:HG13	1:A:208:ASP:CG	2.18	0.63
1:C:68:GLU:CD	1:C:137:ARG:NH2	2.51	0.63
1:C:207:VAL:CG1	1:C:329:ARG:HE	2.12	0.63
1:B:154:PHE:CZ	1:B:156:ARG:HA	2.33	0.63
1:A:292:TYR:CB	1:A:318:SER:O	2.47	0.63
1:A:309:SER:O	1:A:322:ALA:CB	2.46	0.63
1:A:156:ARG:O	1:A:209:PHE:C	2.37	0.63
1:C:154:PHE:CE1	1:C:156:ARG:N	2.66	0.63
1:C:170:TYR:C	1:C:171:ASN:HD22	2.02	0.63
1:B:137:ARG:O	1:B:230:VAL:HG22	1.98	0.63
1:B:185:ILE:HD13	1:B:186:LEU:H	1.53	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:GLY:N	1:B:234:TYR:O	2.31	0.63
1:C:156:ARG:O	1:C:209:PHE:C	2.37	0.63
1:C:119:LEU:CD2	1:C:234:TYR:HE2	2.10	0.63
1:C:82:ILE:O	1:C:83:THR:N	2.29	0.63
1:B:326:VAL:HG12	1:B:327:ALA:CA	2.27	0.63
1:A:206:LEU:O	1:A:206:LEU:CD1	2.45	0.63
1:A:125:GLN:C	1:A:242:THR:HG22	2.19	0.62
1:C:135:ARG:CB	1:C:186:LEU:O	2.47	0.62
1:B:166:LEU:O	1:B:168:SER:N	2.32	0.62
1:B:274:TRP:NE1	1:B:340:GLU:OE1	2.31	0.62
1:B:296:PRO:HG3	1:B:337:THR:HB	1.81	0.62
1:A:166:LEU:O	1:A:168:SER:N	2.32	0.62
1:A:83:THR:CG2	1:A:84:ARG:H	2.08	0.62
1:A:86:GLY:N	1:A:234:TYR:O	2.31	0.62
1:B:83:THR:HG23	1:B:236:VAL:O	2.00	0.62
1:C:68:GLU:CG	1:C:137:ARG:HH22	2.12	0.62
1:C:155:ASP:O	1:C:156:ARG:C	2.36	0.62
1:C:166:LEU:O	1:C:168:SER:N	2.32	0.62
1:C:137:ARG:O	1:C:230:VAL:HG22	1.98	0.62
1:B:163:PRO:HG3	1:B:168:SER:HB3	1.80	0.62
1:C:296:PRO:HG3	1:C:337:THR:HB	1.81	0.62
1:C:206:LEU:N	1:C:329:ARG:HH12	1.96	0.62
1:C:231:ARG:HG3	1:C:232:VAL:H	1.63	0.62
1:C:130:ARG:NH1	1:C:237:GLN:HA	2.10	0.62
1:C:82:ILE:HG23	1:C:83:THR:N	2.15	0.62
1:B:83:THR:CG2	1:B:84:ARG:H	2.08	0.62
1:C:55:VAL:HG22	1:C:56:THR:H	1.60	0.62
1:A:83:THR:HG23	1:A:236:VAL:O	2.00	0.62
1:C:292:TYR:CB	1:C:318:SER:O	2.47	0.62
1:B:213:ILE:O	1:B:214:MET:HG3	2.00	0.62
1:A:170:TYR:C	1:A:171:ASN:HD22	2.02	0.62
1:B:135:ARG:HG3	1:B:233:GLU:CB	2.23	0.62
1:B:82:ILE:HG23	1:B:83:THR:N	2.15	0.62
1:A:136:PHE:CE2	1:A:212:LEU:HD11	2.35	0.62
1:C:136:PHE:CE2	1:C:212:LEU:HD11	2.35	0.62
1:C:157:ASP:O	1:C:157:ASP:OD1	2.18	0.62
1:A:124:ALA:HB1	1:A:244:SER:O	2.00	0.62
1:C:159:ALA:HB3	1:C:328:GLU:HG3	1.72	0.62
1:C:109:ASN:ND2	1:C:197:VAL:HG23	2.14	0.62
1:B:248:ALA:C	1:B:263:VAL:O	2.38	0.62
1:A:157:ASP:OD1	1:A:157:ASP:O	2.18	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ASN:ND2	1:A:197:VAL:HG23	2.14	0.62
1:A:163:PRO:HG3	1:A:168:SER:HB3	1.80	0.62
1:C:112:GLU:O	1:C:114:GLY:N	2.33	0.62
1:A:248:ALA:HB1	1:A:264:SER:HG	1.55	0.62
1:A:308:PHE:HE2	1:A:310:VAL:CG2	1.92	0.62
1:A:112:GLU:O	1:A:114:GLY:N	2.33	0.62
1:C:186:LEU:HD23	1:C:186:LEU:C	2.20	0.62
1:B:136:PHE:CE2	1:B:212:LEU:HD11	2.35	0.62
1:C:201:ILE:HG21	1:C:265:TRP:C	2.20	0.61
1:C:236:VAL:CG1	1:C:237:GLN:N	2.62	0.61
1:C:124:ALA:HB1	1:C:244:SER:O	2.00	0.61
1:C:83:THR:HG23	1:C:236:VAL:O	2.00	0.61
1:B:112:GLU:O	1:B:114:GLY:N	2.33	0.61
1:A:124:ALA:HB2	1:A:245:THR:HG21	1.82	0.61
1:C:98:ASP:OD1	1:C:99:THR:N	2.33	0.61
1:B:188:VAL:HG23	1:B:188:VAL:O	1.99	0.61
1:B:236:VAL:CG1	1:B:237:GLN:N	2.62	0.61
1:B:237:GLN:C	1:B:238:LEU:HD12	2.21	0.61
1:B:124:ALA:HB2	1:B:245:THR:HG21	1.82	0.61
1:B:300:LEU:C	1:B:308:PHE:CZ	2.74	0.61
1:A:120:ILE:CD1	1:A:329:ARG:HH21	2.13	0.61
1:A:185:ILE:HD13	1:A:186:LEU:H	1.53	0.61
1:B:125:GLN:C	1:B:242:THR:HG22	2.19	0.61
1:B:124:ALA:HB1	1:B:244:SER:O	2.00	0.61
1:B:157:ASP:O	1:B:157:ASP:OD1	2.18	0.61
1:A:130:ARG:NH1	1:A:237:GLN:HA	2.10	0.61
1:A:236:VAL:CG1	1:A:237:GLN:N	2.62	0.61
1:A:82:ILE:HG23	1:A:83:THR:N	2.15	0.61
1:A:83:THR:HG23	1:A:130:ARG:NH1	2.15	0.61
1:C:111:SER:N	1:C:350:ARG:NH2	2.45	0.61
1:B:130:ARG:HB3	1:B:237:GLN:H	1.66	0.61
1:A:136:PHE:CE2	1:A:212:LEU:CD1	2.84	0.61
1:A:237:GLN:C	1:A:238:LEU:HD12	2.21	0.61
1:B:169:LEU:HD22	1:B:170:TYR:CD1	2.36	0.61
1:B:186:LEU:C	1:B:186:LEU:HD23	2.20	0.61
1:B:134:LEU:HD23	1:B:188:VAL:CG2	2.31	0.61
1:A:296:PRO:HG3	1:A:337:THR:HB	1.81	0.61
1:A:130:ARG:HB3	1:A:237:GLN:H	1.66	0.61
1:A:144:SER:C	1:A:146:THR:N	2.54	0.61
1:C:188:VAL:O	1:C:188:VAL:HG23	1.99	0.61
1:C:200:GLY:C	1:C:282:GLY:HA2	2.16	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:LEU:C	1:C:308:PHE:CZ	2.74	0.61
1:A:300:LEU:C	1:A:308:PHE:CZ	2.74	0.61
1:C:213:ILE:O	1:C:214:MET:HG3	2.00	0.61
1:A:188:VAL:HG23	1:A:188:VAL:O	1.99	0.61
1:C:136:PHE:CE2	1:C:212:LEU:CD1	2.84	0.61
1:C:237:GLN:C	1:C:238:LEU:HD12	2.21	0.61
1:B:144:SER:C	1:B:146:THR:N	2.54	0.61
1:C:85:SER:C	1:C:234:TYR:CE1	2.74	0.61
1:B:156:ARG:NH1	1:B:173:GLU:OE1	2.34	0.61
1:B:83:THR:HG23	1:B:130:ARG:NH1	2.15	0.61
1:C:130:ARG:HD2	1:C:237:GLN:CG	2.27	0.61
1:C:264:SER:C	1:C:265:TRP:HA	2.21	0.61
1:C:120:ILE:HD12	1:C:351:ILE:O	2.01	0.61
1:B:170:TYR:C	1:B:171:ASN:HD22	2.02	0.61
1:B:311:LEU:N	1:B:311:LEU:HD12	2.16	0.61
1:A:291:PHE:HB2	1:A:346:TRP:CB	2.29	0.61
1:A:213:ILE:O	1:A:214:MET:HG3	2.00	0.61
1:A:198:ALA:HB1	1:A:200:GLY:C	2.14	0.61
1:A:85:SER:C	1:A:234:TYR:CE1	2.74	0.61
1:C:286:PHE:CD2	1:C:350:ARG:HA	2.35	0.61
1:A:290:LEU:CD1	1:A:290:LEU:C	2.69	0.61
1:A:311:LEU:HD12	1:A:311:LEU:N	2.16	0.61
1:C:274:TRP:NE1	1:C:340:GLU:OE1	2.31	0.61
1:C:95:LYS:NZ	1:C:221:ALA:CB	2.64	0.60
1:B:136:PHE:CE2	1:B:212:LEU:CD1	2.84	0.60
1:B:290:LEU:C	1:B:290:LEU:CD1	2.69	0.60
1:A:286:PHE:CD2	1:A:350:ARG:HA	2.35	0.60
1:C:306:SER:O	1:C:307:ASP:C	2.40	0.60
1:A:105:THR:HG1	1:A:211:LYS:HD3	0.78	0.60
1:B:231:ARG:HG3	1:B:232:VAL:H	1.63	0.60
1:B:314:ALA:O	1:B:315:ALA:HB2	2.01	0.60
1:B:85:SER:C	1:B:234:TYR:CE1	2.74	0.60
1:A:338:THR:HG1	1:A:339:GLU:HB2	1.64	0.60
1:B:306:SER:O	1:B:307:ASP:C	2.40	0.60
1:C:124:ALA:HB2	1:C:245:THR:HG21	1.82	0.60
1:C:105:THR:HG1	1:C:211:LYS:HD3	0.79	0.60
1:C:291:PHE:C	1:C:292:TYR:CA	2.67	0.60
1:C:311:LEU:N	1:C:311:LEU:HD12	2.16	0.60
1:C:109:ASN:ND2	1:C:350:ARG:HH21	1.99	0.60
1:C:314:ALA:O	1:C:315:ALA:HB2	2.01	0.60
1:B:129:TYR:CB	1:B:237:GLN:O	2.49	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:TYR:CB	1:A:237:GLN:O	2.49	0.60
1:A:217:TYR:CD1	1:A:217:TYR:N	2.69	0.60
1:C:156:ARG:NH1	1:C:173:GLU:OE1	2.34	0.60
1:C:201:ILE:CG2	1:C:265:TRP:CA	2.80	0.60
1:C:290:LEU:CD1	1:C:290:LEU:C	2.69	0.60
1:B:136:PHE:CD2	1:B:212:LEU:HD21	2.36	0.60
1:B:130:ARG:CB	1:B:237:GLN:CB	2.68	0.60
1:B:286:PHE:CD2	1:B:350:ARG:HA	2.35	0.60
1:A:306:SER:O	1:A:307:ASP:C	2.40	0.60
1:A:156:ARG:NH1	1:A:173:GLU:OE1	2.34	0.60
1:A:186:LEU:HD23	1:A:186:LEU:C	2.20	0.60
1:A:120:ILE:O	1:A:120:ILE:CG1	2.50	0.60
1:A:134:LEU:HD23	1:A:188:VAL:CG2	2.31	0.60
1:C:200:GLY:HA3	1:C:201:ILE:HG22	1.83	0.60
1:B:130:ARG:HD2	1:B:237:GLN:CG	2.27	0.60
1:B:327:ALA:HB2	1:B:331:GLN:OE1	1.96	0.60
1:A:269:LYS:CG	1:A:270:GLY:N	2.58	0.60
1:A:136:PHE:CD2	1:A:212:LEU:HD21	2.37	0.60
1:C:169:LEU:HD22	1:C:170:TYR:CD1	2.36	0.60
1:C:134:LEU:HD23	1:C:188:VAL:CG2	2.31	0.60
1:C:130:ARG:CB	1:C:237:GLN:CB	2.68	0.60
1:B:120:ILE:O	1:B:120:ILE:CG1	2.50	0.60
1:B:179:VAL:HG21	1:B:181:TRP:CD1	2.36	0.60
1:B:217:TYR:CD1	1:B:217:TYR:N	2.69	0.60
1:B:95:LYS:NZ	1:B:221:ALA:CB	2.64	0.60
1:A:179:VAL:HG21	1:A:181:TRP:CD1	2.37	0.60
1:C:83:THR:HG23	1:C:130:ARG:NH1	2.15	0.60
1:C:144:SER:C	1:C:146:THR:N	2.54	0.60
1:B:149:LYS:CD	1:B:177:SER:OG	2.50	0.60
1:A:342:PRO:C	1:A:343:LYS:HD3	2.23	0.60
1:A:169:LEU:HD22	1:A:170:TYR:CD1	2.36	0.60
1:A:95:LYS:NZ	1:A:221:ALA:CB	2.64	0.60
1:C:136:PHE:CD2	1:C:212:LEU:HD21	2.37	0.59
1:B:98:ASP:OD1	1:B:99:THR:N	2.33	0.59
1:A:314:ALA:O	1:A:315:ALA:HB2	2.01	0.59
1:C:138:TYR:HD2	1:C:184:PHE:CE1	2.16	0.59
1:B:163:PRO:CB	1:B:164:ASN:HD22	2.15	0.59
1:C:163:PRO:HB2	1:C:165:ASP:H	1.67	0.59
1:C:129:TYR:CB	1:C:237:GLN:O	2.49	0.59
1:C:277:ASP:HA	1:C:334:LYS:CE	2.32	0.59
1:A:277:ASP:HA	1:A:334:LYS:CE	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:THR:CA	1:C:218:GLY:O	2.50	0.59
1:A:163:PRO:CB	1:A:164:ASN:HD22	2.15	0.59
1:A:130:ARG:CB	1:A:237:GLN:CB	2.68	0.59
1:A:327:ALA:HB2	1:A:331:GLN:OE1	1.96	0.59
1:A:97:THR:CA	1:A:218:GLY:O	2.50	0.59
1:A:163:PRO:HB2	1:A:165:ASP:H	1.66	0.59
1:C:203:ASP:O	1:C:205:LYS:N	2.35	0.59
1:C:206:LEU:N	1:C:329:ARG:NH1	2.48	0.59
1:B:163:PRO:HB2	1:B:165:ASP:H	1.67	0.59
1:A:203:ASP:O	1:A:205:LYS:N	2.34	0.59
1:A:231:ARG:HG3	1:A:232:VAL:H	1.63	0.59
1:A:248:ALA:N	1:A:264:SER:O	2.36	0.59
1:B:97:THR:CA	1:B:218:GLY:O	2.50	0.59
1:A:307:ASP:O	1:A:323:GLY:O	2.21	0.59
1:A:138:TYR:HE2	1:A:180:PRO:HA	1.68	0.59
1:A:207:VAL:HG13	1:A:208:ASP:OD2	2.03	0.59
1:A:98:ASP:OD1	1:A:99:THR:N	2.33	0.59
1:C:230:VAL:HG12	1:C:231:ARG:H	1.68	0.59
1:B:277:ASP:HA	1:B:334:LYS:HZ2	1.68	0.59
1:B:336:VAL:HG13	1:B:336:VAL:O	2.03	0.59
1:C:120:ILE:CG1	1:C:120:ILE:O	2.50	0.59
1:C:246:SER:O	1:C:349:LEU:C	2.40	0.59
1:B:169:LEU:CD2	1:B:169:LEU:C	2.70	0.59
1:B:207:VAL:HG13	1:B:208:ASP:OD2	2.03	0.59
1:B:300:LEU:HB3	1:B:310:VAL:HG21	1.84	0.59
1:A:200:GLY:HA3	1:A:201:ILE:HG22	1.84	0.59
1:C:169:LEU:CD2	1:C:169:LEU:C	2.70	0.59
1:B:300:LEU:HD11	1:B:333:VAL:HG11	1.85	0.59
1:B:307:ASP:O	1:B:323:GLY:O	2.21	0.59
1:C:163:PRO:CB	1:C:164:ASN:HD22	2.15	0.59
1:B:291:PHE:C	1:B:292:TYR:CA	2.67	0.58
1:A:265:TRP:CH2	1:A:348:ALA:O	2.52	0.58
1:C:307:ASP:O	1:C:323:GLY:O	2.21	0.58
1:B:179:VAL:HG13	1:B:181:TRP:CD1	2.38	0.58
1:B:200:GLY:HA3	1:B:201:ILE:HG22	1.83	0.58
1:B:113:PRO:CB	1:B:283:THR:O	2.51	0.58
1:B:203:ASP:O	1:B:205:LYS:N	2.34	0.58
1:C:130:ARG:HB3	1:C:237:GLN:H	1.66	0.58
1:A:179:VAL:HG13	1:A:181:TRP:CD1	2.38	0.58
1:C:202:SER:HA	1:C:281:LEU:HG	1.85	0.58
1:B:264:SER:C	1:B:265:TRP:HA	2.22	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:VAL:O	1:A:336:VAL:HG13	2.03	0.58
1:A:179:VAL:CG1	1:A:181:TRP:HD1	2.14	0.58
1:A:230:VAL:HG12	1:A:231:ARG:H	1.68	0.58
1:C:95:LYS:HZ1	1:C:221:ALA:CA	2.14	0.58
1:B:172:ILE:HG23	1:B:172:ILE:O	2.03	0.58
1:B:230:VAL:HG12	1:B:231:ARG:H	1.68	0.58
1:A:300:LEU:HB3	1:A:310:VAL:HG21	1.84	0.58
1:C:213:ILE:C	1:C:214:MET:HG3	2.24	0.58
1:A:169:LEU:C	1:A:169:LEU:CD2	2.70	0.58
1:A:172:ILE:O	1:A:172:ILE:HG23	2.03	0.58
1:C:112:GLU:O	1:C:113:PRO:C	2.41	0.58
1:C:179:VAL:HG21	1:C:181:TRP:CD1	2.36	0.58
1:C:113:PRO:HD2	1:C:285:ASN:N	2.19	0.58
1:C:291:PHE:HB2	1:C:346:TRP:CB	2.29	0.58
1:C:300:LEU:HB3	1:C:310:VAL:HG21	1.84	0.58
1:B:138:TYR:HE2	1:B:180:PRO:HA	1.68	0.58
1:B:227:LEU:H	1:B:227:LEU:CD1	2.17	0.58
1:B:277:ASP:HA	1:B:334:LYS:CE	2.32	0.58
1:B:315:ALA:HA	1:B:318:SER:HB2	1.84	0.58
1:C:172:ILE:HG23	1:C:172:ILE:O	2.03	0.58
1:C:207:VAL:HG13	1:C:208:ASP:OD2	2.03	0.58
1:C:217:TYR:CD1	1:C:217:TYR:N	2.69	0.58
1:C:296:PRO:HG3	1:C:337:THR:CB	2.27	0.58
1:B:342:PRO:C	1:B:343:LYS:HD3	2.23	0.58
1:C:138:TYR:HE2	1:C:180:PRO:HA	1.68	0.58
1:C:185:ILE:HD12	1:C:186:LEU:H	0.65	0.58
1:A:296:PRO:HG3	1:A:337:THR:CB	2.27	0.58
1:C:197:VAL:HG21	1:C:350:ARG:NH2	1.95	0.58
1:C:315:ALA:HA	1:C:318:SER:HB2	1.84	0.58
1:B:179:VAL:CG1	1:B:181:TRP:HD1	2.14	0.58
1:B:105:THR:HG1	1:B:211:LYS:HD3	0.75	0.58
1:B:83:THR:HA	1:B:236:VAL:O	2.04	0.58
1:C:342:PRO:C	1:C:343:LYS:HD3	2.23	0.58
1:C:113:PRO:HD2	1:C:285:ASN:O	2.04	0.57
1:B:112:GLU:O	1:B:113:PRO:C	2.41	0.57
1:B:280:PHE:HD2	1:B:331:GLN:O	1.86	0.57
1:C:340:GLU:OE1	1:C:340:GLU:HA	2.04	0.57
1:A:136:PHE:HB3	1:A:230:VAL:HG11	1.87	0.57
1:C:302:ASN:CB	1:C:333:VAL:HG22	2.34	0.57
1:C:336:VAL:HG13	1:C:336:VAL:O	2.03	0.57
1:A:340:GLU:OE1	1:A:340:GLU:HA	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:THR:HA	1:A:236:VAL:O	2.04	0.57
1:C:163:PRO:C	1:C:164:ASN:ND2	2.44	0.57
1:C:198:ALA:HB1	1:C:200:GLY:C	2.14	0.57
1:B:302:ASN:CB	1:B:333:VAL:HG22	2.34	0.57
1:A:250:ILE:HA	1:A:347:GLN:HA	1.87	0.57
1:C:83:THR:HA	1:C:236:VAL:O	2.03	0.57
1:C:61:PRO:HD2	1:C:181:TRP:HZ3	1.67	0.57
1:B:138:TYR:HD2	1:B:184:PHE:CE1	2.16	0.57
1:B:313:GLU:CG	1:B:318:SER:HB2	2.19	0.57
1:A:138:TYR:HA	1:A:230:VAL:HG22	1.86	0.57
1:C:136:PHE:HB3	1:C:230:VAL:HG11	1.86	0.57
1:B:151:ALA:CA	1:B:177:SER:HB2	2.17	0.57
1:B:238:LEU:CD1	1:B:238:LEU:N	2.67	0.57
1:A:315:ALA:HA	1:A:318:SER:HB2	1.84	0.57
1:C:238:LEU:N	1:C:238:LEU:CD1	2.67	0.57
1:A:313:GLU:HG3	1:A:318:SER:OG	2.01	0.57
1:B:340:GLU:OE1	1:B:340:GLU:HA	2.04	0.57
1:A:95:LYS:HZ2	1:A:221:ALA:CB	2.17	0.57
1:C:197:VAL:CG2	1:C:350:ARG:CZ	2.80	0.57
1:C:280:PHE:HD2	1:C:331:GLN:O	1.86	0.57
1:B:291:PHE:HB2	1:B:346:TRP:CB	2.29	0.57
1:C:78:ALA:O	1:C:80:ASP:CA	2.52	0.57
1:A:227:LEU:CD1	1:A:227:LEU:H	2.17	0.57
1:C:250:ILE:HA	1:C:347:GLN:HA	1.87	0.57
1:C:197:VAL:HG21	1:C:350:ARG:HH12	1.69	0.57
1:B:136:PHE:HB3	1:B:230:VAL:HG11	1.87	0.57
1:A:258:ASP:CG	1:A:259:GLY:N	2.58	0.57
1:B:124:ALA:CB	1:B:245:THR:HG21	2.35	0.57
1:A:280:PHE:HD2	1:A:331:GLN:O	1.86	0.57
1:A:302:ASN:CB	1:A:333:VAL:HG22	2.34	0.57
1:A:124:ALA:CB	1:A:245:THR:HG21	2.35	0.57
1:A:95:LYS:HZ1	1:A:221:ALA:CA	2.16	0.57
1:C:152:LEU:CD1	1:C:184:PHE:HE2	2.18	0.57
1:B:149:LYS:CE	1:B:151:ALA:HA	2.35	0.57
1:B:302:ASN:HB2	1:B:333:VAL:HG22	1.87	0.57
1:A:149:LYS:CE	1:A:151:ALA:HA	2.35	0.56
1:C:82:ILE:CG2	1:C:238:LEU:HB2	2.32	0.56
1:C:302:ASN:HB2	1:C:333:VAL:HG22	1.87	0.56
1:B:290:LEU:HD12	1:B:290:LEU:C	2.26	0.56
1:A:290:LEU:C	1:A:290:LEU:HD12	2.26	0.56
1:C:154:PHE:CD1	1:C:155:ASP:C	2.78	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:TRP:CH2	1:C:348:ALA:O	2.52	0.56
1:B:152:LEU:HD12	1:B:184:PHE:HE2	1.70	0.56
1:B:86:GLY:N	1:B:234:TYR:CE1	2.74	0.56
1:A:112:GLU:O	1:A:113:PRO:C	2.41	0.56
1:A:154:PHE:CD1	1:A:155:ASP:C	2.78	0.56
1:A:138:TYR:HD2	1:A:184:PHE:CE1	2.16	0.56
1:C:138:TYR:HA	1:C:230:VAL:HG22	1.86	0.56
1:C:198:ALA:CA	1:C:200:GLY:O	2.54	0.56
1:B:120:ILE:O	1:B:120:ILE:HG13	2.05	0.56
1:B:285:ASN:HD22	1:B:286:PHE:N	2.03	0.56
1:B:95:LYS:HZ1	1:B:221:ALA:CA	2.16	0.56
1:A:238:LEU:CD1	1:A:238:LEU:N	2.67	0.56
1:B:154:PHE:CD1	1:B:155:ASP:C	2.78	0.56
1:B:300:LEU:HD12	1:B:333:VAL:CG1	2.36	0.56
1:C:77:THR:CG2	1:C:78:ALA:N	2.49	0.56
1:A:264:SER:C	1:A:265:TRP:HA	2.22	0.56
1:A:291:PHE:C	1:A:292:TYR:CA	2.67	0.56
1:B:250:ILE:HA	1:B:347:GLN:HA	1.87	0.56
1:C:285:ASN:HD22	1:C:286:PHE:N	2.04	0.56
1:C:208:ASP:H	1:C:329:ARG:HH21	1.46	0.56
1:B:138:TYR:HA	1:B:230:VAL:HG22	1.86	0.56
1:B:152:LEU:CD1	1:B:184:PHE:HE2	2.18	0.56
1:A:326:VAL:CG1	1:A:327:ALA:O	2.48	0.56
1:A:300:LEU:HD11	1:A:333:VAL:HG11	1.85	0.56
1:A:152:LEU:HD12	1:A:184:PHE:HE2	1.71	0.56
1:C:200:GLY:O	1:C:282:GLY:HA2	2.06	0.56
1:A:213:ILE:C	1:A:214:MET:HG3	2.24	0.56
1:B:95:LYS:HZ2	1:B:221:ALA:CB	2.18	0.56
1:A:145:THR:O	1:A:145:THR:CG2	2.54	0.56
1:A:152:LEU:CD1	1:A:184:PHE:HE2	2.18	0.56
1:A:82:ILE:CG2	1:A:238:LEU:HB2	2.32	0.56
1:C:152:LEU:HD12	1:C:184:PHE:HE2	1.70	0.56
1:A:300:LEU:CA	1:A:308:PHE:HZ	2.19	0.56
1:B:213:ILE:C	1:B:214:MET:HG3	2.24	0.56
1:C:162:PRO:C	1:C:163:PRO:O	2.42	0.56
1:B:162:PRO:C	1:B:163:PRO:O	2.42	0.56
1:B:198:ALA:HB1	1:B:200:GLY:C	2.14	0.56
1:A:302:ASN:HB2	1:A:333:VAL:HG22	1.87	0.56
1:A:120:ILE:O	1:A:120:ILE:HG13	2.05	0.55
1:A:174:GLY:C	1:A:175:CYS:HG	2.06	0.55
1:C:120:ILE:HG13	1:C:120:ILE:O	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:ASP:HA	1:C:334:LYS:NZ	2.21	0.55
1:C:289:THR:HG23	1:C:321:TRP:CZ3	2.41	0.55
1:C:277:ASP:HA	1:C:334:LYS:HZ2	1.71	0.55
1:B:104:THR:O	1:B:105:THR:O	2.24	0.55
1:A:113:PRO:C	1:A:115:THR:N	2.43	0.55
1:A:162:PRO:C	1:A:163:PRO:O	2.42	0.55
1:B:149:LYS:CD	1:B:170:TYR:HH	1.67	0.55
1:B:170:TYR:HE1	1:B:217:TYR:OH	1.86	0.55
1:B:326:VAL:CG1	1:B:327:ALA:O	2.48	0.55
1:A:274:TRP:CD1	1:A:339:GLU:C	2.80	0.55
1:B:145:THR:O	1:B:145:THR:CG2	2.54	0.55
1:C:145:THR:CG2	1:C:145:THR:O	2.54	0.55
1:C:124:ALA:CB	1:C:245:THR:HG21	2.35	0.55
1:C:300:LEU:HD11	1:C:333:VAL:HG11	1.85	0.55
1:C:71:THR:CG2	1:C:87:SER:CB	2.77	0.55
1:B:163:PRO:C	1:B:164:ASN:ND2	2.44	0.55
1:B:82:ILE:CG2	1:B:238:LEU:HB2	2.32	0.55
1:C:149:LYS:CE	1:C:151:ALA:HA	2.35	0.55
1:C:153:ALA:HB1	1:C:174:GLY:HA3	0.62	0.55
1:C:300:LEU:CA	1:C:308:PHE:HZ	2.19	0.55
1:B:277:ASP:HA	1:B:334:LYS:NZ	2.21	0.55
1:A:121:LYS:HZ3	1:A:350:ARG:NH1	2.03	0.55
1:A:116:PHE:HE2	1:A:234:TYR:CE2	2.24	0.55
1:A:170:TYR:HE1	1:A:217:TYR:OH	1.87	0.55
1:C:258:ASP:CG	1:C:259:GLY:N	2.58	0.55
1:A:289:THR:HG23	1:A:321:TRP:CZ3	2.41	0.55
1:B:274:TRP:CD1	1:B:339:GLU:HA	2.42	0.55
1:A:86:GLY:N	1:A:234:TYR:CE1	2.74	0.55
1:C:179:VAL:CG1	1:C:181:TRP:HD1	2.14	0.55
1:B:116:PHE:HE2	1:B:234:TYR:CE2	2.24	0.55
1:B:300:LEU:CA	1:B:308:PHE:HZ	2.19	0.55
1:C:104:THR:O	1:C:105:THR:O	2.24	0.55
1:C:116:PHE:HE2	1:C:234:TYR:CE2	2.24	0.55
1:C:149:LYS:CD	1:C:177:SER:OG	2.50	0.55
1:B:133:SER:HB3	1:B:235:THR:CG2	2.35	0.55
1:A:313:GLU:CG	1:A:318:SER:HB2	2.19	0.55
1:C:274:TRP:CD1	1:C:339:GLU:C	2.80	0.55
1:A:274:TRP:CD1	1:A:339:GLU:HA	2.42	0.55
1:C:227:LEU:H	1:C:227:LEU:CD1	2.17	0.55
1:C:291:PHE:CE1	1:C:335:MET:CE	2.90	0.55
1:C:96:ASN:C	1:C:98:ASP:N	2.55	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:TYR:C	1:B:242:THR:CG2	2.75	0.55
1:B:198:ALA:CA	1:B:200:GLY:O	2.54	0.55
1:C:297:VAL:HB	1:C:336:VAL:CG1	1.98	0.55
1:A:104:THR:O	1:A:105:THR:O	2.24	0.55
1:A:126:TYR:C	1:A:242:THR:CG2	2.75	0.55
1:C:197:VAL:HG22	1:C:198:ALA:H	1.72	0.55
1:C:201:ILE:CG2	1:C:264:SER:OG	2.55	0.55
1:C:300:LEU:CB	1:C:308:PHE:HZ	2.20	0.55
1:C:326:VAL:CG1	1:C:327:ALA:O	2.48	0.55
1:B:300:LEU:CB	1:B:308:PHE:HZ	2.20	0.55
1:A:291:PHE:CE1	1:A:335:MET:CE	2.90	0.55
1:A:300:LEU:HD12	1:A:333:VAL:CG1	2.36	0.55
1:A:154:PHE:CD1	1:A:155:ASP:CA	2.90	0.55
1:A:198:ALA:CA	1:A:200:GLY:O	2.54	0.55
1:C:100:GLU:O	1:C:101:PRO:O	2.25	0.55
1:C:290:LEU:C	1:C:290:LEU:HD12	2.26	0.55
1:B:304:ASP:CG	1:B:332:GLY:H	2.11	0.55
1:B:97:THR:OG1	1:B:97:THR:O	2.25	0.55
1:A:109:ASN:CA	1:A:129:TYR:OH	2.55	0.54
1:A:197:VAL:HG22	1:A:198:ALA:H	1.72	0.54
1:B:291:PHE:CE1	1:B:335:MET:CE	2.90	0.54
1:A:277:ASP:HA	1:A:334:LYS:NZ	2.21	0.54
1:A:163:PRO:C	1:A:164:ASN:ND2	2.44	0.54
1:C:113:PRO:HD2	1:C:285:ASN:H	1.72	0.54
1:B:197:VAL:HG22	1:B:198:ALA:N	2.23	0.54
1:B:350:ARG:O	1:B:351:ILE:CB	2.53	0.54
1:C:274:TRP:CD1	1:C:339:GLU:HA	2.42	0.54
1:B:341:GLN:O	1:B:343:LYS:HG2	2.07	0.54
1:A:197:VAL:HG22	1:A:198:ALA:N	2.23	0.54
1:C:191:ASP:OD1	1:C:209:PHE:CZ	2.61	0.54
1:C:156:ARG:O	1:C:209:PHE:O	2.26	0.54
1:C:113:PRO:HG3	1:C:351:ILE:HG13	1.90	0.54
1:A:300:LEU:CB	1:A:308:PHE:HZ	2.20	0.54
1:A:130:ARG:O	1:A:131:PHE:HB2	2.08	0.54
1:A:191:ASP:OD1	1:A:209:PHE:CZ	2.61	0.54
1:C:179:VAL:CG1	1:C:181:TRP:NE1	2.54	0.54
1:C:197:VAL:HG22	1:C:198:ALA:N	2.23	0.54
1:C:199:ASP:N	1:C:199:ASP:OD1	2.40	0.54
1:C:304:ASP:CG	1:C:332:GLY:H	2.11	0.54
1:C:86:GLY:N	1:C:234:TYR:CE1	2.74	0.54
1:B:191:ASP:OD1	1:B:209:PHE:CZ	2.61	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:TRP:CD1	1:B:339:GLU:C	2.80	0.54
1:C:306:SER:HB2	1:C:325:LYS:H	1.72	0.54
1:A:120:ILE:HD13	1:A:329:ARG:HH21	1.71	0.54
1:A:339:GLU:O	1:A:340:GLU:HA	2.08	0.54
1:A:149:LYS:CD	1:A:177:SER:OG	2.50	0.54
1:C:133:SER:HB3	1:C:235:THR:CG2	2.35	0.54
1:C:174:GLY:C	1:C:175:CYS:HG	2.04	0.54
1:B:258:ASP:CG	1:B:259:GLY:N	2.58	0.54
1:B:300:LEU:O	1:B:308:PHE:CZ	2.61	0.54
1:A:271:THR:CG2	1:A:275:GLU:OE2	2.56	0.54
1:A:306:SER:HB2	1:A:325:LYS:H	1.72	0.54
1:C:95:LYS:NZ	1:C:221:ALA:HB1	2.22	0.54
1:C:300:LEU:HD12	1:C:333:VAL:CG1	2.36	0.54
1:B:130:ARG:O	1:B:131:PHE:HB2	2.08	0.54
1:B:289:THR:HG23	1:B:321:TRP:CZ3	2.41	0.54
1:A:300:LEU:O	1:A:308:PHE:CZ	2.61	0.54
1:A:304:ASP:CG	1:A:332:GLY:H	2.11	0.54
1:B:306:SER:HB2	1:B:325:LYS:H	1.72	0.54
1:C:173:GLU:HG3	1:C:174:GLY:H	1.73	0.54
1:C:126:TYR:C	1:C:242:THR:CG2	2.75	0.54
1:B:153:ALA:HB1	1:B:174:GLY:HA3	0.62	0.54
1:B:248:ALA:O	1:B:263:VAL:O	2.25	0.54
1:C:213:ILE:O	1:C:214:MET:CG	2.56	0.54
1:A:156:ARG:O	1:A:209:PHE:O	2.26	0.54
1:A:153:ALA:HB1	1:A:174:GLY:HA3	0.62	0.54
1:C:85:SER:C	1:C:234:TYR:CD1	2.82	0.54
1:B:136:PHE:CZ	1:B:212:LEU:CD2	2.91	0.54
1:A:285:ASN:HD22	1:A:286:PHE:N	2.04	0.54
1:C:339:GLU:O	1:C:340:GLU:HA	2.08	0.54
1:A:100:GLU:O	1:A:101:PRO:O	2.25	0.53
1:C:231:ARG:CG	1:C:232:VAL:N	2.61	0.53
1:C:326:VAL:CG1	1:C:327:ALA:N	2.19	0.53
1:B:197:VAL:HG22	1:B:198:ALA:H	1.72	0.53
1:A:179:VAL:HG13	1:A:182:THR:HG22	1.90	0.53
1:C:313:GLU:HB2	1:C:314:ALA:C	2.29	0.53
1:B:213:ILE:O	1:B:214:MET:CG	2.56	0.53
1:A:213:ILE:O	1:A:214:MET:CG	2.56	0.53
1:A:136:PHE:CZ	1:A:212:LEU:CD2	2.91	0.53
1:B:154:PHE:CD1	1:B:155:ASP:CA	2.90	0.53
1:B:179:VAL:HG22	1:B:180:PRO:N	2.23	0.53
1:A:276:HIS:CG	1:A:277:ASP:N	2.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:GLN:O	1:C:343:LYS:HG2	2.08	0.53
1:C:244:SER:O	1:C:245:THR:HB	2.08	0.53
1:C:276:HIS:CG	1:C:277:ASP:N	2.74	0.53
1:B:95:LYS:NZ	1:B:221:ALA:HB1	2.22	0.53
1:A:248:ALA:CB	1:A:265:TRP:N	2.70	0.53
1:B:265:TRP:CH2	1:B:348:ALA:O	2.52	0.53
1:A:341:GLN:O	1:A:343:LYS:HG2	2.07	0.53
1:C:109:ASN:CA	1:C:129:TYR:OH	2.55	0.53
1:C:130:ARG:O	1:C:131:PHE:HB2	2.08	0.53
1:C:170:TYR:HE1	1:C:217:TYR:OH	1.87	0.53
1:C:95:LYS:HZ2	1:C:221:ALA:CB	2.21	0.53
1:C:269:LYS:HB3	1:C:277:ASP:OD2	2.09	0.53
1:B:109:ASN:CA	1:B:129:TYR:OH	2.55	0.53
1:B:156:ARG:O	1:B:209:PHE:O	2.26	0.53
1:B:293:GLU:O	1:B:317:GLY:HA2	2.09	0.53
1:C:142:SER:HB3	1:C:227:LEU:O	2.09	0.53
1:C:300:LEU:O	1:C:308:PHE:CZ	2.61	0.53
1:C:90:ILE:CG2	1:C:90:ILE:O	2.54	0.53
1:B:339:GLU:O	1:B:340:GLU:HA	2.08	0.53
1:A:84:ARG:HG3	1:A:119:LEU:HD11	1.91	0.53
1:A:179:VAL:HG22	1:A:180:PRO:N	2.23	0.53
1:A:154:PHE:CB	1:A:212:LEU:HD12	2.35	0.53
1:C:113:PRO:HG3	1:C:120:ILE:CD1	2.39	0.53
1:C:269:LYS:CG	1:C:270:GLY:N	2.58	0.53
1:B:142:SER:HB3	1:B:227:LEU:O	2.09	0.53
1:A:293:GLU:HA	1:A:317:GLY:HA2	1.91	0.53
1:C:271:THR:CG2	1:C:275:GLU:OE2	2.56	0.53
1:B:179:VAL:HG13	1:B:182:THR:HG22	1.90	0.53
1:B:339:GLU:O	1:B:340:GLU:OE1	2.27	0.53
1:B:199:ASP:N	1:B:199:ASP:OD1	2.40	0.53
1:A:85:SER:C	1:A:234:TYR:CD1	2.82	0.53
1:C:179:VAL:HG22	1:C:180:PRO:N	2.23	0.53
1:B:84:ARG:HG3	1:B:119:LEU:HD11	1.91	0.53
1:B:293:GLU:HA	1:B:317:GLY:HA2	1.91	0.53
1:A:269:LYS:HB3	1:A:277:ASP:OD2	2.09	0.53
1:A:133:SER:HB3	1:A:235:THR:CG2	2.35	0.53
1:A:179:VAL:CG1	1:A:182:THR:HG22	2.39	0.53
1:C:135:ARG:CB	1:C:185:ILE:HD11	2.38	0.53
1:C:82:ILE:HG12	1:C:83:THR:N	2.24	0.53
1:B:173:GLU:HG3	1:B:174:GLY:H	1.73	0.53
1:B:129:TYR:CA	1:B:237:GLN:O	2.57	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LYS:NZ	1:A:221:ALA:HB1	2.22	0.52
1:A:129:TYR:CA	1:A:237:GLN:O	2.57	0.52
1:A:82:ILE:HD12	1:A:126:TYR:CE2	2.44	0.52
1:A:82:ILE:HG12	1:A:83:THR:N	2.24	0.52
1:C:107:VAL:O	1:C:115:THR:CG2	2.56	0.52
1:C:136:PHE:CZ	1:C:212:LEU:CD2	2.91	0.52
1:B:100:GLU:O	1:B:101:PRO:O	2.25	0.52
1:B:113:PRO:HG3	1:B:120:ILE:CD1	2.39	0.52
1:B:112:GLU:HB3	1:B:115:THR:CG2	2.40	0.52
1:B:85:SER:C	1:B:234:TYR:CD1	2.82	0.52
1:B:244:SER:O	1:B:245:THR:HB	2.08	0.52
1:B:300:LEU:CG	1:B:308:PHE:HZ	2.20	0.52
1:C:179:VAL:CG1	1:C:182:THR:HG22	2.39	0.52
1:B:149:LYS:HE2	1:B:151:ALA:CB	2.39	0.52
1:B:179:VAL:CG1	1:B:182:THR:HG22	2.39	0.52
1:B:295:ALA:HB1	1:B:314:ALA:C	2.30	0.52
1:B:82:ILE:HD12	1:B:126:TYR:CE2	2.44	0.52
1:A:152:LEU:HD12	1:A:184:PHE:CE2	2.45	0.52
1:C:94:LYS:O	1:C:95:LYS:C	2.48	0.52
1:B:152:LEU:HD12	1:B:184:PHE:CE2	2.44	0.52
1:B:185:ILE:CD1	1:B:186:LEU:O	2.58	0.52
1:A:236:VAL:CG1	1:A:237:GLN:H	2.23	0.52
1:C:112:GLU:HB3	1:C:115:THR:CG2	2.39	0.52
1:C:126:TYR:C	1:C:242:THR:HG22	2.30	0.52
1:C:293:GLU:HA	1:C:317:GLY:HA2	1.91	0.52
1:B:135:ARG:CB	1:B:185:ILE:HD11	2.38	0.52
1:B:154:PHE:CB	1:B:212:LEU:HD12	2.35	0.52
1:A:350:ARG:O	1:A:351:ILE:CB	2.53	0.52
1:C:339:GLU:O	1:C:340:GLU:OE1	2.27	0.52
1:A:112:GLU:HB3	1:A:115:THR:CG2	2.39	0.52
1:C:128:LYS:O	1:C:129:TYR:HB3	2.10	0.52
1:C:152:LEU:HD12	1:C:184:PHE:CE2	2.45	0.52
1:C:179:VAL:HG13	1:C:182:THR:HG22	1.90	0.52
1:C:95:LYS:HZ1	1:C:221:ALA:HB1	1.74	0.52
1:A:304:ASP:OD2	1:A:332:GLY:N	2.43	0.52
1:A:142:SER:HB3	1:A:227:LEU:O	2.09	0.52
1:A:244:SER:O	1:A:245:THR:HB	2.08	0.52
1:C:82:ILE:HD12	1:C:126:TYR:CE2	2.44	0.52
1:C:166:LEU:C	1:C:168:SER:N	2.61	0.52
1:C:350:ARG:O	1:C:351:ILE:CB	2.53	0.52
1:C:78:ALA:O	1:C:81:GLY:N	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:THR:CG2	1:C:57:ARG:N	2.58	0.52
1:A:149:LYS:HE2	1:A:151:ALA:CB	2.39	0.52
1:A:93:LEU:HD12	1:A:138:TYR:HE1	1.75	0.52
1:B:269:LYS:HB3	1:B:277:ASP:OD2	2.09	0.52
1:A:300:LEU:CG	1:A:308:PHE:HZ	2.21	0.52
1:A:277:ASP:CG	1:A:334:LYS:HZ3	2.13	0.52
1:B:338:THR:HG1	1:B:339:GLU:HB2	1.69	0.52
1:C:54:LYS:O	1:C:55:VAL:HB	2.08	0.52
1:C:239:LYS:O	1:C:240:ASN:O	2.28	0.52
1:A:113:PRO:HG3	1:A:120:ILE:CD1	2.39	0.52
1:C:149:LYS:HE2	1:C:151:ALA:CB	2.39	0.52
1:C:304:ASP:OD2	1:C:332:GLY:N	2.43	0.52
1:C:90:ILE:HD11	1:C:232:VAL:HG22	1.83	0.52
1:B:236:VAL:CG1	1:B:237:GLN:H	2.23	0.52
1:B:313:GLU:HB2	1:B:314:ALA:C	2.29	0.52
1:C:149:LYS:HD3	1:C:217:TYR:HE1	1.73	0.52
1:C:125:GLN:C	1:C:242:THR:HG23	2.30	0.52
1:B:304:ASP:OD2	1:B:332:GLY:N	2.43	0.52
1:B:93:LEU:HD12	1:B:138:TYR:HE1	1.75	0.52
1:A:339:GLU:O	1:A:340:GLU:OE1	2.27	0.52
1:A:125:GLN:C	1:A:242:THR:HG23	2.30	0.52
1:C:138:TYR:CZ	1:C:150:VAL:HG21	2.45	0.52
1:C:185:ILE:CD1	1:C:186:LEU:O	2.58	0.52
1:A:295:ALA:HB2	1:A:315:ALA:CB	2.37	0.52
1:A:185:ILE:CD1	1:A:186:LEU:O	2.58	0.51
1:A:235:THR:O	1:A:235:THR:HG23	2.09	0.51
1:C:300:LEU:O	1:C:308:PHE:CE2	2.63	0.51
1:B:136:PHE:HB3	1:B:230:VAL:CG1	2.40	0.51
1:A:295:ALA:HB1	1:A:314:ALA:C	2.30	0.51
1:A:144:SER:O	1:A:146:THR:N	2.44	0.51
1:A:138:TYR:CZ	1:A:150:VAL:HG21	2.45	0.51
1:C:179:VAL:HG13	1:C:181:TRP:CD1	2.38	0.51
1:C:236:VAL:CG1	1:C:237:GLN:H	2.23	0.51
1:C:285:ASN:HD22	1:C:286:PHE:H	1.58	0.51
1:C:84:ARG:HG3	1:C:119:LEU:HD11	1.91	0.51
1:B:144:SER:O	1:B:146:THR:N	2.44	0.51
1:B:295:ALA:N	1:B:316:ALA:CA	2.40	0.51
1:B:94:LYS:O	1:B:95:LYS:C	2.48	0.51
1:A:103:TYR:CE1	1:A:169:LEU:HD12	2.43	0.51
1:A:103:TYR:CD1	1:A:215:ALA:HB2	2.45	0.51
1:B:82:ILE:HG12	1:B:83:THR:N	2.24	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ILE:O	1:B:83:THR:OG1	2.18	0.51
1:A:293:GLU:O	1:A:317:GLY:HA2	2.09	0.51
1:B:248:ALA:O	1:B:263:VAL:C	2.48	0.51
1:A:221:ALA:O	1:A:225:ALA:HB2	2.10	0.51
1:C:83:THR:CB	1:C:130:ARG:HH12	2.24	0.51
1:B:153:ALA:CA	1:B:174:GLY:HA3	2.33	0.51
1:B:239:LYS:O	1:B:240:ASN:O	2.28	0.51
1:A:166:LEU:C	1:A:168:SER:N	2.61	0.51
1:A:230:VAL:CG1	1:A:231:ARG:N	2.74	0.51
1:A:94:LYS:O	1:A:95:LYS:C	2.48	0.51
1:C:295:ALA:HB1	1:C:314:ALA:C	2.30	0.51
1:B:221:ALA:O	1:B:225:ALA:HB2	2.10	0.51
1:B:125:GLN:C	1:B:242:THR:HG23	2.30	0.51
1:A:297:VAL:HB	1:A:336:VAL:CG1	1.98	0.51
1:C:230:VAL:CG1	1:C:231:ARG:N	2.74	0.51
1:B:128:LYS:HG3	1:B:196:PHE:CD2	2.46	0.51
1:B:243:GLY:O	1:B:244:SER:HB2	2.11	0.51
1:B:285:ASN:HD22	1:B:286:PHE:H	1.58	0.51
1:A:107:VAL:O	1:A:115:THR:CG2	2.56	0.51
1:A:128:LYS:HG3	1:A:196:PHE:CD2	2.46	0.51
1:C:221:ALA:O	1:C:225:ALA:HB2	2.10	0.51
1:C:113:PRO:HG2	1:C:285:ASN:HB3	1.91	0.51
1:C:313:GLU:CG	1:C:318:SER:HB2	2.19	0.51
1:B:235:THR:HG23	1:B:235:THR:O	2.09	0.51
1:B:83:THR:CB	1:B:130:ARG:HH12	2.24	0.51
1:C:241:ARG:H	1:C:241:ARG:CD	2.22	0.51
1:A:291:PHE:CG	1:A:345:LYS:O	2.64	0.51
1:A:198:ALA:C	1:A:200:GLY:N	2.55	0.51
1:C:129:TYR:CA	1:C:237:GLN:O	2.57	0.51
1:C:202:SER:N	1:C:281:LEU:HG	2.26	0.51
1:C:136:PHE:HB3	1:C:230:VAL:CG1	2.40	0.51
1:B:103:TYR:CE1	1:B:169:LEU:HD12	2.43	0.51
1:B:300:LEU:O	1:B:308:PHE:CE2	2.63	0.51
1:A:243:GLY:O	1:A:244:SER:HB2	2.11	0.51
1:A:82:ILE:O	1:A:83:THR:OG1	2.18	0.51
1:C:188:VAL:O	1:C:188:VAL:CG2	2.59	0.51
1:B:101:PRO:CB	1:B:217:TYR:CD2	2.94	0.51
1:A:285:ASN:HD22	1:A:286:PHE:H	1.58	0.51
1:A:300:LEU:O	1:A:308:PHE:CE2	2.63	0.51
1:A:239:LYS:O	1:A:240:ASN:O	2.28	0.51
1:A:136:PHE:HB3	1:A:230:VAL:CG1	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:GLY:O	1:C:244:SER:HB2	2.11	0.51
1:C:295:ALA:HB2	1:C:315:ALA:CB	2.37	0.51
1:B:291:PHE:CG	1:B:345:LYS:O	2.64	0.51
1:A:296:PRO:CD	1:A:337:THR:HG21	2.38	0.51
1:A:107:VAL:HA	1:A:211:LYS:HA	1.93	0.50
1:A:101:PRO:CB	1:A:217:TYR:CD2	2.94	0.50
1:C:109:ASN:ND2	1:C:350:ARG:NH2	2.58	0.50
1:C:128:LYS:HG3	1:C:196:PHE:CD2	2.46	0.50
1:C:85:SER:O	1:C:234:TYR:CE1	2.65	0.50
1:C:235:THR:O	1:C:235:THR:HG23	2.09	0.50
1:C:207:VAL:C	1:C:329:ARG:NH2	2.64	0.50
1:A:313:GLU:HB2	1:A:314:ALA:C	2.29	0.50
1:A:188:VAL:O	1:A:188:VAL:CG2	2.59	0.50
1:C:93:LEU:HD12	1:C:138:TYR:HE1	1.75	0.50
1:B:138:TYR:CZ	1:B:150:VAL:HG21	2.45	0.50
1:B:103:TYR:CD1	1:B:215:ALA:HB2	2.46	0.50
1:B:126:TYR:C	1:B:242:THR:HG22	2.30	0.50
1:A:314:ALA:O	1:A:315:ALA:HB3	2.11	0.50
1:B:241:ARG:H	1:B:241:ARG:CD	2.22	0.50
1:A:128:LYS:O	1:A:129:TYR:HB3	2.10	0.50
1:C:153:ALA:CA	1:C:174:GLY:HA3	2.33	0.50
1:C:154:PHE:CB	1:C:212:LEU:HD12	2.35	0.50
1:C:130:ARG:CB	1:C:237:GLN:N	2.74	0.50
1:C:314:ALA:O	1:C:315:ALA:HB3	2.11	0.50
1:B:230:VAL:CG1	1:B:231:ARG:N	2.74	0.50
1:A:130:ARG:CB	1:A:237:GLN:N	2.74	0.50
1:C:144:SER:O	1:C:146:THR:N	2.44	0.50
1:C:279:HIS:HB3	1:C:280:PHE:N	2.26	0.50
1:C:300:LEU:CG	1:C:308:PHE:HZ	2.20	0.50
1:B:198:ALA:C	1:B:200:GLY:N	2.55	0.50
1:B:119:LEU:HD23	1:B:234:TYR:CE2	2.43	0.50
1:C:77:THR:CG2	1:C:78:ALA:H	2.03	0.50
1:A:157:ASP:C	1:A:157:ASP:OD1	2.50	0.50
1:A:173:GLU:HG3	1:A:174:GLY:H	1.73	0.50
1:A:242:THR:CG2	1:A:243:GLY:H	2.22	0.50
1:C:154:PHE:CD1	1:C:155:ASP:CA	2.90	0.50
1:B:314:ALA:O	1:B:315:ALA:HB3	2.11	0.50
1:B:188:VAL:CG2	1:B:188:VAL:O	2.59	0.50
1:A:83:THR:CB	1:A:130:ARG:HH12	2.24	0.50
1:C:103:TYR:CD1	1:C:215:ALA:HB2	2.46	0.50
1:B:130:ARG:CB	1:B:237:GLN:H	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ALA:HA	1:B:177:SER:CB	2.21	0.50
1:B:157:ASP:C	1:B:157:ASP:OD1	2.50	0.50
1:C:101:PRO:CB	1:C:217:TYR:CD2	2.94	0.50
1:B:107:VAL:HA	1:B:211:LYS:HA	1.93	0.50
1:B:128:LYS:O	1:B:129:TYR:HB3	2.10	0.50
1:B:136:PHE:HD1	1:B:231:ARG:O	1.95	0.50
1:B:290:LEU:HD23	1:B:346:TRP:HB2	1.90	0.50
1:B:271:THR:CG2	1:B:275:GLU:OE2	2.56	0.50
1:A:130:ARG:CB	1:A:237:GLN:H	2.25	0.50
1:A:135:ARG:CB	1:A:185:ILE:HD11	2.38	0.50
1:C:71:THR:OG1	1:C:87:SER:CB	2.59	0.50
1:B:116:PHE:CE2	1:B:234:TYR:CE2	3.00	0.50
1:B:130:ARG:CB	1:B:237:GLN:N	2.74	0.50
1:B:133:SER:N	1:B:235:THR:CG2	2.74	0.50
1:B:279:HIS:HB3	1:B:280:PHE:N	2.27	0.50
1:A:150:VAL:HG23	1:A:227:LEU:HD23	1.94	0.49
1:C:130:ARG:CB	1:C:237:GLN:H	2.25	0.49
1:C:293:GLU:O	1:C:317:GLY:HA2	2.09	0.49
1:B:107:VAL:O	1:B:115:THR:CG2	2.56	0.49
1:B:133:SER:O	1:B:234:TYR:CB	2.60	0.49
1:B:242:THR:CG2	1:B:243:GLY:H	2.22	0.49
1:B:300:LEU:CB	1:B:308:PHE:CZ	2.95	0.49
1:A:241:ARG:H	1:A:241:ARG:CD	2.22	0.49
1:C:107:VAL:HA	1:C:211:LYS:HA	1.93	0.49
1:B:150:VAL:HG23	1:B:227:LEU:HD23	1.94	0.49
1:B:85:SER:O	1:B:234:TYR:CE1	2.65	0.49
1:A:277:ASP:HA	1:A:334:LYS:HZ2	1.75	0.49
1:C:157:ASP:C	1:C:157:ASP:OD1	2.50	0.49
1:A:136:PHE:HD1	1:A:231:ARG:O	1.95	0.49
1:C:100:GLU:O	1:C:101:PRO:C	2.48	0.49
1:C:167:ALA:O	1:C:171:ASN:ND2	2.45	0.49
1:A:300:LEU:CB	1:A:308:PHE:CZ	2.95	0.49
1:A:163:PRO:HB2	1:A:165:ASP:N	2.28	0.49
1:A:116:PHE:CE2	1:A:234:TYR:CE2	3.00	0.49
1:A:126:TYR:C	1:A:242:THR:HG22	2.30	0.49
1:B:150:VAL:CG2	1:B:227:LEU:HD23	2.43	0.49
1:C:151:ALA:HA	1:C:177:SER:CB	2.21	0.49
1:C:204:PRO:CB	1:C:329:ARG:N	2.75	0.49
1:B:269:LYS:CG	1:B:270:GLY:N	2.58	0.49
1:A:133:SER:O	1:A:234:TYR:CB	2.60	0.49
1:A:85:SER:O	1:A:234:TYR:CE1	2.65	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ASN:O	1:C:110:PRO:C	2.51	0.49
1:C:290:LEU:HD23	1:C:346:TRP:HB2	1.90	0.49
1:B:167:ALA:O	1:B:171:ASN:ND2	2.45	0.49
1:A:119:LEU:HD23	1:A:234:TYR:CE2	2.43	0.49
1:A:167:ALA:O	1:A:171:ASN:ND2	2.45	0.49
1:C:107:VAL:HG11	1:C:283:THR:CG2	2.43	0.49
1:C:150:VAL:CG2	1:C:227:LEU:HD23	2.43	0.49
1:C:116:PHE:CE2	1:C:234:TYR:CE2	3.00	0.49
1:C:291:PHE:CG	1:C:345:LYS:O	2.64	0.49
1:B:85:SER:O	1:B:234:TYR:HE1	1.96	0.49
1:C:150:VAL:HG23	1:C:227:LEU:HD23	1.94	0.49
1:B:163:PRO:HB2	1:B:165:ASP:N	2.28	0.49
1:B:244:SER:C	1:B:245:THR:HG22	2.31	0.49
1:B:86:GLY:HA2	1:B:234:TYR:HE1	1.68	0.49
1:A:264:SER:OG	1:A:265:TRP:N	2.45	0.49
1:A:295:ALA:N	1:A:316:ALA:CA	2.40	0.49
1:C:85:SER:O	1:C:234:TYR:HE1	1.96	0.49
1:B:288:LEU:CD1	1:B:290:LEU:CG	2.70	0.49
1:B:278:CYS:CA	1:B:334:LYS:HD3	2.42	0.49
1:A:85:SER:O	1:A:234:TYR:HE1	1.96	0.49
1:C:136:PHE:HD1	1:C:231:ARG:O	1.95	0.49
1:C:119:LEU:HD23	1:C:234:TYR:CE2	2.43	0.49
1:C:201:ILE:CD1	1:C:281:LEU:CD1	2.90	0.49
1:B:244:SER:OG	1:B:245:THR:N	2.46	0.49
1:B:264:SER:OG	1:B:265:TRP:N	2.45	0.49
1:B:241:ARG:CD	1:B:241:ARG:N	2.75	0.49
1:A:150:VAL:CG2	1:A:227:LEU:HD23	2.43	0.48
1:A:244:SER:OG	1:A:245:THR:N	2.46	0.48
1:A:88:GLU:OE2	1:A:118:GLN:HB3	2.13	0.48
1:C:278:CYS:CA	1:C:334:LYS:HD3	2.42	0.48
1:B:92:THR:HG23	1:B:93:LEU:O	2.13	0.48
1:C:241:ARG:CD	1:C:241:ARG:N	2.75	0.48
1:A:279:HIS:HB3	1:A:280:PHE:N	2.27	0.48
1:C:133:SER:O	1:C:234:TYR:CB	2.60	0.48
1:C:264:SER:OG	1:C:265:TRP:N	2.45	0.48
1:C:249:GLN:NE2	1:C:265:TRP:N	2.54	0.48
1:C:291:PHE:C	1:C:292:TYR:HB3	2.33	0.48
1:B:88:GLU:OE2	1:B:118:GLN:HB3	2.13	0.48
1:B:84:ARG:HD2	1:B:119:LEU:HD13	1.94	0.48
1:B:88:GLU:O	1:B:231:ARG:HB3	2.05	0.48
1:A:105:THR:HG23	1:A:105:THR:O	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:O	1:A:186:LEU:CD1	2.55	0.48
1:A:89:LEU:HD23	1:A:90:ILE:N	2.28	0.48
1:C:158:ALA:C	1:C:211:LYS:H	1.93	0.48
1:B:130:ARG:HH11	1:B:236:VAL:C	2.16	0.48
1:A:291:PHE:C	1:A:292:TYR:HB3	2.33	0.48
1:A:333:VAL:C	1:A:334:LYS:CD	2.78	0.48
1:C:336:VAL:O	1:C:337:THR:CG2	2.62	0.48
1:B:204:PRO:N	1:B:205:LYS:HD2	2.28	0.48
1:C:66:TYR:HE2	1:C:183:GLY:HA3	1.73	0.48
1:C:163:PRO:CG	1:C:168:SER:CB	2.92	0.48
1:C:300:LEU:CB	1:C:308:PHE:CZ	2.95	0.48
1:B:83:THR:HG23	1:B:130:ARG:CZ	2.44	0.48
1:B:249:GLN:O	1:B:347:GLN:CA	2.61	0.48
1:C:339:GLU:O	1:C:340:GLU:CA	2.60	0.48
1:A:100:GLU:O	1:A:101:PRO:C	2.48	0.48
1:A:150:VAL:O	1:A:151:ALA:C	2.52	0.48
1:A:84:ARG:HD2	1:A:119:LEU:HD13	1.94	0.48
1:C:150:VAL:O	1:C:151:ALA:C	2.52	0.48
1:C:86:GLY:HA2	1:C:234:TYR:HE1	1.68	0.48
1:B:150:VAL:O	1:B:151:ALA:C	2.52	0.48
1:C:336:VAL:O	1:C:337:THR:HG23	2.14	0.48
1:B:336:VAL:O	1:B:337:THR:HG23	2.14	0.48
1:A:241:ARG:CD	1:A:241:ARG:N	2.75	0.48
1:A:83:THR:HG23	1:A:130:ARG:CZ	2.44	0.48
1:C:103:TYR:CE1	1:C:169:LEU:HD12	2.43	0.48
1:C:83:THR:HG23	1:C:130:ARG:CZ	2.44	0.48
1:C:84:ARG:HD2	1:C:119:LEU:HD13	1.94	0.48
1:B:166:LEU:C	1:B:168:SER:N	2.61	0.48
1:A:163:PRO:CG	1:A:168:SER:CB	2.92	0.48
1:A:92:THR:HG23	1:A:93:LEU:O	2.14	0.48
1:C:159:ALA:HB1	1:C:328:GLU:HB2	1.18	0.48
1:B:95:LYS:HZ1	1:B:221:ALA:HB1	1.78	0.48
1:A:249:GLN:O	1:A:347:GLN:CA	2.61	0.48
1:A:130:ARG:HH11	1:A:236:VAL:C	2.16	0.48
1:C:204:PRO:N	1:C:205:LYS:HD2	2.29	0.48
1:C:101:PRO:CG	1:C:217:TYR:CE2	2.74	0.48
1:B:152:LEU:O	1:B:186:LEU:CD1	2.55	0.48
1:A:339:GLU:O	1:A:340:GLU:CA	2.60	0.48
1:A:204:PRO:N	1:A:205:LYS:HD2	2.29	0.48
1:A:150:VAL:O	1:A:151:ALA:O	2.32	0.48
1:C:89:LEU:HD23	1:C:90:ILE:N	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ASN:OD1	1:A:129:TYR:OH	2.32	0.48
1:C:163:PRO:HB2	1:C:165:ASP:N	2.28	0.48
1:C:101:PRO:CG	1:C:217:TYR:HD2	2.26	0.48
1:C:88:GLU:OE2	1:C:118:GLN:HB3	2.14	0.48
1:B:163:PRO:CG	1:B:168:SER:CB	2.92	0.48
1:A:248:ALA:CA	1:A:264:SER:O	2.58	0.48
1:A:288:LEU:C	1:A:289:THR:OG1	2.49	0.48
1:A:290:LEU:HB2	1:A:346:TRP:HA	1.96	0.48
1:A:336:VAL:O	1:A:337:THR:CG2	2.62	0.48
1:B:296:PRO:CD	1:B:337:THR:HG21	2.38	0.48
1:A:111:SER:HB3	1:A:197:VAL:CG2	2.44	0.47
1:C:134:LEU:CD2	1:C:188:VAL:HG22	2.41	0.47
1:C:152:LEU:O	1:C:186:LEU:CD1	2.56	0.47
1:B:105:THR:HG23	1:B:105:THR:O	2.14	0.47
1:B:109:ASN:OD1	1:B:129:TYR:OH	2.32	0.47
1:B:111:SER:HB3	1:B:197:VAL:CG2	2.44	0.47
1:B:336:VAL:O	1:B:337:THR:CG2	2.62	0.47
1:B:141:MET:CG	1:B:141:MET:O	2.46	0.47
1:A:95:LYS:HZ1	1:A:221:ALA:C	2.18	0.47
1:C:244:SER:OG	1:C:245:THR:N	2.46	0.47
1:C:269:LYS:HG2	1:C:270:GLY:O	2.14	0.47
1:C:92:THR:HG23	1:C:93:LEU:O	2.14	0.47
1:B:179:VAL:CG1	1:B:181:TRP:NE1	2.54	0.47
1:A:163:PRO:CG	1:A:168:SER:HB3	2.44	0.47
1:C:295:ALA:N	1:C:316:ALA:CA	2.40	0.47
1:B:101:PRO:HG2	1:B:166:LEU:HD12	1.94	0.47
1:B:163:PRO:CG	1:B:168:SER:HB3	2.44	0.47
1:B:144:SER:HA	1:B:181:TRP:HB3	1.96	0.47
1:C:343:LYS:HB2	1:C:344:GLY:H	1.13	0.47
1:C:249:GLN:O	1:C:347:GLN:CA	2.61	0.47
1:B:95:LYS:HZ1	1:B:221:ALA:C	2.18	0.47
1:C:130:ARG:HB3	1:C:237:GLN:N	2.30	0.47
1:C:130:ARG:HH11	1:C:236:VAL:C	2.16	0.47
1:C:179:VAL:CG2	1:C:181:TRP:CD1	2.93	0.47
1:C:185:ILE:HD11	1:C:186:LEU:O	2.15	0.47
1:C:278:CYS:N	1:C:333:VAL:O	2.48	0.47
1:B:149:LYS:HE2	1:B:151:ALA:HB2	1.96	0.47
1:B:150:VAL:O	1:B:151:ALA:O	2.32	0.47
1:B:185:ILE:HD11	1:B:186:LEU:O	2.15	0.47
1:A:278:CYS:N	1:A:333:VAL:O	2.48	0.47
1:A:149:LYS:HE2	1:A:151:ALA:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:VAL:CG1	1:A:181:TRP:NE1	2.54	0.47
1:B:203:ASP:OD1	1:B:205:LYS:CG	2.56	0.47
1:A:185:ILE:HD11	1:A:186:LEU:O	2.15	0.47
1:A:136:PHE:CE2	1:A:212:LEU:CD2	2.98	0.47
1:C:136:PHE:CE2	1:C:212:LEU:CD2	2.98	0.47
1:C:150:VAL:O	1:C:151:ALA:O	2.32	0.47
1:C:162:PRO:O	1:C:163:PRO:O	2.33	0.47
1:C:144:SER:HA	1:C:181:TRP:HB3	1.96	0.47
1:B:136:PHE:CE2	1:B:212:LEU:CD2	2.98	0.47
1:B:291:PHE:HD2	1:B:346:TRP:HE3	1.63	0.47
1:B:278:CYS:N	1:B:333:VAL:O	2.48	0.47
1:B:269:LYS:HG2	1:B:270:GLY:O	2.14	0.47
1:B:290:LEU:HB2	1:B:346:TRP:HA	1.96	0.47
1:B:291:PHE:C	1:B:292:TYR:HB3	2.33	0.47
1:A:248:ALA:C	1:A:264:SER:CB	2.82	0.47
1:B:338:THR:OG1	1:B:339:GLU:CA	2.63	0.47
1:A:144:SER:HA	1:A:181:TRP:HB3	1.96	0.47
1:C:313:GLU:HG3	1:C:315:ALA:HA	1.97	0.47
1:A:273:GLY:O	1:A:274:TRP:C	2.53	0.47
1:C:201:ILE:HD13	1:C:266:SER:HA	1.97	0.47
1:C:291:PHE:CD1	1:C:292:TYR:N	2.83	0.47
1:C:277:ASP:CG	1:C:334:LYS:HZ3	2.17	0.47
1:A:269:LYS:HG2	1:A:270:GLY:O	2.14	0.47
1:C:296:PRO:CD	1:C:337:THR:HG21	2.39	0.47
1:C:105:THR:O	1:C:105:THR:HG23	2.14	0.47
1:C:107:VAL:HG22	1:C:211:LYS:HB3	1.97	0.47
1:B:291:PHE:CD1	1:B:292:TYR:N	2.83	0.47
1:B:300:LEU:HD12	1:B:300:LEU:HA	1.28	0.47
1:C:338:THR:OG1	1:C:339:GLU:CA	2.63	0.47
1:A:203:ASP:OD1	1:A:205:LYS:CG	2.56	0.47
1:A:153:ALA:CA	1:A:174:GLY:HA3	2.33	0.46
1:C:149:LYS:O	1:C:216:THR:HA	2.15	0.46
1:C:185:ILE:HD12	1:C:186:LEU:C	2.36	0.46
1:B:115:THR:C	1:B:116:PHE:CD1	2.78	0.46
1:A:291:PHE:CD1	1:A:292:TYR:N	2.83	0.46
1:C:162:PRO:O	1:C:163:PRO:C	2.50	0.46
1:B:100:GLU:C	1:B:101:PRO:O	2.54	0.46
1:B:162:PRO:O	1:B:163:PRO:O	2.33	0.46
1:B:174:GLY:O	1:B:175:CYS:CB	2.64	0.46
1:B:280:PHE:HZ	1:B:324:VAL:HG21	1.81	0.46
1:B:90:ILE:O	1:B:90:ILE:CG2	2.54	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:VAL:O	1:A:337:THR:HG23	2.14	0.46
1:A:100:GLU:C	1:A:101:PRO:O	2.54	0.46
1:A:130:ARG:HB3	1:A:237:GLN:N	2.30	0.46
1:C:174:GLY:O	1:C:175:CYS:CB	2.63	0.46
1:C:290:LEU:HB2	1:C:346:TRP:HA	1.96	0.46
1:C:71:THR:O	1:C:71:THR:HG23	2.16	0.46
1:B:101:PRO:CG	1:B:217:TYR:HD2	2.26	0.46
1:B:279:HIS:CB	1:B:280:PHE:N	2.78	0.46
1:A:289:THR:O	1:A:290:LEU:HG	2.14	0.46
1:C:273:GLY:O	1:C:274:TRP:C	2.53	0.46
1:A:162:PRO:O	1:A:163:PRO:O	2.33	0.46
1:A:230:VAL:CG1	1:A:231:ARG:H	2.28	0.46
1:C:234:TYR:CD2	1:C:236:VAL:HG23	2.51	0.46
1:C:125:GLN:CA	1:C:243:GLY:HA2	2.27	0.46
1:B:230:VAL:CG1	1:B:231:ARG:H	2.28	0.46
1:B:295:ALA:HB2	1:B:315:ALA:CB	2.38	0.46
1:B:89:LEU:HD23	1:B:90:ILE:N	2.28	0.46
1:A:280:PHE:HZ	1:A:324:VAL:HG21	1.81	0.46
1:A:290:LEU:HD23	1:A:346:TRP:HB2	1.90	0.46
1:B:249:GLN:CG	1:B:263:VAL:O	2.64	0.46
1:C:244:SER:C	1:C:245:THR:HG22	2.31	0.46
1:C:289:THR:O	1:C:290:LEU:HG	2.14	0.46
1:B:112:GLU:O	1:B:112:GLU:HG3	2.16	0.46
1:A:291:PHE:HD2	1:A:346:TRP:HE3	1.63	0.46
1:A:112:GLU:O	1:A:112:GLU:HG3	2.16	0.46
1:A:185:ILE:HD12	1:A:186:LEU:C	2.36	0.46
1:C:149:LYS:HE2	1:C:151:ALA:HB2	1.96	0.46
1:C:172:ILE:C	1:C:173:GLU:O	2.51	0.46
1:C:249:GLN:CG	1:C:263:VAL:O	2.64	0.46
1:C:89:LEU:HD23	1:C:89:LEU:O	2.00	0.46
1:B:290:LEU:HD13	1:B:291:PHE:HB3	1.98	0.46
1:B:96:ASN:C	1:B:98:ASP:N	2.55	0.46
1:B:297:VAL:HG12	1:B:336:VAL:HG11	0.97	0.46
1:C:160:LYS:N	1:C:328:GLU:OE1	2.49	0.46
1:C:197:VAL:HG21	1:C:350:ARG:NH1	2.30	0.46
1:C:230:VAL:CG1	1:C:231:ARG:H	2.28	0.46
1:C:201:ILE:CD1	1:C:266:SER:HA	2.46	0.46
1:B:130:ARG:HB3	1:B:237:GLN:N	2.30	0.46
1:B:333:VAL:C	1:B:334:LYS:CD	2.78	0.46
1:A:249:GLN:CG	1:A:263:VAL:O	2.64	0.46
1:A:271:THR:HG23	1:A:275:GLU:HG2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ILE:HD11	1:A:232:VAL:HG22	1.83	0.46
1:C:136:PHE:CE2	1:C:212:LEU:HD21	2.51	0.46
1:C:333:VAL:C	1:C:334:LYS:CD	2.78	0.46
1:B:185:ILE:HD12	1:B:186:LEU:C	2.36	0.46
1:B:269:LYS:CE	1:B:270:GLY:O	2.63	0.46
1:B:276:HIS:CG	1:B:277:ASP:N	2.74	0.46
1:A:174:GLY:O	1:A:175:CYS:CB	2.64	0.46
1:A:185:ILE:HD12	1:A:186:LEU:H	0.65	0.46
1:A:82:ILE:HG21	1:A:82:ILE:HD13	1.78	0.46
1:A:90:ILE:O	1:A:90:ILE:CG2	2.54	0.46
1:C:127:GLU:O	1:C:128:LYS:CG	2.64	0.46
1:C:207:VAL:H	1:C:329:ARG:NH1	2.13	0.46
1:C:95:LYS:HZ1	1:C:221:ALA:CB	2.29	0.46
1:B:109:ASN:O	1:B:110:PRO:C	2.51	0.46
1:B:288:LEU:C	1:B:289:THR:OG1	2.49	0.46
1:B:313:GLU:HG3	1:B:315:ALA:HA	1.97	0.46
1:C:74:ARG:C	1:C:75:VAL:HG23	2.37	0.46
1:A:279:HIS:CB	1:A:280:PHE:N	2.78	0.46
1:B:271:THR:HG23	1:B:275:GLU:HG2	1.97	0.46
1:A:234:TYR:CD2	1:A:236:VAL:HG23	2.50	0.46
1:C:207:VAL:N	1:C:329:ARG:CZ	2.64	0.46
1:C:126:TYR:C	1:C:242:THR:HG21	2.37	0.46
1:A:97:THR:O	1:A:97:THR:OG1	2.25	0.46
1:C:279:HIS:CB	1:C:280:PHE:N	2.78	0.45
1:C:95:LYS:HZ1	1:C:221:ALA:C	2.19	0.45
1:B:289:THR:O	1:B:290:LEU:HG	2.14	0.45
1:C:271:THR:HG23	1:C:275:GLU:HG2	1.97	0.45
1:B:273:GLY:O	1:B:274:TRP:C	2.53	0.45
1:A:107:VAL:HG22	1:A:211:LYS:HB3	1.97	0.45
1:A:101:PRO:CG	1:A:217:TYR:CE2	2.74	0.45
1:C:100:GLU:C	1:C:101:PRO:O	2.54	0.45
1:C:181:TRP:CE3	1:C:181:TRP:O	2.69	0.45
1:C:89:LEU:HA	1:C:230:VAL:O	2.16	0.45
1:C:133:SER:CA	1:C:235:THR:HG22	2.46	0.45
1:B:127:GLU:O	1:B:128:LYS:CG	2.64	0.45
1:B:149:LYS:O	1:B:216:THR:HA	2.15	0.45
1:A:181:TRP:O	1:A:181:TRP:CE3	2.69	0.45
1:A:95:LYS:HZ1	1:A:221:ALA:HB1	1.80	0.45
1:C:201:ILE:HD12	1:C:280:PHE:CA	1.90	0.45
1:C:201:ILE:HG23	1:C:281:LEU:HD23	1.93	0.45
1:A:253:PHE:HZ	1:A:268:THR:HG21	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:ARG:CD	1:C:119:LEU:HD13	2.46	0.45
1:C:163:PRO:CG	1:C:168:SER:HB3	2.44	0.45
1:C:280:PHE:HZ	1:C:324:VAL:HG21	1.81	0.45
1:A:338:THR:OG1	1:A:339:GLU:CA	2.63	0.45
1:A:127:GLU:O	1:A:128:LYS:CG	2.64	0.45
1:A:101:PRO:HG2	1:A:166:LEU:HD12	1.94	0.45
1:C:204:PRO:CG	1:C:328:GLU:HG3	2.05	0.45
1:C:288:LEU:C	1:C:289:THR:OG1	2.49	0.45
1:C:60:ALA:HA	1:C:61:PRO:HD2	1.81	0.45
1:B:84:ARG:CD	1:B:119:LEU:HD13	2.46	0.45
1:B:234:TYR:CD2	1:B:236:VAL:HG23	2.51	0.45
1:B:295:ALA:HB2	1:B:315:ALA:HB3	1.99	0.45
1:A:290:LEU:HD13	1:A:291:PHE:HB3	1.98	0.45
1:A:313:GLU:HG3	1:A:315:ALA:HA	1.97	0.45
1:A:295:ALA:HB2	1:A:315:ALA:HB3	1.99	0.45
1:A:326:VAL:HG13	1:A:331:GLN:OE1	2.17	0.45
1:A:236:VAL:CG1	1:A:238:LEU:CD1	2.94	0.45
1:C:109:ASN:OD1	1:C:129:TYR:OH	2.32	0.45
1:B:181:TRP:CE3	1:B:181:TRP:O	2.69	0.45
1:A:269:LYS:CE	1:A:270:GLY:O	2.63	0.45
1:A:136:PHE:CE2	1:A:212:LEU:HD21	2.51	0.45
1:A:149:LYS:O	1:A:216:THR:HA	2.15	0.45
1:C:153:ALA:HB2	1:C:175:CYS:N	2.32	0.45
1:C:236:VAL:CG1	1:C:238:LEU:CD1	2.94	0.45
1:C:291:PHE:HD2	1:C:346:TRP:HE3	1.63	0.45
1:B:248:ALA:C	1:B:263:VAL:C	2.75	0.45
1:C:337:THR:HG1	1:C:343:LYS:HZ2	1.63	0.45
1:C:288:LEU:CD1	1:C:290:LEU:CG	2.70	0.45
1:C:290:LEU:HD13	1:C:291:PHE:HB3	1.98	0.45
1:C:315:ALA:O	1:C:318:SER:N	2.50	0.45
1:A:149:LYS:HD3	1:A:217:TYR:HE1	1.73	0.45
1:A:89:LEU:HA	1:A:230:VAL:O	2.17	0.45
1:C:112:GLU:O	1:C:112:GLU:HG3	2.16	0.45
1:B:293:GLU:O	1:B:316:ALA:C	2.52	0.45
1:B:90:ILE:HD11	1:B:232:VAL:HG22	1.83	0.45
1:A:269:LYS:O	1:A:277:ASP:CA	2.57	0.45
1:A:315:ALA:O	1:A:318:SER:N	2.50	0.45
1:A:278:CYS:CA	1:A:334:LYS:HD3	2.42	0.45
1:B:271:THR:CG2	1:B:275:GLU:HG2	2.47	0.45
1:B:336:VAL:C	1:B:337:THR:HG23	2.37	0.45
1:A:149:LYS:CG	1:A:217:TYR:HE1	2.29	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:PRO:CD	1:C:285:ASN:O	2.65	0.45
1:C:118:GLN:O	1:C:118:GLN:HG2	2.17	0.45
1:B:100:GLU:O	1:B:101:PRO:C	2.48	0.45
1:C:97:THR:OG1	1:C:97:THR:O	2.25	0.45
1:A:262:LEU:HD23	1:A:262:LEU:HA	1.71	0.45
1:A:84:ARG:CD	1:A:119:LEU:HD13	2.46	0.44
1:B:107:VAL:HG22	1:B:211:LYS:HB3	1.98	0.44
1:B:133:SER:CA	1:B:235:THR:HG22	2.47	0.44
1:B:277:ASP:CG	1:B:334:LYS:HZ3	2.21	0.44
1:B:89:LEU:HA	1:B:230:VAL:O	2.17	0.44
1:A:271:THR:CG2	1:A:275:GLU:HG2	2.47	0.44
1:B:213:ILE:HG23	1:B:214:MET:N	2.32	0.44
1:A:109:ASN:O	1:A:110:PRO:C	2.51	0.44
1:A:133:SER:N	1:A:235:THR:CG2	2.74	0.44
1:C:101:PRO:CD	1:C:217:TYR:HD2	2.30	0.44
1:C:253:PHE:HZ	1:C:268:THR:HG21	1.82	0.44
1:B:118:GLN:HG2	1:B:118:GLN:O	2.17	0.44
1:B:149:LYS:CG	1:B:217:TYR:HE1	2.29	0.44
1:B:315:ALA:O	1:B:318:SER:N	2.50	0.44
1:B:82:ILE:HD13	1:B:82:ILE:HG21	1.78	0.44
1:A:122:GLU:CG	1:A:122:GLU:O	2.64	0.44
1:A:105:THR:HA	1:A:212:LEU:O	2.18	0.44
1:A:133:SER:CA	1:A:235:THR:HG22	2.46	0.44
1:A:96:ASN:C	1:A:98:ASP:N	2.55	0.44
1:C:105:THR:HA	1:C:212:LEU:O	2.18	0.44
1:C:268:THR:CG2	1:C:268:THR:O	2.66	0.44
1:C:326:VAL:HG13	1:C:331:GLN:OE1	2.17	0.44
1:B:101:PRO:HD3	1:B:166:LEU:HD11	0.47	0.44
1:A:101:PRO:CD	1:A:217:TYR:HD2	2.30	0.44
1:C:111:SER:O	1:C:350:ARG:NE	2.48	0.44
1:B:136:PHE:CE2	1:B:212:LEU:HD21	2.51	0.44
1:C:163:PRO:HG3	1:C:168:SER:CB	2.48	0.44
1:B:101:PRO:HB3	1:B:217:TYR:CD2	2.53	0.44
1:B:101:PRO:CD	1:B:217:TYR:HD2	2.30	0.44
1:B:326:VAL:HG13	1:B:331:GLN:OE1	2.17	0.44
1:A:213:ILE:HG23	1:A:214:MET:N	2.32	0.44
1:A:199:ASP:N	1:A:199:ASP:OD1	2.40	0.44
1:A:126:TYR:C	1:A:242:THR:HG21	2.37	0.44
1:C:109:ASN:O	1:C:111:SER:N	2.50	0.44
1:C:133:SER:N	1:C:235:THR:CG2	2.74	0.44
1:C:137:ARG:N	1:C:230:VAL:HG13	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:ALA:HB2	1:C:315:ALA:HB3	1.98	0.44
1:C:56:THR:HG23	1:C:57:ARG:HB3	1.99	0.44
1:A:153:ALA:HB2	1:A:175:CYS:N	2.32	0.44
1:C:101:PRO:HD3	1:C:166:LEU:HD11	0.47	0.44
1:C:159:ALA:CB	1:C:328:GLU:OE1	2.55	0.44
1:B:291:PHE:C	1:B:292:TYR:CB	2.86	0.44
1:B:291:PHE:CE1	1:B:335:MET:HE3	2.53	0.44
1:C:213:ILE:HG23	1:C:214:MET:N	2.32	0.44
1:C:134:LEU:N	1:C:233:GLU:O	2.44	0.44
1:C:291:PHE:C	1:C:292:TYR:CB	2.86	0.44
1:B:158:ALA:C	1:B:211:LYS:H	1.93	0.44
1:B:105:THR:HA	1:B:212:LEU:O	2.18	0.44
1:B:84:ARG:NE	1:B:119:LEU:CD1	2.81	0.44
1:A:291:PHE:CE1	1:A:335:MET:HE3	2.51	0.44
1:B:248:ALA:HB3	1:B:249:GLN:HB3	1.87	0.44
1:C:72:GLN:HE21	1:C:73:PRO:HD2	1.83	0.44
1:A:118:GLN:HG2	1:A:118:GLN:O	2.17	0.44
1:A:158:ALA:C	1:A:211:LYS:H	1.93	0.44
1:B:304:ASP:OD2	1:B:331:GLN:CA	2.57	0.44
1:A:300:LEU:HA	1:A:300:LEU:HD12	1.28	0.44
1:A:252:ASP:OD2	1:A:345:LYS:HG2	2.16	0.44
1:C:336:VAL:C	1:C:337:THR:HG23	2.37	0.44
1:A:336:VAL:C	1:A:337:THR:HG23	2.37	0.44
1:C:262:LEU:HA	1:C:262:LEU:HD23	1.71	0.44
1:A:96:ASN:O	1:A:96:ASN:ND2	2.51	0.43
1:C:154:PHE:CZ	1:C:156:ARG:CA	3.01	0.43
1:C:197:VAL:HG22	1:C:350:ARG:CZ	2.48	0.43
1:C:113:PRO:HD3	1:C:351:ILE:O	2.18	0.43
1:B:105:THR:OG1	1:B:211:LYS:HD2	2.03	0.43
1:B:109:ASN:O	1:B:111:SER:N	2.50	0.43
1:B:134:LEU:CD2	1:B:188:VAL:HG22	2.41	0.43
1:B:153:ALA:HB2	1:B:175:CYS:N	2.32	0.43
1:B:172:ILE:C	1:B:173:GLU:O	2.51	0.43
1:B:236:VAL:CG1	1:B:238:LEU:CD1	2.94	0.43
1:C:76:SER:OG	1:C:77:THR:N	2.50	0.43
1:C:271:THR:CG2	1:C:275:GLU:HG2	2.47	0.43
1:A:109:ASN:O	1:A:111:SER:N	2.50	0.43
1:C:101:PRO:HB3	1:C:217:TYR:CD2	2.53	0.43
1:B:149:LYS:HD3	1:B:217:TYR:HE1	1.73	0.43
1:A:326:VAL:CG1	1:A:327:ALA:N	2.19	0.43
1:A:172:ILE:C	1:A:173:GLU:O	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:LYS:CG	1:C:217:TYR:HE1	2.29	0.43
1:C:243:GLY:O	1:C:244:SER:CB	2.67	0.43
1:B:163:PRO:HG3	1:B:168:SER:CB	2.47	0.43
1:B:253:PHE:HZ	1:B:268:THR:HG21	1.82	0.43
1:B:269:LYS:O	1:B:277:ASP:CA	2.57	0.43
1:B:339:GLU:O	1:B:340:GLU:CA	2.60	0.43
1:A:254:ALA:O	1:A:257:LYS:N	2.38	0.43
1:A:137:ARG:N	1:A:230:VAL:HG13	2.33	0.43
1:C:121:LYS:O	1:C:121:LYS:HG3	2.19	0.43
1:B:96:ASN:ND2	1:B:96:ASN:O	2.51	0.43
1:A:101:PRO:HB3	1:A:217:TYR:CD2	2.53	0.43
1:A:139:SER:HA	1:A:140:PRO:HD3	1.13	0.43
1:A:216:THR:OG1	1:A:227:LEU:HD21	2.18	0.43
1:A:125:GLN:CA	1:A:243:GLY:HA2	2.27	0.43
1:C:126:TYR:O	1:C:242:THR:CG2	2.66	0.43
1:C:293:GLU:O	1:C:316:ALA:C	2.52	0.43
1:C:84:ARG:NE	1:C:119:LEU:CD1	2.81	0.43
1:B:137:ARG:N	1:B:230:VAL:HG13	2.33	0.43
1:A:315:ALA:CA	1:A:318:SER:HB2	2.49	0.43
1:A:325:LYS:O	1:A:325:LYS:HG2	2.18	0.43
1:B:242:THR:CG2	1:B:243:GLY:N	2.73	0.43
1:B:112:GLU:HG2	1:B:329:ARG:HH22	1.83	0.43
1:B:121:LYS:O	1:B:121:LYS:HG3	2.19	0.43
1:A:101:PRO:HD3	1:A:166:LEU:HD11	0.47	0.43
1:B:278:CYS:O	1:B:333:VAL:O	2.37	0.43
1:A:121:LYS:O	1:A:121:LYS:HG3	2.19	0.43
1:A:291:PHE:C	1:A:292:TYR:CB	2.86	0.43
1:C:254:ALA:O	1:C:257:LYS:N	2.38	0.43
1:B:186:LEU:C	1:B:186:LEU:CD2	2.87	0.43
1:A:84:ARG:NE	1:A:119:LEU:CD1	2.81	0.43
1:C:87:SER:HA	1:C:231:ARG:HD2	2.01	0.43
1:B:216:THR:OG1	1:B:227:LEU:HD21	2.18	0.43
1:A:186:LEU:C	1:A:186:LEU:CD2	2.87	0.43
1:C:154:PHE:CE1	1:C:156:ARG:CA	3.02	0.43
1:B:288:LEU:O	1:B:289:THR:OG1	2.37	0.43
1:B:311:LEU:N	1:B:311:LEU:CD1	2.82	0.43
1:B:273:GLY:O	1:B:275:GLU:HB3	2.19	0.43
1:C:325:LYS:O	1:C:325:LYS:HG2	2.18	0.43
1:B:325:LYS:O	1:B:325:LYS:HG2	2.18	0.43
1:C:125:GLN:HA	1:C:243:GLY:N	2.34	0.42
1:B:255:GLY:HA2	1:B:342:PRO:CB	2.25	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLN:HA	1:A:243:GLY:N	2.34	0.42
1:C:137:ARG:O	1:C:230:VAL:HA	2.19	0.42
1:C:266:SER:HA	1:C:280:PHE:HA	2.02	0.42
1:C:309:SER:C	1:C:322:ALA:HA	2.20	0.42
1:C:96:ASN:O	1:C:96:ASN:ND2	2.52	0.42
1:B:258:ASP:OD1	1:B:259:GLY:N	2.52	0.42
1:A:278:CYS:O	1:A:333:VAL:O	2.37	0.42
1:A:137:ARG:O	1:A:230:VAL:HA	2.19	0.42
1:A:242:THR:CG2	1:A:243:GLY:N	2.73	0.42
1:A:113:PRO:HB2	1:A:329:ARG:HG3	1.96	0.42
1:C:236:VAL:CG1	1:C:238:LEU:HD11	2.50	0.42
1:B:111:SER:HB3	1:B:197:VAL:HG21	2.01	0.42
1:B:126:TYR:C	1:B:242:THR:HG21	2.37	0.42
1:A:293:GLU:CA	1:A:317:GLY:HA2	2.50	0.42
1:A:134:LEU:CD2	1:A:188:VAL:HG22	2.41	0.42
1:C:302:ASN:HB3	1:C:308:PHE:CE1	2.55	0.42
1:C:304:ASP:OD2	1:C:331:GLN:CA	2.57	0.42
1:B:137:ARG:O	1:B:230:VAL:HA	2.19	0.42
1:B:259:GLY:C	1:B:260:PRO:CD	2.84	0.42
1:B:293:GLU:CA	1:B:317:GLY:HA2	2.50	0.42
1:A:288:LEU:O	1:A:289:THR:OG1	2.37	0.42
1:C:273:GLY:O	1:C:275:GLU:HB3	2.19	0.42
1:C:341:GLN:O	1:C:342:PRO:C	2.58	0.42
1:A:154:PHE:CE1	1:A:156:ARG:CA	3.02	0.42
1:C:169:LEU:C	1:C:171:ASN:H	2.23	0.42
1:C:293:GLU:CA	1:C:317:GLY:HA2	2.50	0.42
1:B:302:ASN:HB3	1:B:308:PHE:CE1	2.55	0.42
1:A:293:GLU:O	1:A:316:ALA:C	2.52	0.42
1:A:169:LEU:C	1:A:171:ASN:H	2.22	0.42
1:A:243:GLY:O	1:A:244:SER:CB	2.67	0.42
1:C:201:ILE:HG22	1:C:264:SER:OG	2.20	0.42
1:C:112:GLU:CA	1:C:284:GLY:CA	2.96	0.42
1:C:315:ALA:CA	1:C:318:SER:HB2	2.49	0.42
1:C:289:THR:CG2	1:C:321:TRP:CZ3	3.03	0.42
1:C:291:PHE:CE1	1:C:335:MET:HE3	2.54	0.42
1:B:170:TYR:C	1:B:171:ASN:ND2	2.72	0.42
1:A:268:THR:O	1:A:268:THR:CG2	2.66	0.42
1:A:266:SER:HA	1:A:280:PHE:HA	2.02	0.42
1:B:297:VAL:HB	1:B:336:VAL:CG1	1.98	0.42
1:B:343:LYS:HB2	1:B:344:GLY:H	1.13	0.42
1:A:170:TYR:C	1:A:171:ASN:ND2	2.72	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:SER:HA	1:A:231:ARG:HD2	2.01	0.42
1:C:101:PRO:HG2	1:C:166:LEU:HD12	1.94	0.42
1:C:163:PRO:CG	1:C:168:SER:HB2	2.50	0.42
1:C:216:THR:OG1	1:C:227:LEU:HD21	2.18	0.42
1:C:258:ASP:OD1	1:C:259:GLY:N	2.52	0.42
1:C:269:LYS:CG	1:C:270:GLY:H	2.23	0.42
1:B:154:PHE:CE1	1:B:156:ARG:CA	3.02	0.42
1:A:273:GLY:O	1:A:275:GLU:HB3	2.19	0.42
1:A:302:ASN:HB3	1:A:308:PHE:CE1	2.55	0.42
1:A:296:PRO:HD2	1:A:337:THR:CG2	2.49	0.42
1:A:163:PRO:CG	1:A:168:SER:HB2	2.50	0.42
1:B:133:SER:CB	1:B:235:THR:CG2	2.94	0.42
1:B:169:LEU:C	1:B:171:ASN:H	2.23	0.42
1:B:185:ILE:HD12	1:B:186:LEU:O	2.20	0.42
1:B:243:GLY:O	1:B:244:SER:CB	2.66	0.42
1:B:315:ALA:CA	1:B:318:SER:HB2	2.49	0.42
1:B:315:ALA:HB1	1:B:318:SER:HB3	1.72	0.42
1:B:87:SER:HA	1:B:231:ARG:HD2	2.01	0.42
1:B:93:LEU:HD12	1:B:138:TYR:CE1	2.54	0.42
1:C:75:VAL:HG12	1:C:76:SER:N	2.35	0.42
1:A:258:ASP:OD1	1:A:259:GLY:N	2.52	0.42
1:A:279:HIS:O	1:A:280:PHE:N	2.42	0.42
1:A:313:GLU:HB2	1:A:315:ALA:CA	2.50	0.42
1:A:289:THR:CG2	1:A:321:TRP:CZ3	3.03	0.42
1:B:336:VAL:CG1	1:B:336:VAL:O	2.67	0.42
1:A:185:ILE:HD12	1:A:186:LEU:O	2.20	0.42
1:A:101:PRO:CG	1:A:217:TYR:HD2	2.26	0.42
1:A:134:LEU:N	1:A:233:GLU:O	2.44	0.42
1:A:93:LEU:HD12	1:A:138:TYR:CE1	2.54	0.42
1:C:130:ARG:NH1	1:C:236:VAL:C	2.70	0.42
1:C:107:VAL:HG11	1:C:283:THR:HG22	2.02	0.42
1:C:292:TYR:CD1	1:C:292:TYR:C	2.93	0.42
1:C:207:VAL:HG11	1:C:329:ARG:NE	2.24	0.42
1:B:149:LYS:CD	1:B:217:TYR:HE1	2.33	0.42
1:B:95:LYS:HZ1	1:B:221:ALA:CB	2.32	0.42
1:B:236:VAL:CG1	1:B:238:LEU:HD11	2.50	0.42
1:A:248:ALA:HB1	1:A:265:TRP:CA	2.38	0.42
1:A:315:ALA:CA	1:A:318:SER:CB	2.97	0.42
1:C:336:VAL:O	1:C:336:VAL:CG1	2.66	0.42
1:A:244:SER:C	1:A:245:THR:HG22	2.31	0.41
1:C:186:LEU:C	1:C:186:LEU:CD2	2.87	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:LYS:C	1:C:277:ASP:CB	2.63	0.41
1:B:292:TYR:C	1:B:292:TYR:CD1	2.94	0.41
1:A:141:MET:CG	1:A:141:MET:O	2.46	0.41
1:A:130:ARG:HB2	1:A:237:GLN:CA	2.49	0.41
1:A:236:VAL:CG1	1:A:238:LEU:HD11	2.49	0.41
1:C:264:SER:OG	1:C:265:TRP:CA	2.69	0.41
1:C:269:LYS:CE	1:C:270:GLY:O	2.63	0.41
1:C:88:GLU:O	1:C:231:ARG:HB3	2.05	0.41
1:B:315:ALA:CA	1:B:318:SER:CB	2.97	0.41
1:B:289:THR:CG2	1:B:321:TRP:CZ3	3.03	0.41
1:B:254:ALA:O	1:B:257:LYS:N	2.38	0.41
1:A:154:PHE:CZ	1:A:156:ARG:CA	3.01	0.41
1:A:197:VAL:CG2	1:A:198:ALA:H	2.34	0.41
1:A:149:LYS:CD	1:A:217:TYR:HE1	2.34	0.41
1:C:93:LEU:CD1	1:C:138:TYR:HE1	2.33	0.41
1:C:199:ASP:CA	1:C:265:TRP:CD1	3.02	0.41
1:B:125:GLN:HA	1:B:243:GLY:N	2.34	0.41
1:B:139:SER:HA	1:B:140:PRO:HD3	1.13	0.41
1:C:141:MET:O	1:C:141:MET:CG	2.46	0.41
1:A:93:LEU:CD1	1:A:138:TYR:HE1	2.33	0.41
1:A:291:PHE:CD2	1:A:345:LYS:O	2.73	0.41
1:B:264:SER:OG	1:B:265:TRP:CA	2.69	0.41
1:A:130:ARG:CG	1:A:131:PHE:N	2.79	0.41
1:A:151:ALA:HA	1:A:177:SER:CB	2.21	0.41
1:C:185:ILE:HD12	1:C:186:LEU:O	2.20	0.41
1:C:278:CYS:O	1:C:333:VAL:O	2.37	0.41
1:B:154:PHE:CZ	1:B:156:ARG:CA	3.02	0.41
1:B:197:VAL:CG2	1:B:198:ALA:H	2.34	0.41
1:B:125:GLN:CA	1:B:243:GLY:HA2	2.27	0.41
1:C:66:TYR:HE2	1:C:183:GLY:CA	2.33	0.41
1:A:306:SER:HB2	1:A:325:LYS:N	2.33	0.41
1:A:126:TYR:O	1:A:242:THR:CG2	2.66	0.41
1:A:128:LYS:O	1:A:238:LEU:HA	2.21	0.41
1:A:163:PRO:HG3	1:A:168:SER:CB	2.47	0.41
1:C:135:ARG:N	1:C:233:GLU:O	2.54	0.41
1:B:136:PHE:CE2	1:B:212:LEU:HD13	2.56	0.41
1:B:289:THR:O	1:B:290:LEU:CG	2.69	0.41
1:A:341:GLN:O	1:A:342:PRO:C	2.58	0.41
1:C:269:LYS:O	1:C:277:ASP:CA	2.57	0.41
1:C:315:ALA:CA	1:C:318:SER:CB	2.97	0.41
1:B:120:ILE:HG13	1:B:350:ARG:HH12	1.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:GLN:HG3	1:A:263:VAL:O	2.21	0.41
1:B:249:GLN:HG3	1:B:263:VAL:O	2.21	0.41
1:A:297:VAL:HG12	1:A:336:VAL:HG11	0.98	0.41
1:B:337:THR:OG1	1:B:343:LYS:NZ	2.42	0.41
1:C:249:GLN:HG3	1:C:263:VAL:O	2.21	0.41
1:C:289:THR:O	1:C:290:LEU:CG	2.69	0.41
1:C:90:ILE:HD13	1:C:90:ILE:HG21	1.83	0.41
1:B:93:LEU:CD1	1:B:138:TYR:CE1	3.03	0.41
1:A:264:SER:OG	1:A:265:TRP:CA	2.69	0.41
1:A:253:PHE:CZ	1:A:268:THR:HG21	2.56	0.41
1:B:262:LEU:HD23	1:B:262:LEU:HA	1.71	0.41
1:A:111:SER:HB3	1:A:197:VAL:HG21	2.02	0.41
1:A:172:ILE:HG21	1:A:172:ILE:HD13	1.88	0.41
1:A:135:ARG:N	1:A:233:GLU:O	2.54	0.41
1:A:93:LEU:CD1	1:A:138:TYR:CE1	3.03	0.41
1:C:136:PHE:CG	1:C:212:LEU:HD21	2.56	0.41
1:C:191:ASP:HB2	1:C:192:SER:H	1.41	0.41
1:C:231:ARG:CG	1:C:232:VAL:H	2.27	0.41
1:C:253:PHE:CZ	1:C:268:THR:HG21	2.56	0.41
1:C:308:PHE:HE1	1:C:333:VAL:CG1	2.34	0.41
1:C:252:ASP:OD1	1:C:345:LYS:HG2	2.20	0.41
1:C:252:ASP:OD2	1:C:345:LYS:HG2	2.16	0.41
1:C:86:GLY:O	1:C:87:SER:CB	2.69	0.41
1:C:120:ILE:HD13	1:C:120:ILE:HG21	1.87	0.41
1:C:93:LEU:CD1	1:C:138:TYR:CE1	3.03	0.41
1:C:291:PHE:CD2	1:C:345:LYS:O	2.73	0.41
1:C:313:GLU:HB2	1:C:315:ALA:CA	2.50	0.41
1:C:95:LYS:HB3	1:C:96:ASN:H	1.60	0.41
1:B:128:LYS:O	1:B:238:LEU:HA	2.21	0.41
1:B:130:ARG:CG	1:B:131:PHE:N	2.79	0.41
1:B:313:GLU:HB2	1:B:315:ALA:CA	2.50	0.41
1:A:308:PHE:HE1	1:A:333:VAL:CG1	2.34	0.41
1:B:248:ALA:CB	1:B:249:GLN:HB2	2.47	0.41
1:B:296:PRO:HB2	1:B:297:VAL:H	0.85	0.41
1:C:55:VAL:O	1:C:57:ARG:N	2.52	0.41
1:C:130:ARG:HB2	1:C:237:GLN:CA	2.49	0.41
1:C:176:VAL:O	1:C:176:VAL:CG1	2.69	0.41
1:C:128:LYS:O	1:C:238:LEU:HA	2.21	0.41
1:B:93:LEU:CD1	1:B:138:TYR:HE1	2.33	0.41
1:A:289:THR:O	1:A:290:LEU:CG	2.69	0.41
1:C:197:VAL:CG2	1:C:198:ALA:H	2.33	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:PRO:CG	1:B:168:SER:HB2	2.50	0.40
1:B:134:LEU:N	1:B:233:GLU:O	2.44	0.40
1:B:135:ARG:N	1:B:233:GLU:O	2.54	0.40
1:B:302:ASN:HB3	1:B:308:PHE:CD1	2.56	0.40
1:B:291:PHE:CD2	1:B:345:LYS:O	2.73	0.40
1:A:302:ASN:HB3	1:A:308:PHE:CD1	2.56	0.40
1:B:294:LYS:O	1:B:296:PRO:CG	2.65	0.40
1:A:130:ARG:HB3	1:A:131:PHE:H	1.46	0.40
1:A:176:VAL:CG1	1:A:176:VAL:O	2.69	0.40
1:C:82:ILE:HD13	1:C:238:LEU:HD22	2.03	0.40
1:C:71:THR:HG23	1:C:87:SER:OG	2.03	0.40
1:C:75:VAL:CG2	1:C:75:VAL:N	2.84	0.40
1:C:296:PRO:HD2	1:C:337:THR:CG2	2.49	0.40
1:A:136:PHE:CG	1:A:212:LEU:HD21	2.56	0.40
1:C:278:CYS:HB3	1:C:333:VAL:C	2.35	0.40
1:C:302:ASN:HB3	1:C:308:PHE:CD1	2.56	0.40
1:C:313:GLU:HG2	1:C:313:GLU:H	1.62	0.40
1:C:91:THR:HG23	1:C:92:THR:N	2.36	0.40
1:B:136:PHE:CG	1:B:212:LEU:HD21	2.56	0.40
1:B:308:PHE:HE1	1:B:333:VAL:CG1	2.34	0.40
1:B:299:GLY:HA2	1:B:335:MET:HG2	2.03	0.40
1:A:246:SER:CB	1:A:263:VAL:HG13	2.52	0.40
1:C:341:GLN:HE21	1:C:341:GLN:HB2	1.72	0.40
1:A:190:THR:HG22	1:A:191:ASP:O	2.22	0.40
1:A:86:GLY:O	1:A:87:SER:CB	2.69	0.40
1:C:149:LYS:CD	1:C:217:TYR:HE1	2.33	0.40
1:C:93:LEU:HD12	1:C:138:TYR:CE1	2.54	0.40
1:B:149:LYS:HG2	1:B:150:VAL:H	1.87	0.40
1:B:176:VAL:CG1	1:B:176:VAL:O	2.69	0.40
1:B:190:THR:HG22	1:B:191:ASP:O	2.22	0.40
1:C:297:VAL:HG12	1:C:336:VAL:HG11	0.98	0.40
1:A:91:THR:HG23	1:A:92:THR:N	2.36	0.40
1:C:119:LEU:C	1:C:121:LYS:H	2.25	0.40
1:B:86:GLY:O	1:B:87:SER:CB	2.69	0.40
1:A:336:VAL:O	1:A:336:VAL:CG1	2.67	0.40
1:B:341:GLN:O	1:B:342:PRO:C	2.58	0.40
1:A:256:VAL:HG13	1:A:257:LYS:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	263/347 (76%)	144 (55%)	60 (23%)	59 (22%)	0 2
1	B	263/347 (76%)	144 (55%)	60 (23%)	59 (22%)	0 2
1	C	291/347 (84%)	161 (55%)	64 (22%)	66 (23%)	0 2
All	All	817/1041 (78%)	449 (55%)	184 (22%)	184 (22%)	0 2

All (184) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	THR
1	A	87	SER
1	A	90	ILE
1	A	95	LYS
1	A	96	ASN
1	A	97	THR
1	A	119	LEU
1	A	128	LYS
1	A	140	PRO
1	A	157	ASP
1	A	160	LYS
1	A	166	LEU
1	A	173	GLU
1	A	202	SER
1	A	209	PHE
1	A	227	LEU
1	A	240	ASN
1	A	244	SER
1	A	245	THR
1	A	246	SER
1	A	255	GLY
1	A	290	LEU
1	A	293	GLU
1	A	295	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	307	ASP
1	A	316	ALA
1	A	329	ARG
1	A	339	GLU
1	A	341	GLN
1	B	83	THR
1	B	87	SER
1	B	90	ILE
1	B	95	LYS
1	B	96	ASN
1	B	97	THR
1	B	119	LEU
1	B	128	LYS
1	B	140	PRO
1	B	157	ASP
1	B	160	LYS
1	B	166	LEU
1	B	173	GLU
1	B	202	SER
1	B	209	PHE
1	B	227	LEU
1	B	240	ASN
1	B	244	SER
1	B	245	THR
1	B	246	SER
1	B	255	GLY
1	B	290	LEU
1	B	293	GLU
1	B	295	ALA
1	B	307	ASP
1	B	316	ALA
1	B	329	ARG
1	B	339	GLU
1	B	341	GLN
1	C	55	VAL
1	C	56	THR
1	C	77	THR
1	C	79	ARG
1	C	80	ASP
1	C	83	THR
1	C	87	SER
1	C	90	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	95	LYS
1	C	96	ASN
1	C	97	THR
1	C	119	LEU
1	C	128	LYS
1	C	140	PRO
1	C	157	ASP
1	C	160	LYS
1	C	166	LEU
1	C	173	GLU
1	C	202	SER
1	C	209	PHE
1	C	227	LEU
1	C	240	ASN
1	C	244	SER
1	C	245	THR
1	C	246	SER
1	C	255	GLY
1	C	290	LEU
1	C	293	GLU
1	C	295	ALA
1	C	307	ASP
1	C	316	ALA
1	C	329	ARG
1	C	339	GLU
1	C	341	GLN
1	A	101	PRO
1	A	105	THR
1	A	114	GLY
1	A	115	THR
1	A	116	PHE
1	A	151	ALA
1	A	156	ARG
1	A	158	ALA
1	A	167	ALA
1	A	291	PHE
1	A	292	TYR
1	A	296	PRO
1	A	315	ALA
1	B	101	PRO
1	B	105	THR
1	B	114	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	115	THR
1	B	116	PHE
1	B	151	ALA
1	B	156	ARG
1	B	158	ALA
1	B	167	ALA
1	B	291	PHE
1	B	292	TYR
1	B	296	PRO
1	B	315	ALA
1	C	69	VAL
1	C	101	PRO
1	C	105	THR
1	C	114	GLY
1	C	115	THR
1	C	116	PHE
1	C	151	ALA
1	C	156	ARG
1	C	158	ALA
1	C	167	ALA
1	C	291	PHE
1	C	292	TYR
1	C	296	PRO
1	C	315	ALA
1	A	145	THR
1	A	152	LEU
1	A	263	VAL
1	B	145	THR
1	B	152	LEU
1	B	263	VAL
1	C	145	THR
1	C	152	LEU
1	C	263	VAL
1	A	131	PHE
1	A	205	LYS
1	A	298	SER
1	A	343	LYS
1	B	131	PHE
1	B	205	LYS
1	B	298	SER
1	B	343	LYS
1	C	131	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	205	LYS
1	C	298	SER
1	C	343	LYS
1	A	134	LEU
1	A	163	PRO
1	A	201	ILE
1	A	260	PRO
1	A	300	LEU
1	A	314	ALA
1	B	82	ILE
1	B	134	LEU
1	B	163	PRO
1	B	201	ILE
1	B	260	PRO
1	B	300	LEU
1	B	314	ALA
1	C	163	PRO
1	C	201	ILE
1	C	260	PRO
1	C	300	LEU
1	C	314	ALA
1	A	82	ILE
1	A	313	GLU
1	B	313	GLU
1	C	71	THR
1	C	82	ILE
1	C	134	LEU
1	C	313	GLU
1	A	297	VAL
1	B	297	VAL
1	C	297	VAL
1	A	259	GLY
1	B	259	GLY
1	C	259	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	215/282 (76%)	178 (83%)	37 (17%)	2 17
1	B	215/282 (76%)	179 (83%)	36 (17%)	3 19
1	C	238/282 (84%)	200 (84%)	38 (16%)	3 21
All	All	668/846 (79%)	557 (83%)	111 (17%)	6 19

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	LEU
1	A	91	THR
1	A	96	ASN
1	A	97	THR
1	A	108	LEU
1	A	117	ASN
1	A	120	ILE
1	A	129	TYR
1	A	134	LEU
1	A	135	ARG
1	A	145	THR
1	A	146	THR
1	A	150	VAL
1	A	152	LEU
1	A	154	PHE
1	A	164	ASN
1	A	165	ASP
1	A	176	VAL
1	A	185	ILE
1	A	192	SER
1	A	199	ASP
1	A	205	LYS
1	A	206	LEU
1	A	208	ASP
1	A	213	ILE
1	A	217	TYR
1	A	234	TYR
1	A	260	PRO
1	A	264	SER
1	A	275	GLU
1	A	276	HIS
1	A	285	ASN
1	A	290	LEU
1	A	292	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	300	LEU
1	A	313	GLU
1	A	339	GLU
1	B	89	LEU
1	B	91	THR
1	B	96	ASN
1	B	97	THR
1	B	108	LEU
1	B	117	ASN
1	B	120	ILE
1	B	129	TYR
1	B	134	LEU
1	B	135	ARG
1	B	145	THR
1	B	146	THR
1	B	150	VAL
1	B	152	LEU
1	B	154	PHE
1	B	164	ASN
1	B	165	ASP
1	B	176	VAL
1	B	185	ILE
1	B	192	SER
1	B	199	ASP
1	B	205	LYS
1	B	206	LEU
1	B	208	ASP
1	B	213	ILE
1	B	217	TYR
1	B	234	TYR
1	B	264	SER
1	B	275	GLU
1	B	276	HIS
1	B	285	ASN
1	B	290	LEU
1	B	292	TYR
1	B	300	LEU
1	B	313	GLU
1	B	339	GLU
1	C	58	LEU
1	C	79	ARG
1	C	89	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	91	THR
1	C	96	ASN
1	C	97	THR
1	C	108	LEU
1	C	117	ASN
1	C	120	ILE
1	C	129	TYR
1	C	134	LEU
1	C	135	ARG
1	C	145	THR
1	C	146	THR
1	C	150	VAL
1	C	152	LEU
1	C	154	PHE
1	C	164	ASN
1	C	165	ASP
1	C	176	VAL
1	C	185	ILE
1	C	192	SER
1	C	199	ASP
1	C	205	LYS
1	C	206	LEU
1	C	208	ASP
1	C	213	ILE
1	C	217	TYR
1	C	234	TYR
1	C	264	SER
1	C	275	GLU
1	C	276	HIS
1	C	285	ASN
1	C	290	LEU
1	C	292	TYR
1	C	300	LEU
1	C	313	GLU
1	C	339	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	117	ASN
1	A	118	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	125	GLN
1	A	164	ASN
1	A	171	ASN
1	A	226	GLN
1	A	237	GLN
1	A	240	ASN
1	A	285	ASN
1	A	341	GLN
1	B	96	ASN
1	B	109	ASN
1	B	117	ASN
1	B	118	GLN
1	B	125	GLN
1	B	164	ASN
1	B	171	ASN
1	B	226	GLN
1	B	237	GLN
1	B	240	ASN
1	B	285	ASN
1	B	341	GLN
1	C	72	GLN
1	C	96	ASN
1	C	109	ASN
1	C	118	GLN
1	C	125	GLN
1	C	164	ASN
1	C	171	ASN
1	C	226	GLN
1	C	237	GLN
1	C	240	ASN
1	C	249	GLN
1	C	285	ASN
1	C	341	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.