



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:34 PM UTC

PDB ID : 2DHH / pdb_00002dhh
Title : Crystal structure of a multidrug transporter reveal a functionally rotating mechanism
Authors : Murakami, S.; Nakashima, R.; Yamashita, E.; Matsumoto, T.
Deposited on : 2006-03-23
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

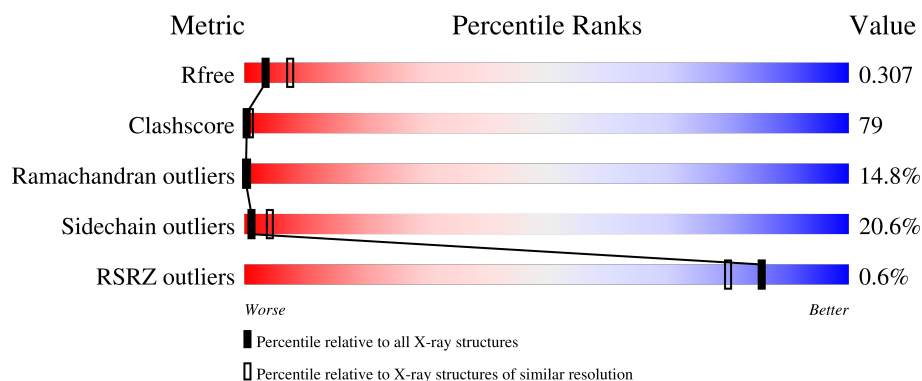
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	1053	
1	B	1053	
1	C	1053	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23378 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ACRB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			
1	B	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			
1	C	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	HIS	-	expression tag	UNP P31224
A	1051	HIS	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
B	1050	HIS	-	expression tag	UNP P31224
B	1051	HIS	-	expression tag	UNP P31224
B	1052	HIS	-	expression tag	UNP P31224
B	1053	HIS	-	expression tag	UNP P31224
C	1050	HIS	-	expression tag	UNP P31224
C	1051	HIS	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224

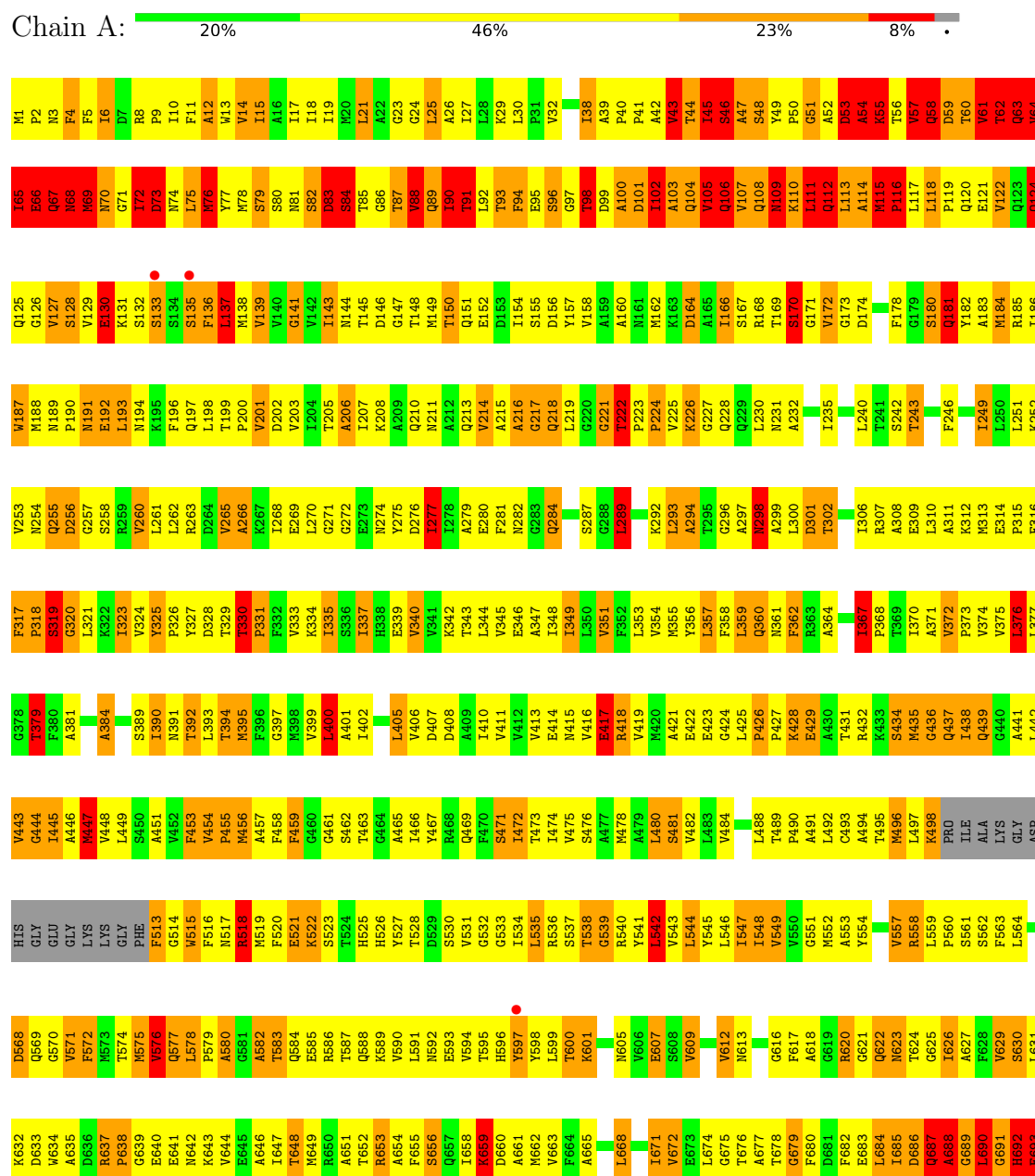
- Molecule 2 is water.

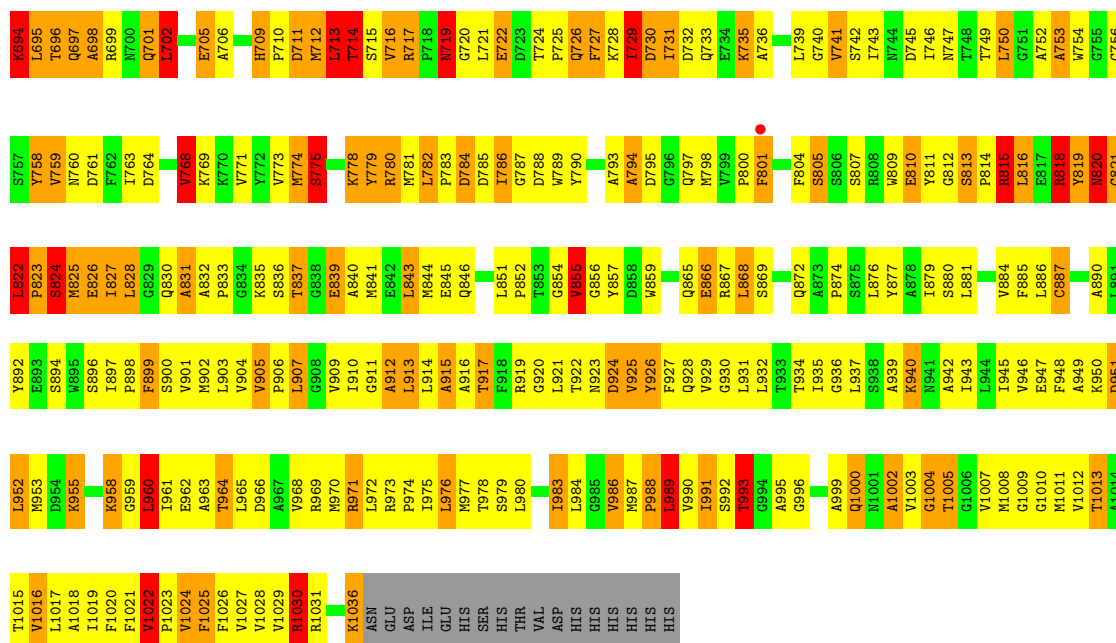
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	22	Total	O	0	0
			22	22		
2	B	8	Total	O	0	0
			8	8		
2	C	26	Total	O	0	0
			26	26		

3 Residue-property plots

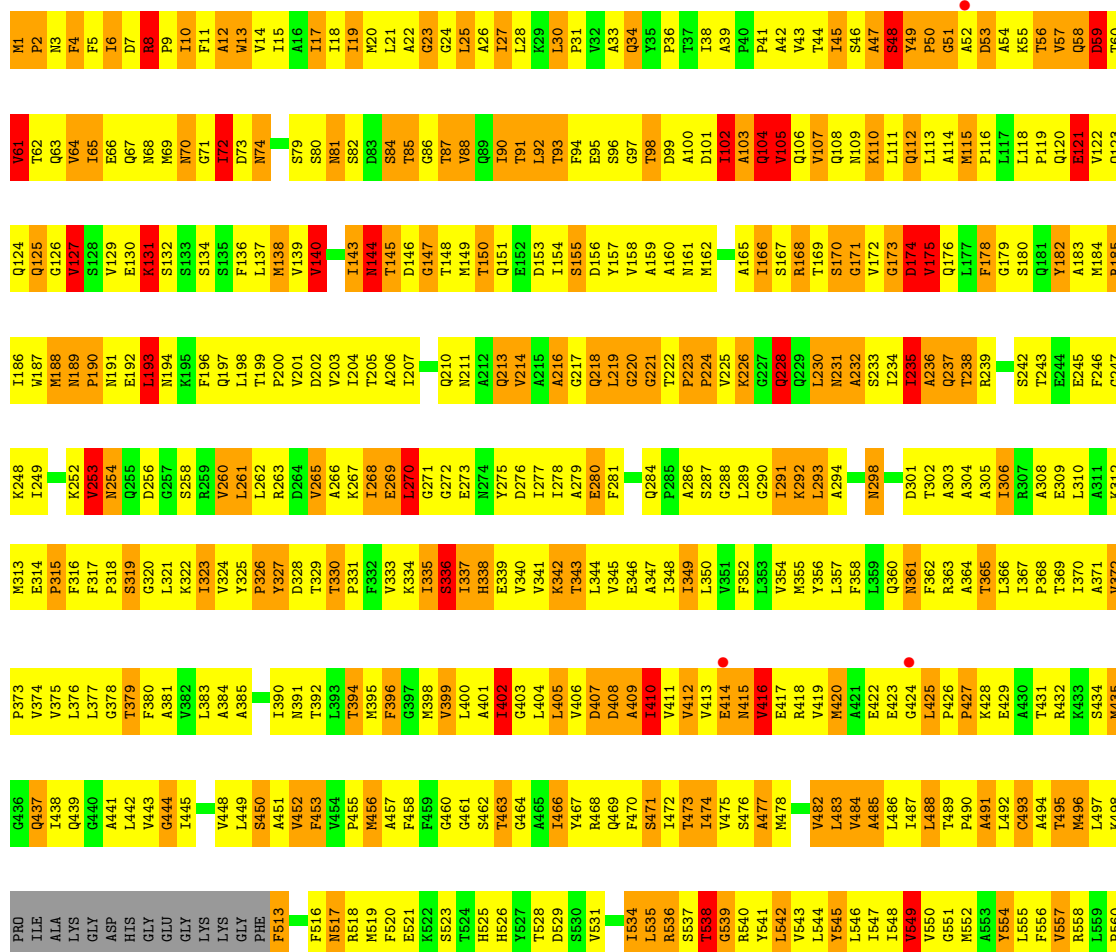
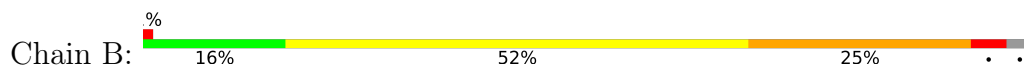
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: ACRB





• Molecule 1: ACRB







4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	225.87Å 134.42Å 163.19Å 90.00° 97.71° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80 10.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (10.00-2.80) 96.7 (10.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.268 , 0.307 0.262 , 0.307	Depositor DCC
R_{free} test set	5752 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	73.4	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 78.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23378	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.97	199/7920 (2.5%)	1.66	169/10756 (1.6%)
1	B	1.29	28/7920 (0.4%)	1.42	101/10756 (0.9%)
1	C	1.98	175/7920 (2.2%)	1.71	209/10756 (1.9%)
All	All	1.78	402/23760 (1.7%)	1.60	479/32268 (1.5%)

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	4
1	B	0	2
1	C	0	6
All	All	0	12

All (402) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	166	ILE	CA-CB	34.30	2.01	1.54
1	C	167	SER	N-CA	31.68	1.87	1.46
1	C	166	ILE	CA-C	-25.56	1.20	1.52
1	C	45	ILE	CA-CB	24.92	1.88	1.54
1	A	68	ASN	CA-CB	24.51	1.94	1.53
1	C	164	ASP	C-O	23.35	1.53	1.24
1	C	161	ASN	N-CA	23.27	1.76	1.46
1	A	67	GLN	CB-CG	21.41	2.16	1.52
1	A	65	ILE	CA-C	20.72	1.79	1.52
1	C	169	THR	CA-CB	19.01	1.85	1.53
1	A	54	ALA	CA-CB	-18.92	1.21	1.53
1	A	68	ASN	N-CA	18.78	1.70	1.46
1	A	823	PRO	C-O	18.26	1.47	1.24
1	A	63	GLN	N-CA	-18.15	1.22	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	VAL	CA-CB	17.86	1.71	1.55
1	A	45	ILE	CA-CB	-17.55	1.30	1.54
1	A	67	GLN	CA-C	-17.27	1.29	1.52
1	C	157	TYR	C-O	16.94	1.45	1.24
1	A	818	ARG	CG-CD	16.71	2.02	1.52
1	A	69	MET	C-O	16.67	1.45	1.24
1	A	70	ASN	CA-C	16.41	1.73	1.52
1	C	160	ALA	CA-CB	-16.00	1.26	1.53
1	A	66	GLU	CA-C	15.83	1.74	1.52
1	A	108	GLN	CA-C	-15.70	1.31	1.52
1	A	65	ILE	C-O	15.64	1.42	1.24
1	C	91	THR	CA-CB	15.02	1.78	1.53
1	C	769	LYS	CA-C	14.94	1.71	1.52
1	A	107	VAL	CA-C	-14.43	1.34	1.52
1	A	823	PRO	N-CA	-14.13	1.29	1.47
1	C	289	LEU	N-CA	-13.99	1.28	1.46
1	A	107	VAL	C-N	13.95	1.53	1.33
1	C	161	ASN	CA-CB	-13.78	1.30	1.53
1	C	129	VAL	CB-CG2	13.47	1.97	1.52
1	C	42	ALA	CA-CB	-13.31	1.30	1.53
1	A	818	ARG	C-N	12.77	1.50	1.33
1	A	110	LYS	N-CA	-12.74	1.29	1.46
1	C	164	ASP	CG-OD2	12.68	1.49	1.25
1	A	105	VAL	C-O	12.46	1.39	1.24
1	C	128	SER	CA-CB	12.41	1.74	1.53
1	C	160	ALA	CA-C	-12.24	1.36	1.52
1	C	127	VAL	CA-CB	12.20	1.75	1.55
1	C	181	GLN	CD-OE1	11.88	1.46	1.23
1	C	166	ILE	N-CA	-11.85	1.31	1.46
1	A	64	VAL	C-N	11.77	1.49	1.33
1	A	816	LEU	N-CA	-11.68	1.31	1.46
1	C	767	ARG	CZ-NH2	-11.43	1.18	1.33
1	A	108	GLN	CB-CG	11.18	1.85	1.52
1	A	111	LEU	N-CA	10.81	1.60	1.46
1	A	822	LEU	CA-C	-10.68	1.42	1.52
1	A	819	TYR	CA-CB	-10.65	1.36	1.53
1	A	727	PHE	CA-C	-10.64	1.39	1.52
1	A	819	TYR	C-O	10.56	1.37	1.23
1	C	104	GLN	CA-CB	10.42	1.71	1.53
1	A	822	LEU	CA-CB	10.33	1.69	1.54
1	C	165	ALA	C-O	10.26	1.37	1.24
1	C	169	THR	C-O	10.24	1.35	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	VAL	CA-C	10.20	1.68	1.53
1	A	129	VAL	N-CA	-10.08	1.34	1.46
1	C	297	ALA	CA-CB	-10.06	1.37	1.53
1	A	65	ILE	CA-CB	-10.02	1.40	1.54
1	A	66	GLU	C-O	-9.97	1.11	1.24
1	A	1022	VAL	CA-CB	9.96	1.60	1.53
1	B	105	VAL	CA-CB	9.90	1.68	1.54
1	A	685	ILE	C-O	-9.89	1.10	1.24
1	A	266	ALA	CA-CB	-9.83	1.46	1.54
1	A	725	PRO	C-O	9.66	1.35	1.23
1	A	826	GLU	CA-C	-9.64	1.40	1.52
1	C	199	THR	CA-CB	9.62	1.65	1.53
1	C	174	ASP	N-CA	9.57	1.57	1.46
1	C	764	ASP	N-CA	9.54	1.57	1.46
1	A	63	GLN	CA-C	-9.51	1.40	1.52
1	C	106	GLN	C-O	9.45	1.35	1.24
1	A	57	VAL	CA-CB	-9.35	1.41	1.54
1	C	107	VAL	CA-CB	9.34	1.66	1.54
1	A	105	VAL	CA-CB	-9.18	1.42	1.54
1	C	46	SER	CA-CB	9.11	1.68	1.53
1	A	696	THR	CA-CB	9.04	1.69	1.53
1	A	79	SER	C-O	9.04	1.36	1.23
1	C	767	ARG	C-O	9.01	1.34	1.23
1	C	164	ASP	CG-OD1	8.99	1.42	1.25
1	A	813	SER	CA-CB	8.99	1.65	1.53
1	A	688	ALA	CA-CB	8.99	1.68	1.53
1	A	62	THR	N-CA	8.94	1.57	1.46
1	A	690	LEU	CA-C	8.85	1.64	1.52
1	A	114	ALA	CA-C	8.85	1.64	1.52
1	A	698	ALA	CA-CB	-8.82	1.39	1.53
1	C	128	SER	CA-C	-8.77	1.42	1.52
1	A	45	ILE	N-CA	-8.73	1.35	1.46
1	A	45	ILE	C-N	8.71	1.45	1.33
1	A	106	GLN	N-CA	8.67	1.57	1.46
1	C	102	ILE	CA-CB	-8.67	1.42	1.54
1	A	73	ASP	CA-C	8.65	1.64	1.52
1	C	44	THR	C-O	8.61	1.34	1.23
1	A	819	TYR	CA-C	-8.59	1.42	1.52
1	B	110	LYS	N-CA	8.57	1.57	1.46
1	C	115	MET	CA-C	-8.55	1.42	1.52
1	C	65	ILE	CA-CB	8.54	1.64	1.54
1	A	825	MET	N-CA	8.52	1.55	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	ILE	C-O	8.49	1.34	1.24
1	A	91	THR	CA-C	8.46	1.63	1.52
1	C	671	ILE	CA-CB	8.44	1.66	1.54
1	A	128	SER	CA-C	8.37	1.62	1.52
1	A	67	GLN	C-O	8.35	1.34	1.24
1	A	180	SER	CA-C	-8.31	1.48	1.52
1	C	291	ILE	CA-CB	-8.28	1.43	1.54
1	A	104	GLN	N-CA	8.20	1.56	1.46
1	A	116	PRO	CA-C	-8.19	1.40	1.52
1	C	74	ASN	C-O	-8.18	1.13	1.24
1	C	235	ILE	CA-CB	8.11	1.65	1.54
1	A	41	PRO	CA-C	-8.10	1.45	1.52
1	C	273	GLU	C-O	-8.09	1.13	1.24
1	A	688	ALA	N-CA	8.02	1.56	1.46
1	A	66	GLU	CA-CB	7.99	1.67	1.53
1	C	991	ILE	CA-CB	7.97	1.63	1.53
1	A	100	ALA	CA-CB	-7.88	1.41	1.53
1	A	725	PRO	CA-C	7.84	1.62	1.52
1	A	46	SER	CA-CB	-7.78	1.41	1.53
1	A	112	GLN	N-CA	-7.76	1.36	1.46
1	A	67	GLN	N-CA	-7.76	1.36	1.46
1	C	57	VAL	CA-CB	7.69	1.63	1.54
1	A	72	ILE	C-O	7.64	1.33	1.24
1	A	93	THR	C-O	7.62	1.33	1.23
1	A	44	THR	CA-CB	-7.62	1.40	1.53
1	A	64	VAL	C-O	-7.62	1.15	1.24
1	C	63	GLN	N-CA	7.62	1.55	1.46
1	C	114	ALA	CA-CB	-7.61	1.42	1.54
1	A	129	VAL	CA-CB	-7.58	1.44	1.54
1	A	44	THR	C-O	7.57	1.33	1.23
1	C	158	VAL	CB-CG2	7.54	1.77	1.52
1	A	692	HIS	CA-C	7.53	1.62	1.52
1	C	306	ILE	CA-C	-7.50	1.44	1.52
1	C	58	GLN	CB-CG	7.48	1.75	1.52
1	C	105	VAL	CA-C	7.46	1.62	1.52
1	C	314	GLU	N-CA	7.44	1.56	1.46
1	B	214	VAL	CA-CB	-7.44	1.44	1.54
1	A	59	ASP	CA-C	-7.41	1.42	1.52
1	A	813	SER	CA-C	7.39	1.62	1.52
1	A	69	MET	CB-CG	7.38	1.74	1.52
1	A	70	ASN	N-CA	7.36	1.54	1.46
1	A	819	TYR	CG-CD1	7.34	1.54	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	ASN	C-O	7.34	1.33	1.24
1	A	79	SER	N-CA	7.26	1.55	1.45
1	A	814	PRO	N-CA	7.26	1.53	1.47
1	C	162	MET	CA-CB	7.25	1.65	1.53
1	C	390	ILE	CA-CB	-7.22	1.45	1.54
1	A	811	TYR	CA-CB	-7.16	1.42	1.53
1	A	101	ASP	CA-C	-7.14	1.43	1.52
1	A	43	VAL	CA-CB	-7.11	1.44	1.54
1	A	768	VAL	CA-CB	-7.11	1.47	1.54
1	A	72	ILE	CB-CG1	7.07	1.67	1.53
1	C	104	GLN	CG-CD	-7.03	1.34	1.52
1	A	821	GLY	N-CA	7.02	1.56	1.44
1	A	41	PRO	C-O	-7.00	1.18	1.24
1	A	103	ALA	CA-CB	6.96	1.64	1.53
1	A	691	GLY	C-O	6.96	1.31	1.23
1	B	47	ALA	CA-C	-6.95	1.44	1.52
1	C	46	SER	C-O	-6.95	1.15	1.24
1	A	76	MET	CA-C	-6.95	1.43	1.52
1	A	43	VAL	C-O	6.94	1.32	1.24
1	A	55	LYS	CD-CE	6.94	1.73	1.52
1	A	687	GLN	CA-CB	6.93	1.65	1.53
1	C	106	GLN	CA-C	-6.93	1.43	1.52
1	C	140	VAL	CA-CB	-6.93	1.44	1.54
1	C	770	LYS	CG-CD	6.87	1.73	1.52
1	B	235	ILE	N-CA	6.87	1.54	1.46
1	A	65	ILE	N-CA	6.86	1.54	1.46
1	A	122	VAL	CA-CB	6.86	1.64	1.54
1	C	67	GLN	N-CA	6.86	1.55	1.46
1	A	70	ASN	CB-CG	-6.80	1.35	1.52
1	A	53	ASP	CA-C	-6.79	1.43	1.52
1	A	107	VAL	C-O	6.78	1.32	1.24
1	C	94	PHE	CA-C	-6.76	1.43	1.53
1	C	67	GLN	CA-C	-6.75	1.43	1.52
1	A	62	THR	CA-CB	-6.72	1.42	1.53
1	A	104	GLN	CG-CD	6.72	1.68	1.52
1	C	78	MET	CA-C	-6.72	1.44	1.52
1	B	140	VAL	CA-CB	6.70	1.63	1.54
1	C	810	GLU	C-O	6.68	1.30	1.24
1	B	178	PHE	CA-C	-6.65	1.45	1.53
1	A	620	ARG	CA-C	-6.61	1.46	1.53
1	B	102	ILE	CA-C	-6.61	1.43	1.52
1	A	58	GLN	N-CA	6.60	1.54	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	757	SER	CA-C	-6.59	1.44	1.52
1	A	696	THR	CA-C	-6.58	1.47	1.52
1	C	96	SER	CA-C	-6.57	1.44	1.52
1	C	945	ILE	CA-CB	6.57	1.63	1.54
1	A	85	THR	N-CA	-6.56	1.37	1.46
1	C	78	MET	C-O	-6.55	1.15	1.23
1	C	419	VAL	CA-CB	6.55	1.63	1.54
1	C	266	ALA	CA-CB	-6.54	1.41	1.52
1	A	825	MET	SD-CE	6.53	1.95	1.79
1	C	140	VAL	C-N	6.52	1.40	1.33
1	A	133	SER	CA-C	6.52	1.60	1.52
1	C	309	GLU	CA-C	-6.50	1.44	1.52
1	A	820	ASN	C-N	6.50	1.43	1.33
1	A	47	ALA	CA-CB	-6.49	1.42	1.53
1	A	118	LEU	CB-CG	6.48	1.66	1.53
1	C	303	ALA	CA-CB	-6.48	1.42	1.53
1	A	719	ASN	CA-C	-6.47	1.44	1.52
1	A	582	ALA	CA-C	6.45	1.61	1.52
1	B	108	GLN	N-CA	6.44	1.54	1.46
1	A	75	LEU	CA-C	6.42	1.61	1.52
1	C	128	SER	N-CA	6.42	1.53	1.46
1	C	92	LEU	C-O	6.42	1.31	1.24
1	B	90	ILE	CA-CB	-6.41	1.46	1.54
1	A	84	SER	CA-C	6.41	1.63	1.52
1	B	267	LYS	CA-C	6.39	1.60	1.53
1	C	113	LEU	N-CA	-6.36	1.38	1.46
1	A	73	ASP	CB-CG	6.34	1.68	1.52
1	C	658	ILE	CA-CB	6.34	1.63	1.54
1	C	111	LEU	C-O	-6.32	1.16	1.24
1	A	367	ILE	CA-C	6.31	1.59	1.52
1	C	172	VAL	CA-CB	6.30	1.63	1.54
1	A	46	SER	CA-C	-6.27	1.44	1.52
1	C	213	GLN	C-O	6.26	1.31	1.23
1	C	66	GLU	CA-CB	6.25	1.63	1.53
1	A	87	THR	CA-CB	-6.24	1.43	1.53
1	A	81	ASN	N-CA	6.23	1.53	1.46
1	A	114	ALA	C-O	6.23	1.31	1.24
1	B	237	GLN	CA-C	-6.19	1.44	1.53
1	C	220	GLY	C-O	-6.15	1.15	1.23
1	A	115	MET	C-O	6.15	1.32	1.24
1	A	815	ARG	N-CA	6.15	1.54	1.46
1	C	162	MET	C-O	6.12	1.31	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	216	ALA	C-O	6.11	1.31	1.23
1	C	104	GLN	CA-C	6.11	1.60	1.52
1	C	174	ASP	C-O	6.11	1.31	1.23
1	A	94	PHE	CA-C	6.11	1.60	1.52
1	A	815	ARG	NE-CZ	6.06	1.39	1.33
1	A	821	GLY	C-N	6.06	1.41	1.33
1	C	311	ALA	CA-CB	-6.05	1.43	1.53
1	C	631	LEU	N-CA	6.04	1.53	1.46
1	C	104	GLN	N-CA	6.03	1.53	1.46
1	A	130	GLU	CA-C	6.01	1.60	1.52
1	C	776	GLU	CA-C	-6.01	1.45	1.52
1	C	103	ALA	CA-CB	-5.99	1.43	1.53
1	C	822	LEU	CA-C	5.99	1.60	1.53
1	A	145	THR	CA-CB	5.99	1.61	1.53
1	C	164	ASP	CB-CG	5.99	1.67	1.52
1	C	316	PHE	CG-CD1	-5.98	1.26	1.38
1	C	156	ASP	CA-C	-5.96	1.44	1.52
1	C	212	ALA	CA-CB	5.92	1.64	1.53
1	A	720	GLY	N-CA	5.91	1.52	1.45
1	A	69	MET	N-CA	-5.91	1.38	1.46
1	C	792	ARG	CA-C	-5.89	1.44	1.52
1	C	54	ALA	CA-C	-5.88	1.44	1.52
1	B	230	LEU	N-CA	5.87	1.53	1.46
1	C	168	ARG	CZ-NH2	5.86	1.41	1.33
1	C	807	SER	N-CA	5.86	1.53	1.45
1	A	109	ASN	CB-CG	5.85	1.66	1.52
1	A	289	LEU	CA-C	5.85	1.59	1.52
1	C	776	GLU	C-O	-5.84	1.17	1.23
1	A	69	MET	CG-SD	5.83	1.95	1.80
1	A	93	THR	N-CA	5.82	1.53	1.46
1	A	70	ASN	CG-OD1	5.82	1.34	1.23
1	A	60	THR	CA-C	-5.81	1.45	1.52
1	A	43	VAL	CB-CG1	-5.81	1.33	1.52
1	A	63	GLN	CD-NE2	5.80	1.45	1.33
1	C	305	ALA	CA-CB	5.80	1.62	1.53
1	A	820	ASN	CA-C	-5.76	1.45	1.52
1	C	1027	VAL	CA-CB	5.75	1.60	1.54
1	A	820	ASN	CA-CB	-5.75	1.43	1.53
1	A	826	GLU	N-CA	-5.75	1.38	1.46
1	C	105	VAL	N-CA	5.74	1.53	1.46
1	C	127	VAL	CA-C	5.74	1.59	1.52
1	C	905	VAL	CA-CB	5.74	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	GLN	C-O	5.72	1.31	1.24
1	C	68	ASN	C-O	-5.72	1.16	1.24
1	A	42	ALA	CA-CB	5.72	1.62	1.53
1	A	88	VAL	CA-CB	-5.71	1.47	1.54
1	C	90	ILE	CA-CB	5.70	1.61	1.54
1	A	113	LEU	CG-CD1	5.69	1.71	1.52
1	A	111	LEU	CG-CD1	5.68	1.71	1.52
1	C	43	VAL	C-O	5.68	1.30	1.24
1	A	127	VAL	CA-CB	5.68	1.61	1.54
1	B	64	VAL	CA-CB	-5.68	1.46	1.54
1	C	287	SER	N-CA	-5.68	1.38	1.46
1	A	55	LYS	CG-CD	5.67	1.69	1.52
1	A	52	ALA	CA-CB	-5.67	1.43	1.53
1	C	321	LEU	N-CA	-5.67	1.39	1.46
1	C	610	PHE	C-O	-5.65	1.16	1.23
1	C	316	PHE	CG-CD2	-5.65	1.26	1.38
1	A	395	MET	CA-C	-5.65	1.47	1.53
1	C	671	ILE	CA-C	5.64	1.59	1.52
1	C	158	VAL	C-O	5.63	1.30	1.24
1	A	57	VAL	C-O	5.62	1.30	1.24
1	A	72	ILE	CA-C	-5.62	1.46	1.52
1	A	42	ALA	CA-C	5.61	1.61	1.53
1	C	763	ILE	CG1-CD1	5.61	1.73	1.51
1	B	402	ILE	CA-C	5.61	1.59	1.52
1	C	159	ALA	CA-CB	-5.60	1.44	1.53
1	A	694	LYS	C-O	5.59	1.31	1.24
1	C	222	THR	C-N	5.58	1.40	1.33
1	A	824	SER	CA-C	5.58	1.60	1.52
1	B	175	VAL	N-CA	5.58	1.53	1.46
1	A	79	SER	CA-C	5.57	1.60	1.53
1	A	747	ASN	CA-C	-5.57	1.45	1.52
1	C	201	VAL	CA-CB	-5.57	1.47	1.54
1	C	260	VAL	CA-CB	-5.57	1.47	1.54
1	B	127	VAL	CA-CB	-5.57	1.46	1.54
1	C	212	ALA	C-O	-5.57	1.16	1.23
1	A	83	ASP	N-CA	5.56	1.53	1.45
1	C	769	LYS	CG-CD	5.56	1.69	1.52
1	A	726	GLN	CA-C	-5.54	1.45	1.52
1	A	698	ALA	N-CA	-5.54	1.39	1.46
1	C	164	ASP	C-N	5.53	1.41	1.33
1	A	822	LEU	C-O	5.53	1.31	1.24
1	A	697	GLN	N-CA	5.52	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	THR	CA-CB	5.52	1.62	1.53
1	C	209	ALA	C-O	-5.51	1.17	1.24
1	B	159	ALA	CA-C	-5.49	1.46	1.52
1	C	764	ASP	CA-C	-5.49	1.46	1.52
1	C	184	MET	C-O	5.48	1.30	1.23
1	C	163	LYS	N-CA	5.47	1.52	1.46
1	A	82	SER	C-O	5.46	1.31	1.23
1	C	580	ALA	CA-C	-5.46	1.46	1.52
1	C	759	VAL	C-O	5.46	1.30	1.24
1	C	825	MET	N-CA	5.45	1.53	1.46
1	A	88	VAL	CA-C	-5.44	1.46	1.52
1	A	113	LEU	CA-C	5.43	1.59	1.52
1	A	83	ASP	C-O	-5.43	1.16	1.23
1	C	157	TYR	CE2-CZ	-5.42	1.25	1.38
1	A	827	ILE	CA-C	-5.42	1.46	1.52
1	C	137	LEU	N-CA	5.40	1.52	1.46
1	A	685	ILE	CG1-CD1	5.40	1.72	1.51
1	C	64	VAL	CA-C	-5.40	1.46	1.52
1	B	253	VAL	CA-CB	5.40	1.61	1.54
1	A	340	VAL	CA-CB	5.39	1.61	1.54
1	C	156	ASP	N-CA	-5.38	1.39	1.46
1	C	131	LYS	CE-NZ	5.37	1.65	1.49
1	A	41	PRO	CG-CD	5.37	1.69	1.50
1	A	87	THR	C-O	-5.36	1.17	1.23
1	C	115	MET	N-CA	-5.34	1.41	1.46
1	A	747	ASN	N-CA	-5.33	1.39	1.46
1	C	626	ILE	CA-C	5.33	1.59	1.52
1	C	165	ALA	CA-C	-5.32	1.45	1.52
1	C	726	GLN	CA-C	-5.32	1.45	1.53
1	A	55	LYS	CB-CG	5.31	1.68	1.52
1	B	303	ALA	CA-CB	-5.31	1.45	1.53
1	A	71	GLY	C-O	-5.31	1.16	1.24
1	A	44	THR	CA-C	5.30	1.60	1.53
1	C	128	SER	C-O	5.30	1.30	1.23
1	C	612	VAL	CA-CB	-5.29	1.48	1.54
1	A	214	VAL	CA-CB	-5.29	1.47	1.54
1	C	46	SER	CA-C	5.28	1.59	1.52
1	A	837	THR	CA-CB	5.28	1.61	1.53
1	C	65	ILE	N-CA	5.28	1.52	1.46
1	C	1016	VAL	CA-CB	5.27	1.60	1.54
1	C	129	VAL	CA-C	5.26	1.59	1.52
1	A	70	ASN	C-O	5.25	1.30	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	78	MET	CB-CG	5.23	1.68	1.52
1	C	183	ALA	CA-CB	-5.23	1.44	1.53
1	B	87	THR	CA-CB	-5.22	1.44	1.53
1	A	78	MET	SD-CE	5.21	1.92	1.79
1	A	73	ASP	N-CA	5.21	1.52	1.46
1	C	139	VAL	CA-CB	-5.20	1.46	1.55
1	A	110	LYS	CA-CB	5.20	1.62	1.53
1	C	176	GLN	N-CA	5.20	1.52	1.45
1	A	724	THR	CA-C	-5.19	1.47	1.52
1	B	107	VAL	N-CA	-5.19	1.40	1.46
1	A	813	SER	C-N	-5.19	1.29	1.33
1	A	46	SER	N-CA	-5.19	1.40	1.45
1	C	747	ASN	C-O	-5.18	1.17	1.24
1	C	286	ALA	CA-CB	-5.18	1.44	1.53
1	A	67	GLN	CD-NE2	-5.17	1.22	1.33
1	A	75	LEU	CG-CD1	5.17	1.69	1.52
1	C	162	MET	CA-C	-5.14	1.45	1.52
1	C	277	ILE	CA-CB	-5.14	1.48	1.54
1	A	917	THR	CA-CB	5.13	1.62	1.53
1	A	77	TYR	CA-CB	-5.13	1.44	1.53
1	B	39	ALA	CA-CB	-5.13	1.44	1.53
1	B	236	ALA	CA-CB	-5.13	1.44	1.53
1	C	64	VAL	N-CA	-5.13	1.41	1.46
1	A	107	VAL	N-CA	-5.12	1.40	1.46
1	A	45	ILE	CG1-CD1	5.12	1.71	1.51
1	C	78	MET	N-CA	5.12	1.52	1.45
1	C	167	SER	C-O	5.11	1.30	1.24
1	C	170	SER	C-O	5.11	1.30	1.23
1	C	375	VAL	CA-CB	-5.11	1.48	1.54
1	C	295	THR	C-O	-5.10	1.17	1.23
1	C	238	THR	CB-CG2	5.10	1.69	1.52
1	C	156	ASP	C-N	-5.09	1.26	1.33
1	A	48	SER	CA-C	-5.09	1.46	1.52
1	C	85	THR	C-O	5.08	1.30	1.24
1	C	110	LYS	CA-CB	-5.08	1.44	1.53
1	C	768	VAL	C-O	5.08	1.28	1.24
1	C	132	SER	N-CA	5.07	1.52	1.45
1	B	216	ALA	C-O	-5.07	1.17	1.24
1	C	93	THR	CA-C	-5.06	1.46	1.52
1	C	833	PRO	CA-C	5.06	1.59	1.52
1	B	112	GLN	N-CA	5.05	1.52	1.46
1	C	129	VAL	CA-CB	-5.05	1.47	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	141	GLY	CA-C	-5.05	1.47	1.52
1	A	381	ALA	CA-CB	-5.04	1.46	1.54
1	C	833	PRO	N-CA	5.04	1.53	1.47
1	A	201	VAL	CA-C	-5.04	1.46	1.52
1	C	316	PHE	CB-CG	5.04	1.62	1.50
1	B	1002	ALA	CA-CB	-5.03	1.45	1.53
1	B	773	VAL	CA-CB	-5.02	1.47	1.54
1	C	176	GLN	CD-OE1	5.01	1.33	1.23
1	C	715	SER	CA-C	5.01	1.59	1.52
1	A	693	GLU	CA-C	5.00	1.59	1.52

All (479) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	VAL	N-CA-C	17.57	128.00	111.48
1	C	767	ARG	CD-NE-CZ	-16.76	100.94	124.40
1	C	126	GLY	N-CA-C	-15.08	88.68	111.00
1	A	696	THR	N-CA-C	-14.55	92.20	112.13
1	A	821	GLY	N-CA-C	-14.09	98.31	115.08
1	C	168	ARG	N-CA-C	13.98	140.57	110.80
1	B	49	TYR	CA-C-N	13.35	136.53	119.84
1	B	49	TYR	C-N-CA	13.35	136.53	119.84
1	A	70	ASN	N-CA-C	-13.31	85.99	108.75
1	A	122	VAL	N-CA-C	-12.72	99.62	111.45
1	C	166	ILE	O-C-N	11.86	137.39	122.57
1	A	110	LYS	N-CA-C	-11.69	98.82	113.55
1	A	317	PHE	CA-C-N	11.23	133.88	119.84
1	A	317	PHE	C-N-CA	11.23	133.88	119.84
1	C	87	THR	N-CA-C	11.18	126.55	108.99
1	C	107	VAL	N-CA-C	-11.17	99.23	110.62
1	A	818	ARG	CA-CB-CG	-10.98	92.14	114.10
1	A	58	GLN	N-CA-C	-10.83	100.08	113.18
1	A	71	GLY	N-CA-C	-10.82	100.18	114.25
1	B	4	PHE	N-CA-C	-10.82	92.75	109.52
1	A	812	GLY	N-CA-C	-10.46	90.78	110.66
1	B	416	VAL	N-CA-C	-10.28	103.49	112.12
1	A	68	ASN	N-CA-CB	-10.19	93.28	110.49
1	A	60	THR	N-CA-C	-10.13	100.66	113.43
1	A	686	ASP	N-CA-C	-9.95	101.15	113.38
1	A	65	ILE	CB-CG1-CD1	-9.77	93.29	113.80
1	C	157	TYR	CA-CB-CG	-9.75	96.36	113.90
1	C	309	GLU	N-CA-C	-9.74	100.22	111.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	818	ARG	CD-NE-CZ	-9.61	110.95	124.40
1	A	111	LEU	CB-CA-C	-9.59	91.33	110.42
1	A	118	LEU	CA-C-N	-9.48	110.09	120.14
1	A	118	LEU	C-N-CA	-9.48	110.09	120.14
1	A	62	THR	N-CA-C	9.46	122.78	111.33
1	B	799	VAL	CA-C-N	9.41	129.17	119.76
1	B	799	VAL	C-N-CA	9.41	129.17	119.76
1	C	167	SER	CA-C-N	-9.35	103.69	121.54
1	C	167	SER	C-N-CA	-9.35	103.69	121.54
1	C	166	ILE	CB-CG1-CD1	-9.28	94.32	113.80
1	C	166	ILE	N-CA-CB	9.21	126.42	111.23
1	B	705	GLU	N-CA-C	-9.18	91.25	110.80
1	A	57	VAL	CB-CA-C	-8.85	99.17	111.65
1	B	1032	ARG	N-CA-C	-8.71	102.67	113.38
1	A	40	PRO	N-CA-C	-8.66	101.31	110.58
1	C	266	ALA	N-CA-C	8.66	122.56	107.49
1	A	89	GLN	N-CA-C	-8.63	95.91	109.72
1	A	124	GLN	N-CA-C	8.53	121.42	111.02
1	B	534	ILE	N-CA-C	-8.50	102.54	110.53
1	C	773	VAL	N-CA-C	-8.50	96.21	108.53
1	A	822	LEU	CA-C-N	8.48	130.44	119.84
1	A	822	LEU	C-N-CA	8.48	130.44	119.84
1	A	128	SER	N-CA-C	8.41	123.18	110.14
1	B	238	THR	N-CA-C	8.37	120.86	108.14
1	C	160	ALA	N-CA-C	8.35	128.59	110.80
1	C	115	MET	CA-C-N	8.34	128.07	119.56
1	C	115	MET	C-N-CA	8.34	128.07	119.56
1	B	1030	ARG	N-CA-C	-8.31	99.55	110.43
1	A	571	VAL	N-CA-C	8.29	118.64	108.53
1	C	127	VAL	N-CA-C	-8.26	95.18	108.90
1	C	168	ARG	CB-CA-C	-8.21	94.09	110.42
1	A	41	PRO	CB-CA-C	-8.18	105.00	111.87
1	C	68	ASN	N-CA-C	8.15	128.17	110.80
1	B	458	PHE	N-CA-C	-8.15	103.80	112.93
1	C	685	ILE	N-CA-C	8.12	119.38	110.21
1	C	763	ILE	N-CA-C	8.08	120.13	107.28
1	A	67	GLN	N-CA-C	8.07	127.98	110.80
1	A	818	ARG	N-CA-CB	8.06	124.11	110.49
1	B	337	ILE	N-CA-C	-8.04	106.07	113.71
1	C	131	LYS	CG-CD-CE	-8.00	92.91	111.30
1	A	222	THR	N-CA-C	-7.91	97.05	109.87
1	C	765	ARG	CB-CA-C	-7.88	100.13	111.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	223	PRO	CA-C-N	7.86	129.66	119.84
1	C	223	PRO	C-N-CA	7.86	129.66	119.84
1	C	785	ASP	N-CA-C	-7.83	103.52	113.23
1	C	265	VAL	CA-C-N	-7.79	109.56	121.40
1	C	265	VAL	C-N-CA	-7.79	109.56	121.40
1	A	39	ALA	CA-C-N	-7.78	114.06	119.66
1	A	39	ALA	C-N-CA	-7.78	114.06	119.66
1	C	57	VAL	N-CA-C	-7.77	101.76	110.62
1	C	277	ILE	N-CA-C	7.77	119.67	108.48
1	B	155	SER	N-CA-C	-7.75	102.52	110.97
1	C	1022	VAL	N-CA-CB	7.70	115.35	110.50
1	A	93	THR	N-CA-C	-7.67	98.08	110.20
1	A	181	GLN	N-CA-C	-7.66	94.48	110.80
1	B	58	GLN	N-CA-C	-7.62	100.45	110.43
1	C	151	GLN	N-CA-C	-7.59	101.45	111.24
1	C	159	ALA	CA-C-N	-7.57	107.08	121.54
1	C	159	ALA	C-N-CA	-7.57	107.08	121.54
1	B	25	LEU	N-CA-C	-7.57	103.11	111.36
1	A	64	VAL	CA-C-N	-7.56	108.36	121.97
1	A	64	VAL	C-N-CA	-7.56	108.36	121.97
1	C	452	VAL	N-CA-C	-7.54	102.74	113.07
1	C	45	ILE	CB-CA-C	-7.53	98.94	111.29
1	C	166	ILE	CB-CA-C	7.49	123.57	111.29
1	B	668	LEU	CA-C-N	7.46	129.16	119.84
1	B	668	LEU	C-N-CA	7.46	129.16	119.84
1	C	864	TYR	N-CA-C	-7.45	102.85	110.97
1	C	66	GLU	N-CA-CB	7.42	120.74	109.91
1	B	988	PRO	N-CA-C	-7.42	100.30	111.57
1	C	166	ILE	CA-C-O	-7.39	111.54	120.78
1	C	306	ILE	N-CA-C	-7.38	102.56	110.23
1	B	410	ILE	N-CA-C	-7.37	104.60	111.45
1	A	735	LYS	N-CA-C	-7.35	103.35	111.36
1	A	93	THR	O-C-N	7.33	131.66	123.01
1	C	851	LEU	CA-C-N	7.32	128.99	119.84
1	C	851	LEU	C-N-CA	7.32	128.99	119.84
1	A	912	ALA	N-CA-C	-7.31	103.24	111.14
1	C	44	THR	CB-CA-C	-7.29	101.76	111.82
1	A	296	GLY	N-CA-C	-7.22	104.87	115.63
1	C	115	MET	N-CA-C	-7.21	102.95	112.75
1	A	727	PHE	N-CA-C	-7.20	97.51	109.24
1	B	912	ALA	N-CA-C	-7.16	104.17	113.12
1	A	816	LEU	N-CA-C	-7.15	96.87	108.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	ILE	N-CA-C	-7.14	97.84	109.12
1	C	717	ARG	CA-C-N	7.09	128.70	119.84
1	C	717	ARG	C-N-CA	7.09	128.70	119.84
1	C	90	ILE	CB-CA-C	-7.07	100.00	110.33
1	C	164	ASP	CB-CG-OD1	-7.05	102.18	118.40
1	C	788	ASP	N-CA-C	-7.04	105.23	113.88
1	C	595	THR	N-CA-C	-7.03	103.37	112.23
1	C	114	ALA	N-CA-C	-7.03	104.59	113.72
1	A	915	ALA	N-CA-C	-7.02	104.74	113.38
1	C	131	LYS	CD-CE-NZ	-7.02	89.43	111.90
1	C	943	ILE	N-CA-C	-7.02	104.01	110.82
1	A	1000	GLN	N-CA-C	-7.01	103.33	110.97
1	B	179	GLY	N-CA-C	-6.97	100.67	110.63
1	A	108	GLN	CB-CA-C	-6.92	96.65	110.42
1	A	819	TYR	CB-CA-C	6.92	122.17	109.71
1	A	724	THR	N-CA-C	-6.87	97.84	108.55
1	C	43	VAL	CA-C-N	-6.86	111.58	122.76
1	C	43	VAL	C-N-CA	-6.86	111.58	122.76
1	A	694	LYS	CA-C-N	-6.85	111.70	122.65
1	A	694	LYS	C-N-CA	-6.85	111.70	122.65
1	A	724	THR	OG1-CB-CG2	-6.84	95.62	109.30
1	A	68	ASN	N-CA-C	-6.80	96.32	110.80
1	C	11	PHE	N-CA-C	-6.80	105.54	114.31
1	C	823	PRO	CA-C-O	-6.79	113.16	121.31
1	A	818	ARG	NE-CZ-NH2	6.76	125.28	119.20
1	C	406	VAL	N-CA-C	-6.73	103.75	110.62
1	A	66	GLU	N-CA-CB	6.72	121.85	110.49
1	A	637	ARG	CA-C-N	6.70	128.21	119.84
1	A	637	ARG	C-N-CA	6.70	128.21	119.84
1	B	570	GLY	N-CA-C	-6.68	106.47	115.36
1	C	94	PHE	N-CA-C	-6.68	100.91	110.59
1	A	85	THR	N-CA-C	-6.66	103.77	114.09
1	C	175	VAL	N-CA-C	6.66	118.11	107.73
1	C	222	THR	CA-C-N	6.65	127.23	120.38
1	C	222	THR	C-N-CA	6.65	127.23	120.38
1	A	62	THR	CA-CB-CG2	-6.63	99.22	110.50
1	C	1004	GLY	N-CA-C	6.62	120.91	112.83
1	C	822	LEU	CB-CA-C	6.62	118.39	108.86
1	A	257	GLY	N-CA-C	-6.61	104.72	114.90
1	A	90	ILE	N-CA-C	-6.61	95.60	109.34
1	A	379	THR	N-CA-C	-6.57	104.19	111.82
1	B	450	SER	N-CA-C	-6.57	105.15	113.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	VAL	N-CA-C	-6.56	95.70	109.34
1	A	58	GLN	CA-C-N	-6.54	111.74	122.54
1	A	58	GLN	C-N-CA	-6.54	111.74	122.54
1	A	437	GLN	N-CA-C	-6.53	105.61	113.97
1	B	47	ALA	N-CA-C	-6.52	100.03	110.14
1	C	758	TYR	N-CA-C	6.52	119.47	107.99
1	C	167	SER	CA-CB-OG	-6.51	98.08	111.10
1	C	315	PRO	CA-C-N	-6.50	111.86	121.99
1	C	315	PRO	C-N-CA	-6.50	111.86	121.99
1	C	397	GLY	N-CA-C	-6.47	104.69	113.37
1	C	710	PRO	N-CA-C	-6.47	106.26	114.35
1	B	222	THR	CA-C-N	6.47	127.04	120.38
1	B	222	THR	C-N-CA	6.47	127.04	120.38
1	C	167	SER	CA-C-O	-6.46	111.28	120.51
1	A	44	THR	CA-CB-CG2	6.44	121.45	110.50
1	C	199	THR	CA-C-N	-6.44	112.20	119.28
1	C	199	THR	C-N-CA	-6.44	112.20	119.28
1	A	824	SER	N-CA-C	6.44	124.51	110.80
1	A	618	ALA	N-CA-C	-6.42	104.67	114.16
1	C	125	GLN	CB-CA-C	6.42	120.89	110.95
1	A	518	ARG	N-CA-C	-6.42	105.49	113.38
1	B	961	ILE	N-CA-C	-6.40	104.37	113.07
1	B	220	GLY	N-CA-C	-6.36	98.10	113.18
1	C	162	MET	CB-CG-SD	-6.36	93.62	112.70
1	A	63	GLN	CA-CB-CG	6.35	126.80	114.10
1	A	141	GLY	CA-C-N	-6.34	115.05	123.17
1	A	141	GLY	C-N-CA	-6.34	115.05	123.17
1	C	118	LEU	CA-C-N	-6.34	113.44	119.85
1	C	118	LEU	C-N-CA	-6.34	113.44	119.85
1	C	123	GLN	N-CA-C	-6.34	97.29	110.80
1	B	867	ARG	N-CA-C	-6.33	103.30	111.02
1	A	70	ASN	O-C-N	-6.32	116.02	123.41
1	C	162	MET	N-CA-C	6.31	124.25	110.80
1	A	576	VAL	CA-C-O	-6.31	116.69	121.68
1	B	102	ILE	N-CA-C	-6.31	105.58	111.45
1	B	174	ASP	CA-C-O	-6.30	113.73	121.67
1	C	167	SER	N-CA-C	-6.30	97.39	110.80
1	B	493	CYS	N-CA-C	-6.29	101.80	110.35
1	B	563	PHE	N-CA-C	6.28	121.83	114.04
1	C	172	VAL	CA-CB-CG1	6.28	121.07	110.40
1	B	463	THR	N-CA-C	-6.27	103.73	112.45
1	C	456	MET	N-CA-C	-6.27	101.18	110.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	ALA	N-CA-C	6.26	119.88	111.24
1	B	231	ASN	CB-CA-C	-6.26	101.53	111.17
1	C	168	ARG	CA-C-N	-6.25	111.00	121.89
1	C	168	ARG	C-N-CA	-6.25	111.00	121.89
1	C	130	GLU	N-CA-C	6.25	118.45	109.14
1	A	719	ASN	CB-CA-C	-6.24	101.12	111.41
1	C	109	ASN	N-CA-C	-6.24	103.20	111.24
1	B	953	MET	N-CA-C	-6.23	104.49	113.21
1	C	865	GLN	N-CA-C	6.23	120.34	112.87
1	A	40	PRO	CB-CA-C	6.21	117.01	111.17
1	A	102	ILE	O-C-N	-6.19	114.54	122.22
1	C	576	VAL	CB-CA-C	-6.19	101.14	111.29
1	A	187	TRP	N-CA-C	6.19	118.53	108.63
1	A	115	MET	N-CA-CB	6.18	121.38	110.37
1	A	696	THR	CB-CA-C	6.17	120.59	110.83
1	B	232	ALA	N-CA-C	6.17	118.80	109.23
1	B	218	GLN	N-CA-C	6.16	119.54	109.06
1	C	755	GLY	N-CA-C	-6.16	98.57	113.18
1	C	1022	VAL	CA-C-N	-6.16	112.57	118.97
1	C	1022	VAL	C-N-CA	-6.16	112.57	118.97
1	C	289	LEU	CA-C-N	6.14	127.47	120.53
1	C	289	LEU	C-N-CA	6.14	127.47	120.53
1	C	753	ALA	O-C-N	6.14	129.15	122.15
1	A	822	LEU	CA-C-O	6.11	127.36	120.46
1	C	184	MET	N-CA-C	-6.10	100.81	109.96
1	A	768	VAL	CB-CA-C	-6.08	102.14	111.08
1	C	165	ALA	CA-C-N	-6.07	111.05	121.97
1	C	165	ALA	C-N-CA	-6.07	111.05	121.97
1	A	456	MET	N-CA-C	-6.05	102.97	110.41
1	B	666	PHE	N-CA-C	6.05	116.23	108.24
1	A	568	ASP	N-CA-C	-6.04	101.47	110.23
1	A	65	ILE	CB-CA-C	6.04	121.19	111.29
1	C	164	ASP	N-CA-CB	-6.04	100.29	110.49
1	C	104	GLN	CA-CB-CG	-6.03	102.04	114.10
1	B	738	ALA	N-CA-C	-6.02	106.91	114.56
1	A	92	LEU	CA-C-N	6.02	130.03	121.42
1	A	92	LEU	C-N-CA	6.02	130.03	121.42
1	B	102	ILE	N-CA-CB	6.02	119.94	110.31
1	A	820	ASN	N-CA-C	5.99	123.56	110.80
1	C	241	THR	N-CA-C	5.99	123.03	114.16
1	A	102	ILE	N-CA-C	5.98	120.36	112.76
1	B	106	GLN	CA-C-O	-5.97	114.52	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	818	ARG	CB-CG-CD	-5.96	97.58	111.30
1	B	641	GLU	N-CA-C	-5.96	102.24	110.35
1	C	771	VAL	CB-CA-C	-5.95	102.03	110.12
1	A	1030	ARG	N-CA-C	-5.94	106.43	113.38
1	A	993	THR	N-CA-C	5.93	117.97	109.14
1	A	823	PRO	CA-N-CD	5.91	120.28	112.00
1	C	449	LEU	N-CA-C	-5.89	104.04	111.11
1	C	905	VAL	CA-C-N	5.89	125.59	119.05
1	C	905	VAL	C-N-CA	5.89	125.59	119.05
1	A	79	SER	N-CA-C	5.88	118.12	110.53
1	B	412	VAL	N-CA-C	-5.88	106.55	113.42
1	C	163	LYS	CA-C-N	5.87	132.75	121.54
1	C	163	LYS	C-N-CA	5.87	132.75	121.54
1	C	110	LYS	O-C-N	-5.84	114.82	122.59
1	C	63	GLN	CB-CA-C	-5.83	101.48	110.81
1	B	1	MET	CA-C-N	5.83	127.13	119.84
1	B	1	MET	C-N-CA	5.83	127.13	119.84
1	A	418	ARG	N-CA-C	-5.82	104.32	112.12
1	A	837	THR	N-CA-C	-5.82	104.13	111.11
1	C	894	SER	N-CA-C	5.82	118.20	108.02
1	B	137	LEU	N-CA-C	-5.81	106.32	113.41
1	B	8	ARG	CA-C-N	5.81	127.10	119.84
1	B	8	ARG	C-N-CA	5.81	127.10	119.84
1	A	547	ILE	N-CA-C	-5.81	104.67	110.30
1	C	292	LYS	CA-C-N	-5.80	115.30	122.84
1	C	292	LYS	C-N-CA	-5.80	115.30	122.84
1	C	494	ALA	N-CA-C	-5.79	103.56	111.56
1	C	792	ARG	CB-CA-C	-5.79	102.01	110.06
1	B	338	HIS	N-CA-C	-5.79	105.05	111.36
1	C	172	VAL	N-CA-C	-5.78	97.32	109.34
1	C	378	GLY	N-CA-C	-5.77	107.51	114.66
1	C	947	GLU	N-CA-C	-5.77	103.73	112.04
1	A	331	PRO	N-CA-C	-5.76	104.45	113.78
1	C	109	ASN	CA-C-O	-5.76	114.76	120.80
1	C	454	VAL	N-CA-C	5.76	121.31	108.88
1	C	130	GLU	CA-C-N	-5.75	114.38	123.24
1	C	130	GLU	C-N-CA	-5.75	114.38	123.24
1	A	104	GLN	CB-CG-CD	-5.74	102.83	112.60
1	A	107	VAL	CB-CA-C	-5.74	101.87	111.29
1	A	989	LEU	N-CA-C	-5.74	104.40	111.75
1	C	161	ASN	CA-C-N	-5.73	110.59	121.54
1	C	161	ASN	C-N-CA	-5.73	110.59	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	115	MET	O-C-N	5.73	125.58	120.48
1	C	168	ARG	O-C-N	-5.73	114.97	122.59
1	C	166	ILE	CA-CB-CG1	-5.72	100.68	110.40
1	C	249	ILE	CA-C-N	5.71	130.01	122.42
1	C	249	ILE	C-N-CA	5.71	130.01	122.42
1	A	416	VAL	N-CA-C	5.70	116.34	110.36
1	C	239	ARG	CG-CD-NE	-5.70	99.47	112.00
1	C	65	ILE	N-CA-C	-5.69	105.18	110.53
1	B	235	ILE	CB-CA-C	-5.69	101.96	111.29
1	A	40	PRO	CA-C-O	-5.69	116.24	120.73
1	A	107	VAL	O-C-N	5.69	129.68	122.57
1	A	454	VAL	CA-C-N	5.68	126.95	119.84
1	A	454	VAL	C-N-CA	5.68	126.95	119.84
1	C	641	GLU	N-CA-C	-5.68	105.08	112.23
1	C	163	LYS	O-C-N	5.67	129.06	122.20
1	A	557	VAL	N-CA-C	-5.67	105.00	110.72
1	C	627	ALA	N-CA-C	5.66	119.50	107.67
1	C	82	SER	N-CA-C	5.66	118.67	108.48
1	C	809	TRP	N-CA-C	-5.66	103.06	110.53
1	C	157	TYR	O-C-N	5.66	130.11	122.59
1	B	144	ASN	N-CA-C	5.65	117.73	108.52
1	A	78	MET	CA-C-O	-5.64	114.27	120.70
1	A	81	ASN	N-CA-C	5.64	118.59	109.40
1	C	594	VAL	N-CA-C	-5.63	104.88	110.62
1	B	110	LYS	CA-C-N	-5.63	112.97	120.79
1	B	110	LYS	C-N-CA	-5.63	112.97	120.79
1	C	764	ASP	CB-CA-C	-5.61	100.86	110.22
1	B	769	LYS	N-CA-C	5.59	117.12	109.18
1	A	821	GLY	O-C-N	-5.59	115.59	122.46
1	A	93	THR	CA-C-N	5.58	131.35	122.59
1	A	93	THR	C-N-CA	5.58	131.35	122.59
1	A	274	ASN	N-CA-C	-5.58	101.19	110.17
1	B	634	TRP	N-CA-C	5.58	117.36	111.28
1	B	998	GLY	N-CA-C	-5.57	99.98	113.18
1	A	201	VAL	N-CA-C	-5.57	105.07	110.42
1	B	415	ASN	N-CA-C	-5.57	104.32	113.50
1	C	279	ALA	CA-C-N	-5.57	114.15	122.39
1	C	279	ALA	C-N-CA	-5.57	114.15	122.39
1	B	420	MET	N-CA-C	-5.56	106.39	114.12
1	A	54	ALA	CA-C-N	-5.55	113.04	120.54
1	A	54	ALA	C-N-CA	-5.55	113.04	120.54
1	C	88	VAL	CB-CA-C	-5.55	101.81	110.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	42	ALA	CA-C-N	5.54	130.25	123.10
1	C	42	ALA	C-N-CA	5.54	130.25	123.10
1	C	153	ASP	CA-C-N	-5.54	117.48	123.08
1	C	153	ASP	C-N-CA	-5.54	117.48	123.08
1	C	127	VAL	CA-C-O	-5.54	116.15	121.63
1	A	64	VAL	CB-CA-C	-5.53	102.22	111.29
1	C	990	VAL	N-CA-C	5.53	120.84	109.34
1	B	106	GLN	N-CA-CB	5.53	118.17	109.94
1	A	81	ASN	CB-CA-C	-5.51	98.84	109.37
1	A	160	ALA	N-CA-C	5.51	117.37	111.36
1	A	695	LEU	CA-C-N	-5.51	114.29	122.56
1	A	695	LEU	C-N-CA	-5.51	114.29	122.56
1	C	168	ARG	CG-CD-NE	-5.51	99.87	112.00
1	C	469	GLN	N-CA-C	-5.51	104.10	112.04
1	B	968	VAL	N-CA-CB	5.51	116.63	110.51
1	C	165	ALA	N-CA-C	5.50	119.97	113.16
1	C	767	ARG	CG-CD-NE	-5.50	99.91	112.00
1	A	91	THR	CA-C-N	5.49	130.71	122.47
1	A	91	THR	C-N-CA	5.49	130.71	122.47
1	C	767	ARG	N-CA-C	-5.49	98.06	107.23
1	A	136	PHE	N-CA-C	5.49	116.31	108.74
1	B	693	GLU	N-CA-C	-5.48	99.13	110.80
1	C	325	TYR	N-CA-C	5.47	118.57	108.94
1	B	782	LEU	CA-C-N	5.47	126.68	119.84
1	B	782	LEU	C-N-CA	5.47	126.68	119.84
1	A	66	GLU	N-CA-C	5.47	122.45	110.80
1	C	72	ILE	CB-CA-C	5.47	117.24	110.73
1	C	763	ILE	N-CA-CB	-5.45	105.03	111.90
1	A	109	ASN	CB-CA-C	-5.45	99.57	110.42
1	C	973	ARG	N-CA-C	-5.44	106.17	113.25
1	C	720	GLY	N-CA-C	5.44	126.06	113.18
1	B	193	LEU	N-CA-C	-5.43	105.27	111.14
1	C	12	ALA	N-CA-C	-5.43	106.79	113.41
1	B	991	ILE	N-CA-C	-5.42	107.45	112.43
1	B	49	TYR	N-CA-C	5.41	120.42	108.73
1	C	106	GLN	CA-CB-CG	-5.41	103.29	114.10
1	C	84	SER	N-CA-C	5.40	119.61	113.19
1	C	557	VAL	N-CA-C	-5.39	106.58	113.22
1	C	769	LYS	CA-C-N	5.38	130.77	120.97
1	C	769	LYS	C-N-CA	5.38	130.77	120.97
1	A	818	ARG	NH1-CZ-NH2	-5.38	112.31	119.30
1	B	707	ALA	N-CA-C	-5.38	102.93	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	567	GLU	N-CA-C	5.38	117.36	109.24
1	C	66	GLU	N-CA-C	-5.37	105.12	110.97
1	B	673	GLU	N-CA-C	5.37	117.75	110.88
1	C	761	ASP	N-CA-C	5.36	118.46	107.69
1	B	222	THR	N-CA-C	5.36	121.65	109.81
1	B	30	LEU	CA-CB-CG	5.35	135.04	116.30
1	B	292	LYS	N-CA-C	5.35	118.79	110.17
1	B	329	THR	CB-CA-C	-5.35	104.64	111.22
1	A	112	GLN	N-CA-C	5.34	122.18	110.80
1	A	690	LEU	CA-C-N	-5.34	114.03	121.67
1	A	690	LEU	C-N-CA	-5.34	114.03	121.67
1	A	940	LYS	N-CA-C	-5.34	105.35	111.07
1	A	242	SER	N-CA-C	5.34	116.64	108.52
1	C	810	GLU	O-C-N	5.33	128.59	123.04
1	A	57	VAL	N-CA-C	5.33	119.86	112.35
1	C	113	LEU	N-CA-CB	-5.33	101.26	110.32
1	C	103	ALA	O-C-N	-5.32	115.52	122.59
1	B	425	LEU	CA-C-N	5.32	125.86	120.38
1	B	425	LEU	C-N-CA	5.32	125.86	120.38
1	C	121	GLU	N-CA-CB	5.32	119.22	110.39
1	A	66	GLU	CB-CA-C	-5.32	99.84	110.42
1	A	426	PRO	CA-C-N	5.32	126.48	119.84
1	A	426	PRO	C-N-CA	5.32	126.48	119.84
1	A	684	LEU	CA-C-N	5.31	131.19	122.64
1	A	684	LEU	C-N-CA	5.31	131.19	122.64
1	B	45	ILE	CB-CA-C	-5.30	104.17	111.49
1	B	121	GLU	N-CA-C	-5.30	105.40	111.07
1	B	692	HIS	N-CA-C	-5.30	99.51	110.80
1	B	488	LEU	N-CA-C	-5.29	105.64	112.68
1	B	228	GLN	N-CA-C	5.29	122.08	110.80
1	A	855	VAL	N-CA-C	5.29	115.97	107.98
1	C	335	ILE	N-CA-C	-5.29	105.56	110.53
1	C	49	TYR	CA-C-N	5.29	126.45	119.84
1	C	49	TYR	C-N-CA	5.29	126.45	119.84
1	B	947	GLU	N-CA-C	-5.28	105.42	111.07
1	C	768	VAL	N-CA-C	-5.28	102.39	109.30
1	C	291	ILE	CB-CA-C	-5.27	102.65	111.29
1	A	813	SER	CB-CA-C	5.26	116.00	108.68
1	B	396	PHE	N-CA-C	-5.26	104.60	111.02
1	C	614	GLY	N-CA-C	-5.26	107.75	114.85
1	A	542	LEU	N-CA-C	-5.25	105.56	111.28
1	A	90	ILE	CB-CG1-CD1	-5.24	102.80	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	SER	N-CA-C	5.24	116.69	109.15
1	A	98	THR	N-CA-C	-5.24	103.62	110.53
1	A	934	THR	N-CA-C	5.24	117.73	111.71
1	A	828	LEU	CB-CG-CD1	-5.22	95.03	110.70
1	B	273	GLU	N-CA-C	-5.22	105.04	111.40
1	A	109	ASN	N-CA-C	5.21	121.90	110.80
1	C	307	ARG	CA-C-N	-5.20	112.03	120.72
1	C	307	ARG	C-N-CA	-5.20	112.03	120.72
1	C	159	ALA	N-CA-CB	-5.19	101.72	110.49
1	A	823	PRO	N-CA-C	-5.19	101.78	112.47
1	C	62	THR	N-CA-CB	5.19	117.50	109.98
1	B	134	SER	N-CA-C	5.18	119.69	112.90
1	A	820	ASN	CB-CA-C	-5.18	100.11	110.42
1	C	275	TYR	CB-CA-C	-5.18	103.66	112.00
1	C	175	VAL	N-CA-CB	-5.18	104.94	111.31
1	B	230	LEU	CA-CB-CG	5.17	134.41	116.30
1	A	88	VAL	CB-CA-C	-5.17	103.09	110.12
1	A	46	SER	N-CA-C	5.17	118.43	110.42
1	A	114	ALA	CA-C-O	-5.17	114.94	120.42
1	A	275	TYR	CA-C-N	-5.16	116.12	123.03
1	A	275	TYR	C-N-CA	-5.16	116.12	123.03
1	B	84	SER	N-CA-C	5.16	117.31	111.02
1	C	768	VAL	CA-C-N	5.15	130.55	122.21
1	C	768	VAL	C-N-CA	5.15	130.55	122.21
1	C	145	THR	N-CA-C	5.14	117.29	111.02
1	C	45	ILE	CA-C-O	-5.13	114.36	120.78
1	A	92	LEU	CB-CA-C	-5.13	103.95	111.23
1	C	107	VAL	O-C-N	5.12	126.84	121.87
1	A	583	THR	CB-CA-C	-5.12	100.24	110.42
1	A	822	LEU	CB-CA-C	-5.12	100.94	108.87
1	A	924	ASP	N-CA-C	5.11	117.64	110.23
1	A	78	MET	CB-CA-C	-5.11	102.44	111.22
1	B	213	GLN	N-CA-C	-5.11	101.83	109.95
1	B	564	LEU	CA-C-N	5.10	125.82	120.11
1	B	564	LEU	C-N-CA	5.10	125.82	120.11
1	C	310	LEU	O-C-N	5.10	128.37	122.20
1	C	171	GLY	CA-C-N	5.09	131.14	121.97
1	C	171	GLY	C-N-CA	5.09	131.14	121.97
1	C	372	VAL	CA-C-N	-5.09	114.36	119.56
1	C	372	VAL	C-N-CA	-5.09	114.36	119.56
1	C	615	PHE	N-CA-C	5.08	116.93	107.99
1	C	775	SER	N-CA-C	5.08	118.23	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	VAL	CB-CA-C	-5.08	107.39	111.71
1	A	729	ILE	N-CA-C	-5.08	98.78	109.34
1	B	1007	VAL	CB-CA-C	-5.08	106.59	111.06
1	A	107	VAL	CA-C-N	5.06	131.21	121.54
1	A	107	VAL	C-N-CA	5.06	131.21	121.54
1	C	168	ARG	CB-CG-CD	-5.06	99.67	111.30
1	C	79	SER	N-CA-C	-5.05	100.04	110.80
1	C	89	GLN	CB-CG-CD	-5.05	104.01	112.60
1	A	298	ASN	N-CA-C	5.05	117.01	108.02
1	A	702	LEU	N-CA-C	5.05	116.86	111.36
1	B	927	PHE	N-CA-C	-5.05	105.06	111.11
1	C	40	PRO	N-CA-C	-5.05	104.54	110.70
1	C	770	LYS	CG-CD-CE	5.05	122.91	111.30
1	A	75	LEU	N-CA-C	5.04	117.00	109.59
1	B	545	TYR	N-CA-C	-5.04	105.44	111.03
1	B	717	ARG	CA-C-N	-5.04	114.57	119.76
1	B	717	ARG	C-N-CA	-5.04	114.57	119.76
1	C	457	ALA	N-CA-C	-5.04	104.47	111.52
1	B	864	TYR	N-CA-C	-5.04	105.31	111.75
1	C	1016	VAL	N-CA-CB	5.04	116.34	110.65
1	B	61	VAL	N-CA-C	-5.03	107.89	112.12
1	C	698	ALA	N-CA-C	-5.03	105.92	111.71
1	B	219	LEU	N-CA-C	-5.03	102.42	109.96
1	B	881	LEU	N-CA-C	-5.03	104.89	111.02
1	C	759	VAL	CA-C-N	-5.02	111.95	121.54
1	C	759	VAL	C-N-CA	-5.02	111.95	121.54
1	C	306	ILE	O-C-N	5.01	127.37	121.96
1	A	653	ARG	N-CA-C	-5.01	104.78	111.24
1	C	240	LEU	CA-C-N	-5.01	112.54	120.70
1	C	240	LEU	C-N-CA	-5.01	112.54	120.70
1	C	9	PRO	N-CA-C	-5.00	102.17	112.47

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	62	THR	Mainchain
1	A	65	ILE	Mainchain
1	A	66	GLU	Peptide
1	A	818	ARG	Mainchain
1	B	102	ILE	Peptide
1	B	706	ALA	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	104	GLN	Mainchain
1	C	160	ALA	Mainchain,Peptide
1	C	166	ILE	Peptide
1	C	168	ARG	Mainchain
1	C	45	ILE	Mainchain

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	7774	0	7931	1227	0
1	B	7774	0	7931	1258	0
1	C	7774	0	7931	1370	0
2	A	22	0	0	31	0
2	B	8	0	0	6	0
2	C	26	0	0	35	0
All	All	23378	0	23793	3741	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 79.

All (3741) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:VAL:CA	1:C:127:VAL:CB	1.75	1.63
1:C:158:VAL:CB	1:C:158:VAL:CG2	1.77	1.60
1:A:69:MET:CB	1:A:69:MET:CG	1.74	1.60
1:A:65:ILE:CA	1:A:65:ILE:C	1.79	1.56
1:C:58:GLN:CB	1:C:58:GLN:CG	1.74	1.55
1:A:68:ASN:N	1:A:68:ASN:CA	1.70	1.55
1:A:108:GLN:CG	1:A:108:GLN:CB	1.86	1.53
1:C:91:THR:CB	1:C:91:THR:CA	1.78	1.53
1:C:169:THR:CA	1:C:169:THR:CB	1.85	1.50
1:C:45:ILE:CA	1:C:45:ILE:CB	1.88	1.49
1:C:161:ASN:N	1:C:161:ASN:CA	1.76	1.45
1:A:61:VAL:O	1:A:65:ILE:CG2	1.66	1.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:VAL:CB	1:C:129:VAL:CG2	1.97	1.43
1:A:68:ASN:CA	1:A:68:ASN:CB	1.94	1.42
1:C:167:SER:N	1:C:167:SER:CA	1.87	1.38
1:C:166:ILE:CA	1:C:166:ILE:CB	2.01	1.36
1:A:818:ARG:CG	1:A:818:ARG:CD	2.02	1.35
1:B:247:GLY:HA2	1:B:268:ILE:CD1	1.63	1.28
1:B:247:GLY:CA	1:B:268:ILE:HD13	1.67	1.23
1:A:67:GLN:CB	1:A:67:GLN:CG	2.16	1.22
1:A:61:VAL:O	1:A:65:ILE:HG22	1.09	1.22
1:C:115:MET:CE	1:C:118:LEU:HD22	1.70	1.22
1:C:159:ALA:HA	2:C:1078:HOH:O	1.05	1.21
1:C:950:LYS:NZ	1:C:1030:ARG:HD3	1.56	1.21
1:C:44:THR:HG22	1:C:91:THR:CB	1.70	1.20
1:A:66:GLU:HG2	2:A:1058:HOH:O	1.40	1.19
1:C:274:ASN:HB2	2:C:1060:HOH:O	1.43	1.19
1:A:108:GLN:HG3	1:B:112:GLN:OE1	1.38	1.18
1:A:686:ASP:HB3	2:A:1059:HOH:O	1.37	1.18
1:C:291:ILE:HD13	1:C:306:ILE:HD13	1.23	1.18
1:C:44:THR:CG2	1:C:91:THR:HB	1.74	1.17
1:B:412:VAL:HG13	1:B:435:MET:HE1	1.23	1.17
1:B:456:MET:HG3	1:B:467:TYR:HB3	1.21	1.17
1:C:110:LYS:HA	1:C:113:LEU:HD12	1.28	1.16
1:C:82:SER:HB3	1:C:88:VAL:HA	1.26	1.15
1:B:1:MET:HB2	1:B:2:PRO:HD2	1.25	1.15
1:C:58:GLN:HB3	2:C:1079:HOH:O	1.45	1.15
1:A:344:LEU:HD23	1:A:402:ILE:HD13	1.15	1.15
1:B:544:LEU:HA	1:B:547:ILE:HD12	1.30	1.14
1:C:713:LEU:HG	1:C:832:ALA:O	1.47	1.14
1:C:166:ILE:HA	1:C:166:ILE:HD13	1.20	1.14
1:C:54:ALA:HB2	1:C:84:SER:HB2	1.30	1.14
1:C:115:MET:HE2	1:C:118:LEU:HD22	1.29	1.14
1:B:1022:VAL:O	1:B:1024:VAL:O	1.66	1.14
1:A:531:VAL:HA	1:A:534:ILE:HD11	1.24	1.13
1:A:690:LEU:HD11	1:A:854:GLY:HA3	1.27	1.13
1:B:445:ILE:HG23	1:B:940:LYS:HG3	1.27	1.13
1:C:190:PRO:HD3	1:C:779:TYR:HD1	1.13	1.12
1:C:432:ARG:HH11	1:C:432:ARG:HG3	1.14	1.12
1:B:990:VAL:HG13	1:B:1005:THR:OG1	1.48	1.11
1:C:69:MET:CE	1:C:92:LEU:HD21	1.78	1.11
1:C:220:GLY:HA3	1:C:231:ASN:ND2	1.65	1.11
1:A:261:LEU:HD12	1:A:263:ARG:HH22	1.08	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ARG:HG2	1:A:970:MET:HE3	1.30	1.11
1:C:699:ARG:HG2	1:C:699:ARG:HH11	1.16	1.11
1:B:894:SER:HB3	1:B:897:ILE:HG12	1.33	1.10
1:C:162:MET:HG2	1:C:313:MET:HE2	1.31	1.10
1:B:987:MET:HA	1:B:987:MET:HE3	1.31	1.10
1:A:400:LEU:HD13	1:A:1003:VAL:HG13	1.27	1.10
1:A:686:ASP:O	1:A:688:ALA:N	1.84	1.09
1:A:713:LEU:HD22	1:A:714:THR:H	1.15	1.09
1:B:441:ALA:HB2	1:B:947:GLU:HG2	1.18	1.09
1:C:188:MET:HE1	1:C:200:PRO:HB3	1.16	1.09
1:C:770:LYS:HG3	2:C:1070:HOH:O	1.48	1.09
1:C:699:ARG:HH11	1:C:699:ARG:CG	1.66	1.09
1:A:729:ILE:HG22	1:A:730:ASP:H	1.14	1.09
1:B:42:ALA:HB2	1:B:93:THR:HG22	1.34	1.08
1:C:847:LEU:HA	1:C:850:LYS:HD3	1.30	1.08
1:C:747:ASN:HA	2:C:1066:HOH:O	1.54	1.08
1:A:443:VAL:HG12	1:A:444:GLY:H	1.19	1.07
1:B:225:VAL:HG22	1:C:781:MET:HE2	1.18	1.07
1:A:945:ILE:HG12	1:A:971:ARG:HG2	1.32	1.07
1:C:427:PRO:HA	1:C:498:LYS:HE3	1.22	1.07
1:A:66:GLU:HA	2:A:1056:HOH:O	1.54	1.06
1:C:1:MET:HB2	1:C:2:PRO:HD2	1.32	1.06
1:C:166:ILE:HA	1:C:166:ILE:CD1	1.85	1.06
1:B:843:LEU:HD23	1:B:847:LEU:HD21	1.07	1.06
1:A:112:GLN:HA	1:A:112:GLN:HE21	1.15	1.05
1:C:162:MET:HB3	1:C:313:MET:HE1	1.38	1.05
1:A:713:LEU:HG	1:A:833:PRO:HD3	1.34	1.05
1:A:649:MET:HB3	1:A:653:ARG:HH21	1.22	1.05
1:C:167:SER:OG	1:C:168:ARG:N	1.85	1.05
1:C:163:LYS:O	1:C:166:ILE:N	1.89	1.04
1:A:54:ALA:HB1	1:A:816:LEU:HG	1.38	1.04
1:A:344:LEU:CD2	1:A:402:ILE:HD13	1.88	1.03
1:C:420:MET:SD	1:C:498:LYS:CE	2.46	1.03
1:A:400:LEU:CD1	1:A:1003:VAL:HG13	1.87	1.03
1:B:574:THR:HG23	1:B:665:ALA:HB2	1.39	1.03
1:B:904:VAL:HG13	1:B:907:LEU:HD12	1.35	1.03
1:C:1022:VAL:HA	1:C:1025:PHE:HD2	1.22	1.03
1:C:713:LEU:HD11	1:C:834:GLY:HA3	1.35	1.03
1:B:431:THR:HG21	1:B:493:CYS:HB3	1.37	1.02
1:A:713:LEU:HB3	1:A:832:ALA:HA	1.37	1.02
1:A:959:GLY:HA3	1:A:962:GLU:HB2	1.41	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:MET:HE1	1:B:127:VAL:HG21	1.42	1.02
1:C:69:MET:HE2	1:C:92:LEU:CD2	1.89	1.02
1:C:712:MET:HB2	1:C:835:LYS:HG3	1.41	1.02
1:A:205:THR:HG22	1:A:205:THR:O	1.54	1.01
1:C:184:MET:HA	1:C:184:MET:HE3	1.41	1.01
1:B:226:LYS:HA	1:B:226:LYS:HE3	1.40	1.01
1:C:238:THR:HG22	1:C:239:ARG:O	1.59	1.01
1:C:415:ASN:ND2	1:C:434:SER:HB2	1.74	1.01
1:B:876:LEU:HD13	1:B:932:LEU:HD11	1.43	1.00
1:C:901:VAL:O	1:C:904:VAL:HG23	1.59	1.00
1:A:713:LEU:O	1:A:714:THR:HG23	1.61	1.00
1:A:713:LEU:CB	1:A:832:ALA:HA	1.91	1.00
1:A:108:GLN:HG3	1:B:112:GLN:CD	1.86	1.00
1:A:559:LEU:HD12	1:A:560:PRO:HD2	1.41	1.00
1:C:188:MET:HE1	1:C:200:PRO:CB	1.92	1.00
1:A:435:MET:HG2	1:A:490:PRO:HB3	1.44	0.99
1:A:536:ARG:HG2	1:A:537:SER:H	1.22	0.99
1:C:115:MET:CE	1:C:118:LEU:CD2	2.40	0.99
1:C:887:CYS:O	1:C:890:ALA:HB3	1.62	0.99
1:C:166:ILE:CB	1:C:166:ILE:HA	1.84	0.99
1:A:328:ASP:OD1	1:A:330:THR:HB	1.62	0.99
1:B:49:TYR:CD2	1:B:122:VAL:HA	1.98	0.99
1:C:159:ALA:O	1:C:161:ASN:N	1.94	0.99
1:B:144:ASN:HB2	1:B:320:GLY:O	1.62	0.99
1:A:818:ARG:HD3	1:A:821:GLY:C	1.88	0.98
1:C:143:ILE:HG23	1:C:284:GLN:NE2	1.77	0.98
1:C:115:MET:HE2	1:C:115:MET:HA	1.41	0.98
1:C:358:PHE:HB3	1:C:977:MET:HE2	1.44	0.98
1:A:819:TYR:H	1:A:824:SER:HB3	1.27	0.98
1:B:523:SER:HA	1:B:526:HIS:HD2	1.29	0.98
1:B:687:GLN:NE2	1:B:856:GLY:HA3	1.79	0.98
1:B:549:VAL:HG22	1:B:550:VAL:N	1.79	0.97
1:C:162:MET:HG2	1:C:313:MET:CE	1.94	0.97
1:A:818:ARG:HD3	1:A:821:GLY:O	1.64	0.97
1:C:729:ILE:HD11	1:C:786:ILE:HD13	1.46	0.97
1:A:687:GLN:NE2	1:A:856:GLY:HA3	1.78	0.97
1:A:251:LEU:HD11	1:A:262:LEU:HA	1.46	0.97
1:C:69:MET:HE2	1:C:92:LEU:HD21	1.00	0.97
1:A:690:LEU:HD11	1:A:854:GLY:CA	1.96	0.96
1:C:588:GLN:HG2	1:C:613:ASN:HD22	1.25	0.96
1:C:111:LEU:HB3	2:C:1056:HOH:O	1.64	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:674:LEU:HD11	1:C:862:MET:HA	1.46	0.96
1:B:704:ALA:O	1:B:705:GLU:HG3	1.66	0.96
1:C:684:LEU:HG	1:C:684:LEU:O	1.64	0.96
1:B:361:ASN:O	1:B:365:THR:HB	1.64	0.96
1:C:164:ASP:O	1:C:167:SER:OG	1.84	0.95
1:A:105:VAL:O	1:A:109:ASN:N	1.99	0.95
1:C:372:VAL:HG13	1:C:373:PRO:HD3	1.48	0.95
1:B:742:SER:HB3	1:B:745:ASP:OD2	1.66	0.95
1:B:843:LEU:CD2	1:B:847:LEU:HD21	1.96	0.95
1:B:537:SER:HB2	1:B:540:ARG:HG2	1.47	0.95
1:B:714:THR:HG21	1:B:833:PRO:HD2	1.49	0.95
1:A:389:SER:O	1:A:394:THR:HG21	1.67	0.95
1:A:790:TYR:HE1	1:A:800:PRO:HG3	1.30	0.95
1:B:712:MET:HB3	1:B:713:LEU:HD12	1.46	0.95
1:A:214:VAL:HG12	1:A:215:ALA:N	1.79	0.95
1:A:979:SER:OG	1:A:1015:THR:HG21	1.66	0.95
1:B:172:VAL:O	1:B:172:VAL:HG12	1.64	0.94
1:B:1022:VAL:HG23	1:B:1023:PRO:HD3	1.48	0.94
1:C:420:MET:SD	1:C:498:LYS:HE2	2.06	0.94
1:A:76:MET:HG2	1:A:95:GLU:OE2	1.66	0.94
1:B:420:MET:HE1	1:B:425:LEU:HD23	1.46	0.94
1:B:431:THR:HG21	1:B:493:CYS:CB	1.96	0.94
1:B:988:PRO:O	1:B:989:LEU:HB3	1.65	0.94
1:C:162:MET:HB3	1:C:313:MET:CE	1.96	0.94
1:C:162:MET:CB	1:C:313:MET:CE	2.45	0.94
1:A:66:GLU:CG	2:A:1058:HOH:O	2.02	0.94
1:A:742:SER:OG	1:A:745:ASP:HB2	1.68	0.94
1:B:807:SER:O	1:B:808:ARG:HG3	1.68	0.94
1:B:930:GLY:O	1:B:934:THR:HG23	1.68	0.94
1:C:535:LEU:HB2	2:C:1076:HOH:O	1.68	0.94
1:C:950:LYS:H	1:C:953:MET:HE2	1.33	0.94
1:A:418:ARG:HD3	1:A:970:MET:HG3	1.46	0.94
1:C:190:PRO:HD3	1:C:779:TYR:CD1	2.02	0.93
1:A:578:LEU:CD2	1:A:587:THR:HG23	1.98	0.93
1:C:58:GLN:HG3	1:C:62:THR:OG1	1.67	0.93
1:C:548:ILE:HD12	1:C:549:VAL:N	1.84	0.93
1:B:962:GLU:O	1:B:966:ASP:HB2	1.69	0.93
1:C:979:SER:O	1:C:983:ILE:HG13	1.68	0.93
1:A:560:PRO:HB2	1:A:922:THR:HG22	1.50	0.92
1:C:222:THR:HB	1:C:223:PRO:HD3	1.50	0.92
1:A:649:MET:HE3	1:A:653:ARG:NH2	1.85	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:MET:CG	1:C:313:MET:CE	2.48	0.92
1:C:3:ASN:HD21	1:C:432:ARG:HD3	1.35	0.92
1:A:64:VAL:O	1:A:65:ILE:C	2.12	0.92
1:A:965:LEU:O	1:A:969:ARG:HG3	1.69	0.92
1:A:919:ARG:HG3	1:A:920:GLY:H	1.33	0.92
1:A:57:VAL:HG12	1:A:58:GLN:N	1.84	0.92
1:B:225:VAL:HG22	1:C:781:MET:CE	1.98	0.92
1:B:406:VAL:O	1:B:408:ASP:O	1.88	0.92
1:A:214:VAL:HG12	1:A:215:ALA:H	1.32	0.92
1:B:549:VAL:HG22	1:B:550:VAL:H	1.33	0.92
1:C:4:PHE:HB3	1:C:8:ARG:HH22	1.34	0.91
1:C:143:ILE:HG23	1:C:284:GLN:HE22	1.35	0.91
1:C:115:MET:HE1	1:C:118:LEU:CD2	2.00	0.91
1:C:1022:VAL:HA	1:C:1025:PHE:CD2	2.05	0.91
1:A:919:ARG:CG	1:A:920:GLY:H	1.82	0.91
1:A:443:VAL:O	1:A:445:ILE:N	2.03	0.91
1:A:495:THR:O	1:A:496:MET:HB2	1.71	0.91
1:C:1025:PHE:O	1:C:1029:VAL:HG23	1.71	0.91
1:A:5:PHE:CD1	1:A:12:ALA:HB2	2.05	0.91
1:A:781:MET:HB3	1:C:228:GLN:OE1	1.70	0.91
1:A:901:VAL:O	1:A:904:VAL:HG23	1.70	0.91
1:B:81:ASN:O	1:B:81:ASN:ND2	2.02	0.91
1:A:585:GLU:OE2	1:C:227:GLY:HA2	1.71	0.91
1:A:128:SER:HB2	1:B:113:LEU:CD2	2.01	0.91
1:A:571:VAL:HG12	1:A:630:SER:HA	1.53	0.91
1:C:459:PHE:H	1:C:459:PHE:HD2	1.13	0.91
1:C:417:GLU:HA	1:C:417:GLU:OE2	1.70	0.91
1:C:431:THR:HG21	1:C:494:ALA:HB2	1.51	0.90
1:C:188:MET:CE	1:C:200:PRO:HB3	2.01	0.90
1:A:578:LEU:HD21	1:A:587:THR:HA	1.52	0.90
1:A:968:VAL:CG2	1:A:1023:PRO:HB3	2.00	0.90
1:C:185:ARG:HG3	1:C:271:GLY:HA3	1.54	0.90
1:C:314:GLU:HB2	1:C:315:PRO:HD3	1.54	0.90
1:B:51:GLY:O	1:B:53:ASP:OD2	1.90	0.90
1:B:911:GLY:HA3	1:B:1013:THR:HG21	1.51	0.90
1:C:951:ASP:C	1:C:953:MET:H	1.79	0.90
1:A:277:ILE:HG23	1:A:277:ILE:O	1.70	0.89
1:C:44:THR:HG22	1:C:91:THR:HB	0.91	0.89
1:B:441:ALA:O	1:B:445:ILE:HG13	1.72	0.89
1:C:418:ARG:O	1:C:420:MET:N	2.04	0.89
1:C:214:VAL:HG12	1:C:215:ALA:N	1.88	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:VAL:CG1	1:A:327:TYR:HB3	2.02	0.89
1:B:49:TYR:CE1	1:B:122:VAL:HG13	2.06	0.89
1:A:190:PRO:HG3	1:A:789:TRP:CE2	2.08	0.89
1:A:968:VAL:HG21	1:A:1023:PRO:HB3	1.52	0.89
1:B:1:MET:CB	1:B:2:PRO:HD2	2.01	0.89
1:B:184:MET:HG3	1:B:184:MET:O	1.71	0.89
1:A:909:VAL:HG12	1:A:913:LEU:HD21	1.55	0.89
1:B:456:MET:HG3	1:B:467:TYR:CB	2.02	0.89
1:C:423:GLU:HB3	1:C:426:PRO:HG3	1.54	0.89
1:B:171:GLY:HA3	1:B:302:THR:CG2	2.03	0.88
1:B:242:SER:HB2	1:B:245:GLU:OE2	1.72	0.88
1:A:818:ARG:HD2	2:A:1054:HOH:O	1.72	0.88
1:C:131:LYS:O	1:C:295:THR:HG22	1.72	0.88
1:A:1024:VAL:HG12	1:A:1025:PHE:H	1.37	0.88
1:B:247:GLY:HA2	1:B:268:ILE:HD13	0.88	0.88
1:C:291:ILE:HD13	1:C:306:ILE:CD1	2.03	0.88
1:C:1017:LEU:O	1:C:1017:LEU:HD23	1.73	0.88
1:B:47:ALA:HB3	1:B:88:VAL:HB	1.56	0.88
1:B:103:ALA:O	1:B:107:VAL:HG23	1.73	0.88
1:C:444:GLY:O	1:C:448:VAL:HG23	1.74	0.88
1:B:171:GLY:HA3	1:B:302:THR:HG22	1.56	0.87
1:C:950:LYS:HZ1	1:C:1030:ARG:HD3	1.31	0.87
1:B:14:VAL:HG11	1:C:890:ALA:HB2	1.54	0.87
1:C:418:ARG:C	1:C:420:MET:H	1.81	0.87
1:C:950:LYS:HZ3	1:C:1030:ARG:HD3	1.33	0.87
1:A:355:MET:CE	1:A:410:ILE:HG12	2.03	0.87
1:A:909:VAL:HG12	1:A:913:LEU:CD2	2.03	0.87
1:C:950:LYS:NZ	1:C:1030:ARG:CD	2.36	0.87
1:A:105:VAL:O	1:A:108:GLN:HB3	1.75	0.87
1:A:228:GLN:HG2	1:B:781:MET:HG2	1.54	0.87
1:C:164:ASP:CG	2:C:1058:HOH:O	2.15	0.87
1:C:452:VAL:O	1:C:932:LEU:HD13	1.73	0.87
1:A:214:VAL:CG1	1:A:215:ALA:H	1.87	0.87
1:A:1009:GLY:O	1:A:1011:MET:N	2.08	0.87
1:C:396:PHE:O	1:C:400:LEU:HD23	1.73	0.87
1:A:528:THR:HG21	1:A:969:ARG:HE	1.38	0.86
1:B:3:ASN:H	1:B:6:ILE:HG12	1.39	0.86
1:B:187:TRP:CZ3	1:B:774:MET:HE3	2.10	0.86
1:C:141:GLY:HA3	1:C:324:VAL:HG22	1.56	0.86
1:C:291:ILE:CD1	1:C:306:ILE:HD13	2.04	0.86
1:B:590:VAL:O	1:B:594:VAL:HG23	1.75	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:TYR:N	1:A:824:SER:HB3	1.89	0.86
1:B:42:ALA:CB	1:B:93:THR:HG22	2.05	0.86
1:B:919:ARG:HG3	1:B:1005:THR:CG2	2.05	0.86
1:A:32:VAL:HG22	1:A:390:ILE:HB	1.57	0.86
1:A:261:LEU:HD12	1:A:263:ARG:NH2	1.89	0.86
1:B:49:TYR:CD1	1:B:122:VAL:HG22	2.10	0.86
1:C:513:PHE:HA	1:C:516:PHE:HB3	1.57	0.86
1:B:714:THR:HG22	1:B:831:ALA:HA	1.57	0.86
1:B:729:ILE:HG13	1:B:730:ASP:N	1.90	0.86
1:B:804:PHE:HD1	1:B:804:PHE:O	1.58	0.86
1:C:181:GLN:OE1	1:C:767:ARG:NE	2.08	0.86
1:B:226:LYS:HA	1:B:226:LYS:CE	2.06	0.86
1:C:743:ILE:H	1:C:743:ILE:HD12	1.38	0.86
1:B:517:ASN:HB3	1:B:521:GLU:OE1	1.75	0.86
1:C:872:GLN:HB2	1:C:875:SER:HB3	1.55	0.86
1:A:756:GLY:HA2	1:A:774:MET:HB2	1.56	0.85
1:A:809:TRP:O	1:A:810:GLU:HB3	1.73	0.85
1:C:686:ASP:OD1	1:C:690:LEU:HB2	1.76	0.85
1:B:690:LEU:HB2	1:B:694:LYS:HB2	1.57	0.85
1:A:139:VAL:HG13	1:A:327:TYR:HB3	1.58	0.85
1:C:314:GLU:HB2	1:C:315:PRO:CD	2.06	0.85
1:C:927:PHE:O	1:C:931:LEU:HB2	1.74	0.85
1:A:729:ILE:HG22	1:A:730:ASP:N	1.88	0.85
1:C:43:VAL:HA	1:C:130:GLU:O	1.74	0.85
1:A:513:PHE:HD1	1:A:517:ASN:ND2	1.73	0.85
1:A:552:MET:HE1	1:A:906:PRO:HA	1.55	0.85
1:A:911:GLY:HA3	1:A:1013:THR:HG21	1.56	0.85
1:C:432:ARG:HG3	1:C:432:ARG:NH1	1.79	0.85
1:A:113:LEU:HD21	1:C:128:SER:HA	1.56	0.85
1:B:623:ASN:HD22	1:B:623:ASN:C	1.82	0.85
1:C:62:THR:HG23	1:C:90:ILE:HD11	1.56	0.85
1:A:298:ASN:HD22	1:A:298:ASN:C	1.84	0.84
1:A:520:PHE:H	1:A:522:LYS:HE3	1.42	0.84
1:A:632:LYS:O	1:A:637:ARG:HD3	1.76	0.84
1:B:431:THR:CG2	1:B:493:CYS:HB3	2.06	0.84
1:B:552:MET:SD	1:B:909:VAL:HG23	2.17	0.84
1:B:115:MET:HE2	1:B:115:MET:HA	1.59	0.84
1:A:10:ILE:HD11	1:B:895:TRP:HB2	1.58	0.84
1:B:605:ASN:HD21	1:B:642:ASN:ND2	1.75	0.84
1:A:103:ALA:O	1:A:107:VAL:HG23	1.76	0.84
1:A:454:VAL:O	1:A:456:MET:O	1.95	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:GLN:HG2	1:C:316:PHE:CG	2.13	0.84
1:B:150:THR:H	1:B:153:ASP:HB3	1.41	0.84
1:B:190:PRO:HG2	1:B:779:TYR:CD1	2.12	0.84
1:B:659:LYS:HD3	1:B:660:ASP:N	1.92	0.84
1:C:685:ILE:HD11	1:C:687:GLN:HA	1.59	0.84
1:A:186:ILE:HB	1:A:773:VAL:HG23	1.60	0.84
1:B:49:TYR:CG	1:B:122:VAL:HA	2.12	0.84
1:C:759:VAL:O	1:C:760:ASN:HB3	1.78	0.84
1:A:441:ALA:O	1:A:445:ILE:HG23	1.77	0.84
1:A:986:VAL:C	1:A:988:PRO:HD2	2.02	0.84
1:B:200:PRO:HD2	1:B:749:THR:HG22	1.58	0.84
1:A:1024:VAL:O	1:A:1026:PHE:N	2.11	0.84
1:B:26:ALA:O	1:B:30:LEU:HD22	1.78	0.84
1:C:72:ILE:HG22	1:C:94:PHE:CE2	2.13	0.84
1:A:154:ILE:HG22	1:A:287:SER:HB3	1.60	0.83
1:A:1029:VAL:HG12	1:A:1030:ARG:H	1.43	0.83
1:B:831:ALA:CB	1:B:840:ALA:HB2	2.08	0.83
1:A:46:SER:O	1:A:127:VAL:HG13	1.78	0.83
1:A:406:VAL:HG13	1:A:407:ASP:N	1.92	0.83
1:A:1020:PHE:O	1:A:1024:VAL:HG23	1.77	0.83
1:B:555:LEU:HB2	1:B:913:LEU:HD23	1.59	0.83
1:A:63:GLN:O	1:A:66:GLU:N	2.10	0.83
1:B:945:ILE:HD12	1:B:1026:PHE:HE2	1.42	0.83
1:C:247:GLY:HA2	1:C:268:ILE:HD13	1.59	0.83
1:A:255:GLN:H	1:A:255:GLN:CD	1.85	0.83
1:C:713:LEU:HD11	1:C:834:GLY:CA	2.07	0.83
1:C:190:PRO:CD	1:C:779:TYR:HD1	1.89	0.83
1:C:699:ARG:HD2	1:C:703:LEU:HD11	1.60	0.83
1:A:498:LYS:O	1:A:498:LYS:NZ	2.11	0.83
1:A:649:MET:HB3	1:A:653:ARG:NH2	1.93	0.83
1:C:4:PHE:CB	1:C:8:ARG:HH22	1.92	0.83
1:B:158:VAL:HA	1:B:162:MET:HG2	1.58	0.83
1:C:420:MET:SD	1:C:498:LYS:NZ	2.52	0.83
1:C:568:ASP:OD1	1:C:634:TRP:NE1	2.10	0.83
1:A:902:MET:O	1:A:905:VAL:HG23	1.79	0.83
1:B:528:THR:O	1:B:531:VAL:HG12	1.79	0.83
1:B:894:SER:CB	1:B:897:ILE:HG12	2.07	0.83
1:B:563:PHE:O	1:B:925:VAL:HG12	1.78	0.83
1:C:164:ASP:O	1:C:168:ARG:HG2	1.78	0.83
1:B:493:CYS:O	1:B:494:ALA:HB3	1.79	0.82
1:B:613:ASN:HD22	1:B:614:GLY:N	1.75	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:713:LEU:HD12	1:B:713:LEU:H	1.44	0.82
1:B:892:TYR:CB	1:B:897:ILE:HD11	2.09	0.82
1:C:165:ALA:HA	1:C:168:ARG:HG3	1.59	0.82
1:A:106:GLN:O	1:A:107:VAL:O	1.97	0.82
1:B:104:GLN:HG3	1:B:105:VAL:N	1.93	0.82
1:A:355:MET:HE3	1:A:410:ILE:HG12	1.59	0.82
1:A:405:LEU:HD22	1:A:406:VAL:N	1.93	0.82
1:C:699:ARG:HG2	1:C:699:ARG:NH1	1.93	0.82
1:C:54:ALA:H	1:C:57:VAL:HG23	1.44	0.82
1:C:562:SER:O	1:C:924:ASP:HA	1.79	0.82
1:B:45:ILE:HD12	1:B:90:ILE:HB	1.61	0.82
1:B:573:MET:HE1	1:B:617:PHE:HE2	1.42	0.82
1:C:55:LYS:HE2	1:C:59:ASP:OD1	1.79	0.82
1:C:686:ASP:HB3	1:C:823:PRO:HG2	1.61	0.82
1:A:342:LYS:HG3	1:A:343:THR:H	1.43	0.82
1:A:820:ASN:O	1:C:168:ARG:NH2	2.13	0.82
1:C:144:ASN:HB3	2:C:1077:HOH:O	1.80	0.82
1:C:962:GLU:O	1:C:965:LEU:HB3	1.79	0.82
1:B:245:GLU:HA	1:B:248:LYS:HG2	1.62	0.82
1:A:443:VAL:HG12	1:A:444:GLY:N	1.95	0.82
1:C:115:MET:CE	1:C:115:MET:HA	2.10	0.82
1:C:166:ILE:CD1	2:C:1075:HOH:O	2.27	0.82
1:A:69:MET:HG2	2:A:1056:HOH:O	1.77	0.82
1:A:545:TYR:HB2	1:A:1021:PHE:CE1	2.14	0.82
1:A:722:GLU:HG3	2:A:1060:HOH:O	1.78	0.82
1:B:1:MET:HB2	1:B:2:PRO:CD	2.09	0.82
1:A:713:LEU:CD2	1:A:714:THR:H	1.92	0.81
1:C:950:LYS:HZ1	1:C:1030:ARG:CD	1.93	0.81
1:A:719:ASN:HD22	1:A:719:ASN:C	1.85	0.81
1:A:276:ASP:HB3	1:C:222:THR:HG23	1.62	0.81
1:A:419:VAL:O	1:A:424:GLY:HA3	1.81	0.81
1:B:104:GLN:CG	1:B:105:VAL:N	2.42	0.81
1:B:276:ASP:O	1:B:614:GLY:HA3	1.81	0.81
1:B:880:SER:O	1:B:884:VAL:HG23	1.81	0.81
1:A:45:ILE:HG22	1:A:45:ILE:O	1.81	0.81
1:A:223:PRO:HD3	1:B:275:TYR:CD2	2.16	0.81
1:B:213:GLN:HE21	1:B:239:ARG:HD2	1.45	0.81
1:B:92:LEU:HD22	1:B:92:LEU:N	1.94	0.81
1:C:164:ASP:O	1:C:168:ARG:CG	2.28	0.81
1:C:644:VAL:HG11	1:C:667:ASN:HD22	1.45	0.81
1:C:888:LEU:HB3	1:C:898:PRO:HB3	1.62	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:LEU:HD23	1:B:675:GLY:N	1.94	0.81
1:B:859:TRP:HB3	1:B:863:SER:HB2	1.61	0.81
1:C:38:ILE:HG21	1:C:466:ILE:HD11	1.61	0.81
1:A:214:VAL:CG1	1:A:215:ALA:N	2.44	0.81
1:A:536:ARG:HG2	1:A:537:SER:N	1.95	0.81
1:A:314:GLU:HA	2:A:1061:HOH:O	1.79	0.81
1:B:405:LEU:HD12	1:B:406:VAL:N	1.96	0.81
1:C:190:PRO:O	1:C:191:ASN:C	2.23	0.81
1:A:205:THR:O	1:A:205:THR:CG2	2.27	0.81
1:A:413:VAL:HG23	1:A:493:CYS:HB2	1.63	0.81
1:A:713:LEU:HB3	1:A:832:ALA:CA	2.11	0.81
1:B:70:ASN:O	1:B:70:ASN:ND2	2.14	0.81
1:B:399:VAL:O	1:B:402:ILE:HG22	1.81	0.81
1:B:314:GLU:H	1:B:315:PRO:HD2	1.44	0.81
1:C:162:MET:CG	1:C:313:MET:HE2	2.07	0.81
1:A:253:VAL:HG23	1:A:258:SER:O	1.80	0.80
1:A:467:TYR:CE1	1:A:925:VAL:HG22	2.16	0.80
1:B:350:LEU:HB3	1:B:984:LEU:HD12	1.61	0.80
1:C:350:LEU:HD13	1:C:984:LEU:CD2	2.11	0.80
1:C:713:LEU:HD21	1:C:835:LYS:H	1.46	0.80
1:A:395:MET:HE2	1:A:395:MET:HA	1.63	0.80
1:A:605:ASN:OD1	1:A:637:ARG:HG2	1.82	0.80
1:A:634:TRP:CE3	1:A:995:ALA:HB1	2.16	0.80
1:A:884:VAL:HG12	1:A:902:MET:HE3	1.63	0.80
1:B:100:ALA:O	1:B:103:ALA:HB3	1.81	0.80
1:B:416:VAL:HG11	1:B:431:THR:HG22	1.64	0.80
1:B:456:MET:CG	1:B:467:TYR:HB3	2.09	0.80
1:B:358:PHE:HB3	1:B:977:MET:HE2	1.63	0.80
1:B:879:ILE:O	1:B:883:VAL:HG23	1.82	0.80
1:C:702:LEU:HB2	1:C:851:LEU:HD21	1.62	0.80
1:A:801:PHE:CD2	1:A:805:SER:OG	2.34	0.80
1:A:951:ASP:O	1:A:955:LYS:HB2	1.81	0.80
1:B:157:TYR:HA	1:B:161:ASN:ND2	1.97	0.80
1:C:156:ASP:O	1:C:157:TYR:C	2.22	0.80
1:B:646:ALA:O	1:B:648:THR:N	2.13	0.80
1:B:849:SER:O	1:B:850:LYS:HD3	1.81	0.80
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.62	0.80
1:A:949:ALA:HB1	1:A:1026:PHE:CE2	2.17	0.80
1:B:11:PHE:O	1:B:14:VAL:HB	1.81	0.80
1:B:945:ILE:HD11	1:B:1022:VAL:HB	1.64	0.80
1:C:346:GLU:OE1	1:C:988:PRO:HG3	1.82	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:PRO:CD	1:C:779:TYR:CD1	2.64	0.80
1:A:406:VAL:HG13	1:A:407:ASP:H	1.45	0.79
1:B:568:ASP:OD1	1:B:644:VAL:HG22	1.82	0.79
1:C:536:ARG:HH11	1:C:961:ILE:HD11	1.47	0.79
1:A:66:GLU:OE2	2:A:1058:HOH:O	1.99	0.79
1:B:230:LEU:HD21	1:C:809:TRP:CH2	2.16	0.79
1:B:830:GLN:H	1:B:830:GLN:HE21	1.30	0.79
1:B:912:ALA:HB2	1:B:1010:GLY:HA3	1.65	0.79
1:C:169:THR:HB	1:C:172:VAL:HG21	1.63	0.79
1:A:105:VAL:O	1:A:108:GLN:CB	2.30	0.79
1:A:685:ILE:HG22	1:A:687:GLN:H	1.48	0.79
1:C:350:LEU:HD12	1:C:985:GLY:HA2	1.64	0.79
1:A:61:VAL:O	1:A:65:ILE:HG23	1.77	0.79
1:A:112:GLN:HE21	1:A:112:GLN:CA	1.95	0.79
1:B:2:PRO:HD3	1:B:486:LEU:HD12	1.65	0.79
1:B:972:LEU:HD13	1:B:976:LEU:HD23	1.64	0.79
1:A:590:VAL:O	1:A:594:VAL:HG23	1.83	0.79
1:A:64:VAL:C	1:A:65:ILE:C	2.50	0.79
1:A:69:MET:HA	1:A:69:MET:HE2	1.64	0.79
1:C:423:GLU:HB3	1:C:426:PRO:CG	2.12	0.79
1:A:568:ASP:OD2	1:A:637:ARG:NH1	2.16	0.79
1:C:183:ALA:O	1:C:185:ARG:HG2	1.82	0.79
1:C:427:PRO:CA	1:C:498:LYS:HE3	2.09	0.79
1:C:728:LYS:HG3	1:C:729:ILE:N	1.97	0.79
1:B:358:PHE:HZ	1:B:976:LEU:HD12	1.47	0.79
1:C:158:VAL:O	1:C:162:MET:N	2.15	0.79
1:C:655:PHE:C	1:C:657:GLN:H	1.91	0.79
1:C:778:LYS:HD2	1:C:779:TYR:HE2	1.48	0.79
1:A:68:ASN:N	1:A:68:ASN:C	2.41	0.78
1:A:584:GLN:H	1:A:622:GLN:HB3	1.48	0.78
1:B:452:VAL:O	1:B:453:PHE:HB2	1.82	0.78
1:C:685:ILE:HG12	1:C:687:GLN:OE1	1.82	0.78
1:A:60:THR:HG21	1:A:119:PRO:HG3	1.65	0.78
1:C:911:GLY:HA3	1:C:1013:THR:HG21	1.63	0.78
1:B:531:VAL:HG13	1:B:965:LEU:HD21	1.64	0.78
1:C:61:VAL:HG12	2:C:1064:HOH:O	1.81	0.78
1:C:252:LYS:O	1:C:260:VAL:HG12	1.82	0.78
1:C:352:PHE:HA	1:C:369:THR:HG21	1.65	0.78
1:B:538:THR:N	1:B:540:ARG:HH21	1.81	0.78
1:B:729:ILE:HG13	1:B:730:ASP:H	1.46	0.78
1:A:61:VAL:HG13	1:A:118:LEU:HD22	1.64	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:MET:C	1:A:70:ASN:HD22	1.91	0.78
1:A:210:GLN:HG3	1:A:249:ILE:HG23	1.63	0.78
1:A:298:ASN:ND2	1:A:300:LEU:H	1.80	0.78
1:B:525:HIS:HA	1:B:528:THR:HG22	1.64	0.78
1:A:400:LEU:HD13	1:A:1003:VAL:CG1	2.11	0.78
1:B:587:THR:O	1:B:591:LEU:HB2	1.83	0.78
1:A:166:ILE:HD13	1:A:166:ILE:N	1.96	0.78
1:A:578:LEU:HD23	1:A:587:THR:HG23	1.66	0.78
1:A:836:SER:OG	1:A:839:GLU:HG2	1.84	0.78
1:A:886:LEU:HD21	1:C:17:ILE:HG21	1.63	0.78
1:B:157:TYR:HA	1:B:161:ASN:HD22	1.49	0.78
1:C:410:ILE:HG22	1:C:411:VAL:N	1.98	0.78
1:C:463:THR:O	1:C:465:ALA:N	2.17	0.78
1:B:987:MET:HE3	1:B:987:MET:CA	2.10	0.78
1:A:520:PHE:N	1:A:522:LYS:HE3	1.99	0.78
1:A:314:GLU:N	1:A:315:PRO:CD	2.47	0.78
1:A:467:TYR:HE1	1:A:925:VAL:HG22	1.46	0.78
1:A:783:PRO:HD3	1:C:219:LEU:HD13	1.65	0.78
1:B:562:SER:O	1:B:924:ASP:HA	1.84	0.78
1:B:602:GLU:OE2	1:B:650:ARG:HD2	1.82	0.78
1:B:987:MET:HA	1:B:987:MET:CE	2.09	0.78
1:C:45:ILE:CB	1:C:45:ILE:C	2.56	0.78
1:C:695:LEU:HD22	1:C:825:MET:HE2	1.66	0.77
1:C:726:GLN:CD	1:C:812:GLY:HA3	2.08	0.77
1:A:115:MET:C	1:A:117:LEU:H	1.92	0.77
1:B:448:VAL:O	1:B:452:VAL:HG22	1.84	0.77
1:C:115:MET:N	1:C:116:PRO:CD	2.47	0.77
1:C:143:ILE:HD11	1:C:286:ALA:HB2	1.67	0.77
1:C:578:LEU:HB3	1:C:579:PRO:HD2	1.65	0.77
1:A:168:ARG:O	1:A:168:ARG:HG3	1.84	0.77
1:A:843:LEU:HA	1:A:846:GLN:NE2	1.98	0.77
1:A:909:VAL:O	1:A:912:ALA:HB3	1.84	0.77
1:B:6:ILE:HD12	1:B:490:PRO:HB2	1.64	0.77
1:B:699:ARG:HG2	1:B:700:ASN:H	1.49	0.77
1:A:54:ALA:CB	1:A:816:LEU:HG	2.15	0.77
1:A:108:GLN:CG	1:B:112:GLN:OE1	2.28	0.77
1:A:495:THR:O	1:A:495:THR:HG22	1.83	0.77
1:B:346:GLU:OE1	1:B:988:PRO:HB3	1.84	0.77
1:B:750:LEU:C	1:B:750:LEU:HD13	2.10	0.77
1:B:345:VAL:HA	1:B:348:ILE:HD12	1.67	0.77
1:B:983:ILE:HD13	1:B:1012:VAL:HG12	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:GLY:CA	1:C:231:ASN:ND2	2.46	0.77
1:C:754:TRP:CZ2	1:C:786:ILE:HG13	2.20	0.77
1:A:115:MET:HA	1:A:115:MET:HE3	1.65	0.77
1:A:522:LYS:N	1:A:522:LYS:HE2	2.00	0.77
1:A:1018:ALA:O	1:A:1022:VAL:HG13	1.85	0.77
1:B:674:LEU:HD13	1:B:860:THR:HG21	1.66	0.77
1:C:84:SER:C	1:C:86:GLY:H	1.92	0.77
1:A:57:VAL:O	1:A:57:VAL:HG13	1.81	0.77
1:A:596:HIS:O	1:A:598:TYR:N	2.18	0.77
1:A:687:GLN:HE21	1:A:856:GLY:HA3	1.47	0.77
1:C:115:MET:HE1	1:C:118:LEU:HD22	1.58	0.77
1:A:514:GLY:O	1:A:518:ARG:HB2	1.84	0.77
1:B:714:THR:HG21	1:B:833:PRO:CD	2.14	0.77
1:C:127:VAL:CA	1:C:127:VAL:CG2	2.60	0.77
1:A:67:GLN:C	1:A:68:ASN:CA	2.57	0.76
1:B:945:ILE:CD1	1:B:1026:PHE:HE2	1.98	0.76
1:C:62:THR:CA	2:C:1064:HOH:O	2.33	0.76
1:A:728:LYS:NZ	1:C:235:ILE:HG22	2.00	0.76
1:C:108:GLN:C	2:C:1056:HOH:O	2.28	0.76
1:C:717:ARG:HH12	1:C:829:GLY:HA2	1.50	0.76
1:A:48:SER:HA	1:A:86:GLY:O	1.85	0.76
1:A:543:VAL:O	1:A:544:LEU:HB3	1.86	0.76
1:A:885:PHE:HD2	1:A:886:LEU:HD12	1.50	0.76
1:B:411:VAL:O	1:B:438:ILE:HG12	1.86	0.76
1:B:707:ALA:O	1:B:708:LYS:HB3	1.83	0.76
1:C:72:ILE:HG22	1:C:94:PHE:HE2	1.49	0.76
1:C:975:ILE:HG21	1:C:1019:ILE:HD13	1.65	0.76
1:B:517:ASN:O	1:B:521:GLU:HG3	1.85	0.76
1:B:520:PHE:HA	1:B:523:SER:OG	1.85	0.76
1:C:82:SER:HB3	1:C:88:VAL:CA	2.13	0.76
1:C:972:LEU:H	1:C:974:PRO:HD2	1.49	0.76
1:A:539:GLY:HA2	1:A:542:LEU:HB2	1.67	0.76
1:B:418:ARG:HG3	1:B:970:MET:CE	2.16	0.76
1:A:522:LYS:HE2	1:A:522:LYS:H	1.50	0.76
1:C:259:ARG:HH11	1:C:259:ARG:HB2	1.46	0.76
1:C:407:ASP:OD2	1:C:940:LYS:NZ	2.17	0.76
1:C:391:ASN:H	1:C:394:THR:CG2	1.97	0.76
1:C:527:TYR:OH	1:C:968:VAL:HG12	1.86	0.76
1:B:136:PHE:HE1	1:B:617:PHE:CZ	2.04	0.76
1:A:60:THR:HG22	1:A:119:PRO:HD3	1.68	0.76
1:A:818:ARG:HA	1:A:824:SER:H	1.49	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:690:LEU:HB2	1:B:694:LYS:CB	2.14	0.76
1:B:894:SER:HB3	1:B:897:ILE:CG1	2.15	0.76
1:A:472:ILE:HD12	1:A:472:ILE:N	1.98	0.76
1:C:713:LEU:HD22	1:C:713:LEU:H	1.51	0.76
1:B:221:GLY:HA3	1:C:780:ARG:NH1	2.02	0.75
1:B:231:ASN:C	1:B:231:ASN:ND2	2.43	0.75
1:B:234:ILE:HG22	1:B:234:ILE:O	1.87	0.75
1:B:269:GLU:O	1:B:270:LEU:HB2	1.86	0.75
1:A:1:MET:N	1:A:2:PRO:HD2	2.01	0.75
1:A:472:ILE:HD12	1:A:472:ILE:H	1.48	0.75
1:A:227:GLY:HA2	1:B:585:GLU:OE1	1.87	0.75
1:A:282:ASN:HD21	1:A:609:VAL:H	1.31	0.75
1:A:515:TRP:HA	1:A:519:MET:SD	2.26	0.75
1:B:328:ASP:HB2	2:B:1059:HOH:O	1.86	0.75
1:C:435:MET:HE2	1:C:490:PRO:HB3	1.68	0.75
1:A:890:ALA:HB1	1:C:11:PHE:CD1	2.22	0.75
1:B:610:PHE:O	1:B:627:ALA:HB1	1.86	0.75
1:B:804:PHE:O	1:B:804:PHE:CD1	2.39	0.75
1:A:713:LEU:HD22	1:A:714:THR:N	1.97	0.75
1:A:790:TYR:CE1	1:A:800:PRO:HG3	2.20	0.75
1:A:818:ARG:CB	1:A:818:ARG:HE	1.98	0.75
1:C:459:PHE:CD2	1:C:459:PHE:N	2.48	0.75
1:A:61:VAL:HG13	1:A:118:LEU:CD2	2.16	0.75
1:B:1022:VAL:HG23	1:B:1023:PRO:CD	2.16	0.75
1:C:166:ILE:C	1:C:172:VAL:HG11	2.11	0.75
1:A:534:ILE:HB	1:A:540:ARG:NH1	2.01	0.75
1:A:661:ALA:O	1:A:663:VAL:HG23	1.87	0.75
1:B:549:VAL:CG2	1:B:550:VAL:N	2.49	0.75
1:A:112:GLN:HA	1:A:112:GLN:NE2	1.97	0.74
1:B:560:PRO:HB2	1:B:836:SER:HB3	1.69	0.74
1:A:73:ASP:HB3	1:A:106:GLN:HE22	1.51	0.74
1:C:489:THR:O	1:C:493:CYS:HB3	1.88	0.74
1:A:599:LEU:O	1:A:600:THR:HB	1.86	0.74
1:A:1023:PRO:O	1:A:1027:VAL:HG23	1.87	0.74
1:C:32:VAL:O	1:C:32:VAL:HG12	1.87	0.74
1:C:975:ILE:HG22	1:C:976:LEU:N	2.00	0.74
1:C:73:ASP:O	1:C:74:ASN:O	2.06	0.74
1:C:424:GLY:HA2	2:C:1073:HOH:O	1.86	0.74
1:C:457:ALA:HB1	1:C:468:ARG:HA	1.67	0.74
1:C:577:GLN:HB3	1:C:624:THR:HG22	1.69	0.74
1:C:643:LYS:O	1:C:647:ILE:HG13	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:LEU:HD12	1:A:560:PRO:CD	2.15	0.74
1:A:578:LEU:HD21	1:A:587:THR:HG23	1.69	0.74
1:B:946:VAL:HG22	1:B:1026:PHE:CZ	2.23	0.74
1:C:1:MET:HE3	1:C:439:GLN:HE22	1.50	0.74
1:C:158:VAL:CG2	1:C:158:VAL:CG1	2.62	0.74
1:B:262:LEU:HB3	1:B:268:ILE:HD11	1.69	0.74
1:C:166:ILE:HG12	2:C:1075:HOH:O	1.88	0.74
1:C:513:PHE:HA	1:C:516:PHE:CB	2.18	0.74
1:C:588:GLN:HG2	1:C:613:ASN:ND2	2.03	0.74
1:C:643:LYS:HG2	1:C:645:GLU:H	1.52	0.74
1:C:655:PHE:HA	1:C:659:LYS:HD3	1.70	0.74
1:C:785:ASP:C	1:C:787:GLY:H	1.93	0.74
1:A:44:THR:O	1:A:45:ILE:HG13	1.88	0.74
1:A:44:THR:O	1:A:45:ILE:CG1	2.36	0.74
1:A:701:GLN:OE1	1:A:852:PRO:HD3	1.87	0.74
1:B:356:TYR:C	1:B:358:PHE:H	1.95	0.74
1:B:686:ASP:HB3	1:B:823:PRO:O	1.87	0.74
1:B:973:ARG:HG2	1:B:974:PRO:HD3	1.70	0.74
1:C:131:LYS:C	1:C:295:THR:HG22	2.12	0.74
1:C:159:ALA:O	1:C:160:ALA:C	2.17	0.74
1:C:680:PHE:CE1	1:C:844:MET:HE2	2.23	0.74
1:A:568:ASP:HB3	1:A:634:TRP:HZ3	1.53	0.74
1:B:228:GLN:CD	1:C:781:MET:HE3	2.13	0.74
1:C:358:PHE:CB	1:C:977:MET:HE2	2.15	0.74
1:C:592:ASN:HD22	1:C:592:ASN:N	1.84	0.74
1:A:919:ARG:HG3	1:A:920:GLY:N	2.03	0.73
1:C:184:MET:HG2	1:C:246:PHE:CD1	2.23	0.73
1:A:578:LEU:O	1:A:623:ASN:ND2	2.20	0.73
1:A:749:THR:O	1:A:753:ALA:HB2	1.88	0.73
1:B:704:ALA:O	1:B:705:GLU:CG	2.35	0.73
1:C:69:MET:CE	1:C:92:LEU:CD2	2.54	0.73
1:C:879:ILE:O	1:C:883:VAL:HG23	1.88	0.73
1:C:950:LYS:O	1:C:954:ASP:HB2	1.88	0.73
1:A:108:GLN:CG	1:B:112:GLN:CD	2.62	0.73
1:A:736:ALA:O	1:A:741:VAL:HG13	1.88	0.73
1:A:993:THR:HG21	1:A:1000:GLN:OE1	1.87	0.73
1:B:945:ILE:CD1	1:B:1026:PHE:CE2	2.72	0.73
1:C:62:THR:HA	2:C:1064:HOH:O	1.86	0.73
1:A:832:ALA:HB3	1:A:835:LYS:HB2	1.70	0.73
1:B:291:ILE:HG21	1:B:306:ILE:HD11	1.69	0.73
1:C:87:THR:CG2	1:C:88:VAL:N	2.51	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ASN:ND2	1:C:149:MET:H	1.86	0.73
1:A:426:PRO:HG2	1:A:429:GLU:OE2	1.88	0.73
1:A:773:VAL:HG13	1:A:773:VAL:O	1.87	0.73
1:A:947:GLU:O	1:A:951:ASP:HB2	1.88	0.73
1:B:350:LEU:HB3	1:B:984:LEU:CD1	2.17	0.73
1:B:790:TYR:HE1	1:B:800:PRO:HB3	1.53	0.73
1:B:970:MET:HA	1:B:970:MET:HE2	1.70	0.73
1:A:190:PRO:HG3	1:A:789:TRP:CD2	2.23	0.73
1:B:423:GLU:OE1	1:B:427:PRO:CD	2.37	0.73
1:C:922:THR:HG22	1:C:923:ASN:H	1.53	0.73
1:B:1018:ALA:O	1:B:1022:VAL:HG22	1.88	0.73
1:C:1:MET:HB2	1:C:2:PRO:CD	2.16	0.73
1:A:428:LYS:HG3	1:A:429:GLU:H	1.52	0.73
1:A:106:GLN:O	1:A:107:VAL:C	2.26	0.73
1:A:461:GLY:O	1:A:463:THR:O	2.06	0.73
1:A:540:ARG:HG3	1:A:541:TYR:H	1.53	0.73
1:A:596:HIS:C	1:A:598:TYR:H	1.95	0.73
1:B:439:GLN:HA	1:B:442:LEU:HD12	1.71	0.73
1:B:759:VAL:HG12	1:B:760:ASN:HB2	1.70	0.73
1:B:7:ASP:O	1:B:8:ARG:HB2	1.89	0.73
1:C:144:ASN:HD21	1:C:149:MET:H	1.33	0.73
1:C:365:THR:O	1:C:368:PRO:HD2	1.88	0.73
1:A:102:ILE:HA	1:A:105:VAL:CG2	2.18	0.72
1:A:801:PHE:HD2	1:A:805:SER:OG	1.70	0.72
1:B:42:ALA:HB2	1:B:93:THR:CG2	2.16	0.72
1:A:90:ILE:HG22	1:A:90:ILE:O	1.85	0.72
1:A:822:LEU:HB3	1:A:823:PRO:HD2	1.69	0.72
1:B:136:PHE:HD2	1:B:290:GLY:O	1.72	0.72
1:B:845:GLU:CG	1:B:857:TYR:OH	2.37	0.72
1:B:65:ILE:O	1:B:69:MET:HG2	1.89	0.72
1:A:10:ILE:HG12	1:B:893:GLU:O	1.90	0.72
1:B:740:GLY:O	1:B:794:ALA:N	2.22	0.72
1:C:358:PHE:HB3	1:C:977:MET:CE	2.19	0.72
1:C:450:SER:O	1:C:451:ALA:CB	2.35	0.72
1:B:642:ASN:H	1:B:650:ARG:HH12	1.38	0.72
1:B:713:LEU:CD1	1:B:843:LEU:HD13	2.19	0.72
1:C:729:ILE:CD1	1:C:786:ILE:HD13	2.18	0.72
1:B:489:THR:O	1:B:492:LEU:HB2	1.89	0.72
1:C:519:MET:HG3	1:C:520:PHE:N	2.03	0.72
1:C:159:ALA:C	1:C:161:ASN:H	1.98	0.72
1:C:946:VAL:O	1:C:946:VAL:HG12	1.90	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:VAL:HG22	1:B:778:LYS:NZ	2.04	0.72
1:A:415:ASN:HB3	1:A:434:SER:OG	1.90	0.72
1:B:30:LEU:HD23	1:B:390:ILE:HD11	1.72	0.72
1:B:48:SER:O	1:B:48:SER:OG	2.00	0.72
1:B:172:VAL:O	1:B:173:GLY:O	2.06	0.72
1:B:944:LEU:O	1:B:971:ARG:HD2	1.89	0.72
1:C:104:GLN:HG3	1:C:131:LYS:HG2	1.72	0.72
1:A:69:MET:O	1:A:70:ASN:ND2	2.19	0.72
1:A:311:ALA:O	1:A:312:LYS:HB2	1.89	0.72
1:A:733:GLN:OE1	1:A:743:ILE:HG12	1.90	0.72
2:B:1060:HOH:O	1:C:110:LYS:HD3	1.90	0.72
1:C:536:ARG:NH1	1:C:961:ILE:HD11	2.05	0.72
1:A:314:GLU:N	1:A:315:PRO:HD3	2.04	0.71
1:A:447:MET:HB3	1:A:887:CYS:SG	2.30	0.71
1:B:136:PHE:HE1	1:B:617:PHE:HZ	1.38	0.71
1:B:235:ILE:H	1:B:235:ILE:HD13	1.55	0.71
1:C:225:VAL:O	1:C:226:LYS:C	2.32	0.71
1:C:613:ASN:C	1:C:613:ASN:OD1	2.32	0.71
1:A:359:LEU:HD12	1:A:417:GLU:HG2	1.72	0.71
1:A:782:LEU:O	1:A:784:ASP:O	2.07	0.71
1:B:92:LEU:N	1:B:92:LEU:CD2	2.53	0.71
1:B:314:GLU:H	1:B:315:PRO:CD	2.03	0.71
1:A:406:VAL:CG1	1:A:407:ASP:H	2.02	0.71
1:A:436:GLY:HA2	1:A:439:GLN:HB2	1.73	0.71
1:A:649:MET:HE3	1:A:653:ARG:CZ	2.19	0.71
1:A:728:LYS:HZ2	1:C:235:ILE:HG22	1.53	0.71
1:A:729:ILE:CG2	1:A:730:ASP:H	1.99	0.71
1:B:714:THR:HG22	1:B:831:ALA:CA	2.20	0.71
1:B:892:TYR:HB3	1:B:897:ILE:HD11	1.71	0.71
1:B:940:LYS:O	1:B:941:ASN:C	2.32	0.71
1:C:108:GLN:HA	2:C:1056:HOH:O	1.89	0.71
1:B:418:ARG:HG3	1:B:970:MET:HE1	1.71	0.71
1:C:327:TYR:HB3	1:C:628:PHE:HB3	1.70	0.71
1:C:764:ASP:OD2	1:C:765:ARG:HD2	1.90	0.71
1:A:896:SER:O	1:A:899:PHE:HB2	1.90	0.71
1:A:904:VAL:HG21	1:A:942:ALA:HB2	1.72	0.71
1:C:542:LEU:HD23	1:C:542:LEU:O	1.89	0.71
1:C:695:LEU:HD22	1:C:825:MET:HG3	1.73	0.71
1:C:713:LEU:CD1	1:C:834:GLY:HA3	2.16	0.71
1:A:11:PHE:CD1	1:B:890:ALA:HB1	2.26	0.71
1:A:69:MET:C	1:A:70:ASN:ND2	2.48	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:LEU:O	1:A:377:LEU:C	2.34	0.71
1:A:644:VAL:O	1:A:648:THR:HG23	1.90	0.71
1:B:115:MET:O	1:B:123:GLN:NE2	2.23	0.71
1:B:116:PRO:HA	1:B:123:GLN:NE2	2.06	0.71
1:B:790:TYR:CE1	1:B:800:PRO:HB3	2.25	0.71
1:C:105:VAL:O	1:C:108:GLN:N	2.23	0.71
1:C:568:ASP:OD2	1:C:644:VAL:HG23	1.88	0.71
1:A:894:SER:OG	1:A:897:ILE:HB	1.90	0.71
1:A:1027:VAL:O	1:A:1029:VAL:O	2.07	0.71
1:B:219:LEU:HD12	1:B:234:ILE:HG12	1.71	0.71
1:C:166:ILE:CG1	2:C:1075:HOH:O	2.38	0.71
1:C:169:THR:HG22	1:C:172:VAL:HG23	1.72	0.71
1:C:777:ALA:O	1:C:779:TYR:N	2.24	0.71
1:C:945:ILE:O	1:C:946:VAL:HG23	1.90	0.71
1:B:518:ARG:HA	1:B:521:GLU:HB2	1.73	0.71
1:C:290:GLY:O	1:C:291:ILE:HG13	1.91	0.71
1:C:317:PHE:HB2	1:C:318:PRO:HD2	1.71	0.71
1:C:418:ARG:HG3	1:C:419:VAL:HG13	1.73	0.71
1:C:463:THR:HG22	1:C:464:GLY:N	2.05	0.71
1:C:476:SER:C	1:C:478:MET:H	1.98	0.71
1:C:696:THR:HA	1:C:825:MET:HE1	1.73	0.71
1:C:951:ASP:C	1:C:953:MET:N	2.48	0.71
1:A:65:ILE:O	1:A:68:ASN:HB2	1.91	0.71
1:B:623:ASN:HD22	1:B:624:THR:N	1.88	0.71
1:C:350:LEU:HD13	1:C:984:LEU:HD23	1.73	0.71
1:C:552:MET:O	1:C:553:ALA:HB3	1.90	0.71
1:C:997:SER:O	1:C:998:GLY:C	2.31	0.71
1:A:189:ASN:HD21	1:A:192:GLU:CB	2.04	0.70
1:A:328:ASP:O	1:A:331:PRO:HD2	1.91	0.70
1:A:687:GLN:HG2	1:C:316:PHE:CD1	2.25	0.70
1:A:818:ARG:CB	1:A:818:ARG:NE	2.54	0.70
1:C:103:ALA:O	1:C:104:GLN:C	2.32	0.70
1:A:9:PRO:HB3	1:A:491:ALA:HB1	1.73	0.70
1:A:551:GLY:O	1:A:554:TYR:HB3	1.91	0.70
1:B:188:MET:SD	1:B:200:PRO:HB3	2.31	0.70
1:B:291:ILE:HG21	1:B:306:ILE:CD1	2.22	0.70
1:C:144:ASN:ND2	1:C:149:MET:HG3	2.07	0.70
1:C:158:VAL:CG2	1:C:158:VAL:CA	2.69	0.70
1:C:189:ASN:CG	1:C:779:TYR:HE1	1.98	0.70
1:C:399:VAL:HA	1:C:402:ILE:CD1	2.21	0.70
1:C:713:LEU:HG	1:C:832:ALA:C	2.17	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:959:GLY:H	1:C:962:GLU:HB2	1.56	0.70
1:B:556:PHE:N	1:B:913:LEU:HD21	2.06	0.70
1:A:228:GLN:HG2	1:B:781:MET:CG	2.22	0.70
1:B:279:ALA:HA	1:B:611:ALA:O	1.91	0.70
1:B:537:SER:HB2	1:B:540:ARG:CG	2.21	0.70
1:B:1005:THR:O	1:B:1005:THR:HG22	1.89	0.70
1:C:12:ALA:HB1	1:C:487:ILE:HG22	1.73	0.70
1:B:418:ARG:HE	1:B:970:MET:HE3	1.56	0.70
1:B:987:MET:O	1:B:990:VAL:HB	1.92	0.70
1:C:102:ILE:O	1:C:103:ALA:C	2.31	0.70
1:B:523:SER:HA	1:B:526:HIS:CD2	2.18	0.70
1:C:192:GLU:O	1:C:195:LYS:N	2.25	0.70
1:A:634:TRP:HE3	1:A:995:ALA:HB1	1.54	0.70
1:B:705:GLU:O	1:B:707:ALA:N	2.23	0.70
1:C:115:MET:HE1	1:C:118:LEU:HD23	1.73	0.70
1:C:380:PHE:CZ	1:C:395:MET:HE1	2.26	0.70
1:A:1013:THR:O	1:A:1017:LEU:HB3	1.91	0.70
1:C:592:ASN:ND2	1:C:592:ASN:H	1.87	0.70
1:A:73:ASP:CB	1:A:106:GLN:HE22	2.05	0.70
1:A:155:SER:HA	1:A:287:SER:OG	1.92	0.70
1:B:328:ASP:C	1:B:328:ASP:OD2	2.35	0.70
1:C:945:ILE:HB	1:C:971:ARG:HG3	1.72	0.70
1:C:1035:ARG:HA	1:C:1035:ARG:HE	1.57	0.70
1:A:68:ASN:O	1:A:70:ASN:N	2.25	0.69
1:A:936:GLY:O	1:A:940:LYS:HB2	1.91	0.69
1:B:542:LEU:HD11	1:B:1028:VAL:HG11	1.74	0.69
1:C:146:ASP:HB2	1:C:148:THR:OG1	1.92	0.69
1:C:166:ILE:CA	1:C:166:ILE:CG1	2.70	0.69
1:A:11:PHE:CE1	1:B:890:ALA:HB1	2.27	0.69
1:B:713:LEU:H	1:B:713:LEU:CD1	2.05	0.69
1:C:169:THR:CB	1:C:169:THR:C	2.64	0.69
1:C:450:SER:O	1:C:451:ALA:HB2	1.92	0.69
1:C:915:ALA:HA	1:C:918:PHE:HB3	1.73	0.69
1:A:114:ALA:O	1:A:117:LEU:HB2	1.92	0.69
1:A:531:VAL:HA	1:A:534:ILE:CD1	2.14	0.69
1:B:118:LEU:HD23	1:B:122:VAL:HG11	1.74	0.69
1:B:188:MET:HE1	1:B:203:VAL:HG21	1.71	0.69
1:B:13:TRP:O	1:B:17:ILE:HG12	1.92	0.69
1:B:225:VAL:H	1:C:781:MET:HE2	1.58	0.69
1:B:646:ALA:C	1:B:648:THR:N	2.46	0.69
1:B:1024:VAL:HG12	1:B:1025:PHE:H	1.56	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:ASP:O	1:C:9:PRO:HD3	1.92	0.69
1:C:247:GLY:CA	1:C:268:ILE:HD13	2.23	0.69
1:A:901:VAL:HG11	1:A:943:ILE:HG12	1.74	0.69
1:B:49:TYR:CG	1:B:122:VAL:HG22	2.27	0.69
1:B:157:TYR:CA	1:B:161:ASN:HD22	2.05	0.69
1:B:851:LEU:N	1:B:852:PRO:HD3	2.08	0.69
1:B:986:VAL:O	1:B:990:VAL:HG23	1.92	0.69
1:C:110:LYS:O	1:C:111:LEU:C	2.35	0.69
1:C:924:ASP:C	1:C:925:VAL:O	2.31	0.69
1:A:340:VAL:HG13	1:A:399:VAL:CG2	2.23	0.69
1:B:380:PHE:CZ	1:B:398:MET:HE2	2.26	0.69
1:B:468:ARG:O	1:B:469:GLN:C	2.34	0.69
1:B:537:SER:C	1:B:540:ARG:HE	2.00	0.69
1:C:163:LYS:HG2	1:C:175:VAL:HG11	1.74	0.69
1:C:402:ILE:O	1:C:406:VAL:HG23	1.92	0.69
1:C:415:ASN:HD21	1:C:434:SER:HB2	1.57	0.69
1:C:556:PHE:HB2	1:C:913:LEU:CD1	2.22	0.69
1:A:115:MET:O	1:A:117:LEU:N	2.25	0.69
1:B:773:VAL:HG13	1:B:773:VAL:O	1.92	0.69
1:B:943:ILE:O	1:B:947:GLU:HB3	1.92	0.69
1:A:653:ARG:O	1:A:656:SER:N	2.24	0.69
1:A:731:ILE:HD12	1:A:731:ILE:N	2.07	0.69
1:A:822:LEU:HD22	1:A:822:LEU:N	2.08	0.69
1:B:572:PHE:CZ	1:B:629:VAL:HG21	2.27	0.69
1:B:845:GLU:HG3	1:B:857:TYR:OH	1.93	0.69
1:B:973:ARG:HG2	1:B:974:PRO:CD	2.22	0.69
1:B:187:TRP:HZ3	1:B:774:MET:HE3	1.56	0.69
1:B:211:ASN:ND2	1:B:246:PHE:HZ	1.91	0.69
1:B:573:MET:HE1	1:B:617:PHE:CE2	2.27	0.69
1:B:929:VAL:O	1:B:933:THR:OG1	2.11	0.69
1:C:82:SER:OG	1:C:88:VAL:HG13	1.93	0.69
1:C:157:TYR:O	1:C:161:ASN:HB2	1.93	0.69
1:C:214:VAL:CG1	1:C:215:ALA:N	2.56	0.69
1:A:124:GLN:HG2	1:A:758:TYR:CE2	2.28	0.69
1:A:200:PRO:HG2	1:A:749:THR:HA	1.73	0.69
1:A:659:LYS:O	1:A:661:ALA:N	2.26	0.69
1:A:279:ALA:HA	1:A:612:VAL:HG12	1.74	0.68
1:B:151:GLN:HE22	1:B:279:ALA:H	1.39	0.68
1:B:425:LEU:HB3	1:B:498:LYS:O	1.93	0.68
1:B:1012:VAL:HG23	1:B:1013:THR:N	2.08	0.68
1:A:406:VAL:CG1	1:A:407:ASP:N	2.56	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:PHE:CE1	1:A:629:VAL:HG13	2.29	0.68
1:B:281:PHE:HE1	1:B:608:SER:HG	1.39	0.68
1:B:335:ILE:C	1:B:337:ILE:H	2.00	0.68
1:B:573:MET:HE3	1:B:626:ILE:HD12	1.75	0.68
1:B:771:VAL:O	1:B:771:VAL:HG12	1.92	0.68
1:C:33:ALA:HB2	1:C:298:ASN:ND2	2.08	0.68
1:C:162:MET:CG	1:C:313:MET:HE3	2.22	0.68
1:A:813:SER:HB3	1:A:816:LEU:HD21	1.73	0.68
1:A:950:LYS:O	1:A:951:ASP:HB3	1.93	0.68
1:B:207:ILE:CG2	1:B:759:VAL:HG11	2.22	0.68
1:B:214:VAL:HG21	1:C:747:ASN:HD21	1.58	0.68
1:C:167:SER:N	1:C:167:SER:C	2.51	0.68
1:C:590:VAL:O	1:C:594:VAL:HG23	1.92	0.68
1:C:592:ASN:O	1:C:593:GLU:CB	2.42	0.68
1:C:894:SER:C	1:C:896:SER:H	2.01	0.68
1:B:109:ASN:HD22	1:B:112:GLN:HE22	1.41	0.68
1:C:939:ALA:O	1:C:943:ILE:CD1	2.42	0.68
1:A:73:ASP:HB3	2:C:1054:HOH:O	1.93	0.68
1:A:199:THR:HB	1:A:200:PRO:HD2	1.76	0.68
1:A:372:VAL:O	1:A:375:VAL:N	2.26	0.68
1:A:413:VAL:HG23	1:A:493:CYS:CB	2.23	0.68
1:B:584:GLN:HB2	1:B:622:GLN:HE21	1.58	0.68
1:A:521:GLU:HB3	1:A:522:LYS:NZ	2.08	0.68
1:B:327:TYR:CD2	1:B:628:PHE:HB3	2.28	0.68
1:C:713:LEU:HD12	1:C:833:PRO:O	1.91	0.68
1:B:659:LYS:HA	1:B:659:LYS:NZ	2.08	0.68
1:C:1016:VAL:O	1:C:1018:ALA:N	2.22	0.68
1:B:739:LEU:O	1:B:793:ALA:HB1	1.94	0.68
1:B:919:ARG:HG3	1:B:1005:THR:HG21	1.76	0.68
1:A:516:PHE:C	1:A:518:ARG:H	2.00	0.68
1:A:773:VAL:O	1:A:773:VAL:CG1	2.42	0.68
1:B:129:VAL:O	1:B:129:VAL:HG12	1.94	0.68
1:B:792:ARG:HB2	1:B:798:MET:HE1	1.75	0.68
1:C:420:MET:SD	1:C:498:LYS:CD	2.81	0.68
1:C:576:VAL:HG12	1:C:663:VAL:HG22	1.74	0.68
1:A:255:GLN:CD	1:A:255:GLN:N	2.52	0.68
1:A:819:TYR:O	1:A:822:LEU:N	2.18	0.68
1:A:822:LEU:HB3	2:A:1059:HOH:O	1.94	0.68
1:A:855:VAL:HG23	1:A:855:VAL:O	1.94	0.68
1:B:591:LEU:O	1:B:595:THR:HG22	1.92	0.68
1:C:177:LEU:HD13	1:C:179:GLY:C	2.18	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:713:LEU:HD22	1:C:713:LEU:N	2.09	0.68
1:C:713:LEU:HB2	1:C:832:ALA:HB3	1.75	0.68
1:A:104:GLN:O	1:A:108:GLN:HB2	1.94	0.67
1:B:120:GLN:HG2	1:B:124:GLN:HG2	1.76	0.67
1:A:901:VAL:O	1:A:904:VAL:CG2	2.41	0.67
1:A:909:VAL:CG1	1:A:913:LEU:HD21	2.22	0.67
1:B:116:PRO:HA	1:B:123:GLN:HE22	1.59	0.67
1:B:119:PRO:HG2	1:B:122:VAL:CG2	2.24	0.67
1:B:358:PHE:CZ	1:B:976:LEU:HD12	2.27	0.67
1:B:404:LEU:HD13	1:B:449:LEU:HD13	1.75	0.67
1:C:110:LYS:O	1:C:112:GLN:N	2.27	0.67
1:C:114:ALA:O	1:C:115:MET:C	2.35	0.67
1:C:221:GLY:O	1:C:222:THR:C	2.37	0.67
1:C:658:ILE:H	1:C:658:ILE:HD12	1.60	0.67
1:C:727:PHE:CZ	1:C:783:PRO:HB3	2.29	0.67
1:A:73:ASP:CG	1:A:106:GLN:NE2	2.53	0.67
1:A:342:LYS:HG3	1:A:343:THR:N	2.10	0.67
1:A:435:MET:HA	1:A:438:ILE:HD11	1.76	0.67
1:B:190:PRO:HG2	1:B:779:TYR:CG	2.30	0.67
1:B:420:MET:CE	1:B:425:LEU:HD23	2.23	0.67
1:B:525:HIS:HA	1:B:528:THR:CG2	2.25	0.67
1:C:58:GLN:OE1	1:C:82:SER:CA	2.43	0.67
1:C:58:GLN:OE1	1:C:82:SER:N	2.26	0.67
1:A:173:GLY:HA3	1:A:294:ALA:HA	1.76	0.67
1:A:815:ARG:CZ	2:A:1071:HOH:O	2.41	0.67
1:B:150:THR:H	1:B:153:ASP:CB	2.08	0.67
1:B:416:VAL:CG2	1:B:431:THR:HA	2.25	0.67
1:B:537:SER:O	1:B:540:ARG:HB2	1.94	0.67
1:C:778:LYS:O	1:C:779:TYR:HD2	1.77	0.67
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.75	0.67
1:A:571:VAL:HG12	1:A:630:SER:CA	2.24	0.67
1:A:818:ARG:HA	1:A:824:SER:N	2.10	0.67
1:B:347:ALA:HB1	1:B:402:ILE:HG21	1.76	0.67
1:C:5:PHE:HE2	1:C:11:PHE:HD2	1.40	0.67
1:C:457:ALA:CB	1:C:468:ARG:HA	2.23	0.67
1:A:201:VAL:HG21	1:A:745:ASP:OD2	1.95	0.67
1:A:742:SER:HG	1:A:745:ASP:HB2	1.57	0.67
1:A:818:ARG:HE	1:A:818:ARG:HB2	1.57	0.67
1:C:426:PRO:HB2	1:C:429:GLU:HB2	1.77	0.67
1:B:94:PHE:HB2	1:B:98:THR:HG21	1.77	0.67
1:C:166:ILE:HA	1:C:166:ILE:CG1	2.24	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:785:ASP:C	1:C:787:GLY:N	2.51	0.67
1:A:536:ARG:H	1:A:536:ARG:HD2	1.60	0.67
1:B:6:ILE:HA	1:B:491:ALA:HA	1.77	0.67
1:B:175:VAL:HG12	1:B:175:VAL:O	1.94	0.67
1:B:178:PHE:HE1	1:B:615:PHE:CE2	2.13	0.67
1:B:298:ASN:O	1:B:302:THR:HG23	1.94	0.67
1:A:688:ALA:O	1:A:689:GLY:C	2.36	0.67
1:A:1018:ALA:HB1	1:A:1022:VAL:CG1	2.24	0.67
1:B:172:VAL:O	1:B:172:VAL:CG1	2.39	0.67
1:C:190:PRO:HG3	1:C:789:TRP:CH2	2.30	0.67
1:C:778:LYS:C	1:C:779:TYR:HD2	2.03	0.67
1:C:925:VAL:C	1:C:927:PHE:H	2.03	0.67
1:A:583:THR:HG22	1:A:585:GLU:H	1.58	0.66
1:B:30:LEU:HD23	1:B:390:ILE:CG1	2.24	0.66
1:B:407:ASP:C	1:B:408:ASP:O	2.37	0.66
1:B:860:THR:HG22	1:B:861:GLY:N	2.10	0.66
1:C:389:SER:OG	1:C:391:ASN:ND2	2.28	0.66
1:A:355:MET:HA	1:A:977:MET:HE3	1.75	0.66
1:A:521:GLU:HB3	1:A:522:LYS:HZ3	1.60	0.66
1:A:674:LEU:HD22	1:A:675:GLY:H	1.61	0.66
1:A:987:MET:N	1:A:988:PRO:HD2	2.10	0.66
1:B:74:ASN:O	1:B:94:PHE:HB3	1.95	0.66
1:B:124:GLN:O	1:B:125:GLN:HB2	1.95	0.66
1:B:125:GLN:O	1:B:125:GLN:HG2	1.94	0.66
1:B:330:THR:N	1:B:331:PRO:HD2	2.11	0.66
1:B:641:GLU:HA	1:B:650:ARG:NH1	2.11	0.66
1:C:457:ALA:N	1:C:459:PHE:CE2	2.61	0.66
1:C:713:LEU:O	1:C:831:ALA:HA	1.95	0.66
1:C:1024:VAL:O	1:C:1028:VAL:HG23	1.95	0.66
1:A:133:SER:HG	1:A:136:PHE:HE1	1.42	0.66
1:A:736:ALA:O	1:A:741:VAL:CG1	2.43	0.66
1:B:671:ILE:O	1:B:673:GLU:HB2	1.95	0.66
1:C:586:ARG:O	1:C:589:LYS:HB2	1.95	0.66
1:C:693:GLU:O	1:C:694:LYS:C	2.38	0.66
1:C:143:ILE:CD1	1:C:286:ALA:HB2	2.25	0.66
1:C:688:ALA:O	1:C:690:LEU:N	2.25	0.66
1:A:55:LYS:HD3	1:A:816:LEU:HD11	1.77	0.66
1:A:243:THR:HG22	1:A:268:ILE:HG22	1.78	0.66
1:B:990:VAL:CG1	1:B:1005:THR:OG1	2.38	0.66
1:C:162:MET:CB	1:C:313:MET:HE3	2.25	0.66
1:C:317:PHE:HB2	1:C:318:PRO:CD	2.26	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:PRO:HG2	1:A:122:VAL:HG23	1.78	0.66
1:A:189:ASN:HD21	1:A:192:GLU:HB3	1.61	0.66
1:A:759:VAL:HG12	1:A:760:ASN:N	2.09	0.66
1:A:693:GLU:O	1:A:696:THR:N	2.23	0.66
1:C:35:TYR:CD1	1:C:671:ILE:HG12	2.31	0.66
1:C:380:PHE:CE1	1:C:398:MET:SD	2.88	0.66
1:C:592:ASN:HD22	1:C:592:ASN:H	1.40	0.66
1:C:1026:PHE:O	1:C:1029:VAL:HB	1.96	0.66
1:A:540:ARG:HD2	1:A:541:TYR:CD2	2.30	0.66
1:C:372:VAL:HG21	1:C:402:ILE:HG23	1.78	0.66
1:C:416:VAL:HG12	1:C:434:SER:OG	1.96	0.66
1:C:714:THR:HG22	1:C:715:SER:H	1.60	0.66
1:C:801:PHE:HA	1:C:804:PHE:CZ	2.31	0.66
1:A:719:ASN:HB2	1:A:828:LEU:HD23	1.78	0.66
1:B:95:GLU:O	1:B:98:THR:HB	1.96	0.66
1:B:238:THR:OG1	1:B:239:ARG:N	2.29	0.66
1:B:646:ALA:O	1:B:647:ILE:C	2.38	0.66
1:B:712:MET:HE3	1:B:712:MET:HA	1.78	0.66
1:B:940:LYS:NZ	1:B:978:THR:HG23	2.10	0.66
1:C:163:LYS:HD2	1:C:177:LEU:HB2	1.76	0.66
1:C:181:GLN:HG2	1:C:769:LYS:HE3	1.78	0.66
1:C:367:ILE:HG23	1:C:368:PRO:HD3	1.78	0.66
1:C:474:ILE:O	1:C:476:SER:O	2.14	0.66
1:C:843:LEU:O	1:C:846:GLN:HB2	1.96	0.66
1:A:111:LEU:O	1:A:113:LEU:N	2.29	0.66
1:A:344:LEU:CD2	1:A:402:ILE:CD1	2.68	0.66
1:B:1026:PHE:O	1:B:1030:ARG:HG3	1.95	0.66
1:C:901:VAL:HG11	1:C:943:ILE:HD13	1.76	0.66
1:B:199:THR:N	1:B:202:ASP:OD2	2.27	0.65
1:C:166:ILE:CA	1:C:166:ILE:HD13	2.12	0.65
1:C:184:MET:HA	1:C:184:MET:CE	2.23	0.65
1:C:423:GLU:O	1:C:426:PRO:HD3	1.97	0.65
1:A:44:THR:HA	1:A:91:THR:HA	1.79	0.65
1:A:706:ALA:HB3	1:A:716:VAL:HG21	1.77	0.65
1:B:30:LEU:HD23	1:B:390:ILE:CD1	2.26	0.65
1:B:517:ASN:C	1:B:521:GLU:HG3	2.22	0.65
1:B:659:LYS:HA	1:B:659:LYS:HZ3	1.60	0.65
1:C:160:ALA:C	1:C:164:ASP:OD2	2.39	0.65
1:C:633:ASP:O	1:C:634:TRP:HB2	1.95	0.65
1:A:171:GLY:O	1:A:172:VAL:C	2.39	0.65
1:A:330:THR:HG23	1:A:334:LYS:HE2	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:MET:HE1	1:A:410:ILE:HG12	1.77	0.65
1:B:902:MET:O	1:B:905:VAL:HG12	1.97	0.65
1:C:688:ALA:C	1:C:690:LEU:H	2.04	0.65
1:C:939:ALA:O	1:C:943:ILE:HD11	1.95	0.65
1:B:157:TYR:C	1:B:161:ASN:HD22	2.04	0.65
1:B:644:VAL:HG23	1:B:645:GLU:H	1.61	0.65
1:C:188:MET:HA	1:C:266:ALA:HB1	1.78	0.65
1:C:657:GLN:C	1:C:659:LYS:H	2.04	0.65
1:A:857:TYR:C	1:A:857:TYR:CD1	2.73	0.65
1:B:495:THR:O	1:B:498:LYS:HE3	1.97	0.65
1:B:775:SER:HB3	1:B:780:ARG:CG	2.27	0.65
1:B:984:LEU:O	1:B:984:LEU:HD13	1.96	0.65
1:A:83:ASP:HB3	2:A:1068:HOH:O	1.96	0.65
1:A:100:ALA:CB	1:A:131:LYS:HE3	2.27	0.65
1:A:108:GLN:CG	1:A:108:GLN:CA	2.74	0.65
1:A:128:SER:HB2	1:B:113:LEU:HD21	1.77	0.65
1:B:405:LEU:HD12	1:B:406:VAL:H	1.60	0.65
1:B:773:VAL:O	1:B:773:VAL:CG1	2.45	0.65
1:C:266:ALA:O	1:C:267:LYS:C	2.40	0.65
1:C:524:THR:O	1:C:527:TYR:HB3	1.97	0.65
1:C:713:LEU:CG	1:C:832:ALA:O	2.36	0.65
1:A:76:MET:CG	1:A:95:GLU:OE2	2.42	0.65
1:A:108:GLN:CB	1:A:108:GLN:CD	2.66	0.65
1:A:128:SER:CB	1:B:113:LEU:CD2	2.75	0.65
1:B:7:ASP:C	1:B:8:ARG:HD2	2.21	0.65
1:B:45:ILE:HG22	1:B:46:SER:N	2.12	0.65
1:B:293:LEU:HD22	1:B:294:ALA:O	1.97	0.65
1:B:330:THR:N	1:B:331:PRO:CD	2.59	0.65
1:B:655:PHE:HA	1:B:658:ILE:HG21	1.79	0.65
1:B:1024:VAL:CG1	1:B:1028:VAL:HG21	2.27	0.65
1:C:45:ILE:CA	1:C:45:ILE:CG2	2.71	0.65
1:C:74:ASN:HB3	1:C:95:GLU:HB2	1.78	0.65
1:C:324:VAL:HG23	1:C:326:PRO:HD3	1.79	0.65
1:A:263:ARG:HB3	1:A:263:ARG:HH21	1.62	0.65
1:A:521:GLU:HG3	2:A:1075:HOH:O	1.97	0.65
1:A:552:MET:HE1	1:A:906:PRO:CA	2.26	0.65
1:B:6:ILE:CD1	1:B:490:PRO:HB2	2.26	0.65
1:B:601:LYS:O	1:B:603:LYS:N	2.30	0.65
1:C:418:ARG:C	1:C:420:MET:N	2.50	0.65
1:A:60:THR:CG2	1:A:119:PRO:HD3	2.26	0.65
1:A:100:ALA:HB1	1:A:131:LYS:HE3	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:THR:HG22	1:A:223:PRO:HD2	1.79	0.65
1:B:49:TYR:CE2	1:B:125:GLN:HB3	2.31	0.65
1:B:160:ALA:HB1	1:B:767:ARG:HD3	1.76	0.65
1:B:572:PHE:HB2	1:B:666:PHE:O	1.97	0.65
1:B:578:LEU:HB2	1:B:623:ASN:HB2	1.79	0.65
1:B:598:TYR:HB3	1:B:606:VAL:HG11	1.78	0.65
1:C:54:ALA:N	1:C:57:VAL:HG23	2.12	0.65
1:C:431:THR:O	1:C:435:MET:HG2	1.96	0.65
1:C:592:ASN:O	1:C:593:GLU:HB3	1.97	0.65
1:C:728:LYS:HG3	1:C:729:ILE:H	1.60	0.65
1:A:56:THR:HG23	1:C:213:GLN:HG3	1.79	0.65
1:A:719:ASN:C	1:A:719:ASN:ND2	2.49	0.65
1:B:561:SER:HB2	1:B:838:GLY:HA3	1.78	0.65
1:B:699:ARG:HB3	1:B:699:ARG:HH11	1.62	0.65
1:B:835:LYS:HB2	1:B:839:GLU:OE2	1.96	0.65
1:C:60:THR:CG2	1:C:61:VAL:HG23	2.26	0.65
1:C:520:PHE:O	1:C:523:SER:N	2.29	0.65
1:C:786:ILE:HG22	1:C:786:ILE:O	1.97	0.65
1:C:1024:VAL:HG12	1:C:1028:VAL:HG21	1.78	0.65
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.78	0.64
1:B:1012:VAL:CG2	1:B:1013:THR:N	2.61	0.64
1:C:236:ALA:O	1:C:237:GLN:C	2.40	0.64
1:C:395:MET:O	1:C:398:MET:N	2.30	0.64
1:C:545:TYR:OH	1:C:1021:PHE:CG	2.49	0.64
1:C:657:GLN:O	1:C:659:LYS:N	2.30	0.64
1:C:844:MET:HA	1:C:847:LEU:HD21	1.78	0.64
1:A:95:GLU:O	1:A:98:THR:HG23	1.97	0.64
1:A:885:PHE:CD2	1:A:886:LEU:HD12	2.32	0.64
1:B:544:LEU:CA	1:B:547:ILE:HD12	2.19	0.64
1:B:960:LEU:HD12	1:B:961:ILE:HG13	1.79	0.64
1:C:64:VAL:HG12	1:C:65:ILE:N	2.11	0.64
1:C:244:GLU:HA	1:C:263:ARG:HH22	1.61	0.64
1:A:418:ARG:CD	1:A:970:MET:HG3	2.25	0.64
1:A:476:SER:O	1:A:480:LEU:HB2	1.96	0.64
1:B:139:VAL:O	1:B:139:VAL:HG12	1.96	0.64
1:B:972:LEU:CD1	1:B:976:LEU:HD23	2.28	0.64
1:C:211:ASN:C	1:C:211:ASN:HD22	2.05	0.64
1:C:222:THR:HB	1:C:223:PRO:CD	2.24	0.64
1:C:545:TYR:OH	1:C:1021:PHE:CB	2.45	0.64
1:A:298:ASN:HD22	1:A:300:LEU:N	1.95	0.64
1:A:534:ILE:HD12	1:A:540:ARG:NH2	2.13	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:THR:HG21	1:A:598:TYR:HE1	1.63	0.64
1:A:727:PHE:O	1:C:234:ILE:HA	1.97	0.64
1:B:654:ALA:O	1:B:656:SER:N	2.31	0.64
1:B:715:SER:HB2	1:B:830:GLN:NE2	2.12	0.64
1:C:62:THR:CB	2:C:1064:HOH:O	2.45	0.64
1:C:418:ARG:HG3	1:C:419:VAL:CG1	2.28	0.64
1:C:899:PHE:N	1:C:899:PHE:CD1	2.65	0.64
1:A:418:ARG:CG	1:A:970:MET:HE3	2.18	0.64
1:A:59:ASP:HB3	1:C:763:ILE:HD11	1.78	0.64
1:A:540:ARG:HG2	2:A:1064:HOH:O	1.96	0.64
1:A:785:ASP:O	1:A:788:ASP:N	2.30	0.64
1:B:314:GLU:N	1:B:315:PRO:HD2	2.12	0.64
1:C:1:MET:CE	1:C:439:GLN:HE22	2.11	0.64
1:C:14:VAL:HG13	1:C:15:ILE:N	2.12	0.64
1:C:710:PRO:O	1:C:712:MET:O	2.16	0.64
1:C:950:LYS:HZ3	1:C:1030:ARG:CD	2.05	0.64
1:A:911:GLY:H	1:A:914:LEU:HD13	1.63	0.64
1:B:2:PRO:CD	1:B:486:LEU:HD12	2.28	0.64
1:B:1012:VAL:CG2	1:B:1013:THR:H	2.10	0.64
1:C:404:LEU:O	1:C:405:LEU:HD23	1.98	0.64
1:B:68:ASN:O	1:B:70:ASN:ND2	2.31	0.64
1:B:99:ASP:C	1:B:99:ASP:OD2	2.39	0.64
1:B:136:PHE:CE1	1:B:617:PHE:HZ	2.16	0.64
1:B:184:MET:O	1:B:184:MET:CG	2.46	0.64
1:C:26:ALA:O	1:C:30:LEU:HG	1.98	0.64
1:C:114:ALA:O	1:C:118:LEU:HD13	1.98	0.64
1:C:115:MET:SD	1:C:123:GLN:NE2	2.71	0.64
1:C:344:LEU:CD2	1:C:402:ILE:HD11	2.28	0.64
1:C:912:ALA:C	1:C:914:LEU:H	2.04	0.64
1:A:949:ALA:HB1	1:A:1026:PHE:CZ	2.33	0.64
1:B:328:ASP:OD2	1:B:330:THR:N	2.31	0.64
1:C:84:SER:C	1:C:86:GLY:N	2.56	0.64
1:C:371:ALA:O	1:C:375:VAL:HG23	1.98	0.64
1:C:850:LYS:O	1:C:851:LEU:O	2.16	0.64
1:A:44:THR:HG22	1:A:89:GLN:HG3	1.80	0.64
1:A:255:GLN:O	1:A:256:ASP:OD1	2.16	0.64
1:A:601:LYS:HG3	1:A:601:LYS:O	1.98	0.64
1:A:692:HIS:O	1:A:696:THR:OG1	2.13	0.64
1:B:9:PRO:O	1:B:12:ALA:HB3	1.97	0.64
1:B:437:GLN:HA	1:B:437:GLN:HE21	1.63	0.64
1:B:463:THR:HG21	1:B:869:SER:HB2	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:GLN:NE2	1:C:620:ARG:HH11	1.96	0.64
1:C:545:TYR:HA	1:C:548:ILE:HG13	1.80	0.64
1:C:672:VAL:O	1:C:672:VAL:HG12	1.98	0.64
1:A:46:SER:HA	1:A:88:VAL:O	1.99	0.63
1:A:225:VAL:HG12	1:A:226:LYS:N	2.12	0.63
1:A:935:ILE:HG22	1:A:935:ILE:O	1.97	0.63
1:B:410:ILE:HG23	1:B:414:GLU:OE2	1.98	0.63
1:B:750:LEU:HD13	1:B:750:LEU:O	1.98	0.63
1:C:687:GLN:HB2	1:C:854:GLY:O	1.97	0.63
1:A:367:ILE:HG12	1:A:413:VAL:HG21	1.80	0.63
1:A:649:MET:CB	1:A:653:ARG:HH21	2.04	0.63
1:B:371:ALA:O	1:B:375:VAL:HG23	1.98	0.63
1:B:953:MET:HG2	1:B:953:MET:O	1.98	0.63
1:C:60:THR:HG23	1:C:61:VAL:HG23	1.80	0.63
1:C:361:ASN:HB2	1:C:364:ALA:HB3	1.80	0.63
1:C:391:ASN:H	1:C:394:THR:HG23	1.63	0.63
1:A:298:ASN:HD22	1:A:300:LEU:H	1.44	0.63
1:A:818:ARG:CD	1:A:818:ARG:CB	2.76	0.63
1:B:314:GLU:N	1:B:315:PRO:CD	2.61	0.63
1:B:416:VAL:HG21	1:B:431:THR:HA	1.80	0.63
1:C:418:ARG:NE	1:C:970:MET:HE2	2.13	0.63
1:C:644:VAL:HG11	1:C:667:ASN:ND2	2.11	0.63
1:A:102:ILE:HA	1:A:105:VAL:HG23	1.80	0.63
1:A:348:ILE:HA	1:A:351:VAL:HG23	1.80	0.63
1:A:443:VAL:CG1	1:A:444:GLY:H	1.98	0.63
1:B:231:ASN:C	1:B:231:ASN:HD22	2.06	0.63
1:C:159:ALA:CA	2:C:1078:HOH:O	1.89	0.63
1:C:465:ALA:O	1:C:469:GLN:HG2	1.99	0.63
1:C:615:PHE:CD2	1:C:615:PHE:O	2.51	0.63
1:B:235:ILE:HD13	1:B:235:ILE:N	2.13	0.63
1:B:452:VAL:O	1:B:453:PHE:CB	2.46	0.63
1:C:15:ILE:O	1:C:16:ALA:C	2.41	0.63
1:C:91:THR:CB	1:C:91:THR:C	2.68	0.63
1:C:598:TYR:CD2	1:C:606:VAL:HG21	2.33	0.63
1:A:968:VAL:HG21	1:A:1023:PRO:CB	2.29	0.63
1:A:983:ILE:HG13	1:A:984:LEU:N	2.14	0.63
1:A:989:LEU:HG	1:A:993:THR:HG23	1.81	0.63
1:B:674:LEU:HD13	1:B:860:THR:CG2	2.28	0.63
1:B:859:TRP:HB3	1:B:863:SER:CB	2.28	0.63
1:A:1024:VAL:HG12	1:A:1025:PHE:N	2.13	0.63
1:B:613:ASN:ND2	1:B:614:GLY:N	2.46	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:GLU:O	1:C:349:ILE:HB	1.99	0.63
1:A:68:ASN:CB	1:A:68:ASN:C	2.72	0.63
1:B:10:ILE:HG13	1:C:893:GLU:O	1.99	0.63
1:C:391:ASN:N	1:C:394:THR:CG2	2.62	0.63
1:A:191:ASN:C	1:A:193:LEU:H	2.07	0.63
1:B:545:TYR:OH	1:B:906:PRO:HG3	1.99	0.63
1:B:601:LYS:C	1:B:603:LYS:H	2.07	0.63
1:B:713:LEU:HD12	1:B:713:LEU:N	2.14	0.63
1:C:159:ALA:C	2:C:1078:HOH:O	2.32	0.63
1:A:54:ALA:O	1:A:58:GLN:N	2.29	0.62
1:B:136:PHE:HA	1:B:292:LYS:HG3	1.81	0.62
1:B:602:GLU:C	1:B:604:ASN:H	2.06	0.62
1:A:154:ILE:O	1:A:158:VAL:HG23	1.99	0.62
1:A:574:THR:OG1	1:A:627:ALA:HB3	1.99	0.62
1:A:644:VAL:C	1:A:646:ALA:H	2.06	0.62
1:B:538:THR:HG23	1:B:540:ARG:NH2	2.14	0.62
1:B:646:ALA:C	1:B:648:THR:H	2.05	0.62
1:B:775:SER:HB3	1:B:780:ARG:HG3	1.80	0.62
1:B:945:ILE:HD12	1:B:1026:PHE:CE2	2.31	0.62
1:C:204:ILE:HG12	1:C:759:VAL:CG1	2.29	0.62
1:C:274:ASN:CB	2:C:1060:HOH:O	2.20	0.62
1:A:5:PHE:CE1	1:A:12:ALA:HB2	2.33	0.62
1:A:64:VAL:O	1:A:65:ILE:O	2.17	0.62
1:A:756:GLY:CA	1:A:774:MET:HB2	2.29	0.62
1:C:457:ALA:H	1:C:459:PHE:HE2	1.42	0.62
1:C:552:MET:HE1	1:C:909:VAL:HG21	1.80	0.62
1:C:686:ASP:CG	1:C:690:LEU:HB2	2.23	0.62
1:A:106:GLN:O	1:A:110:LYS:HB2	1.98	0.62
1:B:252:LYS:HB3	1:B:260:VAL:CG1	2.30	0.62
1:B:831:ALA:HB3	1:B:840:ALA:HB2	1.80	0.62
1:C:187:TRP:HZ3	1:C:774:MET:HE2	1.64	0.62
1:C:190:PRO:HG3	1:C:789:TRP:CZ2	2.34	0.62
1:B:148:THR:O	1:B:148:THR:HG22	2.00	0.62
1:B:589:LYS:O	1:B:592:ASN:HB2	2.00	0.62
1:B:723:ASP:HA	1:B:814:PRO:HD3	1.81	0.62
1:B:850:LYS:C	1:B:852:PRO:HD3	2.24	0.62
1:C:169:THR:O	1:C:170:SER:C	2.42	0.62
1:C:189:ASN:HD22	1:C:190:PRO:N	1.98	0.62
1:C:764:ASP:CG	1:C:765:ARG:HD2	2.24	0.62
1:A:750:LEU:HD11	1:C:216:ALA:HB2	1.82	0.62
1:C:463:THR:HA	1:C:466:ILE:HD13	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:999:ALA:O	1:C:1003:VAL:HG23	1.99	0.62
1:A:184:MET:HB3	1:A:771:VAL:HG13	1.80	0.62
1:B:699:ARG:HG2	1:B:700:ASN:N	2.14	0.62
1:B:831:ALA:HB2	1:B:840:ALA:HB2	1.82	0.62
1:C:104:GLN:NE2	1:C:131:LYS:HE2	2.15	0.62
1:C:830:GLN:OE1	1:C:832:ALA:HA	2.00	0.62
1:A:1:MET:H2	1:A:2:PRO:HD2	1.65	0.62
1:A:318:PRO:O	1:A:319:SER:C	2.42	0.62
1:A:634:TRP:CD1	1:A:634:TRP:H	2.16	0.62
1:A:728:LYS:HG3	1:A:729:ILE:O	2.00	0.62
1:B:534:ILE:HG23	1:B:541:TYR:CZ	2.35	0.62
1:B:852:PRO:HA	1:B:855:VAL:HB	1.80	0.62
1:B:873:ALA:C	1:B:875:SER:H	2.08	0.62
1:C:644:VAL:CG1	1:C:667:ASN:HB2	2.30	0.62
1:A:228:GLN:CG	1:B:781:MET:HG2	2.30	0.62
1:A:655:PHE:C	1:A:656:SER:O	2.41	0.62
1:A:719:ASN:HB2	1:A:828:LEU:CD2	2.29	0.62
1:C:92:LEU:HD22	1:C:107:VAL:HG22	1.82	0.62
1:C:530:SER:O	1:C:534:ILE:HG23	1.99	0.62
1:C:554:TYR:O	1:C:555:LEU:HB2	1.99	0.62
1:C:657:GLN:HB3	1:C:658:ILE:HD12	1.82	0.62
1:C:899:PHE:N	1:C:899:PHE:HD1	1.96	0.62
1:A:113:LEU:CD2	1:C:128:SER:HA	2.27	0.62
1:A:513:PHE:CD1	1:A:517:ASN:ND2	2.63	0.62
1:A:713:LEU:HB3	1:A:831:ALA:O	1.99	0.62
1:B:921:LEU:CD2	1:B:1005:THR:HG22	2.30	0.62
1:C:143:ILE:CG2	1:C:284:GLN:HE22	2.08	0.62
1:C:259:ARG:HH11	1:C:259:ARG:CB	2.13	0.62
1:C:578:LEU:HD22	1:C:661:ALA:CB	2.30	0.62
1:C:703:LEU:O	1:C:706:ALA:HB3	2.00	0.62
1:A:709:HIS:N	1:A:710:PRO:HD3	2.14	0.61
1:C:167:SER:H	1:C:175:VAL:HG21	1.64	0.61
1:C:184:MET:HG2	1:C:246:PHE:CE1	2.35	0.61
1:C:417:GLU:HB3	1:C:973:ARG:HH12	1.64	0.61
1:A:418:ARG:HG2	1:A:970:MET:CE	2.19	0.61
1:B:49:TYR:HE2	1:B:125:GLN:HB3	1.65	0.61
1:B:978:THR:CG2	1:B:979:SER:N	2.62	0.61
1:C:164:ASP:O	1:C:168:ARG:HG3	1.99	0.61
1:C:345:VAL:O	1:C:348:ILE:HG12	2.00	0.61
1:A:61:VAL:HG13	1:A:118:LEU:HD13	1.81	0.61
1:A:340:VAL:HG13	1:A:399:VAL:HG21	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:THR:O	1:A:584:GLN:C	2.43	0.61
1:A:950:LYS:O	1:A:951:ASP:CB	2.47	0.61
1:B:109:ASN:HD22	1:B:112:GLN:NE2	1.98	0.61
1:B:184:MET:HB3	1:B:771:VAL:HG22	1.82	0.61
1:B:280:GLU:CB	1:B:284:GLN:O	2.48	0.61
1:B:585:GLU:O	1:B:588:GLN:N	2.32	0.61
1:B:673:GLU:OE1	1:B:673:GLU:HA	2.00	0.61
1:C:54:ALA:HB2	1:C:84:SER:CB	2.20	0.61
1:C:344:LEU:HD22	1:C:402:ILE:HD11	1.82	0.61
1:C:410:ILE:HG22	1:C:411:VAL:H	1.65	0.61
1:C:607:GLU:HG3	1:C:607:GLU:O	2.00	0.61
1:A:983:ILE:C	1:A:983:ILE:HD12	2.24	0.61
1:C:62:THR:HG23	1:C:90:ILE:CD1	2.28	0.61
1:C:189:ASN:HD22	1:C:189:ASN:C	2.08	0.61
1:C:305:ALA:O	1:C:309:GLU:N	2.33	0.61
1:C:310:LEU:O	1:C:313:MET:N	2.31	0.61
1:A:44:THR:CG2	1:A:89:GLN:HG3	2.31	0.61
1:A:367:ILE:HG13	1:A:368:PRO:HD3	1.83	0.61
1:A:481:SER:O	1:A:484:VAL:N	2.32	0.61
1:A:909:VAL:HG12	1:A:913:LEU:HD23	1.81	0.61
1:A:950:LYS:HA	1:A:953:MET:HB3	1.80	0.61
1:B:280:GLU:HB2	1:B:284:GLN:O	2.01	0.61
1:B:356:TYR:C	1:B:358:PHE:N	2.50	0.61
1:B:697:GLN:O	1:B:699:ARG:O	2.18	0.61
1:B:703:LEU:HA	1:B:706:ALA:HB3	1.82	0.61
1:C:549:VAL:C	1:C:551:GLY:N	2.56	0.61
1:C:600:THR:OG1	1:C:601:LYS:N	2.34	0.61
1:C:705:GLU:O	1:C:707:ALA:N	2.33	0.61
1:A:48:SER:HB2	1:A:125:GLN:HG3	1.83	0.61
1:A:554:TYR:CE1	1:A:558:ARG:HD3	2.36	0.61
1:A:563:PHE:O	1:A:564:LEU:HD12	2.00	0.61
1:B:623:ASN:C	1:B:623:ASN:ND2	2.53	0.61
1:C:57:VAL:CG1	1:C:88:VAL:CG2	2.79	0.61
1:C:131:LYS:HB2	1:C:295:THR:CG2	2.30	0.61
1:C:376:LEU:HD22	1:C:398:MET:HE2	1.83	0.61
1:C:431:THR:HG21	1:C:494:ALA:CB	2.28	0.61
1:A:154:ILE:CG2	1:A:287:SER:HB3	2.27	0.61
1:A:544:LEU:O	1:A:547:ILE:HB	2.01	0.61
1:A:897:ILE:N	1:A:898:PRO:HD2	2.15	0.61
1:B:585:GLU:O	1:B:586:ARG:C	2.42	0.61
1:C:988:PRO:O	1:C:989:LEU:C	2.43	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:975:ILE:H	1:B:975:ILE:HD12	1.65	0.61
1:C:841:MET:HE1	1:C:866:GLU:HG3	1.83	0.61
1:B:187:TRP:O	1:B:266:ALA:HA	2.01	0.61
1:C:161:ASN:N	1:C:164:ASP:OD2	2.34	0.61
1:C:391:ASN:O	1:C:392:THR:C	2.44	0.61
1:C:911:GLY:CA	1:C:1013:THR:HG21	2.31	0.61
1:A:324:VAL:HG12	1:A:325:TYR:N	2.15	0.61
1:B:143:ILE:HD12	1:B:322:LYS:HB3	1.83	0.61
1:B:310:LEU:O	1:B:314:GLU:HG3	2.01	0.61
1:B:709:HIS:N	1:B:710:PRO:HD3	2.15	0.61
1:B:775:SER:HB3	1:B:780:ARG:CD	2.30	0.61
1:C:453:PHE:O	1:C:456:MET:HG2	2.00	0.61
1:C:697:GLN:O	1:C:698:ALA:C	2.41	0.61
1:A:418:ARG:HH12	1:A:973:ARG:HB3	1.65	0.60
1:A:781:MET:HE2	1:C:225:VAL:H	1.65	0.60
1:B:235:ILE:N	1:B:235:ILE:CD1	2.64	0.60
1:C:254:ASN:OD1	1:C:258:SER:O	2.19	0.60
1:C:368:PRO:HG3	1:C:413:VAL:HG11	1.82	0.60
1:C:554:TYR:HD1	1:C:558:ARG:HH21	1.42	0.60
1:C:851:LEU:HD12	1:C:851:LEU:N	2.16	0.60
1:C:908:GLY:HA2	1:C:1014:ALA:HB2	1.81	0.60
1:A:323:ILE:HG12	1:A:325:TYR:HE1	1.65	0.60
1:A:690:LEU:HD11	1:A:854:GLY:C	2.26	0.60
1:A:713:LEU:O	1:A:714:THR:CG2	2.44	0.60
1:B:25:LEU:C	1:B:27:ILE:H	2.09	0.60
1:B:143:ILE:HG23	1:B:286:ALA:HB2	1.84	0.60
1:B:219:LEU:CD2	1:C:783:PRO:HG3	2.31	0.60
1:B:314:GLU:HB2	1:B:315:PRO:HD3	1.82	0.60
1:B:543:VAL:O	1:B:547:ILE:CD1	2.49	0.60
1:C:2:PRO:O	1:C:6:ILE:HG13	2.00	0.60
1:A:58:GLN:HG3	1:A:63:GLN:HE22	1.66	0.60
1:A:255:GLN:O	1:A:256:ASP:CG	2.43	0.60
1:A:391:ASN:H	1:A:394:THR:HG22	1.65	0.60
1:B:360:GLN:O	1:B:361:ASN:HB2	1.99	0.60
1:C:188:MET:HE1	1:C:200:PRO:CA	2.31	0.60
1:C:615:PHE:O	1:C:615:PHE:HD2	1.84	0.60
1:A:51:GLY:O	1:C:215:ALA:HB1	2.01	0.60
1:A:643:LYS:O	1:A:647:ILE:HG13	2.01	0.60
1:A:1011:MET:HA	1:A:1011:MET:HE3	1.83	0.60
1:B:535:LEU:O	1:B:536:ARG:C	2.45	0.60
1:C:57:VAL:HG12	1:C:88:VAL:CG2	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:GLN:HB3	1:C:798:MET:HE3	1.83	0.60
1:C:576:VAL:HG21	1:C:591:LEU:HD22	1.83	0.60
1:C:942:ALA:HA	1:C:945:ILE:HG22	1.84	0.60
1:A:527:TYR:O	1:A:530:SER:OG	2.11	0.60
1:B:591:LEU:CD1	1:B:611:ALA:HB1	2.31	0.60
1:C:552:MET:CE	1:C:909:VAL:HG21	2.31	0.60
1:C:615:PHE:CD2	1:C:615:PHE:C	2.79	0.60
1:A:246:PHE:O	1:A:249:ILE:CD1	2.49	0.60
1:A:686:ASP:C	1:A:688:ALA:H	2.08	0.60
1:A:905:VAL:O	1:A:909:VAL:HG23	2.00	0.60
1:C:10:ILE:HG22	1:C:10:ILE:O	2.00	0.60
1:C:291:ILE:O	1:C:291:ILE:HG22	1.99	0.60
1:C:560:PRO:O	1:C:922:THR:HG22	2.01	0.60
1:C:897:ILE:HG12	1:C:950:LYS:HE3	1.82	0.60
1:C:953:MET:HE1	1:C:1030:ARG:HH22	1.66	0.60
1:A:10:ILE:HD11	1:B:895:TRP:CB	2.29	0.60
1:A:169:THR:O	1:A:170:SER:C	2.43	0.60
1:A:425:LEU:HB3	1:A:426:PRO:HD2	1.82	0.60
1:B:71:GLY:O	1:B:72:ILE:C	2.44	0.60
1:C:545:TYR:OH	1:C:1021:PHE:CD2	2.51	0.60
1:C:663:VAL:O	1:C:664:PHE:HB3	2.02	0.60
1:C:1024:VAL:HG12	1:C:1028:VAL:CG2	2.32	0.60
1:A:758:TYR:O	1:A:758:TYR:CG	2.55	0.60
1:B:574:THR:HG23	1:B:665:ALA:CB	2.22	0.60
1:B:808:ARG:CB	1:B:808:ARG:HH21	2.15	0.60
1:C:485:ALA:O	1:C:490:PRO:HD3	2.02	0.60
1:C:933:THR:O	1:C:937:LEU:HB2	2.02	0.60
1:A:171:GLY:O	1:A:294:ALA:HB2	2.02	0.60
1:A:540:ARG:HD2	1:A:541:TYR:CE2	2.37	0.60
1:A:583:THR:HG22	1:A:585:GLU:N	2.17	0.60
1:A:728:LYS:HD2	1:C:235:ILE:HG22	1.84	0.60
1:A:827:ILE:N	1:A:827:ILE:HD12	2.16	0.60
1:A:952:LEU:HD12	1:A:953:MET:N	2.17	0.60
1:B:2:PRO:C	1:B:4:PHE:H	2.08	0.60
1:B:695:LEU:HD12	1:B:825:MET:HE3	1.83	0.60
1:B:807:SER:C	1:B:808:ARG:HG3	2.27	0.60
1:C:308:ALA:O	1:C:311:ALA:HB3	2.02	0.60
1:C:758:TYR:HB3	1:C:772:TYR:CE2	2.36	0.60
1:C:790:TYR:CD1	1:C:800:PRO:HB3	2.37	0.60
1:A:17:ILE:HG22	1:A:21:LEU:CD2	2.31	0.60
1:A:54:ALA:HB1	1:A:816:LEU:CG	2.24	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:ARG:NH2	1:A:722:GLU:OE1	2.35	0.60
1:B:3:ASN:N	1:B:6:ILE:HG12	2.13	0.60
1:B:165:ALA:O	1:B:166:ILE:C	2.45	0.60
1:B:207:ILE:HG21	1:B:759:VAL:HG11	1.82	0.60
1:B:418:ARG:HH21	1:B:970:MET:CG	2.14	0.60
1:B:785:ASP:O	1:B:786:ILE:C	2.44	0.60
1:C:684:LEU:HD11	1:C:855:VAL:CG1	2.32	0.60
1:A:196:PHE:O	1:A:197:GLN:HB2	2.03	0.59
1:A:528:THR:CG2	1:A:969:ARG:HE	2.10	0.59
1:A:1009:GLY:C	1:A:1011:MET:H	2.07	0.59
1:B:214:VAL:HG21	1:C:747:ASN:ND2	2.16	0.59
1:C:166:ILE:O	1:C:172:VAL:HG11	2.02	0.59
1:C:590:VAL:O	1:C:592:ASN:O	2.20	0.59
1:A:68:ASN:N	1:A:68:ASN:CB	2.65	0.59
1:B:115:MET:HA	1:B:115:MET:CE	2.30	0.59
1:B:346:GLU:OE1	1:B:988:PRO:CB	2.48	0.59
1:B:431:THR:HG21	1:B:493:CYS:HB2	1.84	0.59
1:B:560:PRO:CB	1:B:836:SER:HB3	2.32	0.59
1:B:776:GLU:HG2	1:B:777:ALA:N	2.17	0.59
1:B:952:LEU:HA	1:B:956:GLU:OE2	2.02	0.59
1:C:140:VAL:O	1:C:288:GLY:HA3	2.02	0.59
1:C:200:PRO:HG2	1:C:749:THR:HA	1.83	0.59
1:C:540:ARG:HE	1:C:541:TYR:HE1	1.47	0.59
1:C:886:LEU:O	1:C:890:ALA:HB2	2.02	0.59
1:C:911:GLY:HA3	1:C:1013:THR:CG2	2.32	0.59
1:A:26:ALA:O	1:A:30:LEU:HG	2.02	0.59
1:A:795:ASP:OD1	1:A:797:GLN:HG2	2.03	0.59
1:B:692:HIS:O	1:B:693:GLU:HG3	2.02	0.59
1:B:907:LEU:O	1:B:909:VAL:N	2.35	0.59
1:B:960:LEU:C	1:B:960:LEU:CD1	2.76	0.59
1:B:975:ILE:HD12	1:B:975:ILE:N	2.17	0.59
1:C:847:LEU:O	1:C:850:LYS:HG2	2.03	0.59
1:A:10:ILE:CD1	1:B:895:TRP:HB2	2.29	0.59
1:A:269:GLU:HG3	1:A:270:LEU:O	2.03	0.59
1:A:298:ASN:C	1:A:298:ASN:ND2	2.52	0.59
1:A:321:LEU:CD1	2:A:1061:HOH:O	2.49	0.59
1:A:548:ILE:CG2	1:A:910:ILE:HG12	2.32	0.59
1:A:571:VAL:CG1	1:A:630:SER:HA	2.30	0.59
1:B:281:PHE:CE2	1:B:324:VAL:HG11	2.37	0.59
1:B:330:THR:H	1:B:331:PRO:CD	2.14	0.59
1:C:262:LEU:CD2	1:C:268:ILE:HD11	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:PHE:HA	1:C:369:THR:CG2	2.33	0.59
1:C:778:LYS:C	1:C:779:TYR:CD2	2.80	0.59
1:A:166:ILE:O	1:A:168:ARG:N	2.36	0.59
1:A:223:PRO:HD3	1:B:275:TYR:HB2	1.84	0.59
1:A:435:MET:HA	1:A:438:ILE:CD1	2.32	0.59
1:B:344:LEU:O	1:B:345:VAL:C	2.45	0.59
1:B:568:ASP:O	1:B:634:TRP:CH2	2.55	0.59
1:B:754:TRP:CZ2	1:B:786:ILE:HG12	2.37	0.59
1:C:14:VAL:HG13	1:C:15:ILE:H	1.66	0.59
1:C:72:ILE:CG2	1:C:94:PHE:CE2	2.83	0.59
1:A:576:VAL:HG11	1:A:591:LEU:HD23	1.84	0.59
1:A:687:GLN:HB3	1:A:854:GLY:O	2.03	0.59
1:B:245:GLU:O	1:B:246:PHE:C	2.44	0.59
1:B:371:ALA:HA	1:B:374:VAL:HG12	1.84	0.59
1:B:563:PHE:HB2	1:B:866:GLU:HG2	1.85	0.59
1:B:980:LEU:HD23	1:B:983:ILE:HD12	1.83	0.59
1:B:1024:VAL:HG12	1:B:1028:VAL:HG21	1.84	0.59
1:C:185:ARG:HD3	1:C:272:GLY:O	2.01	0.59
1:A:49:TYR:HE2	1:A:121:GLU:HG2	1.68	0.59
1:A:166:ILE:O	1:A:169:THR:HG23	2.03	0.59
1:A:282:ASN:ND2	1:A:609:VAL:H	2.00	0.59
1:A:534:ILE:HD12	1:A:540:ARG:HH22	1.68	0.59
1:A:781:MET:HE3	1:C:228:GLN:OE1	2.02	0.59
1:A:886:LEU:HD21	1:C:17:ILE:CG2	2.31	0.59
1:B:196:PHE:O	1:B:197:GLN:HB2	2.03	0.59
1:B:1024:VAL:O	1:B:1025:PHE:HB2	2.03	0.59
1:C:94:PHE:O	1:C:95:GLU:O	2.20	0.59
1:C:414:GLU:OE2	1:C:977:MET:SD	2.61	0.59
1:A:30:LEU:HD21	1:A:384:ALA:HB2	1.85	0.59
1:A:90:ILE:O	1:A:90:ILE:CG2	2.50	0.59
1:A:467:TYR:HE1	1:A:925:VAL:CG2	2.15	0.59
1:A:857:TYR:CD1	1:A:857:TYR:O	2.55	0.59
1:B:6:ILE:HD12	1:B:491:ALA:N	2.17	0.59
1:B:606:VAL:HA	1:B:631:LEU:HD23	1.84	0.59
1:B:652:THR:O	1:B:656:SER:HB3	2.02	0.59
1:B:860:THR:CG2	1:B:861:GLY:N	2.66	0.59
1:C:60:THR:HG23	1:C:60:THR:O	2.00	0.59
1:C:459:PHE:O	1:C:460:GLY:O	2.19	0.59
1:C:547:ILE:O	1:C:550:VAL:HG12	2.03	0.59
1:C:633:ASP:O	1:C:633:ASP:CG	2.45	0.59
1:C:925:VAL:O	1:C:927:PHE:N	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:972:LEU:N	1:C:974:PRO:HD2	2.17	0.59
1:A:115:MET:C	1:A:117:LEU:N	2.56	0.59
1:A:193:LEU:HD12	1:A:265:VAL:CG1	2.32	0.59
1:A:709:HIS:H	1:A:710:PRO:HD3	1.68	0.59
1:C:358:PHE:CG	1:C:977:MET:HE2	2.37	0.59
1:A:5:PHE:HD1	1:A:12:ALA:HB2	1.64	0.58
1:A:702:LEU:HD11	1:A:844:MET:CE	2.32	0.58
1:A:855:VAL:O	1:A:855:VAL:CG2	2.51	0.58
1:A:961:ILE:O	1:A:965:LEU:HD23	2.02	0.58
1:B:876:LEU:CD1	1:B:932:LEU:HD11	2.27	0.58
1:B:986:VAL:HG12	1:B:990:VAL:HG23	1.85	0.58
1:C:553:ALA:O	1:C:557:VAL:HG23	2.03	0.58
1:C:907:LEU:O	1:C:910:ILE:HG22	2.03	0.58
1:C:919:ARG:HB3	1:C:921:LEU:HD23	1.83	0.58
1:C:987:MET:HB3	1:C:988:PRO:CD	2.33	0.58
1:A:185:ARG:O	1:A:186:ILE:HG13	2.02	0.58
1:A:277:ILE:O	1:A:277:ILE:CG2	2.43	0.58
1:A:919:ARG:CG	1:A:920:GLY:N	2.52	0.58
1:B:110:LYS:O	1:B:111:LEU:C	2.40	0.58
1:B:138:MET:HE3	1:B:306:ILE:HD13	1.85	0.58
1:B:851:LEU:N	1:B:852:PRO:CD	2.65	0.58
1:B:921:LEU:HD23	1:B:1005:THR:O	2.03	0.58
1:A:375:VAL:O	1:A:379:THR:HG23	2.02	0.58
1:B:48:SER:N	1:B:49:TYR:CE1	2.62	0.58
1:B:80:SER:HB2	1:B:90:ILE:HG23	1.84	0.58
1:C:726:GLN:NE2	1:C:812:GLY:HA3	2.18	0.58
1:A:13:TRP:O	1:A:17:ILE:HG13	2.03	0.58
1:A:124:GLN:HG2	1:A:758:TYR:HE2	1.67	0.58
1:A:190:PRO:HG3	1:A:789:TRP:CZ2	2.38	0.58
1:B:13:TRP:HA	1:B:13:TRP:CE3	2.37	0.58
1:B:200:PRO:CD	1:B:749:THR:HG22	2.30	0.58
1:B:472:ILE:HG23	1:B:473:THR:H	1.68	0.58
1:C:181:GLN:OE1	1:C:767:ARG:NH2	2.37	0.58
1:A:685:ILE:HG22	1:A:687:GLN:N	2.18	0.58
1:B:456:MET:HA	1:B:876:LEU:HD21	1.86	0.58
1:B:842:GLU:O	1:B:846:GLN:HG3	2.04	0.58
1:B:922:THR:OG1	1:B:923:ASN:N	2.26	0.58
1:C:327:TYR:CB	1:C:628:PHE:HB3	2.33	0.58
1:C:705:GLU:O	1:C:706:ALA:C	2.47	0.58
1:C:786:ILE:O	1:C:786:ILE:CG2	2.51	0.58
1:C:847:LEU:HD22	1:C:847:LEU:H	1.69	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:N	1:A:2:PRO:CD	2.66	0.58
1:A:60:THR:HG22	1:A:119:PRO:CD	2.33	0.58
1:A:135:SER:O	1:A:136:PHE:CD2	2.56	0.58
1:B:146:ASP:O	1:B:147:GLY:C	2.44	0.58
1:B:328:ASP:CB	2:B:1059:HOH:O	2.48	0.58
1:C:776:GLU:O	1:C:777:ALA:C	2.46	0.58
1:A:342:LYS:O	1:A:343:THR:C	2.46	0.58
1:A:780:ARG:HG2	1:A:780:ARG:HH11	1.68	0.58
1:B:30:LEU:HD23	1:B:390:ILE:HG13	1.85	0.58
1:B:230:LEU:HD21	1:C:809:TRP:HH2	1.64	0.58
1:B:309:GLU:O	1:B:312:LYS:N	2.36	0.58
1:C:844:MET:HA	1:C:847:LEU:CD2	2.34	0.58
1:C:949:ALA:C	1:C:951:ASP:H	2.11	0.58
1:A:528:THR:O	1:A:532:GLY:N	2.35	0.58
1:A:588:GLN:HG2	1:A:613:ASN:ND2	2.19	0.58
1:A:644:VAL:C	1:A:646:ALA:N	2.58	0.58
1:C:762:PHE:H	1:C:771:VAL:CG2	2.17	0.58
1:A:399:VAL:C	1:A:401:ALA:H	2.12	0.58
1:A:463:THR:O	1:A:465:ALA:N	2.36	0.58
1:B:20:MET:HE3	1:B:373:PRO:C	2.28	0.58
1:B:219:LEU:CD1	1:B:234:ILE:HG12	2.33	0.58
1:B:443:VAL:O	1:B:444:GLY:C	2.44	0.58
1:C:102:ILE:HG22	1:C:103:ALA:N	2.13	0.58
1:C:928:GLN:N	1:C:928:GLN:OE1	2.37	0.58
1:A:292:LYS:O	1:A:293:LEU:O	2.22	0.58
1:A:488:LEU:O	1:A:492:LEU:HB2	2.04	0.58
1:B:419:VAL:O	1:B:426:PRO:HG3	2.04	0.58
1:B:975:ILE:H	1:B:975:ILE:CD1	2.17	0.58
1:C:160:ALA:C	1:C:161:ASN:CA	2.70	0.58
1:C:497:LEU:CD1	1:C:498:LYS:H	2.17	0.58
1:C:1028:VAL:HG12	1:C:1032:ARG:NH1	2.18	0.58
1:B:369:THR:O	1:B:373:PRO:HD3	2.04	0.57
1:B:403:GLY:O	1:B:404:LEU:HD23	2.04	0.57
1:B:531:VAL:CG1	1:B:965:LEU:HD21	2.34	0.57
1:B:613:ASN:ND2	1:B:613:ASN:C	2.62	0.57
1:B:644:VAL:HG23	1:B:645:GLU:N	2.18	0.57
1:B:911:GLY:CA	1:B:1013:THR:HG21	2.30	0.57
1:B:987:MET:HE2	1:B:991:ILE:HG23	1.86	0.57
1:C:185:ARG:HG3	1:C:271:GLY:CA	2.32	0.57
1:C:489:THR:N	1:C:490:PRO:HD2	2.18	0.57
1:C:912:ALA:C	1:C:914:LEU:N	2.59	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ASP:OD1	1:A:164:ASP:N	2.35	0.57
1:A:401:ALA:HB2	1:A:474:ILE:HG12	1.86	0.57
1:A:1021:PHE:O	1:A:1024:VAL:HB	2.04	0.57
1:B:24:GLY:HA2	1:B:27:ILE:HG23	1.85	0.57
1:B:472:ILE:HG23	1:B:473:THR:N	2.20	0.57
1:C:76:MET:HE2	1:C:95:GLU:HA	1.86	0.57
1:C:220:GLY:CA	1:C:231:ASN:HD22	2.15	0.57
1:C:277:ILE:HD11	1:C:620:ARG:NH2	2.18	0.57
1:C:832:ALA:HB1	1:C:833:PRO:HD2	1.85	0.57
1:C:885:PHE:CD1	1:C:886:LEU:N	2.72	0.57
1:B:485:ALA:HA	1:B:489:THR:HB	1.86	0.57
1:C:314:GLU:O	1:C:317:PHE:CE2	2.57	0.57
1:C:399:VAL:HA	1:C:402:ILE:HD11	1.84	0.57
1:C:685:ILE:HD11	1:C:687:GLN:CA	2.33	0.57
1:C:721:LEU:HD12	1:C:815:ARG:O	2.04	0.57
1:A:139:VAL:O	1:A:139:VAL:HG22	2.04	0.57
1:A:843:LEU:HA	1:A:846:GLN:HE21	1.66	0.57
1:C:66:GLU:OE2	1:C:818:ARG:HD3	2.05	0.57
1:A:182:TYR:HB3	1:A:270:LEU:HD12	1.85	0.57
1:A:194:ASN:ND2	1:A:790:TYR:CD2	2.72	0.57
1:A:600:THR:O	1:A:601:LYS:HB2	2.05	0.57
1:B:65:ILE:HD11	1:B:118:LEU:HD21	1.87	0.57
1:B:211:ASN:ND2	1:B:246:PHE:CZ	2.71	0.57
1:B:531:VAL:HA	1:B:534:ILE:HG12	1.86	0.57
1:B:640:GLU:OE2	1:B:640:GLU:N	2.38	0.57
1:B:873:ALA:O	1:B:875:SER:N	2.36	0.57
1:C:57:VAL:O	1:C:61:VAL:HB	2.03	0.57
1:C:831:ALA:HB2	1:C:840:ALA:HB2	1.85	0.57
1:A:108:GLN:CD	1:B:112:GLN:CD	2.72	0.57
1:B:49:TYR:CE2	1:B:122:VAL:HA	2.40	0.57
1:B:663:VAL:O	1:B:663:VAL:HG12	2.05	0.57
1:C:124:GLN:HB3	1:C:758:TYR:HE2	1.68	0.57
1:A:822:LEU:CB	1:A:823:PRO:HD2	2.22	0.57
1:A:911:GLY:N	1:A:914:LEU:HD13	2.19	0.57
1:B:940:LYS:HZ1	1:B:978:THR:HG23	1.69	0.57
1:C:211:ASN:C	1:C:211:ASN:ND2	2.61	0.57
1:A:345:VAL:O	1:A:349:ILE:HD13	2.05	0.57
1:B:622:GLN:CG	1:B:622:GLN:O	2.53	0.57
1:C:214:VAL:HG12	1:C:215:ALA:H	1.67	0.57
1:C:548:ILE:HD12	1:C:549:VAL:H	1.67	0.57
1:A:188:MET:HA	1:A:266:ALA:HB2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:GLN:HG2	1:B:781:MET:SD	2.45	0.57
1:A:406:VAL:O	1:A:407:ASP:C	2.45	0.57
1:B:847:LEU:HD23	1:B:847:LEU:H	1.69	0.57
1:B:910:ILE:O	1:B:914:LEU:HG	2.05	0.57
1:B:1013:THR:HG23	1:B:1013:THR:O	2.05	0.57
1:C:50:PRO:HD3	1:C:125:GLN:HG3	1.86	0.57
1:C:92:LEU:N	1:C:92:LEU:HD12	2.19	0.57
1:C:358:PHE:CD1	1:C:977:MET:HE2	2.40	0.57
1:A:45:ILE:HB	1:A:90:ILE:HB	1.86	0.57
1:A:407:ASP:O	1:A:408:ASP:C	2.48	0.57
1:A:907:LEU:O	1:A:910:ILE:HG13	2.05	0.57
1:A:927:PHE:CE2	1:A:931:LEU:HD22	2.39	0.57
1:B:57:VAL:HG23	1:B:58:GLN:H	1.68	0.57
1:B:380:PHE:CE1	1:B:398:MET:HE2	2.40	0.57
1:B:431:THR:CG2	1:B:493:CYS:CB	2.74	0.57
1:B:439:GLN:HA	1:B:442:LEU:CD1	2.34	0.57
1:B:945:ILE:HD11	1:B:1026:PHE:CE2	2.39	0.57
1:B:966:ASP:O	1:B:970:MET:HB2	2.04	0.57
1:B:1015:THR:O	1:B:1018:ALA:HB3	2.05	0.57
1:C:644:VAL:HG11	1:C:667:ASN:HB2	1.87	0.57
1:C:699:ARG:CD	1:C:703:LEU:HD11	2.32	0.57
1:A:170:SER:O	1:A:170:SER:OG	2.23	0.56
1:A:325:TYR:N	1:A:325:TYR:CD1	2.70	0.56
1:A:649:MET:O	1:A:653:ARG:NE	2.37	0.56
1:B:193:LEU:HD22	1:B:198:LEU:O	2.05	0.56
1:B:210:GLN:HG3	1:B:249:ILE:HG23	1.86	0.56
1:B:845:GLU:HG2	1:B:857:TYR:OH	2.03	0.56
1:C:229:GLN:O	1:C:230:LEU:HB3	2.05	0.56
1:C:699:ARG:CG	1:C:699:ARG:NH1	2.42	0.56
1:A:282:ASN:ND2	1:A:599:LEU:HD11	2.20	0.56
1:A:926:TYR:CE1	1:A:999:ALA:HB2	2.39	0.56
1:B:395:MET:O	1:B:396:PHE:C	2.44	0.56
1:B:651:ALA:O	1:B:655:PHE:CE2	2.58	0.56
1:B:784:ASP:O	1:B:785:ASP:C	2.46	0.56
1:B:785:ASP:O	1:B:787:GLY:N	2.38	0.56
1:C:897:ILE:N	1:C:898:PRO:HD2	2.20	0.56
1:A:11:PHE:O	1:A:14:VAL:N	2.38	0.56
1:A:162:MET:CE	1:A:310:LEU:HD22	2.36	0.56
1:A:191:ASN:O	1:A:193:LEU:N	2.39	0.56
1:A:252:LYS:HB3	1:A:260:VAL:HG21	1.87	0.56
1:A:400:LEU:HG	1:A:929:VAL:HG12	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:PHE:CD1	1:A:517:ASN:N	2.73	0.56
1:A:686:ASP:C	1:A:688:ALA:N	2.62	0.56
1:B:69:MET:HE1	1:B:111:LEU:HB2	1.87	0.56
1:B:221:GLY:HA3	1:C:780:ARG:HH11	1.71	0.56
1:B:541:TYR:C	1:B:543:VAL:H	2.12	0.56
1:B:913:LEU:O	1:B:917:THR:OG1	2.19	0.56
1:B:941:ASN:HD22	1:B:1015:THR:HA	1.70	0.56
1:C:58:GLN:OE1	1:C:82:SER:CB	2.54	0.56
1:C:123:GLN:O	1:C:125:GLN:N	2.37	0.56
1:C:311:ALA:O	1:C:313:MET:N	2.39	0.56
1:C:527:TYR:OH	1:C:1019:ILE:HG13	2.05	0.56
1:A:298:ASN:HB3	1:A:301:ASP:OD1	2.05	0.56
1:A:726:GLN:N	1:A:810:GLU:O	2.38	0.56
1:B:399:VAL:O	1:B:400:LEU:C	2.47	0.56
1:B:418:ARG:HG3	1:B:970:MET:HE3	1.87	0.56
1:B:639:GLY:HA2	1:B:643:LYS:NZ	2.20	0.56
1:C:248:LYS:O	1:C:249:ILE:C	2.48	0.56
1:C:274:ASN:ND2	2:C:1057:HOH:O	2.26	0.56
1:C:379:THR:CG2	1:C:477:ALA:HB2	2.36	0.56
1:C:601:LYS:O	1:C:603:LYS:N	2.37	0.56
1:A:60:THR:CG2	1:A:119:PRO:HG3	2.34	0.56
1:A:223:PRO:HD3	1:B:275:TYR:CG	2.39	0.56
1:A:400:LEU:HD11	1:A:1003:VAL:HG13	1.80	0.56
1:A:428:LYS:HG3	1:A:429:GLU:N	2.20	0.56
1:A:456:MET:O	1:A:457:ALA:HB3	2.05	0.56
1:A:904:VAL:O	1:A:905:VAL:C	2.49	0.56
1:A:911:GLY:HA2	1:A:914:LEU:HD13	1.86	0.56
1:B:571:VAL:O	1:B:572:PHE:HB3	2.05	0.56
1:C:764:ASP:OD2	1:C:765:ARG:CD	2.53	0.56
1:C:792:ARG:HB2	1:C:798:MET:HE1	1.87	0.56
1:A:197:GLN:HA	1:A:798:MET:HE2	1.87	0.56
1:A:263:ARG:NH2	1:A:263:ARG:HB3	2.20	0.56
1:A:268:ILE:N	1:A:268:ILE:HD12	2.20	0.56
1:A:530:SER:O	1:A:534:ILE:HG12	2.06	0.56
1:A:717:ARG:NH1	1:A:830:GLN:HE22	2.02	0.56
1:A:783:PRO:C	1:A:784:ASP:O	2.48	0.56
1:A:819:TYR:O	1:A:820:ASN:C	2.48	0.56
1:B:47:ALA:HB3	1:B:88:VAL:CB	2.31	0.56
1:C:5:PHE:CD2	1:C:12:ALA:HB2	2.41	0.56
1:C:5:PHE:CE2	1:C:11:PHE:HD2	2.22	0.56
1:C:56:THR:O	1:C:60:THR:HB	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:THR:CA	1:C:91:THR:CG2	2.76	0.56
1:C:306:ILE:O	1:C:309:GLU:N	2.38	0.56
1:C:868:LEU:O	1:C:869:SER:HB3	2.06	0.56
1:A:169:THR:O	1:A:172:VAL:HG22	2.06	0.56
1:A:199:THR:HB	1:A:200:PRO:CD	2.35	0.56
1:A:826:GLU:C	1:A:827:ILE:HD12	2.31	0.56
1:A:897:ILE:O	1:A:900:SER:OG	2.20	0.56
1:A:902:MET:C	1:A:904:VAL:H	2.13	0.56
1:B:48:SER:HA	1:B:87:THR:HA	1.86	0.56
1:B:370:ILE:HG22	1:B:370:ILE:O	2.05	0.56
1:B:478:MET:HE3	1:B:478:MET:HA	1.87	0.56
1:C:62:THR:HG21	1:C:80:SER:HB3	1.88	0.56
1:C:409:ALA:O	1:C:413:VAL:HG12	2.04	0.56
1:C:427:PRO:O	1:C:431:THR:HG22	2.06	0.56
1:C:719:ASN:OD1	1:C:719:ASN:N	2.37	0.56
1:A:65:ILE:C	1:A:65:ILE:N	2.61	0.56
1:A:594:VAL:HA	1:A:655:PHE:CE2	2.41	0.56
1:A:687:GLN:HE22	1:A:856:GLY:HA3	1.70	0.56
1:A:901:VAL:HG13	1:A:942:ALA:HB3	1.87	0.56
1:A:911:GLY:HA3	1:A:1013:THR:CG2	2.32	0.56
1:B:104:GLN:CG	1:B:105:VAL:H	2.18	0.56
1:B:441:ALA:CB	1:B:947:GLU:HG2	2.13	0.56
1:B:591:LEU:HD12	1:B:611:ALA:HB1	1.87	0.56
1:B:681:ASP:O	1:B:859:TRP:HE3	1.88	0.56
1:B:701:GLN:HA	1:B:704:ALA:HB3	1.88	0.56
1:B:736:ALA:C	1:B:738:ALA:H	2.12	0.56
1:B:942:ALA:HA	1:B:1022:VAL:HG11	1.88	0.56
1:B:1026:PHE:HB3	1:B:1030:ARG:NH2	2.21	0.56
1:A:731:ILE:N	1:A:731:ILE:CD1	2.69	0.56
1:B:186:ILE:HD13	1:B:262:LEU:HD13	1.88	0.56
1:B:905:VAL:N	1:B:906:PRO:HD2	2.21	0.56
1:B:1024:VAL:HG12	1:B:1025:PHE:N	2.21	0.56
1:C:102:ILE:HG22	1:C:106:GLN:HG3	1.88	0.56
1:C:978:THR:O	1:C:979:SER:C	2.46	0.56
1:A:63:GLN:O	1:A:65:ILE:C	2.49	0.56
1:A:188:MET:HA	1:A:266:ALA:CB	2.36	0.56
1:A:191:ASN:C	1:A:193:LEU:N	2.63	0.56
1:A:418:ARG:HH12	1:A:973:ARG:CB	2.18	0.56
1:A:781:MET:HE3	1:C:228:GLN:CD	2.30	0.56
1:B:71:GLY:O	1:B:72:ILE:O	2.24	0.56
1:B:278:ILE:HD11	1:B:584:GLN:NE2	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:ASN:HD21	1:C:432:ARG:CD	2.15	0.56
1:C:169:THR:CA	1:C:169:THR:CG2	2.79	0.56
1:C:181:GLN:CD	1:C:769:LYS:HD2	2.31	0.56
1:C:399:VAL:C	1:C:401:ALA:H	2.14	0.56
1:C:894:SER:O	1:C:896:SER:N	2.39	0.56
1:C:950:LYS:H	1:C:953:MET:CE	2.13	0.56
1:A:99:ASP:OD1	1:A:101:ASP:HB2	2.06	0.55
1:A:818:ARG:CG	2:A:1062:HOH:O	2.54	0.55
1:A:945:ILE:CG1	1:A:971:ARG:HG2	2.22	0.55
1:B:216:ALA:HB2	1:B:236:ALA:HB2	1.88	0.55
1:B:476:SER:O	1:B:477:ALA:C	2.49	0.55
1:B:632:LYS:O	1:B:637:ARG:HD2	2.05	0.55
1:B:899:PHE:O	1:B:903:LEU:HG	2.06	0.55
1:C:326:PRO:O	1:C:327:TYR:C	2.50	0.55
1:C:847:LEU:CA	1:C:850:LYS:HD3	2.20	0.55
1:C:950:LYS:N	1:C:953:MET:HE2	2.13	0.55
1:A:298:ASN:ND2	1:A:300:LEU:N	2.49	0.55
1:A:699:ARG:NH1	1:A:722:GLU:OE1	2.36	0.55
1:B:146:ASP:O	1:B:148:THR:N	2.39	0.55
1:B:419:VAL:O	1:B:419:VAL:HG12	2.06	0.55
1:B:699:ARG:O	1:B:701:GLN:N	2.38	0.55
1:B:737:GLN:O	1:B:737:GLN:HG2	2.06	0.55
1:B:1027:VAL:O	1:B:1030:ARG:O	2.24	0.55
1:C:415:ASN:HA	1:C:418:ARG:NH1	2.21	0.55
1:C:525:HIS:O	1:C:529:ASP:N	2.38	0.55
1:A:579:PRO:O	1:A:580:ALA:C	2.49	0.55
1:A:691:GLY:O	1:A:692:HIS:C	2.50	0.55
1:A:961:ILE:O	1:A:965:LEU:CD2	2.54	0.55
1:B:91:THR:C	1:B:92:LEU:HD22	2.31	0.55
1:B:325:TYR:O	1:B:326:PRO:O	2.25	0.55
1:C:169:THR:CB	1:C:169:THR:N	2.62	0.55
1:C:192:GLU:O	1:C:194:ASN:N	2.39	0.55
1:C:457:ALA:HB1	1:C:468:ARG:CA	2.35	0.55
1:C:708:LYS:C	1:C:710:PRO:HD3	2.31	0.55
1:C:910:ILE:HG23	1:C:911:GLY:N	2.22	0.55
1:A:200:PRO:CD	1:A:749:THR:HG23	2.37	0.55
1:A:367:ILE:HG13	1:A:368:PRO:CD	2.37	0.55
1:B:485:ALA:HA	1:B:489:THR:CB	2.35	0.55
1:B:544:LEU:HD22	1:B:1021:PHE:HZ	1.72	0.55
1:B:743:ILE:HA	1:B:746:ILE:HD12	1.88	0.55
1:B:898:PRO:C	1:B:900:SER:N	2.63	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:975:ILE:O	1:B:979:SER:HB2	2.07	0.55
1:C:467:TYR:C	1:C:469:GLN:H	2.15	0.55
1:A:29:LYS:HG2	1:A:29:LYS:O	2.07	0.55
1:A:325:TYR:N	1:A:325:TYR:HD1	2.04	0.55
1:A:400:LEU:HG	1:A:929:VAL:CG1	2.36	0.55
1:A:533:GLY:O	1:A:534:ILE:C	2.49	0.55
1:A:596:HIS:C	1:A:598:TYR:N	2.65	0.55
1:B:713:LEU:HD13	1:B:843:LEU:HD13	1.88	0.55
1:B:941:ASN:ND2	1:B:1015:THR:HA	2.21	0.55
1:A:47:ALA:HB2	1:A:127:VAL:HG22	1.88	0.55
1:A:548:ILE:HG23	1:A:910:ILE:HG12	1.87	0.55
1:A:901:VAL:HG13	1:A:942:ALA:CB	2.37	0.55
1:B:335:ILE:HG22	1:B:336:SER:N	2.20	0.55
1:B:545:TYR:O	1:B:547:ILE:N	2.40	0.55
1:B:986:VAL:O	1:B:988:PRO:O	2.24	0.55
1:C:190:PRO:O	1:C:192:GLU:N	2.39	0.55
1:C:598:TYR:HB3	1:C:606:VAL:HG11	1.88	0.55
1:C:742:SER:O	1:C:746:ILE:HG13	2.07	0.55
1:C:819:TYR:O	1:C:820:ASN:HB2	2.05	0.55
1:C:824:SER:O	1:C:825:MET:HG2	2.06	0.55
1:A:513:PHE:HD1	1:A:517:ASN:HD21	1.55	0.55
1:A:696:THR:OG1	1:A:825:MET:HE1	2.07	0.55
1:A:717:ARG:NH2	1:A:828:LEU:HG	2.22	0.55
1:B:493:CYS:O	1:B:494:ALA:CB	2.46	0.55
1:B:674:LEU:HD22	1:B:681:ASP:OD2	2.06	0.55
1:B:898:PRO:O	1:B:900:SER:N	2.40	0.55
1:C:490:PRO:C	1:C:491:ALA:O	2.47	0.55
1:C:767:ARG:O	1:C:769:LYS:HG2	2.07	0.55
1:A:68:ASN:N	1:A:69:MET:N	2.54	0.55
1:A:815:ARG:HD2	2:A:1068:HOH:O	2.06	0.55
1:B:707:ALA:O	1:B:708:LYS:CB	2.51	0.55
1:B:947:GLU:O	1:B:951:ASP:HB2	2.06	0.55
1:B:960:LEU:C	1:B:960:LEU:HD13	2.31	0.55
1:C:383:LEU:HD11	1:C:394:THR:OG1	2.07	0.55
1:C:533:GLY:O	1:C:536:ARG:HB2	2.07	0.55
1:C:570:GLY:O	1:C:571:VAL:HG13	2.07	0.55
1:C:1030:ARG:HA	1:C:1033:PHE:HD2	1.72	0.55
1:A:11:PHE:O	1:A:14:VAL:HG23	2.06	0.55
1:A:73:ASP:CG	1:A:106:GLN:HE22	2.15	0.55
1:A:225:VAL:CG1	1:A:226:LYS:N	2.69	0.55
1:A:399:VAL:C	1:A:401:ALA:N	2.65	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:916:ALA:O	1:A:919:ARG:O	2.25	0.55
1:A:988:PRO:O	1:A:990:VAL:O	2.25	0.55
1:B:639:GLY:HA2	1:B:643:LYS:HZ3	1.70	0.55
1:C:136:PHE:CE2	1:C:292:LYS:HE2	2.41	0.55
1:C:156:ASP:O	1:C:159:ALA:HB3	2.07	0.55
1:C:328:ASP:OD1	1:C:330:THR:HB	2.06	0.55
1:C:549:VAL:O	1:C:551:GLY:N	2.40	0.55
1:C:643:LYS:C	1:C:647:ILE:HG13	2.32	0.55
1:C:680:PHE:HE1	1:C:844:MET:HE2	1.72	0.55
1:C:695:LEU:CD2	1:C:825:MET:HE2	2.34	0.55
1:C:946:VAL:O	1:C:946:VAL:CG1	2.54	0.55
1:A:10:ILE:HG21	1:B:893:GLU:HB2	1.88	0.55
1:A:14:VAL:HG11	1:B:886:LEU:O	2.06	0.55
1:A:54:ALA:HB2	1:A:82:SER:O	2.07	0.55
1:A:354:VAL:O	1:A:355:MET:HB3	2.08	0.55
1:A:635:ALA:C	1:A:637:ARG:H	2.14	0.55
1:B:10:ILE:O	1:B:11:PHE:C	2.48	0.55
1:B:59:ASP:HA	1:B:63:GLN:HB2	1.89	0.55
1:B:324:VAL:C	1:B:326:PRO:HD2	2.32	0.55
1:B:570:GLY:N	1:B:634:TRP:CH2	2.75	0.55
1:C:87:THR:HG22	1:C:88:VAL:N	2.18	0.55
1:C:210:GLN:OE1	1:C:249:ILE:HG23	2.06	0.55
1:C:778:LYS:HD2	1:C:779:TYR:CE2	2.38	0.55
1:C:949:ALA:C	1:C:951:ASP:N	2.64	0.55
1:A:62:THR:O	1:A:63:GLN:O	2.24	0.54
1:A:689:GLY:O	1:A:690:LEU:O	2.25	0.54
1:A:987:MET:N	1:A:988:PRO:CD	2.69	0.54
1:B:228:GLN:HA	1:B:228:GLN:NE2	2.23	0.54
1:B:362:PHE:O	1:B:364:ALA:N	2.40	0.54
1:B:534:ILE:HA	1:B:541:TYR:CE1	2.42	0.54
1:B:557:VAL:O	1:B:557:VAL:HG12	2.06	0.54
1:B:641:GLU:HA	1:B:650:ARG:HH12	1.72	0.54
1:B:952:LEU:HD12	1:B:956:GLU:OE2	2.07	0.54
1:B:1001:ASN:O	1:B:1005:THR:HB	2.06	0.54
1:B:1016:VAL:C	1:B:1018:ALA:H	2.16	0.54
1:C:127:VAL:CB	1:C:127:VAL:C	2.73	0.54
1:C:251:LEU:HB2	1:C:260:VAL:O	2.08	0.54
1:C:311:ALA:O	1:C:312:LYS:C	2.49	0.54
1:C:707:ALA:O	1:C:710:PRO:HD3	2.06	0.54
1:A:186:ILE:CB	1:A:773:VAL:HG23	2.34	0.54
1:A:310:LEU:HD12	1:A:325:TYR:OH	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:GLY:O	1:A:690:LEU:C	2.51	0.54
1:A:740:GLY:O	1:A:793:ALA:HB1	2.08	0.54
1:B:2:PRO:HG3	1:B:435:MET:HG2	1.87	0.54
1:B:356:TYR:O	1:B:358:PHE:N	2.39	0.54
1:B:372:VAL:HG22	1:B:373:PRO:CD	2.38	0.54
1:B:545:TYR:C	1:B:547:ILE:N	2.62	0.54
1:B:703:LEU:O	1:B:704:ALA:C	2.50	0.54
1:B:897:ILE:HG13	1:B:898:PRO:HD3	1.89	0.54
1:C:76:MET:HE3	1:C:93:THR:HG22	1.88	0.54
1:C:190:PRO:HD2	1:C:779:TYR:CD1	2.42	0.54
1:C:645:GLU:O	1:C:648:THR:HG22	2.08	0.54
1:C:847:LEU:O	1:C:851:LEU:HD11	2.07	0.54
1:C:860:THR:HG23	1:C:860:THR:O	2.07	0.54
1:A:329:THR:HG23	1:A:329:THR:O	2.06	0.54
1:B:7:ASP:O	1:B:8:ARG:CB	2.54	0.54
1:B:540:ARG:O	1:B:541:TYR:CD1	2.60	0.54
1:B:891:LEU:HD12	1:B:892:TYR:CE1	2.42	0.54
1:C:398:MET:O	1:C:402:ILE:HG13	2.07	0.54
1:C:475:VAL:CG1	1:C:476:SER:N	2.70	0.54
1:C:913:LEU:HD23	1:C:927:PHE:HZ	1.72	0.54
1:C:1010:GLY:C	1:C:1013:THR:HG22	2.32	0.54
1:A:780:ARG:HG2	1:A:780:ARG:NH1	2.23	0.54
1:A:952:LEU:HD12	1:A:952:LEU:C	2.32	0.54
1:B:131:LYS:O	1:B:132:SER:HB3	2.06	0.54
1:B:156:ASP:OD2	1:B:182:TYR:HB2	2.07	0.54
1:B:399:VAL:HG11	1:B:989:LEU:HG	1.89	0.54
1:B:418:ARG:HE	1:B:970:MET:CE	2.21	0.54
1:B:448:VAL:O	1:B:452:VAL:CG2	2.53	0.54
1:B:945:ILE:HD11	1:B:1026:PHE:CZ	2.42	0.54
1:B:1012:VAL:C	1:B:1014:ALA:H	2.15	0.54
1:C:268:ILE:O	1:C:268:ILE:HG22	2.06	0.54
1:C:317:PHE:N	1:C:317:PHE:CD2	2.71	0.54
1:C:903:LEU:O	1:C:906:PRO:HD2	2.08	0.54
1:A:104:GLN:NE2	1:B:109:ASN:HB3	2.22	0.54
1:A:138:MET:HE3	1:A:306:ILE:HD13	1.88	0.54
1:A:231:ASN:OD1	1:B:622:GLN:OE1	2.26	0.54
1:A:818:ARG:NE	1:A:818:ARG:HB2	2.19	0.54
1:B:49:TYR:CE2	1:B:122:VAL:O	2.61	0.54
1:B:136:PHE:CE1	1:B:617:PHE:CZ	2.90	0.54
1:B:706:ALA:HA	1:B:713:LEU:HD22	1.90	0.54
1:B:940:LYS:O	1:B:943:ILE:N	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ASN:HD21	1:C:149:MET:N	2.05	0.54
1:C:144:ASN:OD1	1:C:320:GLY:O	2.25	0.54
1:C:477:ALA:H	1:C:480:LEU:HD23	1.72	0.54
1:C:847:LEU:HD23	1:C:847:LEU:C	2.33	0.54
1:C:851:LEU:HD12	1:C:851:LEU:H	1.73	0.54
1:A:516:PHE:C	1:A:518:ARG:N	2.66	0.54
1:B:42:ALA:CB	1:B:93:THR:CG2	2.82	0.54
1:B:335:ILE:C	1:B:337:ILE:N	2.66	0.54
1:B:483:LEU:O	1:B:485:ALA:O	2.26	0.54
1:B:640:GLU:O	1:B:643:LYS:HB2	2.07	0.54
1:B:971:ARG:O	1:B:975:ILE:HD13	2.08	0.54
1:B:1010:GLY:HA2	1:B:1013:THR:CG2	2.38	0.54
1:C:731:ILE:HD13	1:C:805:SER:HB3	1.89	0.54
1:C:760:ASN:C	1:C:760:ASN:OD1	2.49	0.54
1:C:801:PHE:HA	1:C:804:PHE:CE1	2.42	0.54
1:C:951:ASP:O	1:C:953:MET:N	2.38	0.54
1:A:203:VAL:HG13	1:A:262:LEU:CD1	2.37	0.54
1:A:686:ASP:O	1:A:687:GLN:C	2.50	0.54
1:A:736:ALA:HA	1:A:741:VAL:CG1	2.38	0.54
1:A:843:LEU:O	1:A:846:GLN:N	2.40	0.54
1:B:130:GLU:OE1	1:C:110:LYS:HE2	2.08	0.54
1:B:431:THR:OG1	1:B:494:ALA:HB2	2.07	0.54
1:B:750:LEU:HB2	1:B:801:PHE:CE1	2.42	0.54
1:C:461:GLY:HA3	1:C:869:SER:OG	2.07	0.54
1:C:713:LEU:HD21	1:C:835:LYS:N	2.19	0.54
1:C:1025:PHE:C	1:C:1029:VAL:HG23	2.33	0.54
1:A:58:GLN:HG3	1:A:63:GLN:NE2	2.22	0.54
1:A:99:ASP:HB3	1:A:102:ILE:HG22	1.90	0.54
1:A:172:VAL:HG23	1:A:172:VAL:O	2.08	0.54
1:A:693:GLU:C	1:A:695:LEU:N	2.65	0.54
1:A:781:MET:HE2	1:C:225:VAL:N	2.23	0.54
1:B:70:ASN:H	1:B:70:ASN:HD22	1.55	0.54
1:B:367:ILE:HG12	1:B:492:LEU:HD13	1.89	0.54
1:B:602:GLU:C	1:B:604:ASN:N	2.65	0.54
1:B:941:ASN:OD1	1:B:979:SER:OG	2.26	0.54
1:C:241:THR:O	1:C:241:THR:OG1	2.25	0.54
1:C:456:MET:O	1:C:457:ALA:HB3	2.07	0.54
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.90	0.54
1:C:778:LYS:HG3	1:C:779:TYR:CE2	2.43	0.54
1:C:861:GLY:H	1:C:864:TYR:HB2	1.73	0.54
1:A:1021:PHE:HB3	1:A:1025:PHE:CE1	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:VAL:HG22	1:B:373:PRO:HD3	1.90	0.54
1:B:740:GLY:HA3	1:B:794:ALA:HB2	1.90	0.54
1:B:885:PHE:CE2	1:B:898:PRO:HB2	2.42	0.54
1:C:87:THR:HG23	1:C:88:VAL:N	2.22	0.54
1:C:137:LEU:HG	1:C:293:LEU:HB2	1.90	0.54
1:A:38:ILE:O	1:A:462:SER:HA	2.08	0.54
1:A:65:ILE:O	1:A:68:ASN:OD1	2.26	0.54
1:A:210:GLN:HG3	1:A:249:ILE:CG2	2.34	0.54
1:A:966:ASP:O	1:A:969:ARG:HB2	2.08	0.54
1:B:143:ILE:CD1	1:B:322:LYS:HB3	2.37	0.54
1:C:115:MET:SD	1:C:127:VAL:HG11	2.48	0.54
1:C:666:PHE:CD2	1:C:666:PHE:O	2.61	0.54
1:C:682:PHE:HE2	1:C:702:LEU:HD11	1.73	0.54
1:C:966:ASP:HA	1:C:969:ARG:HB2	1.90	0.54
1:A:472:ILE:H	1:A:472:ILE:CD1	2.19	0.53
1:A:687:GLN:HA	2:A:1055:HOH:O	2.08	0.53
1:A:713:LEU:HB2	1:A:833:PRO:HD2	1.89	0.53
1:A:939:ALA:O	1:A:943:ILE:HG13	2.08	0.53
1:B:7:ASP:CG	1:B:8:ARG:HH21	2.16	0.53
1:B:119:PRO:HG2	1:B:122:VAL:HG23	1.90	0.53
1:B:178:PHE:HA	1:B:277:ILE:HG21	1.88	0.53
1:B:233:SER:OG	1:C:53:ASP:OD1	2.25	0.53
1:B:416:VAL:HG11	1:B:431:THR:CG2	2.36	0.53
1:B:537:SER:CA	1:B:540:ARG:HE	2.21	0.53
1:B:832:ALA:N	1:B:833:PRO:HD2	2.22	0.53
1:B:925:VAL:HA	1:B:928:GLN:OE1	2.08	0.53
1:C:192:GLU:O	1:C:193:LEU:C	2.51	0.53
1:C:484:VAL:HG12	1:C:489:THR:HG23	1.90	0.53
1:A:43:VAL:HG11	1:A:107:VAL:HG21	1.91	0.53
1:A:58:GLN:NE2	1:A:816:LEU:HD13	2.23	0.53
1:A:63:GLN:O	1:A:64:VAL:C	2.50	0.53
1:A:116:PRO:C	1:A:117:LEU:HD22	2.32	0.53
1:A:149:MET:HE3	1:A:154:ILE:HG12	1.90	0.53
1:A:575:MET:O	1:A:663:VAL:HA	2.08	0.53
1:A:764:ASP:HB3	1:A:769:LYS:HD2	1.90	0.53
1:B:184:MET:HB2	1:B:762:PHE:CE2	2.44	0.53
1:C:186:ILE:O	1:C:188:MET:N	2.41	0.53
1:C:410:ILE:O	1:C:412:VAL:N	2.40	0.53
1:C:476:SER:O	1:C:477:ALA:HB3	2.08	0.53
1:C:714:THR:HG22	1:C:715:SER:N	2.22	0.53
1:C:924:ASP:O	1:C:925:VAL:O	2.25	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:947:GLU:O	1:C:949:ALA:O	2.26	0.53
1:A:116:PRO:HB3	1:C:123:GLN:HG3	1.91	0.53
1:A:344:LEU:HD22	1:A:376:LEU:HD11	1.89	0.53
1:A:568:ASP:O	1:A:634:TRP:HH2	1.91	0.53
1:A:638:PRO:HG2	1:A:639:GLY:H	1.73	0.53
1:A:694:LYS:O	1:A:698:ALA:HB2	2.08	0.53
1:B:525:HIS:CA	1:B:528:THR:HG22	2.38	0.53
1:B:693:GLU:O	1:B:696:THR:OG1	2.26	0.53
1:C:35:TYR:CG	1:C:671:ILE:HG12	2.43	0.53
1:C:100:ALA:O	1:C:101:ASP:C	2.50	0.53
1:C:246:PHE:HZ	1:C:762:PHE:HB2	1.72	0.53
1:C:616:GLY:HA3	1:C:619:GLY:O	2.08	0.53
1:C:673:GLU:O	1:C:674:LEU:HB3	2.07	0.53
1:C:753:ALA:HB1	1:C:789:TRP:CZ2	2.43	0.53
1:C:778:LYS:CD	1:C:779:TYR:HE2	2.19	0.53
1:A:2:PRO:O	1:A:6:ILE:HG23	2.09	0.53
1:A:752:ALA:O	1:A:774:MET:HG3	2.08	0.53
1:A:818:ARG:HD3	1:A:822:LEU:N	2.23	0.53
1:B:261:LEU:HD13	1:B:261:LEU:N	2.23	0.53
1:B:562:SER:HB3	1:B:922:THR:HG21	1.90	0.53
1:B:956:GLU:H	1:B:956:GLU:CD	2.17	0.53
1:B:989:LEU:HA	1:B:992:SER:HB2	1.90	0.53
1:C:65:ILE:O	1:C:66:GLU:C	2.48	0.53
1:C:103:ALA:O	1:C:105:VAL:N	2.41	0.53
1:C:204:ILE:HG12	1:C:759:VAL:HG13	1.90	0.53
1:C:915:ALA:O	1:C:919:ARG:N	2.40	0.53
1:A:402:ILE:O	1:A:405:LEU:HD13	2.08	0.53
1:A:575:MET:SD	1:A:626:ILE:HG13	2.49	0.53
1:A:671:ILE:O	1:A:672:VAL:C	2.51	0.53
1:B:25:LEU:O	1:B:27:ILE:N	2.41	0.53
1:B:291:ILE:CG2	1:B:306:ILE:HD11	2.38	0.53
1:C:80:SER:O	1:C:81:ASN:HB3	2.08	0.53
1:C:743:ILE:H	1:C:743:ILE:CD1	2.04	0.53
1:C:901:VAL:HG12	1:C:942:ALA:HB1	1.90	0.53
1:C:965:LEU:O	1:C:969:ARG:HB2	2.09	0.53
1:A:187:TRP:CZ3	1:A:774:MET:HE3	2.43	0.53
1:A:281:PHE:O	1:A:282:ASN:C	2.51	0.53
1:A:393:LEU:HD11	1:A:466:ILE:HG12	1.91	0.53
1:A:552:MET:C	1:A:554:TYR:H	2.16	0.53
1:A:897:ILE:HG21	1:A:950:LYS:HE2	1.89	0.53
1:A:924:ASP:O	1:A:925:VAL:C	2.50	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:GLN:HA	1:B:62:THR:HB	1.90	0.53
1:B:174:ASP:CG	1:B:175:VAL:H	2.16	0.53
1:B:410:ILE:C	1:B:412:VAL:H	2.15	0.53
1:B:668:LEU:N	1:B:668:LEU:HD23	2.24	0.53
1:B:937:LEU:O	1:B:940:LYS:HB3	2.08	0.53
1:B:962:GLU:O	1:B:966:ASP:CB	2.48	0.53
1:C:157:TYR:CE1	1:C:318:PRO:HD3	2.43	0.53
1:C:175:VAL:O	1:C:175:VAL:HG12	2.08	0.53
1:A:289:LEU:HD23	1:A:289:LEU:C	2.33	0.53
1:A:443:VAL:CG1	1:A:444:GLY:N	2.65	0.53
1:A:472:ILE:N	1:A:472:ILE:CD1	2.72	0.53
1:A:780:ARG:NH2	1:C:223:PRO:HG2	2.24	0.53
1:A:901:VAL:HG11	1:A:943:ILE:CG1	2.38	0.53
1:A:1021:PHE:HB3	1:A:1025:PHE:CZ	2.44	0.53
1:B:6:ILE:HD13	1:B:6:ILE:N	2.24	0.53
1:B:525:HIS:O	1:B:529:ASP:OD2	2.27	0.53
1:B:944:LEU:CB	1:B:975:ILE:HD11	2.39	0.53
1:C:17:ILE:N	1:C:17:ILE:CD1	2.71	0.53
1:C:674:LEU:HD11	1:C:862:MET:CA	2.31	0.53
1:C:894:SER:C	1:C:896:SER:N	2.66	0.53
1:C:914:LEU:O	1:C:915:ALA:HB3	2.09	0.53
1:A:911:GLY:H	1:A:914:LEU:CD1	2.20	0.53
1:B:25:LEU:C	1:B:27:ILE:N	2.64	0.53
1:B:987:MET:N	1:B:988:PRO:CD	2.70	0.53
1:C:520:PHE:O	1:C:523:SER:OG	2.27	0.53
1:A:141:GLY:N	1:A:324:VAL:O	2.38	0.53
1:A:189:ASN:O	1:A:189:ASN:CG	2.52	0.53
1:A:774:MET:O	1:A:775:SER:O	2.26	0.53
1:B:693:GLU:C	1:B:695:LEU:H	2.15	0.53
1:C:4:PHE:O	1:C:8:ARG:HG2	2.09	0.53
1:C:66:GLU:HB3	1:C:78:MET:HE2	1.91	0.53
1:C:492:LEU:HA	1:C:495:THR:HB	1.91	0.53
1:A:143:ILE:HG21	1:A:281:PHE:CD2	2.44	0.53
1:A:444:GLY:O	1:A:448:VAL:HG23	2.09	0.53
1:B:586:ARG:HH22	1:B:660:ASP:HB2	1.74	0.53
1:B:892:TYR:C	1:B:894:SER:H	2.16	0.53
1:C:155:SER:HB3	1:C:180:SER:H	1.74	0.53
1:C:564:LEU:CD2	1:C:671:ILE:HD12	2.39	0.53
1:C:868:LEU:O	1:C:869:SER:CB	2.57	0.53
1:A:64:VAL:O	1:A:68:ASN:OD1	2.27	0.52
1:A:391:ASN:O	1:A:392:THR:C	2.51	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:THR:O	1:A:600:THR:HG22	2.10	0.52
1:B:401:ALA:O	1:B:404:LEU:N	2.41	0.52
1:C:578:LEU:HB3	1:C:579:PRO:CD	2.35	0.52
1:C:699:ARG:HH11	1:C:699:ARG:HG3	1.67	0.52
1:C:974:PRO:O	1:C:975:ILE:C	2.52	0.52
1:A:739:LEU:HD22	1:A:739:LEU:H	1.74	0.52
1:B:613:ASN:HD22	1:B:614:GLY:CA	2.22	0.52
1:C:404:LEU:CD2	1:C:937:LEU:HD13	2.40	0.52
1:C:443:VAL:O	1:C:447:MET:HB2	2.09	0.52
1:C:997:SER:O	1:C:1000:GLN:N	2.42	0.52
1:A:61:VAL:HG22	1:A:118:LEU:HD22	1.90	0.52
1:A:884:VAL:CG1	1:A:902:MET:HE3	2.37	0.52
1:A:986:VAL:O	1:A:991:ILE:HD12	2.09	0.52
1:A:1004:GLY:O	1:A:1005:THR:C	2.52	0.52
1:A:1007:VAL:O	1:A:1011:MET:HB2	2.08	0.52
1:B:362:PHE:C	1:B:364:ALA:H	2.16	0.52
1:C:177:LEU:HD13	1:C:179:GLY:O	2.09	0.52
1:C:389:SER:HG	1:C:391:ASN:HD22	1.52	0.52
1:C:410:ILE:CG2	1:C:411:VAL:N	2.69	0.52
1:C:552:MET:O	1:C:553:ALA:CB	2.56	0.52
1:C:841:MET:O	1:C:845:GLU:HG3	2.10	0.52
1:A:189:ASN:HD21	1:A:192:GLU:HB2	1.72	0.52
1:A:902:MET:O	1:A:904:VAL:N	2.43	0.52
1:A:999:ALA:O	1:A:1002:ALA:HB3	2.10	0.52
1:B:777:ALA:O	1:B:780:ARG:HB2	2.09	0.52
1:B:952:LEU:O	1:B:963:ALA:HB2	2.09	0.52
1:B:961:ILE:O	1:B:965:LEU:HB2	2.09	0.52
1:C:6:ILE:HA	1:C:491:ALA:HB2	1.90	0.52
1:C:159:ALA:C	1:C:161:ASN:N	2.56	0.52
1:A:107:VAL:O	1:A:110:LYS:CB	2.58	0.52
1:A:111:LEU:O	1:A:112:GLN:C	2.47	0.52
1:A:399:VAL:O	1:A:401:ALA:N	2.43	0.52
1:A:538:THR:C	1:A:540:ARG:H	2.17	0.52
1:A:568:ASP:CG	1:A:637:ARG:HH12	2.16	0.52
1:A:572:PHE:N	1:A:572:PHE:CD1	2.78	0.52
1:A:616:GLY:HA3	1:A:624:THR:OG1	2.09	0.52
1:B:41:PRO:HG2	1:B:98:THR:HG22	1.90	0.52
1:B:162:MET:HB2	1:B:313:MET:SD	2.50	0.52
1:B:551:GLY:O	1:B:554:TYR:HB2	2.09	0.52
1:B:687:GLN:CD	1:B:856:GLY:HA3	2.34	0.52
1:C:110:LYS:CA	1:C:113:LEU:HD12	2.20	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ASN:N	1:C:161:ASN:CB	2.59	0.52
1:C:459:PHE:HD2	1:C:459:PHE:N	1.89	0.52
1:C:945:ILE:C	1:C:945:ILE:HD12	2.34	0.52
1:A:128:SER:HB2	1:B:113:LEU:HD22	1.90	0.52
1:A:133:SER:OG	1:A:136:PHE:HE1	1.91	0.52
1:A:644:VAL:O	1:A:646:ALA:N	2.43	0.52
1:B:87:THR:HG21	1:B:620:ARG:NH1	2.25	0.52
1:B:649:MET:O	1:B:653:ARG:HB2	2.10	0.52
1:C:324:VAL:CG2	1:C:326:PRO:HD3	2.39	0.52
1:C:419:VAL:HA	1:C:422:GLU:HB3	1.91	0.52
1:C:432:ARG:HH11	1:C:432:ARG:CG	2.02	0.52
1:A:246:PHE:O	1:A:249:ILE:HD12	2.09	0.52
1:B:20:MET:HE2	1:B:377:LEU:HD12	1.91	0.52
1:B:34:GLN:HB2	1:B:333:VAL:HG22	1.92	0.52
1:B:365:THR:O	1:B:368:PRO:HD2	2.10	0.52
1:B:450:SER:O	1:B:451:ALA:C	2.50	0.52
1:B:740:GLY:HA3	1:B:794:ALA:CB	2.39	0.52
1:B:960:LEU:HD11	1:B:1027:VAL:CG1	2.39	0.52
1:C:352:PHE:CA	1:C:369:THR:HG21	2.37	0.52
1:C:939:ALA:O	1:C:943:ILE:HG12	2.10	0.52
1:A:58:GLN:HG2	1:A:59:ASP:OD1	2.09	0.52
1:A:59:ASP:CB	1:C:763:ILE:HD11	2.38	0.52
1:A:67:GLN:NE2	2:A:1063:HOH:O	2.12	0.52
1:A:113:LEU:CD2	1:C:127:VAL:O	2.58	0.52
1:A:246:PHE:O	1:A:249:ILE:HD13	2.10	0.52
1:A:717:ARG:HH11	1:A:830:GLN:HE22	1.55	0.52
1:B:518:ARG:HA	1:B:521:GLU:CB	2.40	0.52
1:B:570:GLY:N	1:B:634:TRP:HH2	2.07	0.52
1:B:763:ILE:HD11	1:C:59:ASP:HB3	1.91	0.52
1:B:973:ARG:CG	1:B:974:PRO:HD3	2.37	0.52
1:C:71:GLY:C	1:C:72:ILE:HG13	2.33	0.52
1:C:752:ALA:O	1:C:774:MET:HA	2.10	0.52
1:C:877:TYR:O	1:C:880:SER:HB3	2.09	0.52
1:A:183:ALA:N	1:A:271:GLY:O	2.43	0.52
1:A:761:ASP:OD2	1:A:761:ASP:N	2.42	0.52
1:B:4:PHE:O	1:B:5:PHE:HB2	2.10	0.52
1:B:304:ALA:O	1:B:308:ALA:HB2	2.10	0.52
1:B:335:ILE:O	1:B:337:ILE:N	2.43	0.52
1:B:572:PHE:CE2	1:B:629:VAL:HG21	2.45	0.52
1:C:287:SER:OG	1:C:288:GLY:N	2.43	0.52
1:C:314:GLU:CB	1:C:315:PRO:CD	2.79	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:LEU:O	1:C:445:ILE:HG13	2.10	0.52
1:C:519:MET:O	1:C:523:SER:OG	2.24	0.52
1:C:572:PHE:CZ	1:C:629:VAL:HG11	2.45	0.52
1:C:599:LEU:O	1:C:603:LYS:HB2	2.10	0.52
1:C:1024:VAL:CG1	1:C:1028:VAL:CG2	2.88	0.52
1:A:65:ILE:C	1:A:65:ILE:HD12	2.34	0.52
1:A:1015:THR:C	1:A:1017:LEU:H	2.18	0.52
1:B:168:ARG:HD3	1:C:69:MET:O	2.10	0.52
1:B:968:VAL:O	1:B:972:LEU:HB2	2.09	0.52
1:C:300:LEU:O	1:C:301:ASP:C	2.53	0.52
1:C:945:ILE:CB	1:C:971:ARG:HG3	2.40	0.52
1:A:102:ILE:HA	1:A:105:VAL:HG21	1.92	0.51
1:A:114:ALA:O	1:A:115:MET:C	2.53	0.51
1:A:711:ASP:C	1:A:713:LEU:H	2.18	0.51
1:A:1004:GLY:O	1:A:1007:VAL:N	2.43	0.51
1:B:228:GLN:NE2	1:C:781:MET:HE3	2.25	0.51
1:B:360:GLN:O	1:B:361:ASN:CB	2.58	0.51
1:C:393:LEU:C	1:C:395:MET:H	2.18	0.51
1:A:68:ASN:H	1:A:69:MET:N	2.08	0.51
1:A:100:ALA:HB1	1:A:131:LYS:CE	2.39	0.51
1:A:150:THR:O	1:A:151:GLN:C	2.54	0.51
1:A:354:VAL:HG13	1:A:980:LEU:HD23	1.92	0.51
1:A:578:LEU:HD21	1:A:587:THR:CA	2.34	0.51
1:A:911:GLY:CA	1:A:914:LEU:HD13	2.38	0.51
1:B:6:ILE:HD12	1:B:490:PRO:CB	2.39	0.51
1:B:25:LEU:O	1:B:28:LEU:HG	2.10	0.51
1:B:55:LYS:O	1:B:57:VAL:N	2.43	0.51
1:B:659:LYS:HD3	1:B:660:ASP:H	1.72	0.51
1:C:695:LEU:O	1:C:696:THR:C	2.54	0.51
1:C:1035:ARG:HA	1:C:1035:ARG:NE	2.25	0.51
1:A:837:THR:HG22	1:A:841:MET:HE3	1.92	0.51
1:B:556:PHE:HA	1:B:913:LEU:HD11	1.92	0.51
1:B:712:MET:HB3	1:B:713:LEU:CD1	2.29	0.51
1:B:729:ILE:CG1	1:B:730:ASP:N	2.70	0.51
1:B:978:THR:HG22	1:B:979:SER:H	1.76	0.51
1:C:165:ALA:C	2:C:1075:HOH:O	2.52	0.51
1:C:214:VAL:CG1	1:C:215:ALA:H	2.23	0.51
1:C:641:GLU:O	1:C:650:ARG:NH1	2.41	0.51
1:C:682:PHE:CE2	1:C:702:LEU:HD11	2.46	0.51
1:A:221:GLY:C	1:A:222:THR:O	2.50	0.51
1:A:922:THR:C	1:A:924:ASP:H	2.18	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:ASP:CG	1:B:175:VAL:N	2.69	0.51
1:B:594:VAL:HG22	1:B:663:VAL:HG11	1.91	0.51
1:C:121:GLU:O	1:C:758:TYR:OH	2.27	0.51
1:C:263:ARG:HG3	1:C:263:ARG:O	2.08	0.51
1:A:116:PRO:HA	2:A:1072:HOH:O	2.10	0.51
1:A:148:THR:HG21	1:A:319:SER:OG	2.10	0.51
1:A:311:ALA:O	1:A:312:LYS:CB	2.53	0.51
1:A:314:GLU:H	1:A:315:PRO:HD3	1.74	0.51
1:A:335:ILE:HD12	1:A:335:ILE:C	2.36	0.51
1:B:105:VAL:O	1:B:109:ASN:N	2.35	0.51
1:B:1022:VAL:CG2	1:B:1023:PRO:CD	2.86	0.51
1:B:1026:PHE:HB3	1:B:1030:ARG:NE	2.25	0.51
1:C:105:VAL:HG12	1:C:106:GLN:N	2.18	0.51
1:C:341:VAL:O	1:C:345:VAL:HG23	2.11	0.51
1:A:11:PHE:CD1	1:B:890:ALA:CB	2.94	0.51
1:A:138:MET:HE3	1:A:306:ILE:CD1	2.40	0.51
1:A:280:GLU:HB2	1:A:284:GLN:O	2.09	0.51
1:A:543:VAL:O	1:A:544:LEU:CB	2.55	0.51
1:A:621:GLY:O	1:A:623:ASN:N	2.43	0.51
1:A:822:LEU:O	1:A:823:PRO:C	2.52	0.51
1:B:104:GLN:HG2	1:B:105:VAL:H	1.74	0.51
1:B:330:THR:O	1:B:334:LYS:HG3	2.09	0.51
1:B:420:MET:HA	1:B:423:GLU:O	2.09	0.51
1:B:583:THR:HG22	1:B:586:ARG:HG3	1.93	0.51
1:B:898:PRO:O	1:B:899:PHE:C	2.53	0.51
1:B:1027:VAL:O	1:B:1031:ARG:HB3	2.10	0.51
1:C:52:ALA:O	1:C:53:ASP:CG	2.53	0.51
1:C:705:GLU:C	1:C:707:ALA:N	2.67	0.51
1:C:1022:VAL:O	1:C:1023:PRO:C	2.50	0.51
1:A:158:VAL:HA	1:A:162:MET:HG2	1.92	0.51
1:A:651:ALA:O	1:A:655:PHE:HD1	1.93	0.51
1:A:687:GLN:O	1:A:688:ALA:HB2	2.09	0.51
1:A:831:ALA:HB2	1:A:837:THR:HA	1.93	0.51
1:A:978:THR:C	1:A:980:LEU:H	2.16	0.51
1:B:420:MET:HE2	1:B:426:PRO:HD3	1.92	0.51
1:B:908:GLY:C	1:B:910:ILE:H	2.17	0.51
1:C:115:MET:N	1:C:116:PRO:HD3	2.23	0.51
1:C:792:ARG:HG2	1:C:793:ALA:O	2.11	0.51
1:A:69:MET:CG	1:A:69:MET:CA	2.80	0.51
1:A:166:ILE:N	1:A:166:ILE:CD1	2.67	0.51
1:A:488:LEU:HG	1:A:492:LEU:HD22	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ILE:HG23	1:B:266:ALA:HB1	1.91	0.51
1:B:778:LYS:O	1:B:779:TYR:HB2	2.11	0.51
1:B:974:PRO:O	1:B:976:LEU:N	2.44	0.51
1:B:986:VAL:HG12	1:B:990:VAL:CG2	2.40	0.51
1:B:1024:VAL:HG13	1:B:1028:VAL:HG21	1.93	0.51
1:C:129:VAL:CG2	1:C:129:VAL:CA	2.84	0.51
1:C:321:LEU:C	1:C:321:LEU:HD13	2.36	0.51
1:C:696:THR:O	1:C:697:GLN:C	2.52	0.51
1:A:11:PHE:C	1:A:13:TRP:H	2.18	0.51
1:A:14:VAL:CG1	1:B:886:LEU:HB3	2.41	0.51
1:A:109:ASN:CG	1:C:108:GLN:OE1	2.53	0.51
1:B:552:MET:SD	1:B:909:VAL:CG2	2.96	0.51
1:B:863:SER:O	1:B:866:GLU:N	2.44	0.51
1:C:392:THR:O	1:C:395:MET:N	2.42	0.51
1:C:482:VAL:O	1:C:486:LEU:HG	2.11	0.51
1:C:549:VAL:HG12	1:C:550:VAL:N	2.25	0.51
1:C:701:GLN:O	1:C:704:ALA:N	2.44	0.51
1:C:1016:VAL:O	1:C:1019:ILE:HG22	2.11	0.51
1:A:584:GLN:N	1:A:622:GLN:HB3	2.23	0.51
1:A:639:GLY:O	1:A:640:GLU:C	2.54	0.51
1:A:750:LEU:HD11	1:C:216:ALA:CB	2.41	0.51
1:A:818:ARG:NH1	1:A:821:GLY:O	2.43	0.51
1:B:168:ARG:HH11	1:C:69:MET:HB2	1.75	0.51
1:B:470:PHE:O	1:B:471:SER:C	2.52	0.51
1:B:819:TYR:O	1:B:820:ASN:C	2.54	0.51
1:C:16:ALA:O	1:C:20:MET:HG3	2.10	0.51
1:C:50:PRO:CD	1:C:125:GLN:HG3	2.41	0.51
1:C:280:GLU:HB3	1:C:284:GLN:O	2.11	0.51
1:C:713:LEU:CD1	1:C:833:PRO:O	2.59	0.51
1:C:734:GLU:O	1:C:738:ALA:N	2.44	0.51
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.46	0.51
1:C:911:GLY:O	1:C:914:LEU:O	2.29	0.51
1:A:65:ILE:HG13	1:A:66:GLU:N	2.26	0.50
1:A:443:VAL:O	1:A:444:GLY:C	2.54	0.50
1:A:583:THR:HB	1:A:586:ARG:HG3	1.93	0.50
1:A:732:ASP:HB3	1:A:735:LYS:HB2	1.93	0.50
1:B:231:ASN:CG	1:B:231:ASN:O	2.52	0.50
1:B:946:VAL:HG22	1:B:1026:PHE:CE1	2.45	0.50
1:C:111:LEU:C	1:C:111:LEU:HD13	2.35	0.50
1:C:425:LEU:N	1:C:426:PRO:HD3	2.26	0.50
1:C:655:PHE:O	1:C:657:GLN:N	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:907:LEU:HG	1:C:1017:LEU:HD23	1.93	0.50
1:A:44:THR:C	1:A:45:ILE:HG13	2.35	0.50
1:A:107:VAL:O	1:A:110:LYS:HB3	2.11	0.50
1:A:658:ILE:O	1:A:659:LYS:O	2.27	0.50
1:A:988:PRO:O	1:A:989:LEU:C	2.54	0.50
1:B:149:MET:SD	1:B:154:ILE:HG22	2.51	0.50
1:B:316:PHE:CZ	1:C:687:GLN:HG3	2.46	0.50
1:B:595:THR:HB	1:B:609:VAL:HG11	1.93	0.50
1:B:693:GLU:C	1:B:695:LEU:N	2.68	0.50
1:B:705:GLU:C	1:B:707:ALA:N	2.70	0.50
1:B:987:MET:N	1:B:988:PRO:HD2	2.26	0.50
1:C:58:GLN:C	2:C:1079:HOH:O	2.54	0.50
1:C:356:TYR:C	1:C:358:PHE:H	2.18	0.50
1:A:371:ALA:O	1:A:372:VAL:C	2.54	0.50
1:A:418:ARG:NH1	1:A:973:ARG:HB3	2.26	0.50
1:A:527:TYR:CD2	1:A:972:LEU:HG	2.47	0.50
1:A:599:LEU:O	1:A:600:THR:CB	2.59	0.50
1:B:462:SER:OG	1:B:865:GLN:NE2	2.44	0.50
1:C:188:MET:HA	1:C:266:ALA:CB	2.40	0.50
1:C:247:GLY:HA2	1:C:268:ILE:CD1	2.38	0.50
1:C:446:ALA:C	1:C:448:VAL:H	2.20	0.50
1:C:556:PHE:HB2	1:C:913:LEU:HD11	1.93	0.50
1:C:666:PHE:CD2	1:C:666:PHE:N	2.79	0.50
1:C:785:ASP:O	1:C:787:GLY:N	2.44	0.50
1:A:54:ALA:O	1:A:55:LYS:C	2.50	0.50
1:A:76:MET:SD	1:A:95:GLU:OE2	2.70	0.50
1:A:276:ASP:CB	1:C:222:THR:HG23	2.35	0.50
1:B:25:LEU:O	1:B:28:LEU:N	2.36	0.50
1:B:228:GLN:HA	1:B:228:GLN:HE21	1.76	0.50
1:B:602:GLU:CD	1:B:650:ARG:HH21	2.19	0.50
1:B:679:GLY:HA2	1:B:830:GLN:HB3	1.94	0.50
1:C:44:THR:O	1:C:45:ILE:C	2.54	0.50
1:C:102:ILE:O	1:C:105:VAL:HB	2.12	0.50
1:A:254:ASN:O	1:A:258:SER:OG	2.20	0.50
1:A:421:ALA:O	1:A:423:GLU:N	2.44	0.50
1:A:428:LYS:CG	1:A:429:GLU:H	2.22	0.50
1:A:569:GLN:O	1:A:570:GLY:C	2.55	0.50
1:A:913:LEU:C	1:A:915:ALA:H	2.20	0.50
1:A:1016:VAL:O	1:A:1016:VAL:HG12	2.10	0.50
1:B:170:SER:C	1:B:172:VAL:H	2.19	0.50
1:B:539:GLY:C	1:B:541:TYR:H	2.20	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:TYR:C	1:B:547:ILE:H	2.20	0.50
1:B:578:LEU:HD12	1:B:586:ARG:NH2	2.26	0.50
1:B:633:ASP:CG	1:B:634:TRP:N	2.68	0.50
1:C:226:LYS:HA	2:C:1072:HOH:O	2.11	0.50
1:C:343:THR:O	1:C:344:LEU:C	2.55	0.50
1:C:549:VAL:C	1:C:551:GLY:H	2.18	0.50
1:C:726:GLN:N	1:C:810:GLU:O	2.38	0.50
1:A:552:MET:SD	1:A:909:VAL:HG11	2.52	0.50
1:B:49:TYR:CD1	1:B:122:VAL:HG13	2.46	0.50
1:B:174:ASP:C	1:B:175:VAL:HG23	2.37	0.50
1:B:317:PHE:CD1	1:B:321:LEU:HD23	2.47	0.50
1:B:728:LYS:HD3	1:B:810:GLU:OE1	2.12	0.50
1:C:169:THR:CB	1:C:172:VAL:HG21	2.38	0.50
1:C:191:ASN:O	1:C:194:ASN:HB2	2.11	0.50
1:C:536:ARG:NH1	1:C:961:ILE:CD1	2.75	0.50
1:C:644:VAL:O	1:C:648:THR:HG22	2.12	0.50
1:C:674:LEU:HD12	1:C:865:GLN:OE1	2.12	0.50
1:C:695:LEU:CD2	1:C:825:MET:HG3	2.41	0.50
1:C:758:TYR:H	1:C:758:TYR:HD1	1.55	0.50
1:A:75:LEU:HD12	1:A:76:MET:N	2.26	0.50
1:A:193:LEU:HA	1:A:265:VAL:HG13	1.94	0.50
1:A:235:ILE:O	1:A:235:ILE:HG22	2.11	0.50
1:A:371:ALA:O	1:A:372:VAL:O	2.30	0.50
1:A:534:ILE:HD12	1:A:540:ARG:NH1	2.26	0.50
1:A:588:GLN:O	1:A:591:LEU:N	2.43	0.50
1:A:709:HIS:N	1:A:710:PRO:CD	2.74	0.50
1:B:833:PRO:HG2	1:B:834:GLY:H	1.77	0.50
1:C:243:THR:OG1	1:C:244:GLU:N	2.45	0.50
1:C:422:GLU:OE2	1:C:423:GLU:HG3	2.12	0.50
1:C:428:LYS:O	1:C:432:ARG:HB2	2.12	0.50
1:C:735:LYS:O	1:C:738:ALA:HB3	2.11	0.50
1:A:186:ILE:HD12	1:A:207:ILE:HD13	1.94	0.50
1:A:200:PRO:HG2	1:A:749:THR:HG23	1.93	0.50
1:A:578:LEU:H	1:A:578:LEU:HD22	1.76	0.50
1:B:8:ARG:H	1:B:9:PRO:HD3	1.76	0.50
1:B:572:PHE:HA	1:B:668:LEU:HD21	1.93	0.50
1:B:659:LYS:HD3	1:B:659:LYS:C	2.36	0.50
1:B:1019:ILE:O	1:B:1023:PRO:HG3	2.11	0.50
1:C:393:LEU:O	1:C:395:MET:N	2.45	0.50
1:C:463:THR:HG22	1:C:464:GLY:H	1.73	0.50
1:C:540:ARG:HG3	1:C:541:TYR:CD1	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:559:LEU:HD13	1:C:917:THR:HG23	1.94	0.50
1:C:711:ASP:CG	1:C:712:MET:N	2.70	0.50
1:C:997:SER:O	1:C:999:ALA:N	2.45	0.50
1:A:133:SER:HB3	1:A:136:PHE:CD1	2.46	0.50
1:B:129:VAL:H	1:C:109:ASN:HD21	1.58	0.50
1:B:680:PHE:CD1	1:B:680:PHE:C	2.90	0.50
1:B:830:GLN:H	1:B:830:GLN:NE2	2.04	0.50
1:B:863:SER:O	1:B:864:TYR:C	2.55	0.50
1:C:934:THR:O	1:C:935:ILE:C	2.52	0.50
1:C:934:THR:O	1:C:936:GLY:N	2.45	0.50
1:C:1016:VAL:C	1:C:1018:ALA:H	2.16	0.50
1:A:218:GLN:HB3	1:A:231:ASN:HD21	1.77	0.49
1:B:115:MET:HA	1:B:118:LEU:HD13	1.94	0.49
1:B:401:ALA:HA	1:B:404:LEU:HB2	1.93	0.49
1:B:547:ILE:O	1:B:550:VAL:O	2.30	0.49
1:B:600:THR:OG1	1:B:601:LYS:HE2	2.13	0.49
1:B:868:LEU:O	1:B:869:SER:C	2.55	0.49
1:B:1017:LEU:O	1:B:1021:PHE:HB2	2.12	0.49
1:B:1022:VAL:CG2	1:B:1023:PRO:HD3	2.33	0.49
1:C:260:VAL:O	1:C:260:VAL:HG13	2.11	0.49
1:C:1032:ARG:HG2	1:C:1032:ARG:O	2.11	0.49
1:B:408:ASP:C	1:B:410:ILE:H	2.20	0.49
1:B:542:LEU:HD11	1:B:1028:VAL:CG1	2.40	0.49
1:B:973:ARG:N	1:B:974:PRO:HD2	2.27	0.49
1:C:88:VAL:HG11	2:C:1064:HOH:O	2.12	0.49
1:C:242:SER:O	1:C:243:THR:C	2.55	0.49
1:C:519:MET:CG	1:C:520:PHE:N	2.75	0.49
1:C:657:GLN:C	1:C:659:LYS:N	2.71	0.49
1:C:688:ALA:C	1:C:690:LEU:N	2.66	0.49
1:C:966:ASP:HA	1:C:969:ARG:CB	2.42	0.49
1:A:372:VAL:O	1:A:373:PRO:C	2.55	0.49
1:A:455:PRO:HB2	1:A:877:TYR:CE1	2.48	0.49
1:A:790:TYR:HE1	1:A:800:PRO:CG	2.14	0.49
1:B:100:ALA:HB1	1:B:131:LYS:HD2	1.94	0.49
1:B:413:VAL:HG13	1:B:414:GLU:N	2.27	0.49
1:C:104:GLN:CD	1:C:131:LYS:HE2	2.38	0.49
1:C:847:LEU:HD22	1:C:847:LEU:N	2.28	0.49
1:A:38:ILE:HD11	1:A:671:ILE:HG21	1.94	0.49
1:A:102:ILE:C	1:A:105:VAL:HG23	2.37	0.49
1:A:298:ASN:O	1:A:299:ALA:C	2.55	0.49
1:A:359:LEU:CD1	1:A:417:GLU:HG2	2.41	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:ASP:HB3	1:A:634:TRP:CZ3	2.41	0.49
1:A:613:ASN:HA	1:A:625:GLY:HA3	1.95	0.49
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.48	0.49
1:A:702:LEU:HD11	1:A:844:MET:HE2	1.94	0.49
1:B:119:PRO:HG2	1:B:122:VAL:HG21	1.95	0.49
1:B:690:LEU:HB2	1:B:694:LYS:HB3	1.94	0.49
1:C:184:MET:HB3	1:C:771:VAL:HG13	1.94	0.49
1:C:219:LEU:O	1:C:220:GLY:O	2.30	0.49
1:C:333:VAL:O	1:C:337:ILE:HD12	2.12	0.49
1:C:561:SER:HA	1:C:923:ASN:CB	2.43	0.49
1:A:552:MET:C	1:A:554:TYR:N	2.69	0.49
1:A:719:ASN:N	1:A:826:GLU:O	2.46	0.49
1:A:843:LEU:O	1:A:844:MET:C	2.56	0.49
1:A:843:LEU:HD23	1:A:846:GLN:NE2	2.27	0.49
1:A:1024:VAL:HG12	1:A:1028:VAL:HG23	1.94	0.49
1:B:158:VAL:HA	1:B:162:MET:CG	2.36	0.49
1:B:371:ALA:O	1:B:372:VAL:C	2.55	0.49
1:B:435:MET:HA	1:B:435:MET:HE3	1.94	0.49
1:B:643:LYS:C	1:B:647:ILE:HG13	2.38	0.49
1:C:23:GLY:O	1:C:27:ILE:HG13	2.13	0.49
1:C:40:PRO:CB	1:C:76:MET:HE1	2.43	0.49
1:C:166:ILE:CA	1:C:166:ILE:CD1	2.75	0.49
1:C:389:SER:O	1:C:394:THR:HG21	2.12	0.49
1:C:454:VAL:O	1:C:456:MET:O	2.31	0.49
1:C:461:GLY:CA	1:C:869:SER:OG	2.61	0.49
1:C:1022:VAL:N	1:C:1023:PRO:CD	2.75	0.49
1:A:330:THR:H	1:A:331:PRO:HD2	1.78	0.49
1:A:533:GLY:O	1:A:535:LEU:HB2	2.12	0.49
1:A:537:SER:O	1:A:538:THR:C	2.55	0.49
1:A:574:THR:HG21	1:A:598:TYR:CE1	2.44	0.49
1:A:754:TRP:CZ2	1:A:786:ILE:HG12	2.48	0.49
1:B:139:VAL:O	1:B:140:VAL:C	2.55	0.49
1:B:155:SER:O	1:B:156:ASP:C	2.55	0.49
1:B:314:GLU:C	1:B:316:PHE:H	2.20	0.49
1:B:343:THR:O	1:B:347:ALA:N	2.39	0.49
1:B:701:GLN:HB3	1:B:851:LEU:HD13	1.95	0.49
1:B:1026:PHE:HB3	1:B:1030:ARG:CZ	2.42	0.49
1:C:8:ARG:HG2	1:C:8:ARG:HH21	1.78	0.49
1:C:166:ILE:CA	1:C:166:ILE:CG2	2.85	0.49
1:C:314:GLU:HA	1:C:317:PHE:CZ	2.47	0.49
1:C:354:VAL:C	1:C:356:TYR:H	2.20	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:VAL:HA	1:C:402:ILE:HD12	1.92	0.49
1:C:492:LEU:O	1:C:496:MET:HG2	2.13	0.49
1:C:545:TYR:CZ	1:C:1021:PHE:CD2	3.01	0.49
1:C:781:MET:O	1:C:782:LEU:HD23	2.13	0.49
1:A:68:ASN:H	1:A:69:MET:H	1.61	0.49
1:A:219:LEU:HD23	1:B:754:TRP:HZ3	1.78	0.49
1:A:313:MET:C	1:A:315:PRO:CD	2.85	0.49
1:A:372:VAL:HB	1:A:373:PRO:CD	2.37	0.49
1:A:978:THR:C	1:A:980:LEU:N	2.70	0.49
1:A:999:ALA:HA	1:A:1002:ALA:CB	2.43	0.49
1:B:619:GLY:H	1:B:721:LEU:CD1	2.26	0.49
1:C:513:PHE:CA	1:C:516:PHE:HB3	2.33	0.49
1:C:562:SER:OG	1:C:922:THR:HG21	2.12	0.49
1:C:685:ILE:HD11	1:C:687:GLN:CD	2.38	0.49
1:C:912:ALA:O	1:C:914:LEU:N	2.46	0.49
1:A:631:LEU:HD11	1:A:644:VAL:HG22	1.94	0.49
1:A:818:ARG:HG3	2:A:1062:HOH:O	2.11	0.49
1:A:963:ALA:O	1:A:965:LEU:N	2.46	0.49
1:B:20:MET:HG3	1:B:374:VAL:HG23	1.94	0.49
1:B:150:THR:O	1:B:151:GLN:C	2.55	0.49
1:B:404:LEU:HD13	1:B:449:LEU:CD1	2.42	0.49
1:B:471:SER:O	1:B:475:VAL:HB	2.13	0.49
1:C:80:SER:O	1:C:89:GLN:O	2.31	0.49
1:C:568:ASP:OD1	1:C:634:TRP:CD1	2.65	0.49
1:C:650:ARG:O	1:C:653:ARG:HG2	2.12	0.49
1:C:685:ILE:HD12	1:C:686:ASP:N	2.28	0.49
1:C:705:GLU:O	1:C:708:LYS:N	2.45	0.49
1:A:521:GLU:CG	2:A:1075:HOH:O	2.57	0.49
1:A:971:ARG:C	1:A:974:PRO:HD2	2.38	0.49
1:B:125:GLN:O	1:B:125:GLN:CG	2.59	0.49
1:B:183:ALA:H	1:B:272:GLY:HA2	1.78	0.49
1:B:490:PRO:O	1:B:493:CYS:O	2.30	0.49
1:B:642:ASN:N	1:B:650:ARG:HH12	2.05	0.49
1:C:102:ILE:O	1:C:105:VAL:N	2.46	0.49
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.94	0.49
1:A:83:ASP:OD1	1:A:83:ASP:C	2.56	0.49
1:A:171:GLY:O	1:A:173:GLY:N	2.45	0.49
1:A:356:TYR:C	1:A:358:PHE:H	2.21	0.49
1:A:736:ALA:CA	1:A:741:VAL:HG13	2.42	0.49
1:A:832:ALA:CB	1:A:835:LYS:HB2	2.40	0.49
1:A:1020:PHE:C	1:A:1023:PRO:HD2	2.38	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:PHE:HA	1:B:365:THR:HG22	1.95	0.49
1:B:453:PHE:HA	1:B:456:MET:SD	2.52	0.49
1:B:485:ALA:HA	1:B:489:THR:OG1	2.13	0.49
1:B:583:THR:HG23	1:B:585:GLU:H	1.78	0.49
1:B:905:VAL:N	1:B:906:PRO:CD	2.76	0.49
1:C:4:PHE:HB3	1:C:8:ARG:NH2	2.16	0.49
1:C:396:PHE:HA	1:C:399:VAL:HB	1.94	0.49
1:C:548:ILE:HD12	1:C:548:ILE:C	2.38	0.49
1:C:574:THR:O	1:C:626:ILE:HD13	2.12	0.49
1:A:67:GLN:CB	2:A:1057:HOH:O	2.60	0.48
1:A:193:LEU:HB2	1:A:265:VAL:HG13	1.95	0.48
1:A:621:GLY:C	1:A:623:ASN:H	2.21	0.48
1:B:118:LEU:O	1:B:119:PRO:C	2.56	0.48
1:B:355:MET:O	1:B:365:THR:OG1	2.30	0.48
1:B:369:THR:O	1:B:372:VAL:HG13	2.13	0.48
1:B:578:LEU:HD12	1:B:586:ARG:CZ	2.42	0.48
1:B:586:ARG:NH2	1:B:660:ASP:HB2	2.26	0.48
1:B:638:PRO:HG2	1:B:639:GLY:H	1.78	0.48
1:B:900:SER:O	1:B:903:LEU:N	2.39	0.48
1:B:942:ALA:O	1:B:945:ILE:HG12	2.13	0.48
1:B:969:ARG:HG2	1:B:969:ARG:HH11	1.78	0.48
1:C:379:THR:HB	1:C:398:MET:HE3	1.94	0.48
1:C:414:GLU:OE1	1:C:977:MET:HE3	2.12	0.48
1:C:925:VAL:C	1:C:927:PHE:N	2.68	0.48
1:A:64:VAL:HG12	1:A:65:ILE:N	2.27	0.48
1:A:449:LEU:O	1:A:453:PHE:HD1	1.96	0.48
1:A:534:ILE:HD12	1:A:540:ARG:CZ	2.43	0.48
1:A:554:TYR:HE1	1:A:558:ARG:HD3	1.76	0.48
1:B:218:GLN:HA	1:B:234:ILE:HG13	1.95	0.48
1:B:261:LEU:HD13	1:B:261:LEU:H	1.78	0.48
1:B:261:LEU:CD2	1:B:263:ARG:HB2	2.43	0.48
1:B:743:ILE:HD12	1:B:743:ILE:H	1.78	0.48
1:C:324:VAL:HG23	1:C:325:TYR:N	2.27	0.48
1:C:395:MET:C	1:C:397:GLY:N	2.69	0.48
1:C:449:LEU:O	1:C:452:VAL:N	2.26	0.48
1:C:470:PHE:O	1:C:471:SER:C	2.55	0.48
1:C:576:VAL:HG21	1:C:591:LEU:CD2	2.43	0.48
1:C:753:ALA:HB1	1:C:775:SER:HB2	1.95	0.48
1:C:893:GLU:O	1:C:893:GLU:HG3	2.13	0.48
1:A:72:ILE:O	1:A:72:ILE:HG22	2.13	0.48
1:A:525:HIS:O	1:A:526:HIS:C	2.53	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:PHE:O	1:B:6:ILE:N	2.44	0.48
1:B:341:VAL:CG1	1:B:342:LYS:N	2.76	0.48
1:B:712:MET:HA	1:B:712:MET:CE	2.42	0.48
1:C:110:LYS:HA	1:C:113:LEU:CD1	2.20	0.48
1:C:127:VAL:CA	1:C:127:VAL:CG1	2.83	0.48
1:C:192:GLU:C	1:C:194:ASN:N	2.64	0.48
1:C:252:LYS:O	1:C:260:VAL:CG1	2.57	0.48
1:C:435:MET:HA	1:C:438:ILE:HG22	1.95	0.48
1:C:545:TYR:OH	1:C:1021:PHE:HB3	2.13	0.48
1:C:655:PHE:C	1:C:657:GLN:N	2.58	0.48
1:A:69:MET:HE2	1:A:69:MET:CA	2.39	0.48
1:A:190:PRO:HG2	1:A:788:ASP:HB3	1.95	0.48
1:A:819:TYR:N	1:A:822:LEU:O	2.45	0.48
1:B:197:GLN:O	1:B:792:ARG:NH2	2.45	0.48
1:B:220:GLY:O	1:B:221:GLY:O	2.30	0.48
1:B:423:GLU:OE1	1:B:427:PRO:HD3	2.10	0.48
1:B:610:PHE:O	1:B:627:ALA:CB	2.59	0.48
1:C:4:PHE:CB	1:C:8:ARG:NH2	2.68	0.48
1:C:163:LYS:O	1:C:165:ALA:N	2.46	0.48
1:A:60:THR:CG2	1:A:119:PRO:CD	2.90	0.48
1:A:189:ASN:ND2	1:A:192:GLU:HB3	2.27	0.48
1:A:309:GLU:O	1:A:311:ALA:O	2.32	0.48
1:A:531:VAL:CA	1:A:534:ILE:HD11	2.17	0.48
1:A:600:THR:O	1:A:601:LYS:CB	2.61	0.48
1:B:26:ALA:O	1:B:30:LEU:HB2	2.14	0.48
1:B:362:PHE:C	1:B:364:ALA:N	2.72	0.48
1:B:709:HIS:N	1:B:710:PRO:CD	2.76	0.48
1:B:912:ALA:HB1	1:B:1006:GLY:O	2.13	0.48
1:C:386:PHE:O	1:C:388:PHE:HD1	1.96	0.48
1:C:403:GLY:C	1:C:405:LEU:H	2.21	0.48
1:C:417:GLU:HB3	1:C:973:ARG:NH1	2.28	0.48
1:C:466:ILE:N	1:C:466:ILE:HD12	2.28	0.48
1:C:711:ASP:CG	1:C:712:MET:H	2.22	0.48
1:C:950:LYS:HZ3	1:C:1030:ARG:NH1	2.11	0.48
1:C:964:THR:O	1:C:967:ALA:HB3	2.13	0.48
1:A:56:THR:HG22	1:A:56:THR:O	2.12	0.48
1:A:105:VAL:HA	1:B:109:ASN:HD21	1.79	0.48
1:A:255:GLN:N	1:A:255:GLN:OE1	2.46	0.48
1:A:818:ARG:CD	1:A:821:GLY:O	2.51	0.48
1:B:327:TYR:HD2	1:B:628:PHE:HB3	1.75	0.48
1:B:538:THR:C	1:B:540:ARG:H	2.20	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:648:THR:HG21	1:B:666:PHE:HA	1.95	0.48
1:B:742:SER:CB	1:B:745:ASP:OD2	2.52	0.48
1:B:974:PRO:C	1:B:976:LEU:N	2.70	0.48
1:C:58:GLN:CB	1:C:58:GLN:CD	2.79	0.48
1:C:997:SER:HA	1:C:1000:GLN:OE1	2.12	0.48
1:C:1018:ALA:HA	1:C:1021:PHE:HB2	1.94	0.48
1:B:407:ASP:O	1:B:410:ILE:HG22	2.13	0.48
1:B:416:VAL:HG22	1:B:431:THR:HA	1.94	0.48
1:B:831:ALA:C	1:B:833:PRO:HD2	2.39	0.48
1:B:932:LEU:HA	1:B:935:ILE:HD12	1.95	0.48
1:C:34:GLN:C	1:C:35:TYR:CG	2.91	0.48
1:C:528:THR:O	1:C:531:VAL:HG22	2.14	0.48
1:C:758:TYR:CD2	1:C:770:LYS:HE2	2.49	0.48
1:C:841:MET:O	1:C:842:GLU:C	2.56	0.48
1:C:846:GLN:O	1:C:849:SER:OG	2.29	0.48
1:C:881:LEU:O	1:C:882:ILE:C	2.57	0.48
1:C:910:ILE:CG2	1:C:911:GLY:N	2.77	0.48
1:C:953:MET:HE1	1:C:1030:ARG:NH2	2.28	0.48
1:C:958:LYS:HD2	1:C:958:LYS:N	2.29	0.48
1:A:99:ASP:O	1:A:102:ILE:HG22	2.13	0.48
1:A:158:VAL:O	1:A:158:VAL:HG12	2.13	0.48
1:A:578:LEU:HD21	1:A:587:THR:CG2	2.42	0.48
1:A:702:LEU:HA	1:A:705:GLU:HB2	1.96	0.48
1:A:988:PRO:C	1:A:990:VAL:N	2.67	0.48
1:B:252:LYS:HB3	1:B:260:VAL:HG11	1.95	0.48
1:B:485:ALA:O	1:B:486:LEU:HB3	2.14	0.48
1:C:350:LEU:HD12	1:C:985:GLY:CA	2.39	0.48
1:C:399:VAL:C	1:C:401:ALA:N	2.70	0.48
1:C:850:LYS:O	1:C:851:LEU:C	2.57	0.48
1:C:896:SER:C	1:C:898:PRO:HD2	2.39	0.48
1:C:913:LEU:HD23	1:C:927:PHE:CZ	2.49	0.48
1:A:218:GLN:OE1	1:A:221:GLY:HA3	2.14	0.48
1:A:307:ARG:NH1	1:A:325:TYR:CD2	2.82	0.48
1:A:498:LYS:HA	1:A:498:LYS:HE2	1.95	0.48
1:A:841:MET:O	1:A:844:MET:HB3	2.14	0.48
1:B:101:ASP:O	1:B:105:VAL:HG23	2.14	0.48
1:B:298:ASN:HB2	1:B:301:ASP:OD1	2.14	0.48
1:B:409:ALA:HB2	1:B:485:ALA:HB2	1.94	0.48
1:B:873:ALA:C	1:B:875:SER:N	2.71	0.48
1:B:904:VAL:C	1:B:906:PRO:HD2	2.39	0.48
1:B:1030:ARG:C	1:B:1032:ARG:H	2.22	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:644:VAL:HG12	1:C:667:ASN:HB2	1.95	0.48
1:A:113:LEU:C	1:A:116:PRO:HD2	2.39	0.48
1:B:145:THR:O	1:B:146:ASP:CG	2.56	0.48
1:B:219:LEU:HD12	1:B:219:LEU:H	1.79	0.48
1:B:324:VAL:O	1:B:326:PRO:HD2	2.13	0.48
1:B:341:VAL:HG13	1:B:342:LYS:N	2.29	0.48
1:B:423:GLU:OE1	1:B:427:PRO:CG	2.60	0.48
1:B:438:ILE:CD1	1:B:971:ARG:NH1	2.77	0.48
1:B:830:GLN:HE21	1:B:830:GLN:N	2.06	0.48
1:B:833:PRO:O	1:B:834:GLY:O	2.31	0.48
1:C:104:GLN:HG3	1:C:131:LYS:CG	2.42	0.48
1:C:121:GLU:N	1:C:121:GLU:OE2	2.44	0.48
1:C:246:PHE:HZ	1:C:762:PHE:CB	2.27	0.48
1:C:262:LEU:HD23	1:C:268:ILE:HD11	1.95	0.48
1:C:420:MET:SD	1:C:498:LYS:HD3	2.53	0.48
1:C:536:ARG:HH21	1:C:536:ARG:HG2	1.79	0.48
1:C:545:TYR:HH	1:C:1021:PHE:CB	2.26	0.48
1:C:878:ALA:C	1:C:880:SER:N	2.70	0.48
1:A:251:LEU:CD1	1:A:262:LEU:HA	2.29	0.47
1:A:781:MET:CE	1:C:225:VAL:H	2.26	0.47
1:B:366:LEU:O	1:B:369:THR:N	2.41	0.47
1:B:525:HIS:O	1:B:529:ASP:HB2	2.14	0.47
1:B:562:SER:HA	1:B:837:THR:OG1	2.14	0.47
1:B:626:ILE:HD11	1:B:628:PHE:CZ	2.49	0.47
1:B:665:ALA:O	1:B:666:PHE:CG	2.67	0.47
1:C:115:MET:HB2	1:C:116:PRO:HD3	1.95	0.47
1:C:181:GLN:OE1	1:C:767:ARG:CZ	2.62	0.47
1:C:244:GLU:O	1:C:263:ARG:NH2	2.47	0.47
1:C:653:ARG:O	1:C:655:PHE:O	2.32	0.47
1:C:686:ASP:OD1	1:C:686:ASP:C	2.55	0.47
1:A:66:GLU:CD	2:A:1054:HOH:O	2.56	0.47
1:A:418:ARG:HH21	1:A:970:MET:HA	1.78	0.47
1:A:574:THR:HG22	1:A:665:ALA:HB2	1.96	0.47
1:A:639:GLY:O	1:A:642:ASN:N	2.37	0.47
1:A:729:ILE:O	1:A:730:ASP:HB2	2.13	0.47
1:A:964:THR:HG22	1:A:964:THR:O	2.12	0.47
1:B:58:GLN:HB2	1:B:82:SER:CB	2.44	0.47
1:B:247:GLY:HA2	1:B:268:ILE:HD11	1.78	0.47
1:B:249:ILE:O	1:B:261:LEU:HB2	2.14	0.47
1:B:280:GLU:CA	1:B:284:GLN:O	2.62	0.47
1:B:339:GLU:HB3	1:B:1000:GLN:HE22	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:ASN:H	1:B:394:THR:HG1	1.57	0.47
1:B:556:PHE:C	1:B:558:ARG:H	2.22	0.47
1:B:575:MET:O	1:B:663:VAL:HA	2.14	0.47
1:B:984:LEU:CD1	1:B:984:LEU:O	2.60	0.47
1:C:131:LYS:HB2	1:C:295:THR:HG21	1.96	0.47
1:C:950:LYS:HE2	1:C:1030:ARG:CZ	2.45	0.47
1:C:1024:VAL:CG1	1:C:1028:VAL:HG21	2.44	0.47
1:A:102:ILE:CA	1:A:105:VAL:HG23	2.44	0.47
1:A:184:MET:HE3	1:A:246:PHE:CD2	2.49	0.47
1:A:362:PHE:C	1:A:364:ALA:H	2.21	0.47
1:A:592:ASN:O	1:A:595:THR:HB	2.14	0.47
1:A:779:TYR:N	1:A:779:TYR:CD1	2.82	0.47
1:A:845:GLU:CD	1:A:859:TRP:HE1	2.22	0.47
1:A:920:GLY:O	1:A:921:LEU:HD23	2.14	0.47
1:A:999:ALA:HA	1:A:1002:ALA:HB3	1.97	0.47
1:A:1023:PRO:C	1:A:1024:VAL:O	2.58	0.47
1:B:330:THR:H	1:B:331:PRO:HD2	1.74	0.47
1:B:415:ASN:ND2	1:B:438:ILE:HD13	2.29	0.47
1:B:489:THR:N	1:B:490:PRO:HD2	2.29	0.47
1:B:560:PRO:O	1:B:922:THR:OG1	2.32	0.47
1:B:669:PRO:HB2	1:B:862:MET:HE2	1.95	0.47
1:B:889:ALA:O	1:B:892:TYR:O	2.33	0.47
1:B:987:MET:CA	1:B:987:MET:CE	2.82	0.47
1:B:988:PRO:O	1:B:989:LEU:CB	2.45	0.47
1:B:1024:VAL:O	1:B:1025:PHE:CB	2.62	0.47
1:C:13:TRP:O	1:C:17:ILE:HD13	2.14	0.47
1:C:57:VAL:CG1	1:C:88:VAL:HG23	2.45	0.47
1:C:300:LEU:O	1:C:303:ALA:N	2.48	0.47
1:A:113:LEU:HD23	1:C:127:VAL:O	2.14	0.47
1:A:455:PRO:HB2	1:A:877:TYR:HE1	1.79	0.47
1:A:481:SER:OG	1:A:482:VAL:N	2.46	0.47
1:A:1019:ILE:O	1:A:1023:PRO:HG3	2.14	0.47
1:B:20:MET:O	1:B:23:GLY:O	2.32	0.47
1:B:48:SER:C	1:B:49:TYR:CG	2.93	0.47
1:B:281:PHE:O	1:B:284:GLN:HB3	2.15	0.47
1:B:418:ARG:NE	1:B:970:MET:SD	2.87	0.47
1:B:548:ILE:HD13	1:B:1017:LEU:HD23	1.95	0.47
1:B:709:HIS:C	1:B:711:ASP:N	2.72	0.47
1:B:953:MET:HA	1:B:958:LYS:HA	1.96	0.47
1:B:972:LEU:CD1	1:B:976:LEU:CD2	2.92	0.47
1:C:169:THR:C	1:C:169:THR:CG2	2.87	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:MET:HE3	1:C:932:LEU:CD1	2.44	0.47
1:C:701:GLN:O	1:C:702:LEU:C	2.58	0.47
1:C:978:THR:O	1:C:981:ALA:N	2.47	0.47
1:A:96:SER:OG	1:A:97:GLY:N	2.44	0.47
1:A:156:ASP:O	1:A:157:TYR:C	2.55	0.47
1:A:277:ILE:HA	1:A:613:ASN:O	2.13	0.47
1:A:438:ILE:HD13	1:A:438:ILE:H	1.79	0.47
1:A:736:ALA:HA	1:A:741:VAL:HG13	1.95	0.47
1:A:877:TYR:OH	1:A:932:LEU:HD11	2.15	0.47
1:B:185:ARG:NH2	2:B:1054:HOH:O	2.47	0.47
1:B:600:THR:O	1:B:603:LYS:HG2	2.15	0.47
1:B:987:MET:CE	1:B:987:MET:O	2.62	0.47
1:C:66:GLU:HB3	1:C:78:MET:CE	2.45	0.47
1:C:438:ILE:O	1:C:441:ALA:HB3	2.14	0.47
1:C:532:GLY:C	1:C:534:ILE:N	2.71	0.47
1:A:25:LEU:HD13	1:A:25:LEU:C	2.40	0.47
1:A:471:SER:O	1:A:472:ILE:C	2.57	0.47
1:A:593:GLU:O	1:A:594:VAL:C	2.55	0.47
1:B:126:GLY:C	1:B:127:VAL:HG23	2.39	0.47
1:B:158:VAL:CA	1:B:162:MET:HG2	2.36	0.47
1:B:355:MET:SD	1:B:368:PRO:HB2	2.54	0.47
1:B:568:ASP:HA	1:B:644:VAL:HG21	1.96	0.47
1:B:715:SER:O	1:B:716:VAL:C	2.57	0.47
1:B:729:ILE:CG1	1:B:730:ASP:H	2.24	0.47
1:B:863:SER:C	1:B:865:GLN:N	2.71	0.47
1:B:864:TYR:O	1:B:868:LEU:HB2	2.14	0.47
1:B:892:TYR:HB2	1:B:897:ILE:HD11	1.95	0.47
1:B:944:LEU:HB2	1:B:975:ILE:HD11	1.96	0.47
1:C:18:ILE:O	1:C:19:ILE:C	2.56	0.47
1:C:418:ARG:HD2	1:C:970:MET:HE3	1.96	0.47
1:C:474:ILE:O	1:C:478:MET:HB2	2.15	0.47
1:C:699:ARG:O	1:C:700:ASN:C	2.56	0.47
1:C:767:ARG:HG2	1:C:769:LYS:HD3	1.96	0.47
1:C:925:VAL:O	1:C:926:TYR:HB2	2.14	0.47
1:A:65:ILE:CA	1:A:66:GLU:N	2.66	0.47
1:A:95:GLU:O	1:A:98:THR:CG2	2.62	0.47
1:A:130:GLU:HG2	1:B:113:LEU:HD11	1.97	0.47
1:A:200:PRO:CG	1:A:749:THR:HG23	2.45	0.47
1:A:344:LEU:HD22	1:A:402:ILE:CD1	2.45	0.47
1:A:674:LEU:HD13	1:A:675:GLY:N	2.30	0.47
1:A:995:ALA:O	1:A:996:GLY:C	2.57	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1026:PHE:O	1:A:1030:ARG:HB2	2.14	0.47
1:B:85:THR:HG23	1:B:87:THR:HB	1.95	0.47
1:B:114:ALA:O	1:B:115:MET:C	2.58	0.47
1:B:144:ASN:OD1	1:B:149:MET:HG3	2.15	0.47
1:B:166:ILE:HG22	1:B:167:SER:N	2.30	0.47
1:B:314:GLU:C	1:B:316:PHE:N	2.72	0.47
1:B:314:GLU:HA	1:B:317:PHE:CD2	2.50	0.47
1:B:467:TYR:O	1:B:470:PHE:HB2	2.14	0.47
1:B:612:VAL:HG23	1:B:626:ILE:O	2.15	0.47
1:B:978:THR:HG23	1:B:979:SER:N	2.30	0.47
1:C:1:MET:CB	1:C:2:PRO:HD2	2.21	0.47
1:C:62:THR:O	1:C:66:GLU:HG3	2.15	0.47
1:C:184:MET:HE1	1:C:270:LEU:N	2.28	0.47
1:C:327:TYR:HD1	1:C:571:VAL:HB	1.80	0.47
1:C:415:ASN:HD21	1:C:434:SER:CB	2.27	0.47
1:C:417:GLU:OE2	1:C:417:GLU:CA	2.55	0.47
1:C:491:ALA:C	1:C:493:CYS:H	2.22	0.47
1:C:607:GLU:HB2	1:C:632:LYS:HD3	1.97	0.47
1:C:987:MET:SD	1:C:1008:MET:HE1	2.55	0.47
1:B:12:ALA:O	1:B:13:TRP:C	2.58	0.47
1:B:17:ILE:HG21	1:C:886:LEU:HD21	1.97	0.47
1:B:314:GLU:O	1:B:316:PHE:N	2.47	0.47
1:B:354:VAL:HG21	1:B:981:ALA:HA	1.96	0.47
1:B:418:ARG:HH21	1:B:970:MET:HG2	1.80	0.47
1:B:425:LEU:HA	1:B:426:PRO:HD3	1.70	0.47
1:B:472:ILE:O	1:B:473:THR:C	2.55	0.47
1:B:904:VAL:HG13	1:B:907:LEU:CD1	2.25	0.47
1:B:915:ALA:C	1:B:917:THR:H	2.23	0.47
1:B:945:ILE:HG13	1:B:946:VAL:N	2.30	0.47
1:C:12:ALA:C	1:C:14:VAL:H	2.23	0.47
1:C:305:ALA:O	1:C:306:ILE:C	2.55	0.47
1:A:8:ARG:O	1:A:8:ARG:HG3	2.15	0.47
1:A:223:PRO:HD3	1:B:275:TYR:CB	2.45	0.47
1:A:298:ASN:HB3	1:A:301:ASP:HB2	1.97	0.47
1:A:426:PRO:CB	1:A:427:PRO:HD2	2.45	0.47
1:A:695:LEU:HG	1:A:695:LEU:O	2.14	0.47
1:A:831:ALA:HA	1:A:840:ALA:CB	2.45	0.47
1:B:343:THR:HG21	1:B:1000:GLN:OE1	2.15	0.47
1:B:588:GLN:OE1	1:B:588:GLN:HA	2.14	0.47
1:B:692:HIS:CE1	1:B:723:ASP:OD1	2.68	0.47
1:C:32:VAL:O	1:C:32:VAL:CG1	2.56	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:LYS:C	1:C:165:ALA:N	2.71	0.47
1:C:331:PRO:O	1:C:332:PHE:C	2.56	0.47
1:C:355:MET:HA	1:C:355:MET:CE	2.45	0.47
1:C:685:ILE:HD12	1:C:686:ASP:C	2.39	0.47
1:A:118:LEU:HA	1:A:118:LEU:HD23	1.50	0.47
1:A:635:ALA:C	1:A:637:ARG:N	2.73	0.47
1:B:57:VAL:HG11	1:B:86:GLY:HA2	1.97	0.47
1:B:262:LEU:HD22	1:B:266:ALA:HB3	1.96	0.47
1:B:428:LYS:O	1:B:432:ARG:HB2	2.15	0.47
1:B:455:PRO:C	1:B:457:ALA:N	2.72	0.47
1:B:469:GLN:O	1:B:473:THR:OG1	2.32	0.47
1:B:653:ARG:C	1:B:654:ALA:O	2.55	0.47
1:B:790:TYR:HD1	1:B:800:PRO:N	2.13	0.47
1:B:898:PRO:C	1:B:900:SER:H	2.23	0.47
1:C:476:SER:C	1:C:478:MET:N	2.66	0.47
1:C:666:PHE:CD2	1:C:666:PHE:C	2.92	0.47
1:C:721:LEU:HD23	1:C:721:LEU:O	2.15	0.47
1:C:857:TYR:CD1	1:C:857:TYR:C	2.92	0.47
1:A:58:GLN:HE21	1:A:816:LEU:CD1	2.28	0.46
1:A:713:LEU:HB2	1:A:833:PRO:CD	2.45	0.46
1:B:538:THR:H	1:B:540:ARG:HH21	1.61	0.46
1:B:556:PHE:CA	1:B:913:LEU:HD21	2.46	0.46
1:C:315:PRO:HB2	1:C:316:PHE:CD1	2.50	0.46
1:C:332:PHE:CE1	1:C:569:GLN:HG2	2.50	0.46
1:C:549:VAL:O	1:C:550:VAL:C	2.57	0.46
1:C:578:LEU:CD2	1:C:590:VAL:HG21	2.45	0.46
1:C:713:LEU:CD2	1:C:835:LYS:H	2.24	0.46
1:C:729:ILE:HD11	1:C:786:ILE:CD1	2.33	0.46
1:C:872:GLN:HB2	1:C:875:SER:CB	2.37	0.46
1:A:515:TRP:C	1:A:515:TRP:CD1	2.93	0.46
1:B:217:GLY:HA3	1:C:754:TRP:O	2.16	0.46
1:B:375:VAL:HG22	1:B:484:VAL:HG21	1.97	0.46
1:B:462:SER:OG	1:B:865:GLN:CD	2.58	0.46
1:B:538:THR:HG23	1:B:540:ARG:HH22	1.77	0.46
1:B:546:LEU:O	1:B:550:VAL:HB	2.15	0.46
1:B:690:LEU:HD22	1:B:694:LYS:HB2	1.97	0.46
1:B:743:ILE:O	1:B:747:ASN:ND2	2.48	0.46
1:B:986:VAL:C	1:B:988:PRO:HD2	2.39	0.46
1:C:77:TYR:CE1	1:C:860:THR:OG1	2.68	0.46
1:C:169:THR:CG2	1:C:172:VAL:CG2	2.93	0.46
1:C:259:ARG:CB	1:C:259:ARG:NH1	2.77	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:ALA:HA	1:C:611:ALA:O	2.16	0.46
1:C:356:TYR:C	1:C:358:PHE:N	2.72	0.46
1:C:399:VAL:O	1:C:401:ALA:N	2.49	0.46
1:C:445:ILE:HD13	1:C:940:LYS:HE3	1.97	0.46
1:C:719:ASN:N	2:C:1063:HOH:O	2.26	0.46
1:A:104:GLN:O	1:A:105:VAL:C	2.57	0.46
1:A:113:LEU:HD13	1:C:108:GLN:HE22	1.80	0.46
1:A:572:PHE:CD1	1:A:629:VAL:HG13	2.50	0.46
1:A:909:VAL:O	1:A:912:ALA:CB	2.59	0.46
1:B:42:ALA:HA	1:B:93:THR:HA	1.97	0.46
1:B:189:ASN:HB3	1:B:192:GLU:HB3	1.98	0.46
1:B:345:VAL:HG12	1:B:349:ILE:CD1	2.45	0.46
1:B:355:MET:CE	1:B:369:THR:HG22	2.46	0.46
1:B:366:LEU:O	1:B:370:ILE:HG13	2.15	0.46
1:B:474:ILE:O	1:B:475:VAL:C	2.59	0.46
1:B:644:VAL:O	1:B:645:GLU:C	2.58	0.46
1:B:804:PHE:O	1:B:805:SER:CB	2.63	0.46
1:B:941:ASN:O	1:B:942:ALA:C	2.58	0.46
1:C:16:ALA:HB2	1:C:488:LEU:HD22	1.97	0.46
1:C:26:ALA:O	1:C:30:LEU:CG	2.64	0.46
1:C:536:ARG:C	1:C:538:THR:H	2.22	0.46
1:C:559:LEU:HD13	1:C:917:THR:CG2	2.45	0.46
1:C:674:LEU:HD21	1:C:862:MET:N	2.29	0.46
1:C:989:LEU:HD12	1:C:1000:GLN:HA	1.96	0.46
1:A:114:ALA:C	1:A:116:PRO:HD2	2.41	0.46
1:A:135:SER:O	1:A:136:PHE:CG	2.69	0.46
1:A:316:PHE:O	1:A:321:LEU:HD11	2.15	0.46
1:A:741:VAL:HG22	1:A:746:ILE:HD11	1.97	0.46
1:A:822:LEU:HG	2:A:1055:HOH:O	2.15	0.46
1:B:11:PHE:O	1:B:14:VAL:N	2.48	0.46
1:B:316:PHE:CE2	1:C:687:GLN:HG3	2.50	0.46
1:C:169:THR:HG22	1:C:172:VAL:CG2	2.41	0.46
1:C:281:PHE:O	1:C:282:ASN:C	2.57	0.46
1:C:470:PHE:CD2	1:C:929:VAL:HG11	2.50	0.46
1:C:897:ILE:HD13	1:C:950:LYS:HG3	1.98	0.46
1:A:203:VAL:HG13	1:A:262:LEU:HD11	1.97	0.46
1:A:713:LEU:CG	1:A:832:ALA:HA	2.46	0.46
1:A:729:ILE:HD13	1:C:234:ILE:HG23	1.97	0.46
1:A:1015:THR:OG1	1:A:1016:VAL:N	2.48	0.46
1:B:41:PRO:HG2	1:B:98:THR:CG2	2.46	0.46
1:B:104:GLN:HG2	1:B:105:VAL:N	2.27	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:SER:OG	1:B:288:GLY:N	2.49	0.46
1:B:413:VAL:C	1:B:415:ASN:H	2.23	0.46
1:B:518:ARG:HA	1:B:521:GLU:CG	2.46	0.46
1:B:518:ARG:O	1:B:520:PHE:N	2.48	0.46
1:B:1020:PHE:O	1:B:1023:PRO:HG2	2.15	0.46
2:B:1060:HOH:O	1:C:110:LYS:CD	2.59	0.46
1:C:60:THR:HG22	1:C:61:VAL:HG23	1.97	0.46
1:C:144:ASN:CG	1:C:149:MET:HG3	2.40	0.46
1:C:467:TYR:C	1:C:469:GLN:N	2.71	0.46
1:A:44:THR:C	1:A:45:ILE:CG1	2.89	0.46
1:A:102:ILE:O	1:A:102:ILE:HG23	2.01	0.46
1:A:166:ILE:HG22	1:A:172:VAL:HG11	1.98	0.46
1:A:252:LYS:HB3	1:A:260:VAL:CG2	2.45	0.46
1:A:552:MET:HB2	1:A:910:ILE:HG23	1.96	0.46
1:A:572:PHE:CE1	1:A:629:VAL:CG1	2.99	0.46
1:A:820:ASN:HB3	1:C:168:ARG:NH2	2.31	0.46
1:B:174:ASP:OD1	1:B:175:VAL:N	2.49	0.46
1:B:613:ASN:O	1:B:625:GLY:HA2	2.16	0.46
1:B:693:GLU:O	1:B:695:LEU:N	2.49	0.46
1:C:166:ILE:C	1:C:167:SER:C	2.83	0.46
1:C:355:MET:CE	1:C:977:MET:HG2	2.45	0.46
1:C:418:ARG:NH2	1:C:948:PHE:HZ	2.14	0.46
1:C:666:PHE:N	1:C:666:PHE:HD2	2.13	0.46
1:C:895:TRP:HA	1:C:895:TRP:CE3	2.51	0.46
1:A:58:GLN:NE2	1:A:816:LEU:CD1	2.78	0.46
1:A:349:ILE:N	1:A:349:ILE:CD1	2.79	0.46
1:B:213:GLN:CG	1:C:56:THR:HG23	2.45	0.46
1:B:252:LYS:HG2	1:B:253:VAL:H	1.80	0.46
1:B:920:GLY:O	1:B:921:LEU:O	2.34	0.46
1:C:188:MET:HE1	1:C:200:PRO:HA	1.98	0.46
1:C:395:MET:O	1:C:396:PHE:C	2.58	0.46
1:C:400:LEU:HD12	1:C:930:GLY:HA2	1.98	0.46
1:C:663:VAL:HG12	1:C:664:PHE:N	2.30	0.46
1:A:187:TRP:HH2	1:C:223:PRO:HG3	1.79	0.46
1:A:572:PHE:N	1:A:572:PHE:HD1	2.13	0.46
1:A:576:VAL:HG11	1:A:591:LEU:CD2	2.45	0.46
1:B:219:LEU:HD21	1:C:783:PRO:HG3	1.97	0.46
1:B:344:LEU:O	1:B:347:ALA:HB3	2.16	0.46
1:B:671:ILE:HB	1:B:672:VAL:H	1.50	0.46
1:B:716:VAL:HA	1:B:828:LEU:O	2.16	0.46
1:B:897:ILE:HG13	1:B:898:PRO:CD	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:973:ARG:CG	1:B:974:PRO:CD	2.92	0.46
1:B:988:PRO:C	1:B:990:VAL:H	2.24	0.46
1:A:23:GLY:O	1:A:27:ILE:HG12	2.16	0.46
1:A:66:GLU:OE2	1:A:818:ARG:HD2	2.16	0.46
1:A:661:ALA:O	1:A:662:MET:C	2.58	0.46
1:B:396:PHE:CD2	1:B:1003:VAL:HG21	2.50	0.46
1:B:429:GLU:HA	1:B:432:ARG:HB3	1.97	0.46
1:B:575:MET:HA	1:B:626:ILE:HG22	1.96	0.46
1:B:778:LYS:O	1:B:779:TYR:CB	2.64	0.46
1:C:49:TYR:HB3	1:C:52:ALA:HB3	1.98	0.46
1:C:66:GLU:O	1:C:69:MET:N	2.49	0.46
1:C:165:ALA:O	1:C:166:ILE:O	2.34	0.46
1:C:307:ARG:HA	1:C:310:LEU:HD12	1.98	0.46
1:C:514:GLY:O	1:C:518:ARG:HG3	2.16	0.46
1:C:545:TYR:CZ	1:C:1025:PHE:CZ	3.04	0.46
1:C:901:VAL:O	1:C:902:MET:C	2.58	0.46
1:A:171:GLY:O	1:A:294:ALA:CB	2.64	0.46
1:A:428:LYS:HE3	1:A:429:GLU:OE2	2.15	0.46
1:A:453:PHE:O	1:A:454:VAL:C	2.59	0.46
1:A:521:GLU:N	1:A:522:LYS:HE2	2.31	0.46
1:A:543:VAL:HG22	1:A:544:LEU:H	1.80	0.46
1:A:902:MET:C	1:A:904:VAL:N	2.74	0.46
1:B:686:ASP:CB	1:B:823:PRO:O	2.62	0.46
1:C:228:GLN:NE2	1:C:230:LEU:O	2.49	0.46
1:C:367:ILE:HG13	1:C:368:PRO:N	2.30	0.46
1:C:759:VAL:O	1:C:760:ASN:CB	2.47	0.46
1:C:818:ARG:NH2	1:C:821:GLY:O	2.47	0.46
1:C:945:ILE:CG2	1:C:1022:VAL:HG11	2.46	0.46
1:A:49:TYR:O	1:A:50:PRO:C	2.59	0.45
1:A:427:PRO:HG3	1:A:497:LEU:O	2.16	0.45
1:A:493:CYS:C	1:A:494:ALA:O	2.59	0.45
1:A:975:ILE:O	1:A:976:LEU:C	2.59	0.45
1:B:45:ILE:CG2	1:B:46:SER:N	2.79	0.45
1:B:74:ASN:O	1:B:94:PHE:CB	2.62	0.45
1:B:112:GLN:HB2	2:B:1055:HOH:O	2.16	0.45
1:B:157:TYR:O	1:B:161:ASN:ND2	2.45	0.45
1:B:162:MET:CB	1:B:313:MET:SD	3.04	0.45
1:B:189:ASN:HD22	1:B:190:PRO:HD2	1.81	0.45
1:B:193:LEU:HD23	1:B:265:VAL:HG21	1.98	0.45
1:B:340:VAL:O	1:B:341:VAL:C	2.59	0.45
1:B:485:ALA:C	1:B:487:ILE:H	2.24	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:PRO:HD3	1:B:660:ASP:O	2.16	0.45
1:B:597:TYR:CE1	1:B:654:ALA:CB	2.99	0.45
1:B:714:THR:HG22	1:B:831:ALA:N	2.30	0.45
1:B:907:LEU:O	1:B:910:ILE:HG22	2.16	0.45
1:B:939:ALA:O	1:B:943:ILE:HB	2.15	0.45
1:B:975:ILE:N	1:B:975:ILE:CD1	2.78	0.45
1:B:1005:THR:CG2	1:B:1005:THR:O	2.60	0.45
1:C:9:PRO:C	1:C:11:PHE:H	2.24	0.45
1:C:88:VAL:HG12	1:C:89:GLN:N	2.32	0.45
1:C:114:ALA:HA	1:C:117:LEU:HD12	1.97	0.45
1:C:143:ILE:CG2	1:C:284:GLN:NE2	2.64	0.45
1:C:246:PHE:O	1:C:249:ILE:HG13	2.17	0.45
1:C:350:LEU:HD13	1:C:984:LEU:HD22	1.93	0.45
1:C:491:ALA:O	1:C:493:CYS:N	2.38	0.45
1:C:939:ALA:O	1:C:943:ILE:CG1	2.64	0.45
1:A:189:ASN:HB2	1:A:779:TYR:CZ	2.51	0.45
1:A:243:THR:HG22	1:A:268:ILE:CG2	2.46	0.45
1:A:541:TYR:C	1:A:543:VAL:O	2.59	0.45
1:A:1018:ALA:HB1	1:A:1022:VAL:HG13	1.95	0.45
1:B:513:PHE:N	1:B:513:PHE:CD1	2.83	0.45
1:B:702:LEU:C	1:B:703:LEU:O	2.58	0.45
1:C:162:MET:O	1:C:166:ILE:HG12	2.16	0.45
1:C:344:LEU:O	1:C:345:VAL:C	2.59	0.45
1:C:547:ILE:HA	1:C:550:VAL:HG12	1.98	0.45
1:C:626:ILE:HD13	1:C:627:ALA:H	1.80	0.45
1:C:764:ASP:O	1:C:765:ARG:C	2.59	0.45
1:C:907:LEU:HD23	1:C:1018:ALA:HA	1.99	0.45
1:C:1017:LEU:O	1:C:1017:LEU:CD2	2.56	0.45
1:A:696:THR:O	1:A:699:ARG:N	2.49	0.45
1:C:159:ALA:HB1	1:C:181:GLN:HG3	1.98	0.45
1:C:363:ARG:O	1:C:367:ILE:HG22	2.15	0.45
1:C:416:VAL:O	1:C:420:MET:HE2	2.16	0.45
1:C:535:LEU:O	1:C:535:LEU:HG	2.16	0.45
1:C:904:VAL:O	1:C:905:VAL:C	2.58	0.45
1:A:552:MET:O	1:A:554:TYR:N	2.50	0.45
1:A:696:THR:O	1:A:697:GLN:C	2.58	0.45
1:A:1022:VAL:N	1:A:1023:PRO:HD2	2.31	0.45
1:B:97:GLY:O	1:B:98:THR:O	2.34	0.45
1:B:602:GLU:O	1:B:604:ASN:N	2.50	0.45
1:B:972:LEU:HD13	1:B:976:LEU:CD2	2.41	0.45
1:C:108:GLN:HG3	1:C:129:VAL:HG21	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ALA:HA	1:C:767:ARG:CZ	2.47	0.45
1:C:410:ILE:O	1:C:411:VAL:C	2.59	0.45
1:C:614:GLY:HA2	1:C:621:GLY:O	2.17	0.45
1:C:790:TYR:C	1:C:791:VAL:HG23	2.40	0.45
1:C:858:ASP:OD1	1:C:859:TRP:N	2.50	0.45
1:A:294:ALA:HB3	1:A:297:ALA:HB3	1.97	0.45
1:A:461:GLY:O	1:A:462:SER:C	2.58	0.45
1:A:740:GLY:O	1:A:794:ALA:N	2.43	0.45
1:B:58:GLN:C	1:B:60:THR:H	2.25	0.45
1:B:358:PHE:HB3	1:B:977:MET:CE	2.39	0.45
1:B:776:GLU:CG	1:B:777:ALA:N	2.79	0.45
1:C:140:VAL:HB	1:C:289:LEU:HB2	1.99	0.45
1:C:218:GLN:HG2	1:C:232:ALA:O	2.17	0.45
1:C:685:ILE:CG1	1:C:687:GLN:OE1	2.61	0.45
1:C:889:ALA:O	1:C:890:ALA:C	2.59	0.45
1:C:897:ILE:HG12	1:C:950:LYS:CE	2.47	0.45
1:A:281:PHE:CZ	1:A:324:VAL:HG11	2.52	0.45
1:A:405:LEU:O	1:A:406:VAL:C	2.57	0.45
1:A:607:GLU:HB2	1:A:631:LEU:O	2.17	0.45
1:A:693:GLU:O	1:A:694:LYS:C	2.59	0.45
1:B:26:ALA:HB1	1:B:384:ALA:HB2	1.98	0.45
1:B:65:ILE:HG23	1:B:111:LEU:HD13	1.98	0.45
1:B:569:GLN:OE1	1:B:569:GLN:HA	2.16	0.45
1:B:700:ASN:C	1:B:702:LEU:N	2.75	0.45
1:B:709:HIS:O	1:B:711:ASP:N	2.50	0.45
1:B:725:PRO:HB2	1:B:809:TRP:CZ3	2.51	0.45
1:B:847:LEU:HD23	1:B:847:LEU:N	2.29	0.45
1:C:114:ALA:O	1:C:115:MET:O	2.34	0.45
1:C:203:VAL:O	1:C:204:ILE:C	2.58	0.45
1:C:447:MET:O	1:C:447:MET:HE3	2.16	0.45
1:C:577:GLN:HB3	1:C:624:THR:CG2	2.42	0.45
1:C:714:THR:CG2	1:C:716:VAL:HG23	2.46	0.45
1:C:721:LEU:CD1	1:C:815:ARG:O	2.64	0.45
1:C:937:LEU:O	1:C:940:LYS:HB3	2.16	0.45
1:C:940:LYS:HA	1:C:943:ILE:HG12	1.99	0.45
1:A:1:MET:H3	1:A:2:PRO:HD2	1.75	0.45
1:A:492:LEU:HD12	1:A:492:LEU:HA	1.64	0.45
1:A:684:LEU:HD11	1:A:851:LEU:HD13	1.98	0.45
1:A:822:LEU:HA	1:A:823:PRO:HD3	1.32	0.45
1:A:1036:LYS:HD2	1:A:1036:LYS:C	2.42	0.45
1:B:228:GLN:CG	1:C:781:MET:HE3	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:LEU:O	1:B:379:THR:N	2.49	0.45
1:B:418:ARG:NH2	1:B:970:MET:CG	2.79	0.45
1:B:987:MET:CE	1:B:990:VAL:HB	2.47	0.45
1:B:1018:ALA:O	1:B:1020:PHE:N	2.50	0.45
1:C:950:LYS:NZ	1:C:1030:ARG:NE	2.65	0.45
1:C:957:GLY:C	1:C:958:LYS:HD2	2.42	0.45
1:A:65:ILE:O	1:A:68:ASN:CB	2.63	0.45
1:B:51:GLY:C	1:B:53:ASP:OD2	2.58	0.45
1:B:187:TRP:CZ3	1:B:774:MET:CE	2.94	0.45
1:B:269:GLU:HB3	1:B:270:LEU:H	1.61	0.45
1:B:490:PRO:C	1:B:492:LEU:N	2.75	0.45
1:C:14:VAL:CG1	1:C:15:ILE:N	2.79	0.45
1:C:34:GLN:HA	1:C:333:VAL:CG1	2.47	0.45
1:C:140:VAL:O	1:C:140:VAL:HG12	2.13	0.45
1:C:176:GLN:HE21	1:C:620:ARG:HH11	1.64	0.45
1:C:249:ILE:HD13	1:C:249:ILE:HG21	1.61	0.45
1:C:310:LEU:HD22	1:C:323:ILE:HD13	1.99	0.45
1:C:746:ILE:O	1:C:747:ASN:C	2.59	0.45
1:C:758:TYR:HA	1:C:772:TYR:HA	1.98	0.45
1:C:774:MET:HG2	1:C:775:SER:N	2.31	0.45
1:C:779:TYR:N	1:C:779:TYR:CD2	2.83	0.45
1:A:73:ASP:O	1:A:75:LEU:N	2.42	0.45
1:A:82:SER:HB2	1:A:816:LEU:HB2	1.99	0.45
1:A:400:LEU:HD21	1:A:1003:VAL:HG22	1.98	0.45
1:A:418:ARG:NH2	1:A:970:MET:HA	2.32	0.45
1:A:713:LEU:CG	1:A:714:THR:H	2.30	0.45
1:B:271:GLY:HA3	1:B:275:TYR:OH	2.17	0.45
1:B:345:VAL:HG12	1:B:349:ILE:HD13	1.98	0.45
1:B:690:LEU:CB	1:B:694:LYS:HB2	2.38	0.45
1:B:775:SER:CB	1:B:780:ARG:HG3	2.46	0.45
1:C:163:LYS:HG2	1:C:175:VAL:CG1	2.45	0.45
1:C:404:LEU:C	1:C:405:LEU:HD23	2.42	0.45
1:C:439:GLN:HG3	1:C:440:GLY:N	2.32	0.45
1:C:463:THR:CG2	1:C:464:GLY:H	2.28	0.45
1:C:680:PHE:HB2	1:C:859:TRP:HZ3	1.82	0.45
1:C:753:ALA:O	1:C:775:SER:CB	2.65	0.45
1:A:102:ILE:O	1:A:106:GLN:HG3	2.16	0.45
1:A:208:LYS:HA	1:A:760:ASN:HD21	1.82	0.45
1:A:219:LEU:HD12	1:A:232:ALA:HB3	1.99	0.45
1:A:355:MET:HE1	1:A:410:ILE:HA	1.99	0.45
1:A:407:ASP:OD2	1:A:978:THR:HG21	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ARG:HH11	1:A:973:ARG:NE	2.14	0.45
1:A:820:ASN:HB3	1:C:168:ARG:CZ	2.46	0.45
1:A:836:SER:OG	1:A:839:GLU:CG	2.62	0.45
1:A:897:ILE:HG21	1:A:950:LYS:CE	2.47	0.45
1:B:438:ILE:HD12	1:B:971:ARG:NH1	2.32	0.45
1:B:640:GLU:H	1:B:643:LYS:HG3	1.82	0.45
1:B:762:PHE:HE1	1:B:764:ASP:HB2	1.82	0.45
1:B:819:TYR:CE1	1:B:860:THR:OG1	2.70	0.45
1:C:99:ASP:OD2	1:C:99:ASP:C	2.60	0.45
1:C:456:MET:HE3	1:C:932:LEU:HD11	1.99	0.45
1:C:497:LEU:HD13	1:C:498:LYS:H	1.81	0.45
1:C:682:PHE:HE2	1:C:702:LEU:CD1	2.29	0.45
1:A:115:MET:N	1:A:116:PRO:CD	2.80	0.44
1:A:330:THR:N	1:A:331:PRO:HD2	2.32	0.44
1:A:846:GLN:HE21	1:A:846:GLN:HB2	1.60	0.44
1:A:930:GLY:O	1:A:931:LEU:C	2.59	0.44
1:B:341:VAL:HG23	1:B:395:MET:CE	2.47	0.44
1:B:420:MET:HE2	1:B:425:LEU:HA	1.99	0.44
1:B:518:ARG:C	1:B:520:PHE:N	2.75	0.44
1:B:592:ASN:HA	1:B:595:THR:HG23	2.00	0.44
1:B:640:GLU:N	1:B:643:LYS:HG3	2.32	0.44
1:B:762:PHE:CE1	1:B:764:ASP:HB2	2.52	0.44
1:B:864:TYR:C	1:B:864:TYR:CD1	2.95	0.44
1:B:900:SER:O	1:B:901:VAL:C	2.59	0.44
1:C:72:ILE:CG2	1:C:94:PHE:CZ	3.00	0.44
1:C:117:LEU:O	1:C:118:LEU:C	2.58	0.44
1:C:130:GLU:OE1	1:C:174:ASP:HB2	2.17	0.44
1:C:157:TYR:C	1:C:157:TYR:CD2	2.95	0.44
1:C:166:ILE:HD11	2:C:1075:HOH:O	2.05	0.44
1:C:934:THR:HG22	1:C:1011:MET:SD	2.57	0.44
1:A:94:PHE:HZ	1:A:107:VAL:HG22	1.82	0.44
1:A:185:ARG:NH2	1:A:774:MET:HE2	2.32	0.44
1:A:393:LEU:HD13	1:A:466:ILE:HG23	1.98	0.44
1:A:562:SER:HB3	1:A:924:ASP:HB3	1.99	0.44
1:A:713:LEU:HB2	1:A:832:ALA:HA	1.90	0.44
1:A:790:TYR:CE1	1:A:800:PRO:CG	2.96	0.44
1:B:778:LYS:HZ2	1:B:778:LYS:HB3	1.82	0.44
1:B:843:LEU:O	1:B:844:MET:C	2.59	0.44
1:B:891:LEU:HD12	1:B:892:TYR:CD1	2.52	0.44
1:C:58:GLN:NE2	1:C:82:SER:O	2.50	0.44
1:C:303:ALA:O	1:C:304:ALA:C	2.58	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ILE:HD13	1:C:634:TRP:CZ3	2.51	0.44
1:C:418:ARG:NH2	1:C:948:PHE:CZ	2.85	0.44
1:C:873:ALA:O	1:C:876:LEU:N	2.50	0.44
1:A:207:ILE:HG22	1:A:207:ILE:O	2.17	0.44
1:A:362:PHE:C	1:A:364:ALA:N	2.74	0.44
1:A:545:TYR:HE1	1:A:907:LEU:HD11	1.82	0.44
1:A:678:THR:O	1:A:679:GLY:O	2.35	0.44
1:A:1029:VAL:HG12	1:A:1030:ARG:N	2.21	0.44
1:B:401:ALA:O	1:B:402:ILE:C	2.59	0.44
1:B:696:THR:O	1:B:699:ARG:HB3	2.17	0.44
1:B:703:LEU:O	1:B:705:GLU:HB2	2.17	0.44
1:B:740:GLY:O	1:B:794:ALA:HB2	2.17	0.44
1:B:967:ALA:O	1:B:968:VAL:C	2.61	0.44
1:C:323:ILE:HG22	1:C:324:VAL:O	2.17	0.44
1:C:527:TYR:O	1:C:531:VAL:HG13	2.17	0.44
1:C:758:TYR:CD1	1:C:758:TYR:N	2.83	0.44
1:C:801:PHE:CD1	1:C:804:PHE:HE1	2.36	0.44
1:C:912:ALA:O	1:C:914:LEU:O	2.34	0.44
1:C:931:LEU:O	1:C:935:ILE:HB	2.17	0.44
1:C:948:PHE:O	1:C:952:LEU:HB2	2.16	0.44
1:A:94:PHE:CZ	1:A:103:ALA:HB1	2.52	0.44
1:A:178:PHE:N	1:A:178:PHE:HD1	2.15	0.44
1:A:324:VAL:C	1:A:325:TYR:CD1	2.95	0.44
1:A:340:VAL:HG13	1:A:399:VAL:HG23	1.96	0.44
1:A:540:ARG:O	1:A:543:VAL:HG12	2.18	0.44
1:A:658:ILE:C	1:A:659:LYS:O	2.60	0.44
1:A:1018:ALA:HB1	1:A:1022:VAL:HG11	1.98	0.44
1:B:44:THR:HG22	1:B:45:ILE:O	2.17	0.44
1:B:79:SER:O	1:B:79:SER:OG	2.26	0.44
1:B:188:MET:HB2	1:B:775:SER:HA	1.99	0.44
1:B:362:PHE:O	1:B:365:THR:N	2.43	0.44
1:B:520:PHE:O	1:B:523:SER:N	2.43	0.44
1:B:682:PHE:HD1	1:B:859:TRP:CZ3	2.36	0.44
1:B:785:ASP:O	1:B:788:ASP:N	2.47	0.44
1:B:804:PHE:O	1:B:805:SER:HB3	2.17	0.44
1:B:835:LYS:HD2	1:B:839:GLU:OE1	2.18	0.44
1:B:945:ILE:O	1:B:949:ALA:N	2.32	0.44
1:C:286:ALA:HB1	1:C:287:SER:H	1.48	0.44
1:C:355:MET:CA	1:C:355:MET:HE3	2.47	0.44
1:C:392:THR:O	1:C:393:LEU:C	2.59	0.44
1:C:395:MET:O	1:C:397:GLY:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLU:HB3	2:A:1074:HOH:O	2.17	0.44
1:A:307:ARG:NH1	1:A:325:TYR:CE2	2.86	0.44
1:A:407:ASP:OD1	1:A:940:LYS:NZ	2.40	0.44
1:A:437:GLN:HG2	1:A:948:PHE:CE2	2.52	0.44
1:A:520:PHE:C	1:A:522:LYS:H	2.25	0.44
1:A:687:GLN:HG2	1:C:316:PHE:CD2	2.49	0.44
1:A:746:ILE:HD13	1:A:804:PHE:CE1	2.52	0.44
1:A:781:MET:HE2	1:C:225:VAL:HG13	1.99	0.44
1:A:820:ASN:HB3	1:C:168:ARG:NH1	2.33	0.44
1:B:26:ALA:O	1:B:30:LEU:CB	2.65	0.44
1:B:404:LEU:C	1:B:406:VAL:N	2.75	0.44
1:B:601:LYS:C	1:B:603:LYS:N	2.70	0.44
1:B:702:LEU:HD22	1:B:702:LEU:HA	1.78	0.44
1:B:802:SER:C	1:B:804:PHE:H	2.25	0.44
1:B:1021:PHE:HB3	1:B:1025:PHE:CE1	2.53	0.44
1:C:181:GLN:HG2	1:C:769:LYS:CE	2.46	0.44
1:C:197:GLN:HB3	1:C:197:GLN:HE21	1.57	0.44
1:C:434:SER:O	1:C:438:ILE:HB	2.17	0.44
1:C:986:VAL:O	1:C:987:MET:C	2.60	0.44
1:A:87:THR:HG21	1:A:620:ARG:NH2	2.33	0.44
1:A:254:ASN:O	1:A:256:ASP:N	2.50	0.44
1:A:323:ILE:HG12	1:A:325:TYR:CE1	2.49	0.44
1:A:521:GLU:O	1:A:521:GLU:HG2	2.18	0.44
1:A:687:GLN:HE21	1:A:687:GLN:HB2	1.18	0.44
1:A:729:ILE:N	1:A:729:ILE:CD1	2.78	0.44
1:B:53:ASP:HB2	1:B:56:THR:HB	1.99	0.44
1:B:58:GLN:NE2	1:B:818:ARG:HH11	2.15	0.44
1:B:970:MET:SD	1:B:970:MET:C	3.00	0.44
1:C:2:PRO:C	1:C:6:ILE:HG13	2.42	0.44
1:C:35:TYR:HB3	1:C:36:PRO:HD2	2.00	0.44
1:C:262:LEU:HG	1:C:268:ILE:HD11	2.00	0.44
1:C:379:THR:HB	1:C:398:MET:CE	2.47	0.44
1:C:686:ASP:HB2	1:C:695:LEU:HD12	1.98	0.44
1:C:901:VAL:HG12	1:C:942:ALA:CB	2.47	0.44
1:A:3:ASN:O	1:A:6:ILE:HD13	2.18	0.44
1:A:979:SER:O	1:A:983:ILE:HG22	2.17	0.44
1:B:338:HIS:O	1:B:341:VAL:HG12	2.18	0.44
1:B:378:GLY:O	1:B:381:ALA:HB3	2.18	0.44
1:B:549:VAL:O	1:B:550:VAL:C	2.60	0.44
1:B:682:PHE:HD1	1:B:859:TRP:CH2	2.35	0.44
1:B:709:HIS:C	1:B:711:ASP:H	2.25	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:712:MET:SD	1:B:839:GLU:HB3	2.57	0.44
1:B:767:ARG:HG2	1:B:769:LYS:HE3	2.00	0.44
1:B:938:SER:C	1:B:940:LYS:N	2.76	0.44
1:C:169:THR:O	1:C:172:VAL:HG23	2.18	0.44
1:C:182:TYR:HA	1:C:271:GLY:O	2.18	0.44
1:C:198:LEU:HA	1:C:792:ARG:NH2	2.33	0.44
1:C:538:THR:O	1:C:540:ARG:HG2	2.18	0.44
1:C:696:THR:O	1:C:699:ARG:N	2.50	0.44
1:C:888:LEU:O	1:C:891:LEU:HB3	2.17	0.44
1:A:3:ASN:HA	1:A:6:ILE:HD12	1.99	0.44
1:A:313:MET:C	1:A:315:PRO:HD2	2.42	0.44
1:A:594:VAL:HA	1:A:655:PHE:CZ	2.53	0.44
1:A:621:GLY:C	1:A:623:ASN:N	2.73	0.44
1:A:1024:VAL:CG1	1:A:1025:PHE:H	2.09	0.44
1:B:38:ILE:O	1:B:462:SER:HB2	2.18	0.44
1:B:58:GLN:NE2	1:B:818:ARG:NH1	2.66	0.44
1:C:87:THR:HG23	1:C:88:VAL:H	1.82	0.44
1:C:124:GLN:HB3	1:C:758:TYR:CE2	2.50	0.44
1:C:338:HIS:ND1	1:C:338:HIS:C	2.76	0.44
1:C:432:ARG:NH1	1:C:432:ARG:CG	2.62	0.44
1:C:710:PRO:O	1:C:711:ASP:C	2.61	0.44
1:C:892:TYR:OH	1:C:943:ILE:HG23	2.17	0.44
1:C:1010:GLY:HA2	1:C:1013:THR:CG2	2.48	0.44
1:A:11:PHE:C	1:A:13:TRP:N	2.75	0.44
1:A:256:ASP:HB2	1:A:258:SER:HB3	1.99	0.44
1:A:339:GLU:HA	1:A:342:LYS:HG2	1.99	0.44
1:A:395:MET:HA	1:A:395:MET:CE	2.41	0.44
1:A:520:PHE:O	1:A:522:LYS:N	2.51	0.44
1:A:540:ARG:NH1	1:A:541:TYR:CZ	2.86	0.44
1:A:623:ASN:ND2	1:A:623:ASN:C	2.76	0.44
1:A:722:GLU:HA	2:A:1060:HOH:O	2.17	0.44
1:A:935:ILE:O	1:A:935:ILE:CG2	2.64	0.44
1:A:1009:GLY:C	1:A:1011:MET:N	2.67	0.44
1:A:1015:THR:C	1:A:1017:LEU:N	2.76	0.44
1:B:13:TRP:HA	1:B:13:TRP:HE3	1.80	0.44
1:B:534:ILE:HG23	1:B:541:TYR:CE2	2.53	0.44
1:C:58:GLN:C	1:C:60:THR:H	2.26	0.44
1:C:163:LYS:O	1:C:166:ILE:CA	2.61	0.44
1:C:385:ALA:C	1:C:387:GLY:H	2.26	0.44
1:C:832:ALA:HB1	1:C:833:PRO:CD	2.48	0.44
1:C:874:PRO:O	1:C:875:SER:C	2.61	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:928:GLN:O	1:C:932:LEU:HG	2.18	0.44
1:C:941:ASN:O	1:C:945:ILE:HG22	2.18	0.44
1:A:216:ALA:O	1:A:217:GLY:O	2.36	0.43
1:A:431:THR:O	1:A:432:ARG:C	2.60	0.43
1:A:478:MET:SD	1:A:478:MET:C	3.01	0.43
1:A:541:TYR:O	1:A:543:VAL:O	2.36	0.43
1:B:225:VAL:H	1:C:781:MET:CE	2.28	0.43
1:B:355:MET:HE3	1:B:369:THR:CG2	2.48	0.43
1:B:699:ARG:NH2	1:B:722:GLU:OE1	2.51	0.43
1:B:881:LEU:HD21	1:B:905:VAL:HG21	1.99	0.43
1:B:921:LEU:CD2	1:B:1005:THR:CG2	2.96	0.43
1:C:267:LYS:HE3	1:C:267:LYS:HB2	1.71	0.43
1:C:391:ASN:CG	1:C:394:THR:HG22	2.43	0.43
1:C:692:HIS:HE1	1:C:721:LEU:HD21	1.83	0.43
1:A:116:PRO:CA	1:A:117:LEU:HD22	2.48	0.43
1:A:455:PRO:O	1:A:876:LEU:HD13	2.18	0.43
1:A:536:ARG:C	1:A:538:THR:H	2.25	0.43
1:A:583:THR:CG2	1:A:584:GLN:N	2.80	0.43
1:A:680:PHE:C	1:A:680:PHE:CD1	2.96	0.43
1:A:958:LYS:HB3	1:A:959:GLY:H	1.64	0.43
1:B:612:VAL:HG23	1:B:626:ILE:HG13	2.00	0.43
1:B:654:ALA:O	1:B:655:PHE:C	2.61	0.43
1:B:686:ASP:OD2	1:B:686:ASP:C	2.61	0.43
1:B:732:ASP:HB2	1:B:735:LYS:HG3	2.00	0.43
1:B:818:ARG:HH11	1:B:818:ARG:HG3	1.82	0.43
1:B:885:PHE:HE2	1:B:898:PRO:HB2	1.83	0.43
1:B:1031:ARG:O	1:B:1035:ARG:HB2	2.17	0.43
1:C:72:ILE:CG2	1:C:94:PHE:HE2	2.23	0.43
1:C:191:ASN:HA	1:C:194:ASN:OD1	2.18	0.43
1:C:226:LYS:HG2	2:C:1072:HOH:O	2.17	0.43
1:C:262:LEU:O	1:C:264:ASP:N	2.51	0.43
1:C:379:THR:HG23	1:C:477:ALA:HB2	1.99	0.43
1:C:699:ARG:HB3	1:C:825:MET:HE3	1.99	0.43
1:C:713:LEU:HD11	1:C:835:LYS:H	1.82	0.43
1:A:72:ILE:O	1:A:73:ASP:O	2.37	0.43
1:A:178:PHE:N	1:A:178:PHE:CD1	2.86	0.43
1:A:943:ILE:O	1:A:947:GLU:HB2	2.17	0.43
1:B:185:ARG:NH1	1:B:772:TYR:HB3	2.33	0.43
1:B:199:THR:C	1:B:201:VAL:N	2.75	0.43
1:B:453:PHE:CZ	1:B:474:ILE:HD13	2.53	0.43
1:B:538:THR:O	1:B:540:ARG:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:699:ARG:O	1:B:700:ASN:HB2	2.18	0.43
1:B:801:PHE:HA	1:B:804:PHE:CE1	2.54	0.43
1:B:987:MET:HB3	1:B:988:PRO:HD3	1.99	0.43
1:B:999:ALA:O	1:B:1003:VAL:HG23	2.19	0.43
1:C:51:GLY:O	1:C:53:ASP:OD2	2.36	0.43
1:C:532:GLY:O	1:C:534:ILE:HD12	2.19	0.43
1:C:681:ASP:OD2	1:C:828:LEU:HD11	2.18	0.43
1:C:719:ASN:O	1:C:721:LEU:N	2.52	0.43
1:C:764:ASP:OD2	1:C:765:ARG:NE	2.51	0.43
1:C:790:TYR:CE1	1:C:800:PRO:HB3	2.52	0.43
1:C:987:MET:O	1:C:988:PRO:C	2.60	0.43
1:A:53:ASP:O	1:A:53:ASP:CG	2.61	0.43
1:A:111:LEU:C	1:A:113:LEU:N	2.76	0.43
1:A:778:LYS:HB2	1:A:778:LYS:HE2	1.48	0.43
1:A:946:VAL:O	1:A:946:VAL:HG12	2.18	0.43
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.62	0.43
1:B:183:ALA:N	1:B:271:GLY:O	2.52	0.43
1:B:758:TYR:CD2	1:B:758:TYR:C	2.95	0.43
1:B:979:SER:O	1:B:1011:MET:HE3	2.19	0.43
1:C:591:LEU:HA	1:C:591:LEU:HD13	1.67	0.43
1:C:996:GLY:O	1:C:997:SER:C	2.61	0.43
1:A:785:ASP:C	1:A:787:GLY:N	2.75	0.43
1:A:818:ARG:NH2	1:A:823:PRO:HG3	2.33	0.43
1:A:857:TYR:O	1:A:857:TYR:CG	2.71	0.43
1:B:9:PRO:O	1:B:13:TRP:N	2.42	0.43
1:B:18:ILE:HG22	1:B:19:ILE:N	2.34	0.43
1:B:58:GLN:HA	1:B:62:THR:CB	2.48	0.43
1:B:234:ILE:O	1:B:234:ILE:CG2	2.50	0.43
1:B:326:PRO:HB2	1:B:327:TYR:H	1.55	0.43
1:C:197:GLN:CA	1:C:798:MET:HE3	2.49	0.43
1:C:238:THR:CG2	1:C:239:ARG:N	2.82	0.43
1:C:764:ASP:CB	1:C:765:ARG:HD2	2.49	0.43
1:C:936:GLY:O	1:C:937:LEU:C	2.61	0.43
1:A:222:THR:HG22	1:A:223:PRO:CD	2.48	0.43
1:A:454:VAL:N	1:A:455:PRO:HD2	2.33	0.43
1:A:904:VAL:HG21	1:A:942:ALA:CB	2.45	0.43
1:B:109:ASN:ND2	1:B:112:GLN:HE22	2.14	0.43
1:B:207:ILE:HG22	1:B:759:VAL:HG11	1.97	0.43
1:B:396:PHE:HE2	1:B:999:ALA:HB1	1.82	0.43
1:B:405:LEU:HD12	1:B:405:LEU:C	2.43	0.43
1:B:776:GLU:HG2	1:B:777:ALA:H	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:819:TYR:O	1:B:822:LEU:N	2.51	0.43
1:B:1018:ALA:C	1:B:1020:PHE:N	2.77	0.43
1:C:4:PHE:CG	1:C:8:ARG:NH2	2.87	0.43
1:C:44:THR:HG22	1:C:91:THR:CA	2.47	0.43
1:C:82:SER:CB	1:C:88:VAL:HA	2.19	0.43
1:C:91:THR:CA	1:C:91:THR:HB	2.20	0.43
1:C:123:GLN:C	1:C:125:GLN:N	2.73	0.43
1:C:299:ALA:O	1:C:300:LEU:C	2.59	0.43
1:C:382:VAL:O	1:C:383:LEU:C	2.58	0.43
1:C:436:GLY:C	1:C:438:ILE:H	2.26	0.43
1:C:674:LEU:C	1:C:674:LEU:CD1	2.92	0.43
1:C:695:LEU:O	1:C:696:THR:O	2.37	0.43
1:C:768:VAL:O	1:C:768:VAL:CG1	2.66	0.43
1:C:1007:VAL:O	1:C:1008:MET:C	2.61	0.43
1:A:11:PHE:O	1:A:13:TRP:N	2.52	0.43
1:A:65:ILE:HG13	1:A:66:GLU:H	1.83	0.43
1:A:330:THR:O	1:A:331:PRO:C	2.59	0.43
1:A:418:ARG:O	1:A:421:ALA:HB3	2.19	0.43
1:A:449:LEU:CB	1:A:478:MET:HE2	2.49	0.43
1:A:574:THR:HA	1:A:665:ALA:HA	2.01	0.43
1:A:809:TRP:O	1:A:810:GLU:CB	2.51	0.43
1:A:818:ARG:HG2	2:A:1062:HOH:O	2.16	0.43
1:A:865:GLN:O	1:A:866:GLU:C	2.62	0.43
1:A:983:ILE:O	1:A:984:LEU:C	2.62	0.43
1:B:245:GLU:O	1:B:248:LYS:N	2.51	0.43
1:B:415:ASN:O	1:B:434:SER:OG	2.28	0.43
1:B:639:GLY:O	1:B:641:GLU:O	2.37	0.43
1:B:692:HIS:ND1	1:B:692:HIS:C	2.77	0.43
1:C:17:ILE:N	1:C:17:ILE:HD12	2.34	0.43
1:C:118:LEU:N	1:C:118:LEU:CD1	2.82	0.43
1:C:534:ILE:H	1:C:534:ILE:HG13	1.55	0.43
1:C:544:LEU:HD12	1:C:1021:PHE:HZ	1.83	0.43
1:C:578:LEU:HA	1:C:661:ALA:HB1	2.00	0.43
1:C:963:ALA:O	1:C:964:THR:C	2.61	0.43
1:A:2:PRO:O	1:A:6:ILE:N	2.51	0.43
1:A:13:TRP:CZ2	1:A:492:LEU:HD11	2.54	0.43
1:A:43:VAL:HA	1:A:130:GLU:O	2.19	0.43
1:A:359:LEU:HD13	1:A:359:LEU:HA	1.81	0.43
1:A:822:LEU:N	1:A:822:LEU:CD2	2.81	0.43
1:B:228:GLN:HE21	1:B:228:GLN:CA	2.32	0.43
1:B:231:ASN:HD22	1:B:232:ALA:N	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:VAL:CA	1:B:348:ILE:HD12	2.43	0.43
1:B:466:ILE:O	1:B:467:TYR:C	2.60	0.43
1:B:490:PRO:C	1:B:492:LEU:H	2.27	0.43
1:C:393:LEU:C	1:C:395:MET:N	2.77	0.43
1:A:166:ILE:HD13	1:A:166:ILE:H	1.78	0.43
1:A:324:VAL:C	1:A:325:TYR:HD1	2.27	0.43
1:A:367:ILE:HD13	1:A:489:THR:HG23	2.00	0.43
1:B:144:ASN:O	1:B:144:ASN:ND2	2.52	0.43
1:B:327:TYR:HB2	1:B:628:PHE:HB3	1.99	0.43
1:B:492:LEU:O	1:B:496:MET:HB2	2.18	0.43
1:B:892:TYR:CG	1:B:897:ILE:HD11	2.54	0.43
1:B:1022:VAL:HB	1:B:1026:PHE:CZ	2.54	0.43
1:C:14:VAL:CG1	1:C:15:ILE:H	2.31	0.43
1:C:529:ASP:O	1:C:531:VAL:O	2.36	0.43
1:C:591:LEU:HD23	1:C:613:ASN:HB2	1.99	0.43
1:C:728:LYS:CG	1:C:729:ILE:N	2.76	0.43
1:A:182:TYR:CB	1:A:270:LEU:HD12	2.49	0.43
1:A:531:VAL:O	1:A:534:ILE:HG13	2.19	0.43
1:B:173:GLY:H	1:B:294:ALA:H	1.65	0.43
1:B:204:ILE:O	1:B:205:THR:C	2.60	0.43
1:B:328:ASP:OD2	1:B:330:THR:HB	2.19	0.43
1:B:411:VAL:HG12	1:B:974:PRO:HB3	2.00	0.43
1:B:489:THR:HB	1:B:490:PRO:CD	2.49	0.43
1:B:819:TYR:CZ	1:B:860:THR:OG1	2.72	0.43
1:C:47:ALA:HB1	1:C:122:VAL:CG1	2.49	0.43
1:C:56:THR:O	1:C:57:VAL:C	2.62	0.43
1:C:158:VAL:HG12	1:C:159:ALA:N	2.29	0.43
1:C:163:LYS:HB2	2:C:1078:HOH:O	2.18	0.43
1:C:166:ILE:HG21	1:C:291:ILE:HD11	2.01	0.43
1:C:194:ASN:HB3	2:C:1059:HOH:O	2.19	0.43
1:C:247:GLY:O	1:C:263:ARG:HB2	2.19	0.43
1:C:778:LYS:CD	1:C:779:TYR:CE2	3.01	0.43
1:A:59:ASP:HB3	1:C:763:ILE:CD1	2.47	0.42
1:A:66:GLU:O	1:A:68:ASN:N	2.52	0.42
1:A:83:ASP:OD1	1:A:84:SER:N	2.52	0.42
1:A:108:GLN:HG3	1:B:112:GLN:NE2	2.30	0.42
1:A:152:GLU:H	1:A:152:GLU:CD	2.26	0.42
1:A:308:ALA:O	1:A:311:ALA:HB3	2.19	0.42
1:A:449:LEU:O	1:A:451:ALA:O	2.37	0.42
1:A:910:ILE:C	1:A:912:ALA:H	2.27	0.42
1:B:330:THR:O	1:B:330:THR:CG2	2.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:760:ASN:O	1:B:771:VAL:HB	2.19	0.42
1:B:858:ASP:OD1	1:B:859:TRP:N	2.52	0.42
1:B:982:PHE:O	1:B:983:ILE:C	2.62	0.42
1:C:92:LEU:HD22	1:C:107:VAL:CG2	2.47	0.42
1:C:354:VAL:HG13	1:C:980:LEU:HD23	2.01	0.42
1:C:532:GLY:O	1:C:534:ILE:N	2.52	0.42
1:C:781:MET:C	1:C:782:LEU:HG	2.42	0.42
1:A:57:VAL:HG12	1:A:58:GLN:CA	2.49	0.42
1:A:206:ALA:C	1:A:208:LYS:N	2.74	0.42
1:A:208:LYS:HA	1:A:760:ASN:ND2	2.34	0.42
1:A:219:LEU:HD22	1:B:781:MET:O	2.18	0.42
1:A:337:ILE:O	1:A:339:GLU:O	2.38	0.42
1:A:351:VAL:HG13	1:A:410:ILE:HD11	2.00	0.42
1:A:453:PHE:CZ	1:A:474:ILE:HG21	2.53	0.42
1:A:545:TYR:HB2	1:A:1021:PHE:CZ	2.53	0.42
1:A:947:GLU:O	1:A:951:ASP:CB	2.63	0.42
1:A:978:THR:HG23	1:A:979:SER:N	2.33	0.42
1:B:45:ILE:HD13	1:B:65:ILE:CG2	2.50	0.42
1:B:318:PRO:HD2	1:B:321:LEU:HD22	2.00	0.42
1:B:384:ALA:O	1:B:385:ALA:C	2.61	0.42
1:B:418:ARG:NH2	1:B:970:MET:HG3	2.35	0.42
1:C:54:ALA:CB	1:C:84:SER:HB2	2.22	0.42
1:C:159:ALA:CB	1:C:181:GLN:HG3	2.49	0.42
1:C:409:ALA:O	1:C:410:ILE:O	2.37	0.42
1:C:484:VAL:HG13	1:C:488:LEU:HB3	2.00	0.42
1:C:653:ARG:HG3	1:C:654:ALA:N	2.34	0.42
1:A:108:GLN:OE1	1:B:112:GLN:NE2	2.53	0.42
1:A:276:ASP:HB3	1:C:222:THR:CG2	2.42	0.42
1:A:348:ILE:O	1:A:349:ILE:C	2.61	0.42
1:A:532:GLY:HA2	1:A:965:LEU:HD11	2.01	0.42
1:A:937:LEU:HD12	1:A:1011:MET:SD	2.59	0.42
1:A:948:PHE:CD2	1:A:948:PHE:N	2.86	0.42
1:A:952:LEU:C	1:A:952:LEU:CD1	2.92	0.42
1:A:1029:VAL:C	1:A:1031:ARG:N	2.76	0.42
1:B:64:VAL:O	1:B:65:ILE:C	2.62	0.42
1:B:404:LEU:O	1:B:406:VAL:N	2.53	0.42
1:B:639:GLY:C	1:B:640:GLU:OE2	2.62	0.42
1:B:1004:GLY:O	1:B:1007:VAL:HG12	2.18	0.42
1:C:21:LEU:O	1:C:24:GLY:N	2.50	0.42
1:C:123:GLN:HB3	1:C:124:GLN:H	1.68	0.42
1:C:332:PHE:O	1:C:333:VAL:C	2.61	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:HIS:C	1:C:338:HIS:HD1	2.28	0.42
1:C:344:LEU:O	1:C:348:ILE:HG23	2.19	0.42
1:C:524:THR:O	1:C:527:TYR:N	2.50	0.42
1:C:547:ILE:O	1:C:551:GLY:N	2.52	0.42
1:C:750:LEU:HD23	1:C:750:LEU:HA	1.53	0.42
1:C:983:ILE:HG23	1:C:1008:MET:HG3	2.01	0.42
1:A:455:PRO:HG3	1:A:880:SER:HB2	2.02	0.42
1:A:562:SER:OG	1:A:563:PHE:N	2.51	0.42
1:B:18:ILE:O	1:B:19:ILE:C	2.62	0.42
1:B:410:ILE:C	1:B:412:VAL:N	2.76	0.42
1:B:671:ILE:H	1:B:671:ILE:HG12	1.71	0.42
1:B:778:LYS:HZ2	1:B:778:LYS:H	1.66	0.42
1:B:870:GLY:O	1:B:872:GLN:N	2.52	0.42
1:B:885:PHE:CD2	1:B:898:PRO:HB2	2.55	0.42
1:B:970:MET:HE2	1:B:970:MET:CA	2.44	0.42
1:C:61:VAL:O	1:C:62:THR:C	2.61	0.42
1:C:144:ASN:HA	1:C:320:GLY:O	2.20	0.42
1:C:415:ASN:C	1:C:417:GLU:N	2.77	0.42
1:C:417:GLU:OE2	1:C:420:MET:CE	2.67	0.42
1:C:894:SER:OG	1:C:897:ILE:N	2.33	0.42
1:C:959:GLY:O	1:C:960:LEU:C	2.62	0.42
1:A:116:PRO:HB2	1:A:117:LEU:HD22	2.02	0.42
1:A:225:VAL:CG2	1:B:778:LYS:NZ	2.80	0.42
1:A:346:GLU:O	1:A:347:ALA:C	2.62	0.42
1:A:407:ASP:O	1:A:411:VAL:HG23	2.20	0.42
1:B:396:PHE:O	1:B:399:VAL:N	2.44	0.42
1:C:491:ALA:C	1:C:493:CYS:N	2.77	0.42
1:C:775:SER:HG	1:C:789:TRP:HZ2	1.66	0.42
1:C:1021:PHE:N	1:C:1023:PRO:HD2	2.35	0.42
1:A:47:ALA:HB3	1:A:88:VAL:CG2	2.50	0.42
1:A:515:TRP:HD1	1:A:516:PHE:HB2	1.84	0.42
1:B:182:TYR:HD1	1:B:271:GLY:O	2.02	0.42
1:B:578:LEU:HD13	1:B:661:ALA:HB2	2.00	0.42
1:B:987:MET:HE3	1:B:987:MET:O	2.20	0.42
1:C:44:THR:HA	1:C:91:THR:HA	2.01	0.42
1:C:55:LYS:CE	1:C:59:ASP:OD1	2.60	0.42
1:C:123:GLN:C	1:C:125:GLN:H	2.28	0.42
1:C:417:GLU:CB	1:C:973:ARG:HH12	2.32	0.42
1:C:457:ALA:CB	1:C:468:ARG:CA	2.93	0.42
1:C:545:TYR:CZ	1:C:1021:PHE:CG	3.08	0.42
1:A:68:ASN:CA	1:A:68:ASN:CG	2.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:ILE:HD12	1:A:540:ARG:HH12	1.85	0.42
1:A:547:ILE:O	1:A:551:GLY:N	2.47	0.42
1:A:924:ASP:O	1:A:927:PHE:HB3	2.20	0.42
1:B:578:LEU:HB3	1:B:579:PRO:HD2	2.00	0.42
1:B:596:HIS:O	1:B:597:TYR:C	2.61	0.42
1:B:683:GLU:O	1:B:857:TYR:HA	2.18	0.42
1:C:474:ILE:O	1:C:475:VAL:C	2.63	0.42
1:C:699:ARG:HG2	1:C:825:MET:HE1	2.01	0.42
1:C:702:LEU:HD12	1:C:851:LEU:HD21	2.02	0.42
1:C:910:ILE:HG23	1:C:1013:THR:OG1	2.18	0.42
1:A:105:VAL:HB	1:A:106:GLN:H	1.63	0.42
1:A:180:SER:O	1:A:181:GLN:HB2	2.20	0.42
1:A:187:TRP:CH2	1:C:223:PRO:HG3	2.55	0.42
1:A:820:ASN:O	1:A:822:LEU:CD2	2.68	0.42
1:B:84:SER:C	1:B:86:GLY:H	2.27	0.42
1:B:463:THR:HA	1:B:466:ILE:HG13	2.00	0.42
1:B:873:ALA:HB3	1:B:874:PRO:CD	2.50	0.42
1:C:352:PHE:CD1	1:C:369:THR:HG21	2.55	0.42
1:C:489:THR:N	1:C:490:PRO:CD	2.81	0.42
1:C:696:THR:HG22	1:C:699:ARG:HH12	1.85	0.42
1:C:777:ALA:HA	1:C:780:ARG:CZ	2.50	0.42
1:A:104:GLN:HB2	1:A:131:LYS:NZ	2.35	0.42
1:A:186:ILE:HD13	1:A:262:LEU:HD21	2.02	0.42
1:A:469:GLN:O	1:A:473:THR:OG1	2.31	0.42
1:A:728:LYS:HD2	1:C:235:ILE:CG2	2.49	0.42
1:A:983:ILE:HD13	1:A:1008:MET:SD	2.60	0.42
1:A:983:ILE:CG1	1:A:984:LEU:N	2.81	0.42
1:B:407:ASP:O	1:B:408:ASP:O	2.38	0.42
1:B:674:LEU:CD1	1:B:860:THR:HG21	2.43	0.42
1:C:17:ILE:O	1:C:20:MET:HB2	2.20	0.42
1:C:58:GLN:CD	1:C:82:SER:CB	2.93	0.42
1:C:478:MET:O	1:C:481:SER:HB3	2.19	0.42
1:C:775:SER:HB3	1:C:780:ARG:HD3	2.02	0.42
1:C:816:LEU:HD23	1:C:816:LEU:HA	1.83	0.42
1:C:972:LEU:O	1:C:973:ARG:C	2.62	0.42
1:C:986:VAL:O	1:C:986:VAL:HG12	2.20	0.42
1:A:298:ASN:HB3	1:A:301:ASP:CG	2.44	0.42
1:A:348:ILE:O	1:A:351:VAL:N	2.53	0.42
1:A:571:VAL:HG12	1:A:629:VAL:O	2.19	0.42
1:A:653:ARG:O	1:A:655:PHE:N	2.52	0.42
1:A:753:ALA:HB3	1:A:754:TRP:H	1.61	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:TRP:CZ3	1:A:780:ARG:HA	2.54	0.42
1:A:760:ASN:O	1:A:771:VAL:HB	2.19	0.42
1:B:64:VAL:C	1:B:66:GLU:N	2.78	0.42
1:B:68:ASN:HD22	1:B:114:ALA:HB2	1.85	0.42
1:B:336:SER:O	1:B:392:THR:HG22	2.20	0.42
1:B:355:MET:HE3	1:B:369:THR:HG23	2.02	0.42
1:B:470:PHE:CD2	1:B:929:VAL:HG11	2.55	0.42
1:B:808:ARG:HH21	1:B:808:ARG:HB3	1.85	0.42
1:B:841:MET:O	1:B:845:GLU:HB2	2.20	0.42
1:B:907:LEU:O	1:B:908:GLY:C	2.63	0.42
1:B:1021:PHE:O	1:B:1024:VAL:HB	2.20	0.42
1:C:50:PRO:O	1:C:52:ALA:N	2.49	0.42
1:C:246:PHE:O	1:C:249:ILE:N	2.33	0.42
1:C:328:ASP:OD1	1:C:328:ASP:C	2.63	0.42
1:C:380:PHE:CE2	1:C:395:MET:HE1	2.54	0.42
1:C:415:ASN:OD1	1:C:418:ARG:CZ	2.67	0.42
1:C:865:GLN:O	1:C:868:LEU:O	2.38	0.42
1:C:880:SER:O	1:C:884:VAL:HG23	2.20	0.42
1:C:922:THR:HG22	1:C:923:ASN:N	2.26	0.42
1:A:198:LEU:HD22	1:A:202:ASP:HB3	2.00	0.41
1:A:466:ILE:O	1:A:469:GLN:N	2.50	0.41
1:A:605:ASN:O	1:A:632:LYS:N	2.52	0.41
1:A:753:ALA:O	1:A:774:MET:CG	2.68	0.41
1:A:1015:THR:O	1:A:1017:LEU:N	2.53	0.41
1:B:305:ALA:O	1:B:306:ILE:C	2.62	0.41
1:B:544:LEU:O	1:B:547:ILE:HB	2.19	0.41
1:B:750:LEU:C	1:B:750:LEU:CD1	2.82	0.41
1:B:972:LEU:HD21	1:B:1019:ILE:HG12	2.02	0.41
1:B:986:VAL:O	1:B:987:MET:C	2.60	0.41
1:B:1021:PHE:HB3	1:B:1025:PHE:HE1	1.84	0.41
1:C:353:LEU:O	1:C:356:TYR:HB3	2.19	0.41
1:C:532:GLY:O	1:C:533:GLY:C	2.63	0.41
1:C:1015:THR:O	1:C:1019:ILE:HB	2.20	0.41
1:A:144:ASN:ND2	1:A:320:GLY:O	2.53	0.41
1:A:211:ASN:ND2	1:A:760:ASN:OD1	2.53	0.41
1:A:330:THR:CG2	1:A:334:LYS:HE2	2.47	0.41
1:A:545:TYR:HB2	1:A:1021:PHE:HE1	1.76	0.41
1:A:578:LEU:CD2	1:A:587:THR:HA	2.37	0.41
1:A:712:MET:C	1:A:713:LEU:O	2.63	0.41
1:A:894:SER:CB	1:A:897:ILE:HD13	2.50	0.41
1:B:23:GLY:C	1:B:25:LEU:H	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ALA:HB3	1:B:88:VAL:CG2	2.50	0.41
1:B:47:ALA:CB	1:B:61:VAL:HG21	2.50	0.41
1:B:352:PHE:HE1	1:B:365:THR:HG23	1.84	0.41
1:B:354:VAL:O	1:B:358:PHE:HB2	2.20	0.41
1:B:544:LEU:HD22	1:B:1021:PHE:CZ	2.54	0.41
1:B:648:THR:O	1:B:652:THR:N	2.40	0.41
1:B:674:LEU:HD23	1:B:674:LEU:C	2.45	0.41
1:C:375:VAL:HG23	1:C:375:VAL:H	1.64	0.41
1:C:375:VAL:HB	1:C:405:LEU:HD13	2.02	0.41
1:C:417:GLU:O	1:C:420:MET:HB3	2.20	0.41
1:C:527:TYR:O	1:C:529:ASP:N	2.53	0.41
1:A:61:VAL:HG13	1:A:118:LEU:CD1	2.46	0.41
1:A:115:MET:C	2:A:1072:HOH:O	2.62	0.41
1:A:185:ARG:HD3	1:A:272:GLY:O	2.20	0.41
1:A:594:VAL:HA	1:A:655:PHE:HE2	1.85	0.41
1:A:596:HIS:O	1:A:599:LEU:O	2.37	0.41
1:A:831:ALA:HA	1:A:840:ALA:HB1	2.01	0.41
1:A:879:ILE:H	1:A:879:ILE:HG13	1.64	0.41
1:A:988:PRO:HB2	1:A:989:LEU:H	1.57	0.41
1:B:84:SER:O	1:B:86:GLY:N	2.54	0.41
1:B:144:ASN:HD22	1:B:144:ASN:H	1.68	0.41
1:B:410:ILE:O	1:B:413:VAL:HG12	2.20	0.41
1:B:455:PRO:O	1:B:456:MET:C	2.62	0.41
1:B:541:TYR:C	1:B:543:VAL:N	2.77	0.41
1:B:907:LEU:C	1:B:910:ILE:HG22	2.45	0.41
1:B:1016:VAL:C	1:B:1018:ALA:N	2.79	0.41
1:C:485:ALA:HA	1:C:489:THR:OG1	2.21	0.41
1:C:673:GLU:O	1:C:674:LEU:CB	2.67	0.41
1:C:775:SER:O	1:C:776:GLU:C	2.59	0.41
1:C:973:ARG:N	1:C:974:PRO:CD	2.83	0.41
1:A:583:THR:O	1:A:586:ARG:N	2.54	0.41
1:A:683:GLU:OE1	1:A:826:GLU:HB2	2.20	0.41
1:A:686:ASP:HB2	1:A:823:PRO:HB2	2.02	0.41
1:A:690:LEU:CD1	1:A:854:GLY:HA3	2.20	0.41
1:A:978:THR:O	1:A:980:LEU:N	2.53	0.41
1:A:1029:VAL:C	1:A:1031:ARG:H	2.28	0.41
1:B:156:ASP:CG	1:B:182:TYR:CD2	2.99	0.41
1:B:468:ARG:HA	1:B:471:SER:HB2	2.01	0.41
1:B:669:PRO:HB2	1:B:670:ALA:H	1.65	0.41
1:B:730:ASP:O	1:B:805:SER:HA	2.20	0.41
1:B:732:ASP:O	1:B:734:GLU:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:750:LEU:HB2	1:B:801:PHE:HE1	1.82	0.41
1:B:961:ILE:O	1:B:965:LEU:CB	2.68	0.41
1:C:533:GLY:HA3	2:C:1068:HOH:O	2.20	0.41
1:C:680:PHE:HB2	1:C:859:TRP:CZ3	2.55	0.41
1:C:873:ALA:O	1:C:874:PRO:C	2.63	0.41
1:C:914:LEU:HA	1:C:917:THR:OG1	2.20	0.41
1:A:72:ILE:CG1	1:A:107:VAL:HA	2.51	0.41
1:A:72:ILE:HG13	1:A:106:GLN:HB2	2.02	0.41
1:A:254:ASN:O	1:A:255:GLN:C	2.63	0.41
1:A:294:ALA:HB3	1:A:297:ALA:CB	2.51	0.41
1:A:307:ARG:NH2	1:A:328:ASP:OD2	2.49	0.41
1:A:356:TYR:C	1:A:358:PHE:N	2.79	0.41
1:A:405:LEU:HD13	1:A:405:LEU:H	1.85	0.41
1:A:493:CYS:O	1:A:497:LEU:HB2	2.21	0.41
1:A:768:VAL:C	1:A:769:LYS:HG3	2.45	0.41
1:B:43:VAL:O	1:B:92:LEU:N	2.42	0.41
1:B:170:SER:C	1:B:172:VAL:N	2.78	0.41
1:B:280:GLU:HB2	1:B:284:GLN:C	2.45	0.41
1:B:404:LEU:HD21	1:B:937:LEU:HD21	2.02	0.41
1:B:788:ASP:N	1:B:788:ASP:OD1	2.52	0.41
1:B:908:GLY:C	1:B:910:ILE:N	2.79	0.41
1:C:253:VAL:HG12	1:C:259:ARG:HG3	2.03	0.41
1:C:544:LEU:HD12	1:C:1021:PHE:CZ	2.56	0.41
1:C:681:ASP:OD2	1:C:828:LEU:CD1	2.68	0.41
1:C:775:SER:OG	1:C:789:TRP:HZ2	2.03	0.41
1:A:116:PRO:N	2:A:1072:HOH:O	2.54	0.41
1:A:126:GLY:HA3	1:B:116:PRO:HB3	2.01	0.41
1:A:298:ASN:O	1:A:302:THR:HG23	2.20	0.41
1:A:466:ILE:O	1:A:467:TYR:C	2.63	0.41
1:A:583:THR:HG22	1:A:584:GLN:N	2.31	0.41
1:A:589:LYS:HA	1:A:592:ASN:ND2	2.36	0.41
1:A:959:GLY:O	1:A:960:LEU:C	2.63	0.41
1:B:339:GLU:O	1:B:340:VAL:C	2.62	0.41
1:B:482:VAL:HG13	1:B:483:LEU:HD23	2.02	0.41
1:B:498:LYS:HE2	1:B:498:LYS:HB3	1.66	0.41
1:B:518:ARG:C	1:B:520:PHE:H	2.29	0.41
1:B:543:VAL:O	1:B:543:VAL:HG12	2.20	0.41
1:B:763:ILE:HD11	1:C:59:ASP:CB	2.50	0.41
1:B:989:LEU:CA	1:B:992:SER:HB2	2.50	0.41
1:C:143:ILE:HA	1:C:143:ILE:HD13	1.26	0.41
1:C:193:LEU:HA	1:C:193:LEU:HD23	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:ALA:C	1:C:313:MET:N	2.77	0.41
1:C:425:LEU:H	1:C:426:PRO:HD3	1.84	0.41
1:C:528:THR:O	1:C:528:THR:HG22	2.20	0.41
1:C:894:SER:OG	1:C:897:ILE:HG13	2.20	0.41
1:A:324:VAL:CG1	1:A:325:TYR:N	2.81	0.41
1:A:370:ILE:O	1:A:370:ILE:HG22	2.19	0.41
1:A:426:PRO:HB2	1:A:427:PRO:HD2	2.03	0.41
1:B:62:THR:O	1:B:63:GLN:C	2.63	0.41
1:B:836:SER:OG	1:B:838:GLY:N	2.54	0.41
1:B:1014:ALA:O	1:B:1018:ALA:HB2	2.20	0.41
1:B:1026:PHE:HB3	1:B:1030:ARG:HE	1.85	0.41
1:C:4:PHE:HD2	1:C:8:ARG:HH12	1.69	0.41
1:C:115:MET:CB	1:C:116:PRO:HD3	2.48	0.41
1:C:372:VAL:HG23	1:C:376:LEU:HG	2.02	0.41
1:C:989:LEU:HB3	1:C:1004:GLY:HA3	2.02	0.41
1:A:193:LEU:HD12	1:A:265:VAL:HG11	2.02	0.41
1:A:668:LEU:HD12	1:A:668:LEU:C	2.45	0.41
1:A:1022:VAL:N	1:A:1023:PRO:CD	2.83	0.41
1:B:213:GLN:HG3	1:C:56:THR:HG23	2.03	0.41
1:B:470:PHE:CE2	1:B:929:VAL:HG11	2.55	0.41
1:B:741:VAL:HG22	1:B:793:ALA:HA	2.03	0.41
1:B:850:LYS:CA	1:B:852:PRO:HD3	2.51	0.41
1:B:896:SER:O	1:B:899:PHE:HB2	2.20	0.41
1:B:901:VAL:HG21	1:B:943:ILE:HD13	2.02	0.41
1:B:1026:PHE:HB3	1:B:1030:ARG:HH21	1.82	0.41
1:C:189:ASN:C	1:C:189:ASN:ND2	2.77	0.41
1:C:197:GLN:CB	1:C:798:MET:HE3	2.50	0.41
1:C:894:SER:HB3	1:C:897:ILE:HD12	2.03	0.41
1:C:1030:ARG:HE	1:C:1030:ARG:HB3	1.21	0.41
1:A:24:GLY:O	1:A:27:ILE:HB	2.20	0.41
1:A:137:LEU:O	1:A:329:THR:HG22	2.21	0.41
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.92	0.41
1:A:360:GLN:HE21	1:A:360:GLN:HB3	1.58	0.41
1:A:472:ILE:HA	1:A:475:VAL:HG12	2.01	0.41
1:A:539:GLY:CA	1:A:542:LEU:HB2	2.45	0.41
1:A:655:PHE:O	1:A:658:ILE:HG12	2.20	0.41
1:A:685:ILE:CG2	1:A:687:GLN:H	2.27	0.41
1:A:736:ALA:O	1:A:741:VAL:HG12	2.20	0.41
1:A:991:ILE:HG13	1:A:1004:GLY:HA3	2.03	0.41
1:B:14:VAL:O	1:B:15:ILE:C	2.62	0.41
1:B:33:ALA:O	1:B:337:ILE:HD11	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:VAL:O	1:B:66:GLU:N	2.54	0.41
1:B:66:GLU:OE2	1:B:818:ARG:HD3	2.21	0.41
1:B:121:GLU:H	1:B:121:GLU:HG2	1.41	0.41
1:B:194:ASN:C	1:B:194:ASN:ND2	2.79	0.41
1:B:216:ALA:CB	1:B:236:ALA:HB2	2.50	0.41
1:B:484:VAL:C	1:B:485:ALA:O	2.63	0.41
1:B:578:LEU:H	1:B:578:LEU:CD2	2.33	0.41
1:B:743:ILE:H	1:B:743:ILE:CD1	2.32	0.41
1:B:770:LYS:HZ2	1:B:770:LYS:HG3	1.79	0.41
1:B:935:ILE:O	1:B:935:ILE:HG22	2.20	0.41
1:B:945:ILE:HG13	1:B:946:VAL:H	1.86	0.41
1:B:974:PRO:O	1:B:975:ILE:C	2.64	0.41
1:C:9:PRO:C	1:C:11:PHE:N	2.79	0.41
1:C:66:GLU:O	1:C:67:GLN:C	2.64	0.41
1:C:66:GLU:OE1	1:C:821:GLY:HA2	2.20	0.41
1:C:137:LEU:N	1:C:291:ILE:O	2.53	0.41
1:C:166:ILE:HG22	1:C:172:VAL:CG1	2.51	0.41
1:C:202:ASP:CG	1:C:792:ARG:HH22	2.28	0.41
1:C:218:GLN:HG3	1:C:233:SER:HA	2.03	0.41
1:C:322:LYS:HG2	1:C:323:ILE:N	2.34	0.41
1:C:418:ARG:HD2	1:C:970:MET:CE	2.51	0.41
1:C:568:ASP:OD1	1:C:568:ASP:C	2.63	0.41
1:C:826:GLU:O	2:C:1063:HOH:O	2.22	0.41
1:C:844:MET:O	1:C:847:LEU:CD2	2.69	0.41
1:C:934:THR:C	1:C:936:GLY:N	2.78	0.41
1:C:1014:ALA:O	1:C:1018:ALA:HB3	2.21	0.41
1:A:183:ALA:O	1:A:185:ARG:N	2.54	0.41
1:A:370:ILE:O	1:A:370:ILE:CG2	2.68	0.41
1:A:428:LYS:CG	1:A:429:GLU:N	2.83	0.41
1:A:456:MET:HG2	1:A:459:PHE:HE1	1.86	0.41
1:A:542:LEU:HD23	1:A:1028:VAL:HG21	2.02	0.41
1:A:633:ASP:O	1:A:634:TRP:C	2.63	0.41
1:A:729:ILE:CG2	1:A:730:ASP:N	2.62	0.41
1:B:38:ILE:HD12	1:B:466:ILE:CD1	2.52	0.41
1:B:139:VAL:O	1:B:326:PRO:HG2	2.21	0.41
1:B:720:GLY:C	1:B:721:LEU:HD12	2.46	0.41
1:B:775:SER:OG	1:B:776:GLU:N	2.54	0.41
1:B:1011:MET:O	1:B:1012:VAL:C	2.64	0.41
1:C:75:LEU:HD22	1:C:77:TYR:O	2.21	0.41
1:C:188:MET:CE	1:C:200:PRO:HA	2.51	0.41
1:C:202:ASP:O	1:C:205:THR:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:MET:HE2	1:C:977:MET:HG2	2.03	0.41
1:C:593:GLU:O	1:C:597:TYR:N	2.32	0.41
1:C:713:LEU:HD23	1:C:831:ALA:C	2.46	0.41
1:A:44:THR:O	1:A:45:ILE:HG12	2.17	0.40
1:A:198:LEU:HD11	1:A:252:LYS:HB2	2.03	0.40
1:A:333:VAL:O	1:A:337:ILE:HD13	2.21	0.40
1:A:554:TYR:C	1:A:554:TYR:CD1	2.99	0.40
1:A:750:LEU:C	1:A:750:LEU:HD13	2.46	0.40
1:A:815:ARG:NH2	2:A:1071:HOH:O	2.54	0.40
1:A:897:ILE:HG21	1:A:950:LYS:NZ	2.36	0.40
1:B:120:GLN:O	1:B:121:GLU:C	2.62	0.40
1:B:327:TYR:CD1	1:B:327:TYR:C	2.99	0.40
1:B:572:PHE:CD1	1:B:572:PHE:C	2.98	0.40
1:B:592:ASN:O	1:B:595:THR:HG23	2.21	0.40
1:B:640:GLU:N	1:B:640:GLU:CD	2.79	0.40
1:C:165:ALA:C	1:C:166:ILE:HD13	2.47	0.40
1:C:178:PHE:CD1	1:C:610:PHE:HE2	2.38	0.40
1:C:317:PHE:CB	1:C:318:PRO:CD	2.92	0.40
1:C:663:VAL:CG1	1:C:664:PHE:N	2.84	0.40
1:C:712:MET:HE1	1:C:839:GLU:HB3	2.02	0.40
1:C:900:SER:HA	1:C:1029:VAL:HG21	2.03	0.40
1:C:919:ARG:HD2	1:C:919:ARG:HA	1.92	0.40
1:C:949:ALA:O	1:C:951:ASP:N	2.55	0.40
1:A:4:PHE:HD2	1:A:4:PHE:HA	1.80	0.40
1:A:193:LEU:CB	1:A:265:VAL:HG13	2.50	0.40
1:A:240:LEU:HD12	1:A:240:LEU:N	2.37	0.40
1:A:545:TYR:HA	1:A:548:ILE:HG12	2.03	0.40
1:A:753:ALA:O	1:A:774:MET:HG3	2.21	0.40
1:A:952:LEU:HD11	1:A:963:ALA:HB1	2.03	0.40
1:B:206:ALA:O	1:B:207:ILE:C	2.64	0.40
1:B:418:ARG:HH21	1:B:970:MET:HG3	1.85	0.40
1:B:756:GLY:HA2	1:B:773:VAL:O	2.20	0.40
1:B:974:PRO:O	1:B:978:THR:HG22	2.21	0.40
1:C:30:LEU:HA	1:C:31:PRO:HD3	1.95	0.40
1:C:315:PRO:HB2	1:C:316:PHE:CE1	2.56	0.40
1:C:337:ILE:N	1:C:337:ILE:HD13	2.36	0.40
1:C:568:ASP:OD1	1:C:568:ASP:O	2.39	0.40
1:C:760:ASN:O	1:C:771:VAL:HG23	2.21	0.40
1:C:885:PHE:O	1:C:888:LEU:N	2.53	0.40
1:A:462:SER:HB2	1:A:674:LEU:CD2	2.52	0.40
1:A:790:TYR:CE1	1:A:800:PRO:HB3	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:971:ARG:O	1:A:974:PRO:HD2	2.20	0.40
1:B:223:PRO:HA	1:B:224:PRO:HD3	1.98	0.40
1:B:460:GLY:HA2	1:B:872:GLN:OE1	2.21	0.40
1:C:400:LEU:O	1:C:933:THR:HG21	2.21	0.40
1:C:551:GLY:O	1:C:554:TYR:HB2	2.21	0.40
1:C:754:TRP:CE3	1:C:780:ARG:HB2	2.56	0.40
1:C:758:TYR:CG	1:C:758:TYR:O	2.70	0.40
1:C:817:GLU:O	1:C:818:ARG:HG2	2.21	0.40
1:A:243:THR:CG2	1:A:268:ILE:HG22	2.49	0.40
1:A:489:THR:HB	1:A:490:PRO:HD3	2.03	0.40
1:A:713:LEU:HG	1:A:833:PRO:CD	2.25	0.40
1:A:959:GLY:HA3	1:A:962:GLU:CB	2.30	0.40
1:B:11:PHE:O	1:B:12:ALA:C	2.64	0.40
1:B:202:ASP:O	1:B:203:VAL:C	2.63	0.40
1:B:317:PHE:CE2	1:B:323:ILE:HD11	2.56	0.40
1:B:598:TYR:HD1	1:B:606:VAL:HG21	1.85	0.40
1:B:641:GLU:CA	1:B:650:ARG:HH12	2.33	0.40
1:B:921:LEU:HD22	1:B:1005:THR:HG22	2.02	0.40
1:C:4:PHE:CD2	1:C:8:ARG:NH1	2.89	0.40
1:C:360:GLN:OE1	1:C:516:PHE:HE2	2.04	0.40
1:C:475:VAL:HG12	1:C:476:SER:N	2.35	0.40
1:C:713:LEU:HD11	1:C:835:LYS:N	2.36	0.40
1:C:844:MET:O	1:C:848:ALA:N	2.53	0.40
1:C:885:PHE:O	1:C:886:LEU:C	2.65	0.40
1:A:65:ILE:HD13	1:A:111:LEU:HD23	2.02	0.40
1:A:114:ALA:O	1:A:117:LEU:CD2	2.70	0.40
1:A:151:GLN:NE2	1:A:279:ALA:H	2.19	0.40
1:A:300:LEU:O	1:A:301:ASP:C	2.64	0.40
1:A:463:THR:C	1:A:465:ALA:N	2.80	0.40
1:A:493:CYS:O	1:A:494:ALA:C	2.62	0.40
1:A:541:TYR:CD2	1:A:541:TYR:N	2.89	0.40
1:A:607:GLU:O	1:A:607:GLU:OE2	2.40	0.40
1:B:194:ASN:ND2	1:B:194:ASN:O	2.55	0.40
1:B:345:VAL:O	1:B:348:ILE:HB	2.21	0.40
1:B:552:MET:HA	1:B:910:ILE:HD12	2.04	0.40
1:B:776:GLU:CG	1:B:777:ALA:H	2.35	0.40
1:B:945:ILE:CD1	1:B:1022:VAL:CG2	3.00	0.40
1:C:5:PHE:HA	1:C:8:ARG:O	2.22	0.40
1:C:714:THR:HG22	1:C:716:VAL:H	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1018/1053 (97%)	621 (61%)	243 (24%)	154 (15%)	0	0
1	B	1018/1053 (97%)	611 (60%)	259 (25%)	148 (14%)	0	0
1	C	1018/1053 (97%)	642 (63%)	225 (22%)	151 (15%)	0	0
All	All	3054/3159 (97%)	1874 (61%)	727 (24%)	453 (15%)	0	0

All (453) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ASP
1	A	63	GLN
1	A	64	VAL
1	A	65	ILE
1	A	67	GLN
1	A	69	MET
1	A	73	ASP
1	A	74	ASN
1	A	76	MET
1	A	96	SER
1	A	105	VAL
1	A	112	GLN
1	A	137	LEU
1	A	146	ASP
1	A	167	SER
1	A	172	VAL
1	A	181	GLN
1	A	255	GLN
1	A	277	ILE
1	A	293	LEU
1	A	294	ALA
1	A	318	PRO
1	A	330	THR
1	A	376	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	422	GLU
1	A	439	GLN
1	A	443	VAL
1	A	444	GLY
1	A	521	GLU
1	A	538	THR
1	A	597	TYR
1	A	601	LYS
1	A	638	PRO
1	A	659	LYS
1	A	660	ASP
1	A	672	VAL
1	A	676	THR
1	A	677	ALA
1	A	687	GLN
1	A	690	LEU
1	A	713	LEU
1	A	715	SER
1	A	730	ASP
1	A	759	VAL
1	A	775	SER
1	A	820	ASN
1	A	868	LEU
1	A	925	VAL
1	A	988	PRO
1	A	991	ILE
1	A	1016	VAL
1	A	1024	VAL
1	B	8	ARG
1	B	50	PRO
1	B	51	GLY
1	B	54	ALA
1	B	56	THR
1	B	72	ILE
1	B	85	THR
1	B	98	THR
1	B	104	GLN
1	B	147	GLY
1	B	173	GLY
1	B	175	VAL
1	B	228	GLN
1	B	258	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	268	ILE
1	B	270	LEU
1	B	326	PRO
1	B	361	ASN
1	B	363	ARG
1	B	517	ASN
1	B	519	MET
1	B	535	LEU
1	B	536	ARG
1	B	538	THR
1	B	549	VAL
1	B	602	GLU
1	B	606	VAL
1	B	647	ILE
1	B	654	ALA
1	B	655	PHE
1	B	671	ILE
1	B	688	ALA
1	B	689	GLY
1	B	693	GLU
1	B	703	LEU
1	B	705	GLU
1	B	712	MET
1	B	733	GLN
1	B	820	ASN
1	B	831	ALA
1	B	871	ASN
1	B	891	LEU
1	B	907	LEU
1	B	908	GLY
1	B	921	LEU
1	B	1012	VAL
1	B	1019	ILE
1	B	1034	SER
1	C	52	ALA
1	C	61	VAL
1	C	68	ASN
1	C	95	GLU
1	C	110	LYS
1	C	111	LEU
1	C	157	TYR
1	C	160	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	167	SER
1	C	187	TRP
1	C	226	LYS
1	C	311	ALA
1	C	312	LYS
1	C	314	GLU
1	C	319	SER
1	C	394	THR
1	C	410	ILE
1	C	411	VAL
1	C	419	VAL
1	C	464	GLY
1	C	540	ARG
1	C	601	LYS
1	C	658	ILE
1	C	720	GLY
1	C	778	LYS
1	C	851	LEU
1	C	869	SER
1	C	871	ASN
1	C	895	TRP
1	C	925	VAL
1	C	946	VAL
1	C	960	LEU
1	C	965	LEU
1	C	975	ILE
1	C	989	LEU
1	C	993	THR
1	C	1035	ARG
1	A	12	ALA
1	A	54	ALA
1	A	66	GLU
1	A	90	ILE
1	A	135	SER
1	A	147	GLY
1	A	170	SER
1	A	218	GLN
1	A	221	GLY
1	A	256	ASP
1	A	265	VAL
1	A	400	LEU
1	A	435	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	446	ALA
1	A	453	PHE
1	A	455	PRO
1	A	459	PHE
1	A	496	MET
1	A	548	ILE
1	A	553	ALA
1	A	580	ALA
1	A	582	ALA
1	A	600	THR
1	A	622	GLN
1	A	654	ALA
1	A	679	GLY
1	A	688	ALA
1	A	689	GLY
1	A	784	ASP
1	A	866	GLU
1	A	869	SER
1	A	903	LEU
1	A	926	TYR
1	A	951	ASP
1	A	958	LYS
1	A	964	THR
1	A	971	ARG
1	A	1010	GLY
1	A	1012	VAL
1	A	1025	PHE
1	B	22	ALA
1	B	103	ALA
1	B	125	GLN
1	B	221	GLY
1	B	254	ASN
1	B	265	VAL
1	B	291	ILE
1	B	424	GLY
1	B	453	PHE
1	B	471	SER
1	B	539	GLY
1	B	557	VAL
1	B	567	GLU
1	B	603	LYS
1	B	638	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	659	LYS
1	B	669	PRO
1	B	715	SER
1	B	723	ASP
1	B	794	ALA
1	B	805	SER
1	B	834	GLY
1	B	852	PRO
1	B	899	PHE
1	B	901	VAL
1	B	918	PHE
1	B	966	ASP
1	B	975	ILE
1	B	1013	THR
1	C	10	ILE
1	C	34	GLN
1	C	51	GLY
1	C	74	ASN
1	C	164	ASP
1	C	182	TYR
1	C	217	GLY
1	C	220	GLY
1	C	243	THR
1	C	258	SER
1	C	263	ARG
1	C	396	PHE
1	C	404	LEU
1	C	418	ARG
1	C	451	ALA
1	C	460	GLY
1	C	468	ARG
1	C	536	ARG
1	C	576	VAL
1	C	656	SER
1	C	678	THR
1	C	690	LEU
1	C	696	THR
1	C	706	ALA
1	C	715	SER
1	C	803	ALA
1	C	872	GLN
1	C	935	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	998	GLY
1	C	1017	LEU
1	C	1029	VAL
1	A	192	GLU
1	A	206	ALA
1	A	301	ASP
1	A	317	PHE
1	A	319	SER
1	A	320	GLY
1	A	353	LEU
1	A	357	LEU
1	A	372	VAL
1	A	428	LYS
1	A	447	MET
1	A	458	PHE
1	A	515	TRP
1	A	535	LEU
1	A	656	SER
1	A	694	LYS
1	A	753	ALA
1	A	831	ALA
1	A	881	LEU
1	B	2	PRO
1	B	48	SER
1	B	171	GLY
1	B	319	SER
1	B	336	SER
1	B	357	LEU
1	B	405	LEU
1	B	408	ASP
1	B	422	GLU
1	B	491	ALA
1	B	495	THR
1	B	601	LYS
1	B	640	GLU
1	B	675	GLY
1	B	788	ASP
1	B	804	PHE
1	B	1011	MET
1	C	190	PRO
1	C	191	ASN
1	C	193	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	327	TYR
1	C	336	SER
1	C	386	PHE
1	C	422	GLU
1	C	427	PRO
1	C	463	THR
1	C	491	ALA
1	C	497	LEU
1	C	530	SER
1	C	593	GLU
1	C	600	THR
1	C	639	GLY
1	C	671	ILE
1	C	675	GLY
1	C	747	ASN
1	C	760	ASN
1	C	801	PHE
1	C	950	LYS
1	C	952	LEU
1	C	983	ILE
1	C	994	GLY
1	C	1010	GLY
1	A	68	ASN
1	A	116	PRO
1	A	184	MET
1	A	217	GLY
1	A	362	PHE
1	A	384	ALA
1	A	434	SER
1	A	436	GLY
1	A	577	GLN
1	A	712	MET
1	A	810	GLU
1	A	907	LEU
1	A	923	ASN
1	A	960	LEU
1	A	1004	GLY
1	A	1005	THR
1	B	12	ALA
1	B	36	PRO
1	B	59	ASP
1	B	131	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	327	TYR
1	B	407	ASP
1	B	414	GLU
1	B	427	PRO
1	B	461	GLY
1	B	485	ALA
1	B	656	SER
1	B	694	LYS
1	B	870	GLY
1	B	941	ASN
1	B	950	LYS
1	B	959	GLY
1	B	960	LEU
1	B	1014	ALA
1	B	1026	PHE
1	C	54	ALA
1	C	81	ASN
1	C	124	GLN
1	C	159	ALA
1	C	343	THR
1	C	490	PRO
1	C	520	PHE
1	C	620	ARG
1	C	664	PHE
1	C	674	LEU
1	C	777	ALA
1	C	967	ALA
1	C	974	PRO
1	C	976	LEU
1	C	988	PRO
1	A	19	ILE
1	A	174	ASP
1	A	216	ALA
1	A	224	PRO
1	A	392	THR
1	A	417	GLU
1	A	549	VAL
1	A	692	HIS
1	A	714	THR
1	A	818	ARG
1	A	1002	ALA
1	B	10	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	409	ALA
1	B	542	LEU
1	B	618	ALA
1	B	716	VAL
1	B	777	ALA
1	B	849	SER
1	B	851	LEU
1	B	909	VAL
1	B	954	ASP
1	B	1006	GLY
1	B	1017	LEU
1	C	192	GLU
1	C	237	GLN
1	C	332	PHE
1	C	392	THR
1	C	425	LEU
1	C	438	ILE
1	C	458	PHE
1	C	519	MET
1	C	528	THR
1	C	546	LEU
1	C	640	GLU
1	C	716	VAL
1	C	837	THR
1	C	850	LYS
1	C	852	PRO
1	C	963	ALA
1	A	18	ILE
1	A	109	ASN
1	A	191	ASN
1	A	397	GLY
1	A	471	SER
1	A	794	ALA
1	A	892	TYR
1	B	23	GLY
1	B	65	ILE
1	B	105	VAL
1	B	127	VAL
1	B	474	ILE
1	B	477	ALA
1	B	674	LEU
1	B	786	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	942	ALA
1	B	1016	VAL
1	C	80	SER
1	C	106	GLN
1	C	207	ILE
1	C	315	PRO
1	C	333	VAL
1	C	399	VAL
1	C	447	MET
1	C	537	SER
1	C	796	GLY
1	C	926	TYR
1	C	1007	VAL
1	A	709	HIS
1	B	315	PRO
1	B	444	GLY
1	B	484	VAL
1	B	710	PRO
1	B	821	GLY
1	C	19	ILE
1	C	32	VAL
1	C	223	PRO
1	C	426	PRO
1	C	550	VAL
1	A	51	GLY
1	A	539	GLY
1	B	19	ILE
1	B	31	PRO
1	B	190	PRO
1	B	771	VAL
1	C	709	HIS
1	A	729	ILE
1	A	874	PRO
1	B	224	PRO
1	B	974	PRO
1	C	9	PRO
1	C	50	PRO
1	C	291	ILE
1	C	533	GLY
1	A	15	ILE
1	A	716	VAL
1	A	905	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	464	GLY
1	C	15	ILE
1	C	424	GLY
1	C	448	VAL
1	C	571	VAL
1	C	786	ILE
1	C	800	PRO
1	A	326	PRO
1	B	783	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	833/859 (97%)	655 (79%)	178 (21%)	1	4
1	B	833/859 (97%)	664 (80%)	169 (20%)	1	4
1	C	833/859 (97%)	666 (80%)	167 (20%)	1	4
All	All	2499/2577 (97%)	1985 (79%)	514 (21%)	1	4

All (514) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	6	ILE
1	A	14	VAL
1	A	15	ILE
1	A	21	LEU
1	A	25	LEU
1	A	38	ILE
1	A	43	VAL
1	A	45	ILE
1	A	46	SER
1	A	55	LYS
1	A	57	VAL
1	A	58	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	61	VAL
1	A	62	THR
1	A	63	GLN
1	A	65	ILE
1	A	66	GLU
1	A	69	MET
1	A	72	ILE
1	A	79	SER
1	A	80	SER
1	A	83	ASP
1	A	84	SER
1	A	88	VAL
1	A	91	THR
1	A	93	THR
1	A	98	THR
1	A	102	ILE
1	A	105	VAL
1	A	106	GLN
1	A	109	ASN
1	A	111	LEU
1	A	112	GLN
1	A	115	MET
1	A	120	GLN
1	A	124	GLN
1	A	130	GLU
1	A	137	LEU
1	A	139	VAL
1	A	143	ILE
1	A	150	THR
1	A	164	ASP
1	A	166	ILE
1	A	170	SER
1	A	193	LEU
1	A	213	GLN
1	A	222	THR
1	A	226	LYS
1	A	230	LEU
1	A	243	THR
1	A	249	ILE
1	A	260	VAL
1	A	277	ILE
1	A	284	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	289	LEU
1	A	298	ASN
1	A	302	THR
1	A	319	SER
1	A	323	ILE
1	A	325	TYR
1	A	330	THR
1	A	335	ILE
1	A	337	ILE
1	A	349	ILE
1	A	351	VAL
1	A	357	LEU
1	A	359	LEU
1	A	360	GLN
1	A	361	ASN
1	A	367	ILE
1	A	374	VAL
1	A	376	LEU
1	A	379	THR
1	A	390	ILE
1	A	394	THR
1	A	400	LEU
1	A	405	LEU
1	A	414	GLU
1	A	417	GLU
1	A	429	GLU
1	A	438	ILE
1	A	442	LEU
1	A	445	ILE
1	A	447	MET
1	A	472	ILE
1	A	480	LEU
1	A	481	SER
1	A	498	LYS
1	A	513	PHE
1	A	518	ARG
1	A	522	LYS
1	A	523	SER
1	A	542	LEU
1	A	544	LEU
1	A	546	LEU
1	A	549	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	557	VAL
1	A	558	ARG
1	A	561	SER
1	A	572	PHE
1	A	575	MET
1	A	576	VAL
1	A	577	GLN
1	A	578	LEU
1	A	597	TYR
1	A	607	GLU
1	A	609	VAL
1	A	612	VAL
1	A	617	PHE
1	A	623	ASN
1	A	626	ILE
1	A	629	VAL
1	A	630	SER
1	A	641	GLU
1	A	648	THR
1	A	652	THR
1	A	659	LYS
1	A	668	LEU
1	A	671	ILE
1	A	687	GLN
1	A	690	LEU
1	A	693	GLU
1	A	701	GLN
1	A	702	LEU
1	A	705	GLU
1	A	711	ASP
1	A	713	LEU
1	A	714	THR
1	A	717	ARG
1	A	719	ASN
1	A	721	LEU
1	A	722	GLU
1	A	729	ILE
1	A	731	ILE
1	A	741	VAL
1	A	750	LEU
1	A	758	TYR
1	A	763	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	768	VAL
1	A	774	MET
1	A	775	SER
1	A	778	LYS
1	A	779	TYR
1	A	780	ARG
1	A	782	LEU
1	A	786	ILE
1	A	801	PHE
1	A	805	SER
1	A	807	SER
1	A	815	ARG
1	A	818	ARG
1	A	822	LEU
1	A	824	SER
1	A	839	GLU
1	A	843	LEU
1	A	855	VAL
1	A	867	ARG
1	A	868	LEU
1	A	872	GLN
1	A	887	CYS
1	A	899	PHE
1	A	913	LEU
1	A	917	THR
1	A	928	GLN
1	A	952	LEU
1	A	955	LYS
1	A	960	LEU
1	A	976	LEU
1	A	983	ILE
1	A	986	VAL
1	A	989	LEU
1	A	992	SER
1	A	993	THR
1	A	1013	THR
1	A	1022	VAL
1	A	1030	ARG
1	A	1036	LYS
1	B	6	ILE
1	B	8	ARG
1	B	13	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	17	ILE
1	B	21	LEU
1	B	27	ILE
1	B	34	GLN
1	B	48	SER
1	B	50	PRO
1	B	53	ASP
1	B	57	VAL
1	B	59	ASP
1	B	61	VAL
1	B	67	GLN
1	B	70	ASN
1	B	72	ILE
1	B	73	ASP
1	B	74	ASN
1	B	81	ASN
1	B	88	VAL
1	B	91	THR
1	B	92	LEU
1	B	93	THR
1	B	96	SER
1	B	102	ILE
1	B	104	GLN
1	B	115	MET
1	B	121	GLU
1	B	127	VAL
1	B	131	LYS
1	B	138	MET
1	B	140	VAL
1	B	143	ILE
1	B	144	ASN
1	B	145	THR
1	B	150	THR
1	B	166	ILE
1	B	168	ARG
1	B	169	THR
1	B	170	SER
1	B	174	ASP
1	B	176	GLN
1	B	180	SER
1	B	182	TYR
1	B	185	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	188	MET
1	B	189	ASN
1	B	191	ASN
1	B	193	LEU
1	B	223	PRO
1	B	226	LYS
1	B	228	GLN
1	B	235	ILE
1	B	237	GLN
1	B	243	THR
1	B	253	VAL
1	B	254	ASN
1	B	256	ASP
1	B	260	VAL
1	B	261	LEU
1	B	269	GLU
1	B	270	LEU
1	B	280	GLU
1	B	289	LEU
1	B	293	LEU
1	B	298	ASN
1	B	306	ILE
1	B	319	SER
1	B	323	ILE
1	B	330	THR
1	B	335	ILE
1	B	336	SER
1	B	342	LYS
1	B	343	THR
1	B	349	ILE
1	B	365	THR
1	B	372	VAL
1	B	379	THR
1	B	383	LEU
1	B	394	THR
1	B	399	VAL
1	B	402	ILE
1	B	410	ILE
1	B	416	VAL
1	B	417	GLU
1	B	435	MET
1	B	437	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	452	VAL
1	B	456	MET
1	B	466	ILE
1	B	473	THR
1	B	482	VAL
1	B	483	LEU
1	B	488	LEU
1	B	496	MET
1	B	497	LEU
1	B	513	PHE
1	B	516	PHE
1	B	538	THR
1	B	549	VAL
1	B	554	TYR
1	B	562	SER
1	B	574	THR
1	B	591	LEU
1	B	595	THR
1	B	601	LYS
1	B	607	GLU
1	B	612	VAL
1	B	623	ASN
1	B	624	THR
1	B	629	VAL
1	B	641	GLU
1	B	647	ILE
1	B	649	MET
1	B	653	ARG
1	B	655	PHE
1	B	659	LYS
1	B	668	LEU
1	B	671	ILE
1	B	672	VAL
1	B	673	GLU
1	B	692	HIS
1	B	696	THR
1	B	702	LEU
1	B	712	MET
1	B	743	ILE
1	B	757	SER
1	B	759	VAL
1	B	760	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	764	ASP
1	B	770	LYS
1	B	778	LYS
1	B	781	MET
1	B	782	LEU
1	B	786	ILE
1	B	788	ASP
1	B	799	VAL
1	B	808	ARG
1	B	830	GLN
1	B	847	LEU
1	B	864	TYR
1	B	868	LEU
1	B	871	ASN
1	B	876	LEU
1	B	879	ILE
1	B	884	VAL
1	B	891	LEU
1	B	895	TRP
1	B	900	SER
1	B	921	LEU
1	B	933	THR
1	B	943	ILE
1	B	946	VAL
1	B	947	GLU
1	B	951	ASP
1	B	956	GLU
1	B	960	LEU
1	B	965	LEU
1	B	966	ASP
1	B	970	MET
1	B	972	LEU
1	B	978	THR
1	B	984	LEU
1	B	987	MET
1	B	989	LEU
1	B	993	THR
1	B	1012	VAL
1	B	1027	VAL
1	B	1036	LYS
1	C	10	ILE
1	C	13	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	17	ILE
1	C	19	ILE
1	C	37	THR
1	C	45	ILE
1	C	46	SER
1	C	48	SER
1	C	58	GLN
1	C	60	THR
1	C	63	GLN
1	C	64	VAL
1	C	65	ILE
1	C	70	ASN
1	C	74	ASN
1	C	75	LEU
1	C	82	SER
1	C	83	ASP
1	C	89	GLN
1	C	90	ILE
1	C	91	THR
1	C	102	ILE
1	C	104	GLN
1	C	107	VAL
1	C	108	GLN
1	C	110	LYS
1	C	111	LEU
1	C	117	LEU
1	C	118	LEU
1	C	134	SER
1	C	137	LEU
1	C	140	VAL
1	C	143	ILE
1	C	146	ASP
1	C	148	THR
1	C	149	MET
1	C	152	GLU
1	C	155	SER
1	C	162	MET
1	C	168	ARG
1	C	169	THR
1	C	170	SER
1	C	177	LEU
1	C	184	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	185	ARG
1	C	186	ILE
1	C	189	ASN
1	C	192	GLU
1	C	194	ASN
1	C	207	ILE
1	C	210	GLN
1	C	211	ASN
1	C	228	GLN
1	C	233	SER
1	C	235	ILE
1	C	239	ARG
1	C	253	VAL
1	C	258	SER
1	C	259	ARG
1	C	265	VAL
1	C	268	ILE
1	C	269	GLU
1	C	274	ASN
1	C	293	LEU
1	C	295	THR
1	C	313	MET
1	C	316	PHE
1	C	317	PHE
1	C	324	VAL
1	C	337	ILE
1	C	341	VAL
1	C	351	VAL
1	C	355	MET
1	C	367	ILE
1	C	372	VAL
1	C	377	LEU
1	C	400	LEU
1	C	413	VAL
1	C	416	VAL
1	C	417	GLU
1	C	419	VAL
1	C	425	LEU
1	C	432	ARG
1	C	437	GLN
1	C	438	ILE
1	C	454	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	458	PHE
1	C	459	PHE
1	C	475	VAL
1	C	492	LEU
1	C	497	LEU
1	C	521	GLU
1	C	535	LEU
1	C	536	ARG
1	C	538	THR
1	C	544	LEU
1	C	546	LEU
1	C	549	VAL
1	C	568	ASP
1	C	576	VAL
1	C	577	GLN
1	C	578	LEU
1	C	588	GLN
1	C	591	LEU
1	C	592	ASN
1	C	613	ASN
1	C	617	PHE
1	C	622	GLN
1	C	624	THR
1	C	626	ILE
1	C	650	ARG
1	C	662	MET
1	C	666	PHE
1	C	668	LEU
1	C	674	LEU
1	C	676	THR
1	C	685	ILE
1	C	696	THR
1	C	699	ARG
1	C	713	LEU
1	C	719	ASN
1	C	721	LEU
1	C	722	GLU
1	C	724	THR
1	C	733	GLN
1	C	743	ILE
1	C	745	ASP
1	C	750	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	759	VAL
1	C	762	PHE
1	C	768	VAL
1	C	770	LYS
1	C	778	LYS
1	C	782	LEU
1	C	799	VAL
1	C	808	ARG
1	C	813	SER
1	C	826	GLU
1	C	828	LEU
1	C	847	LEU
1	C	850	LYS
1	C	867	ARG
1	C	868	LEU
1	C	872	GLN
1	C	876	LEU
1	C	885	PHE
1	C	899	PHE
1	C	904	VAL
1	C	907	LEU
1	C	921	LEU
1	C	922	THR
1	C	929	VAL
1	C	931	LEU
1	C	935	ILE
1	C	941	ASN
1	C	945	ILE
1	C	952	LEU
1	C	958	LYS
1	C	960	LEU
1	C	968	VAL
1	C	984	LEU
1	C	989	LEU
1	C	993	THR
1	C	1021	PHE
1	C	1030	ARG
1	C	1035	ARG
1	C	1036	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	67	GLN
1	A	68	ASN
1	A	70	ASN
1	A	89	GLN
1	A	106	GLN
1	A	108	GLN
1	A	109	ASN
1	A	161	ASN
1	A	181	GLN
1	A	191	ASN
1	A	197	GLN
1	A	210	GLN
1	A	213	GLN
1	A	231	ASN
1	A	254	ASN
1	A	274	ASN
1	A	282	ASN
1	A	284	GLN
1	A	298	ASN
1	A	360	GLN
1	A	415	ASN
1	A	437	GLN
1	A	569	GLN
1	A	577	GLN
1	A	622	GLN
1	A	623	ASN
1	A	687	GLN
1	A	719	ASN
1	A	737	GLN
1	A	830	GLN
1	A	846	GLN
1	A	865	GLN
1	A	871	ASN
1	A	1001	ASN
1	B	58	GLN
1	B	68	ASN
1	B	70	ASN
1	B	74	ASN
1	B	104	GLN
1	B	106	GLN
1	B	109	ASN
1	B	112	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	120	GLN
1	B	125	GLN
1	B	151	GLN
1	B	161	ASN
1	B	189	ASN
1	B	210	GLN
1	B	213	GLN
1	B	218	GLN
1	B	228	GLN
1	B	231	ASN
1	B	237	GLN
1	B	254	ASN
1	B	274	ASN
1	B	415	ASN
1	B	437	GLN
1	B	439	GLN
1	B	517	ASN
1	B	526	HIS
1	B	577	GLN
1	B	584	GLN
1	B	613	ASN
1	B	623	ASN
1	B	642	ASN
1	B	726	GLN
1	B	744	ASN
1	B	760	ASN
1	B	830	GLN
1	B	846	GLN
1	B	865	GLN
1	B	1001	ASN
1	C	3	ASN
1	C	68	ASN
1	C	104	GLN
1	C	106	GLN
1	C	120	GLN
1	C	125	GLN
1	C	144	ASN
1	C	176	GLN
1	C	189	ASN
1	C	191	ASN
1	C	197	GLN
1	C	211	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	231	ASN
1	C	237	GLN
1	C	284	GLN
1	C	391	ASN
1	C	439	GLN
1	C	588	GLN
1	C	592	ASN
1	C	605	ASN
1	C	667	ASN
1	C	747	ASN
1	C	872	GLN
1	C	941	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1022/1053 (97%)	-0.41	4 (0%) 88 84	5, 97, 116, 127	0
1	B	1022/1053 (97%)	-0.34	6 (0%) 85 80	49, 102, 116, 127	0
1	C	1022/1053 (97%)	-0.38	7 (0%) 84 77	5, 94, 118, 127	0
All	All	3066/3159 (97%)	-0.38	17 (0%) 85 80	5, 99, 117, 127	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	52	ALA	5.4
1	B	1034	SER	5.1
1	C	538	THR	4.3
1	C	194	ASN	3.6
1	B	414	GLU	3.3
1	C	670	ALA	2.9
1	C	870	GLY	2.9
1	A	801	PHE	2.8
1	B	563	PHE	2.8
1	C	419	VAL	2.6
1	C	414	GLU	2.5
1	C	164	ASP	2.3
1	A	135	SER	2.1
1	A	133	SER	2.1
1	B	704	ALA	2.1
1	B	424	GLY	2.0
1	A	597	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.