



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 03:02 PM EST

PDB ID : 1O1F
EMDB ID : EMD-1001
Title : MOLECULAR MODELS OF AVERAGED RIGOR CROSSBRIDGES FROM
TOMOGRAMS OF INSECT FLIGHT MUSCLE
Authors : Chen, L.F.; Winkler, H.; Reedy, M.K.; Reedy, M.C.; Taylor, K.A.
Deposited on : 2002-11-15
Resolution : 70.00 Å (reported)
Based on initial models : 1ATN, 2MYS

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

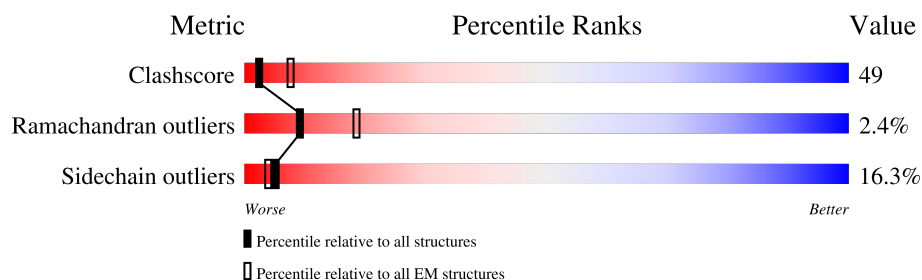
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 70.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	840	<div> <div>100%</div> <div>26% 50% 20% .</div> </div>
1	D	840	<div> <div>99%</div> <div>26% 51% 20% .</div> </div>
1	G	840	<div> <div>100%</div> <div>25% 51% 20% .</div> </div>
1	J	840	<div> <div>99%</div> <div>25% 51% 20% .</div> </div>
2	B	145	<div> <div>100%</div> <div>66% 26% 6% .</div> </div>
2	E	145	<div> <div>100%</div> <div>63% 28% 6% .</div> </div>
2	H	145	<div> <div>100%</div> <div>63% 28% 6% .</div> </div>
2	K	145	<div> <div>100%</div> <div>65% 26% 6% .</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain		
3	C	147	100%	61%	37%
3	F	147	90%	61%	38%
3	I	147	100%	61%	37%
3	L	147	73%	61%	37%
4	0	375	99%	65%	27% 6% ..
4	1	375	99%	64%	27% 7% ..
4	2	375	99%	63%	28% 7% ..
4	3	375	99%	63%	29% 6% ..
4	4	375	95%	58%	32% 8% ..
4	5	375	99%	58%	32% 8% ..
4	6	375	98%	56%	33% 9% ..
4	7	375	99%	56%	34% 8% ..
4	8	375	93%	60%	30% 7% ..
4	V	375	99%	61%	30% 6% ..
4	W	375	99%	63%	28% 7% ..
4	X	375	99%	63%	28% 6% ..
4	Y	375	99%	64%	28% 6% ..
4	Z	375	99%	64%	28% 6% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MLY	A	505	-	-	X	-
1	MLY	A	553	-	-	X	-
1	MLY	A	764	-	-	X	-
1	MLY	A	768	-	-	X	-
1	MLY	A	839	-	-	X	-
1	MLY	D	553	-	-	X	-
1	MLY	D	782	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MLY	D	839	-	-	X	-
1	MLY	G	553	-	-	X	-
1	MLY	G	764	-	-	X	-
1	MLY	G	768	-	-	X	-
1	MLY	G	84	-	-	X	-
1	MLY	J	553	-	-	X	-
1	MLY	J	764	-	-	X	-
1	MLY	J	768	-	-	X	-
1	MLY	J	84	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 76872 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called SKELETAL MUSCLE MYOSIN II.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	840	Total	C	N	O	S	0	0
			6797	4382	1135	1243	37		
1	D	840	Total	C	N	O	S	0	0
			6797	4382	1135	1243	37		
1	G	840	Total	C	N	O	S	0	0
			6797	4382	1135	1243	37		
1	J	840	Total	C	N	O	S	0	0
			6797	4382	1135	1243	37		

- Molecule 2 is a protein called SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		
2	E	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		
2	H	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		
2	K	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		

- Molecule 3 is a protein called SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	147	Total	C	N	O	S	0	0
			1123	698	188	230	7		
3	F	147	Total	C	N	O	S	0	0
			1123	698	188	230	7		
3	I	147	Total	C	N	O	S	0	0
			1123	698	188	230	7		
3	L	147	Total	C	N	O	S	0	0
			1123	698	188	230	7		

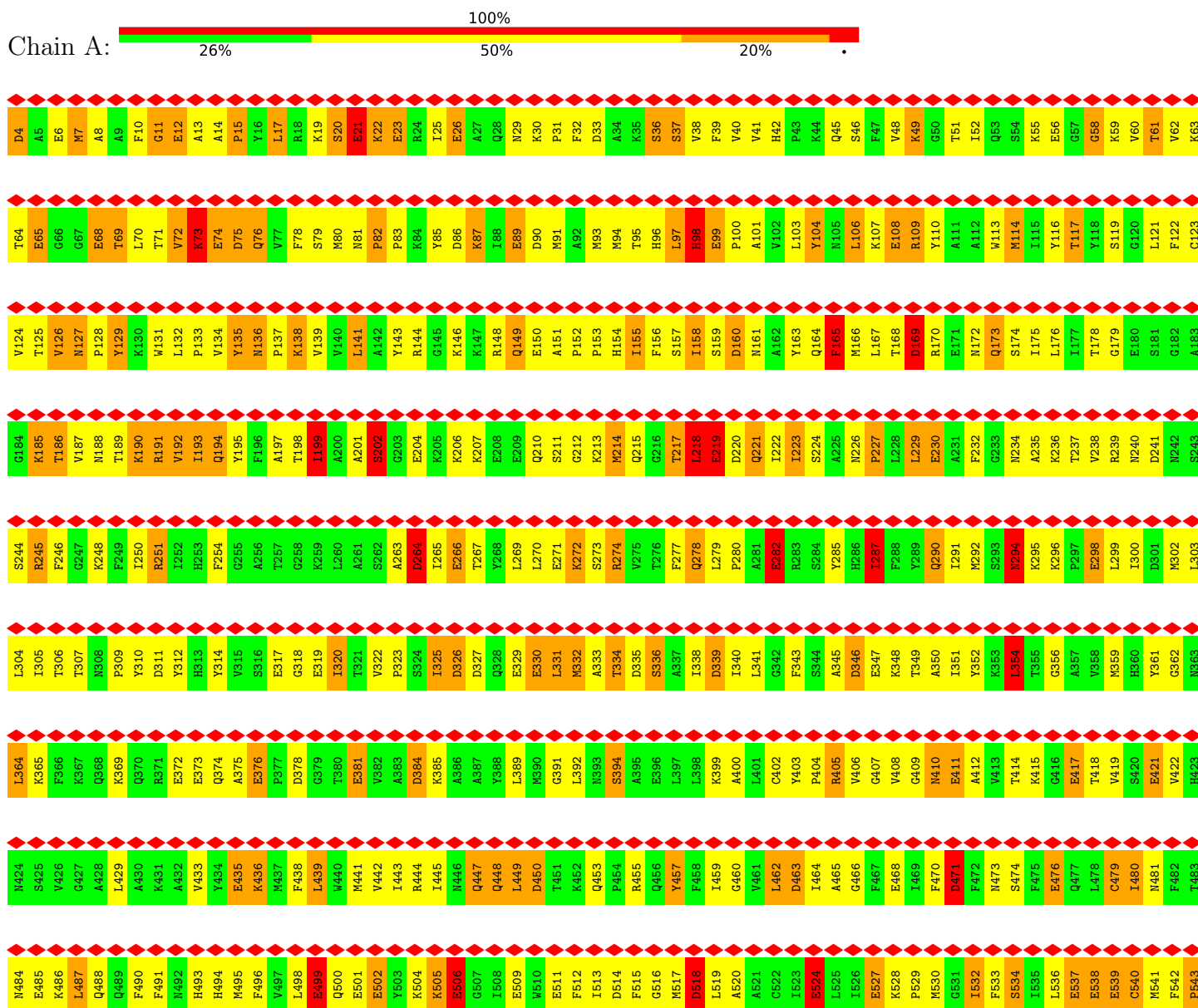
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

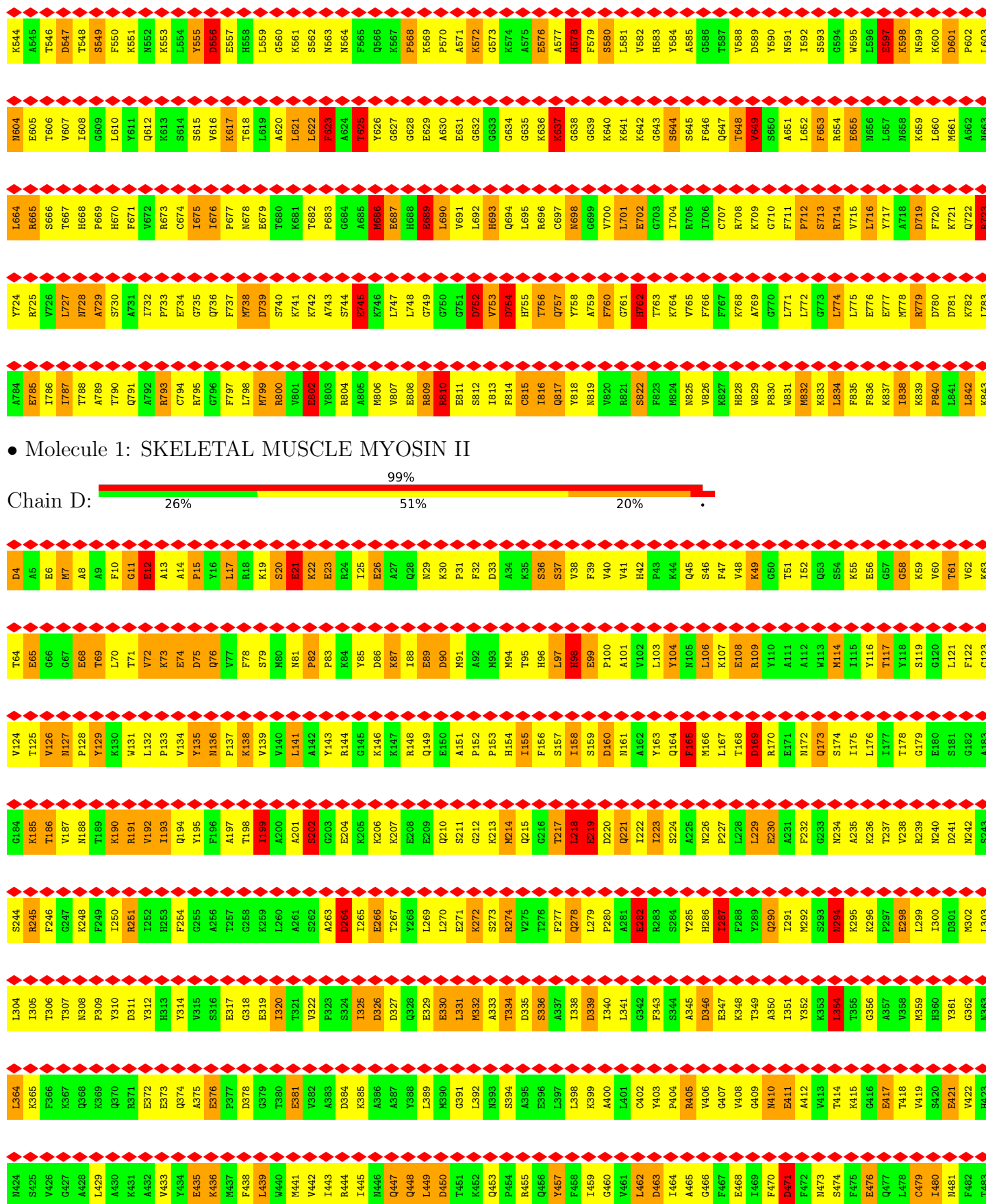
Mol	Chain	Residues	Atoms					AltConf	Trace
4	0	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	1	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	2	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	3	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	4	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	5	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	6	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	7	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	8	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	V	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	W	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	X	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	Y	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	Z	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		

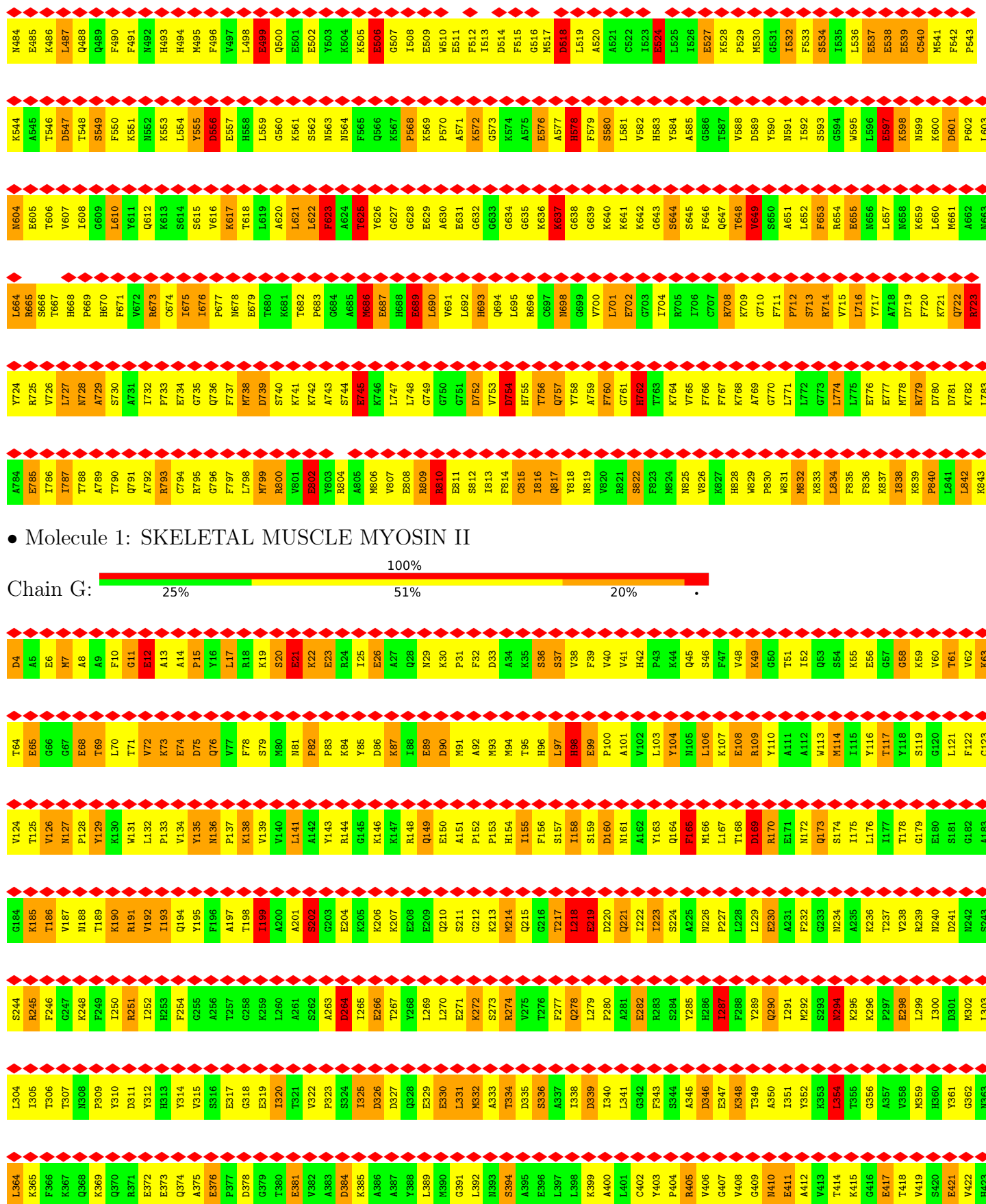
3 Residue-property plots

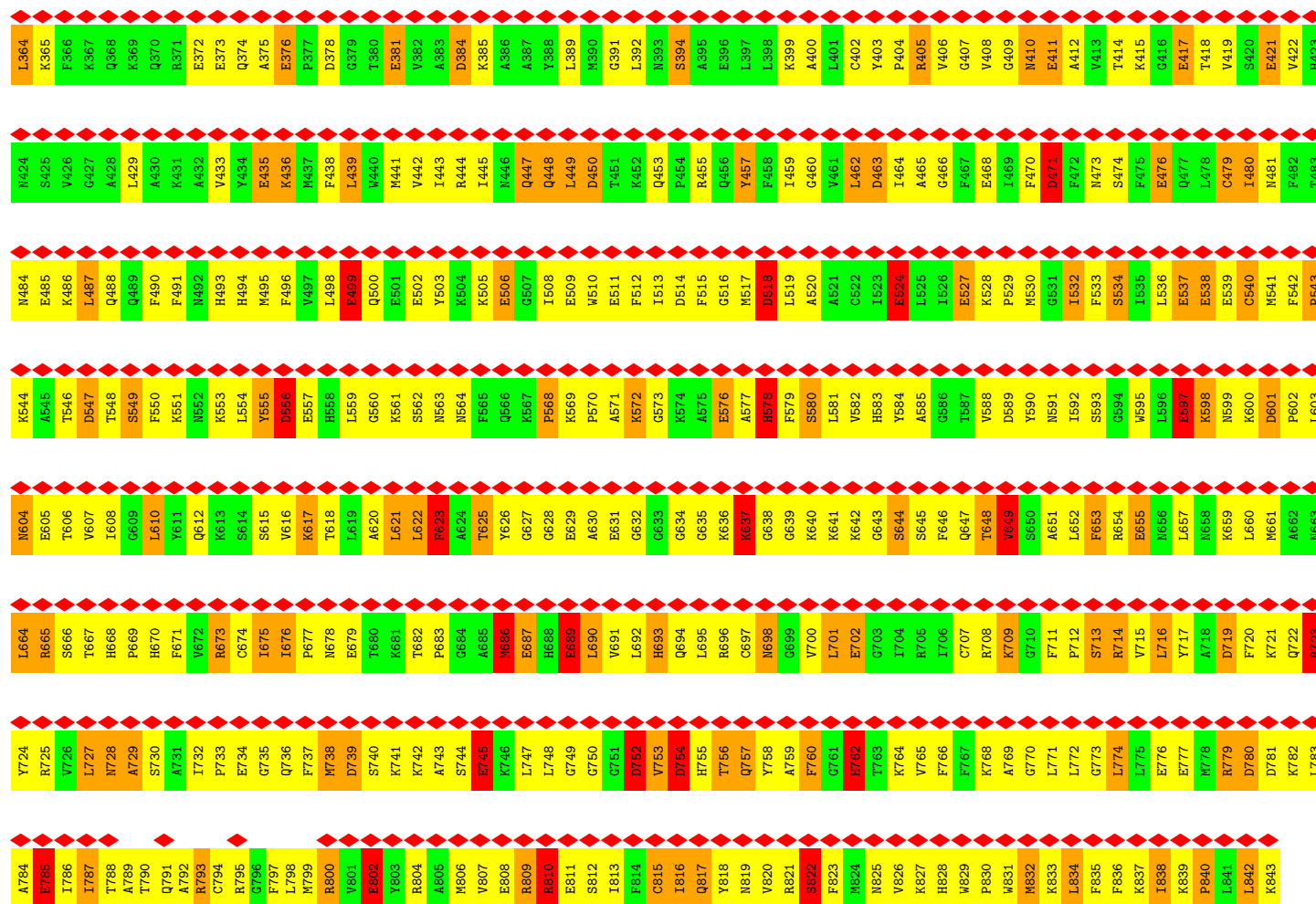
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: SKELETAL MUSCLE MYOSIN II

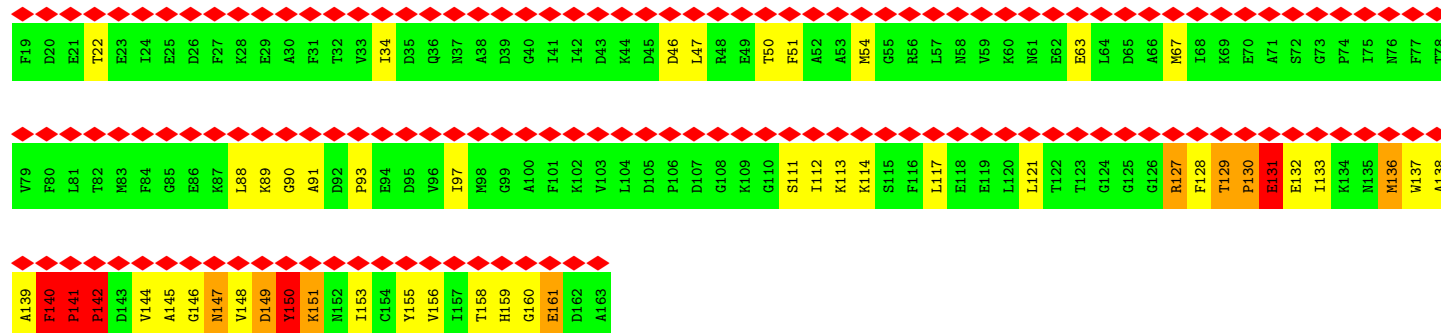






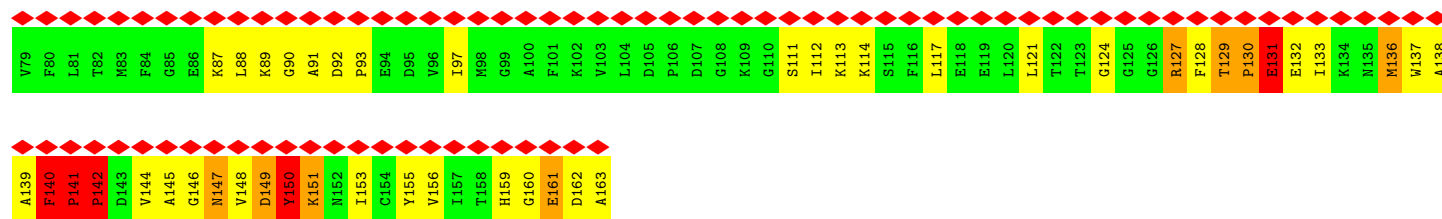


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

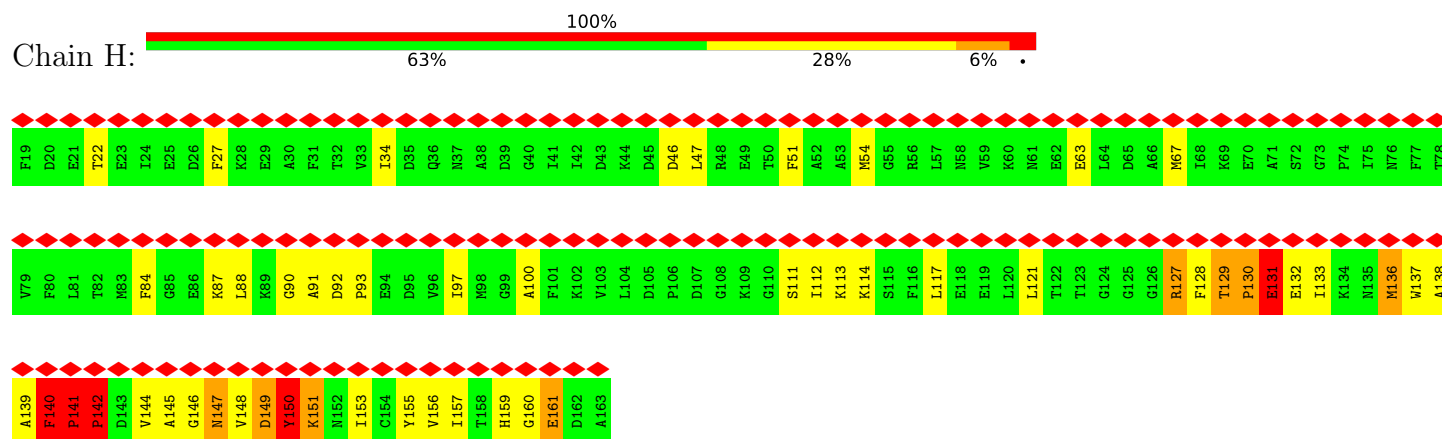


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

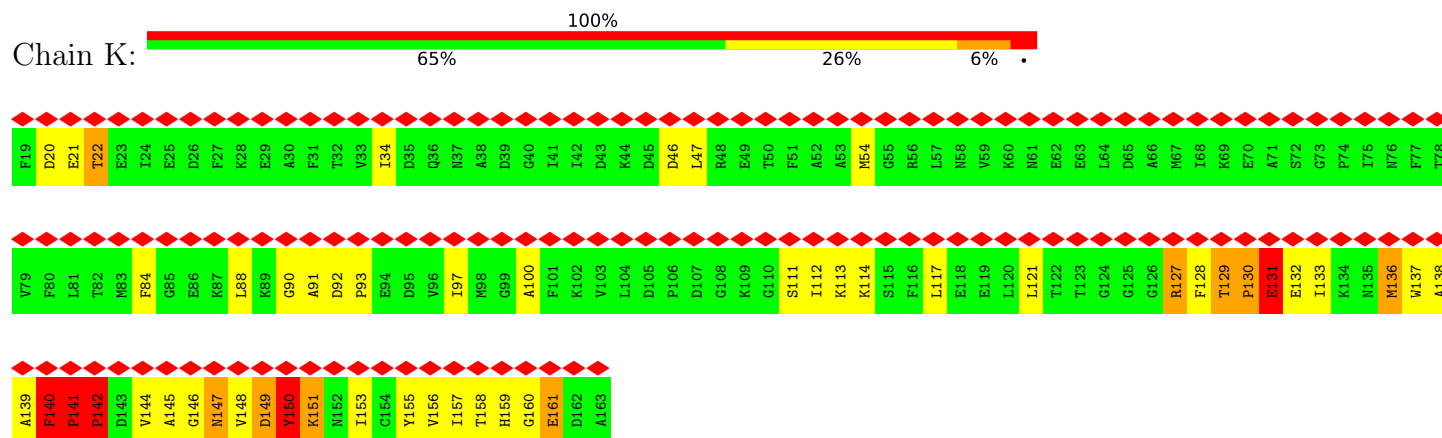




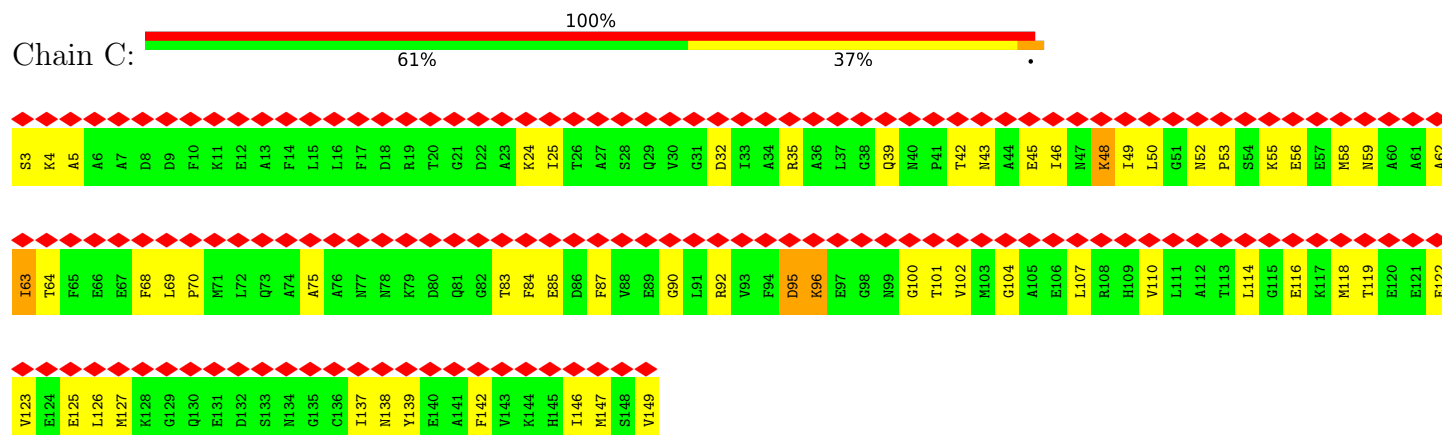
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



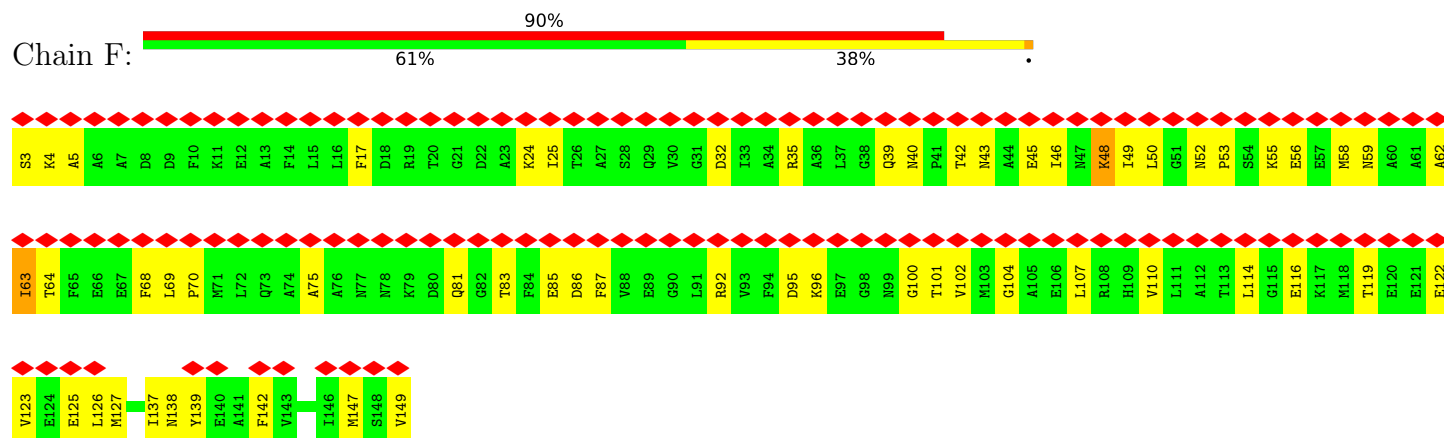
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



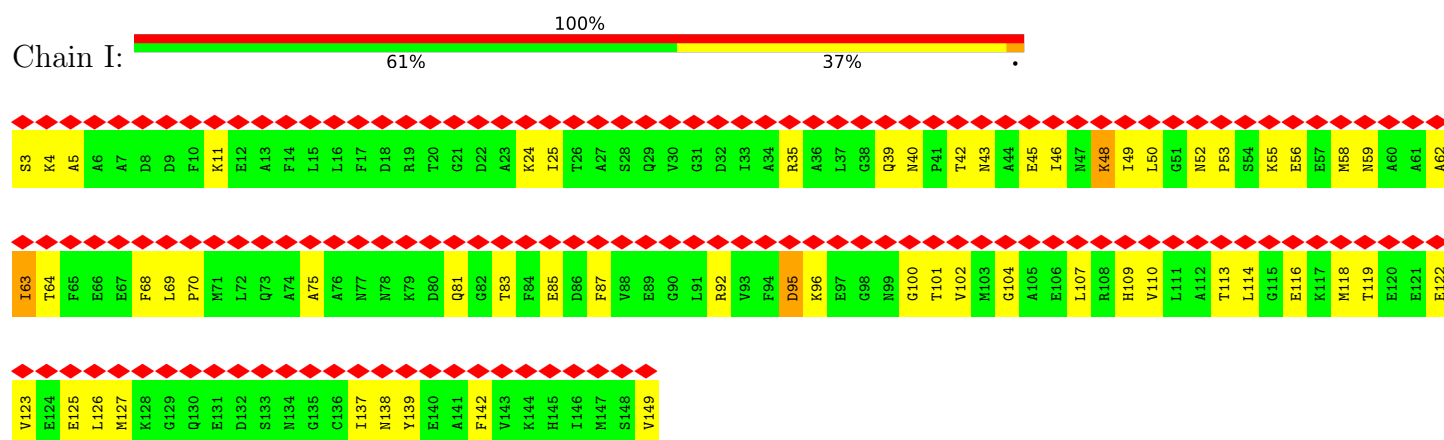
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



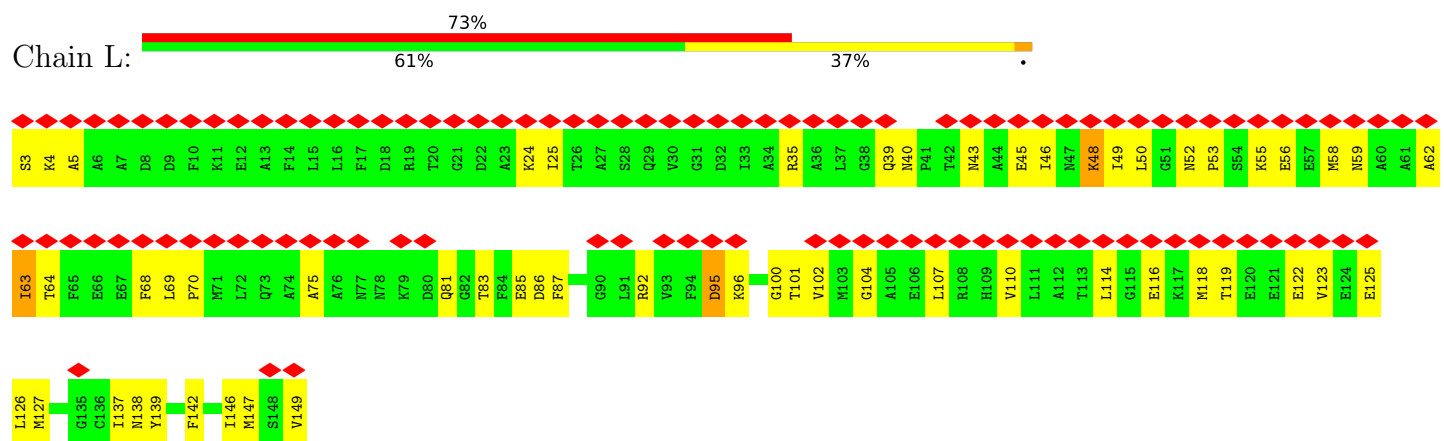
● Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



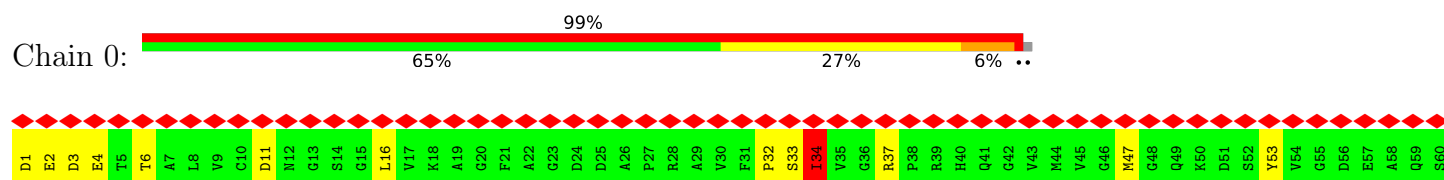
● Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

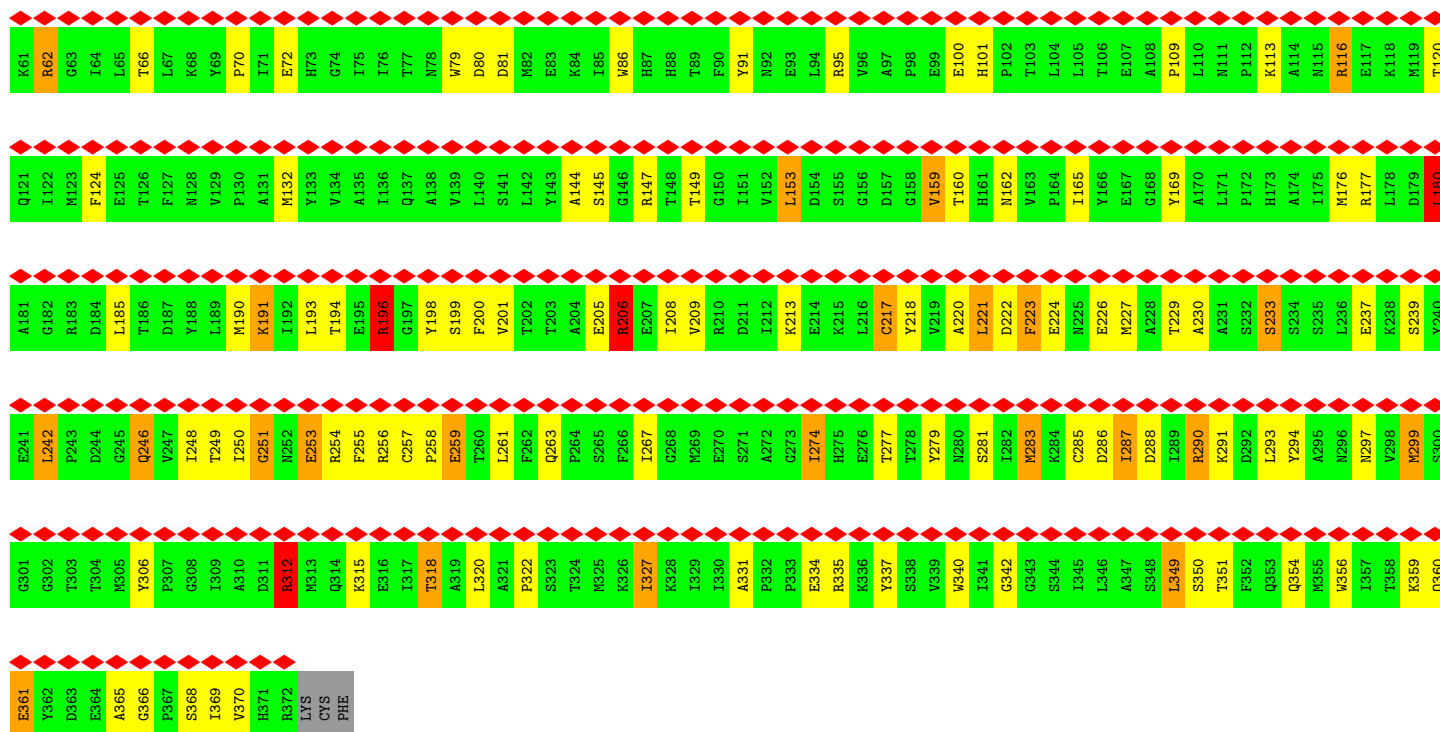


● Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

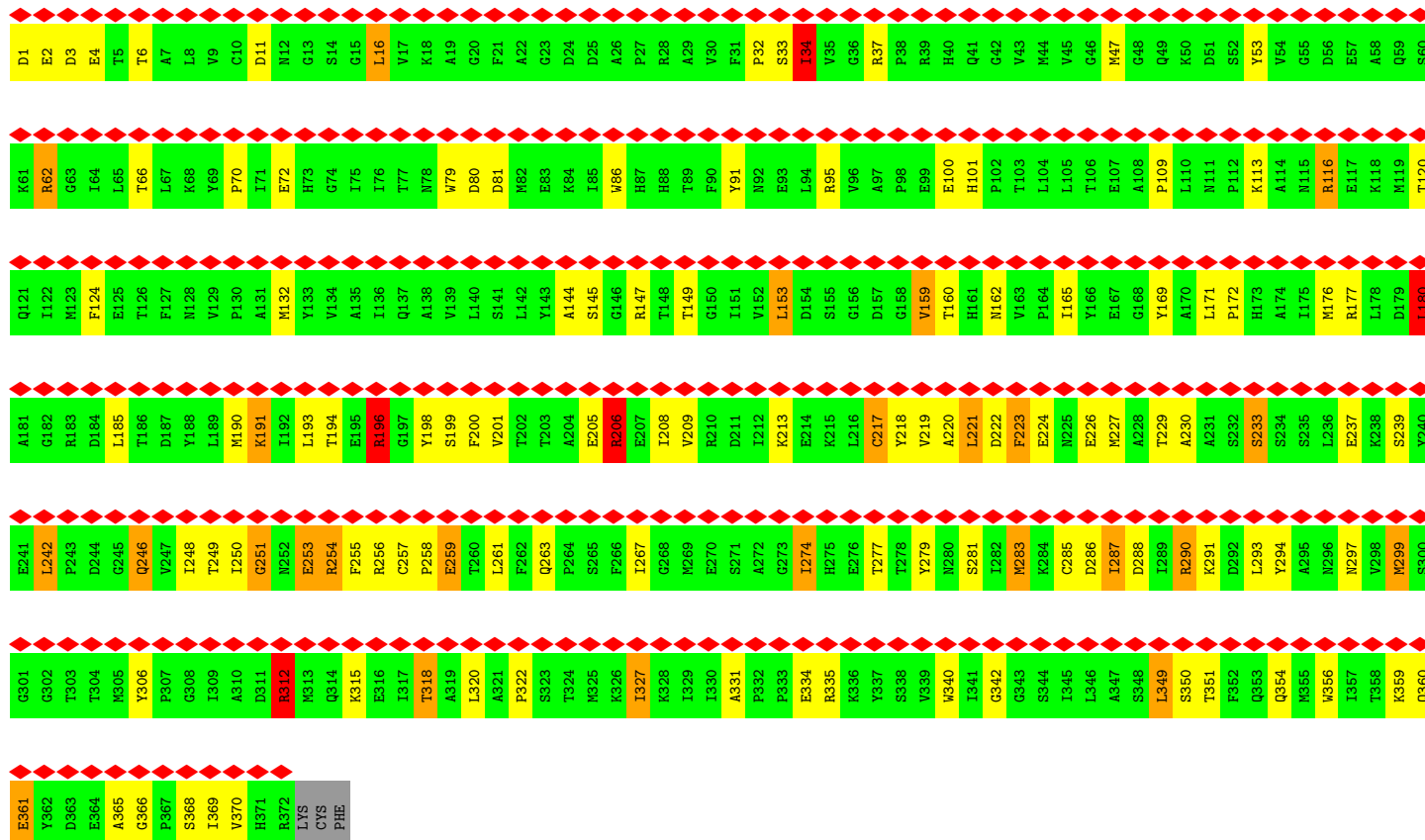


● Molecule 4: SKELETAL MUSCLE ACTIN

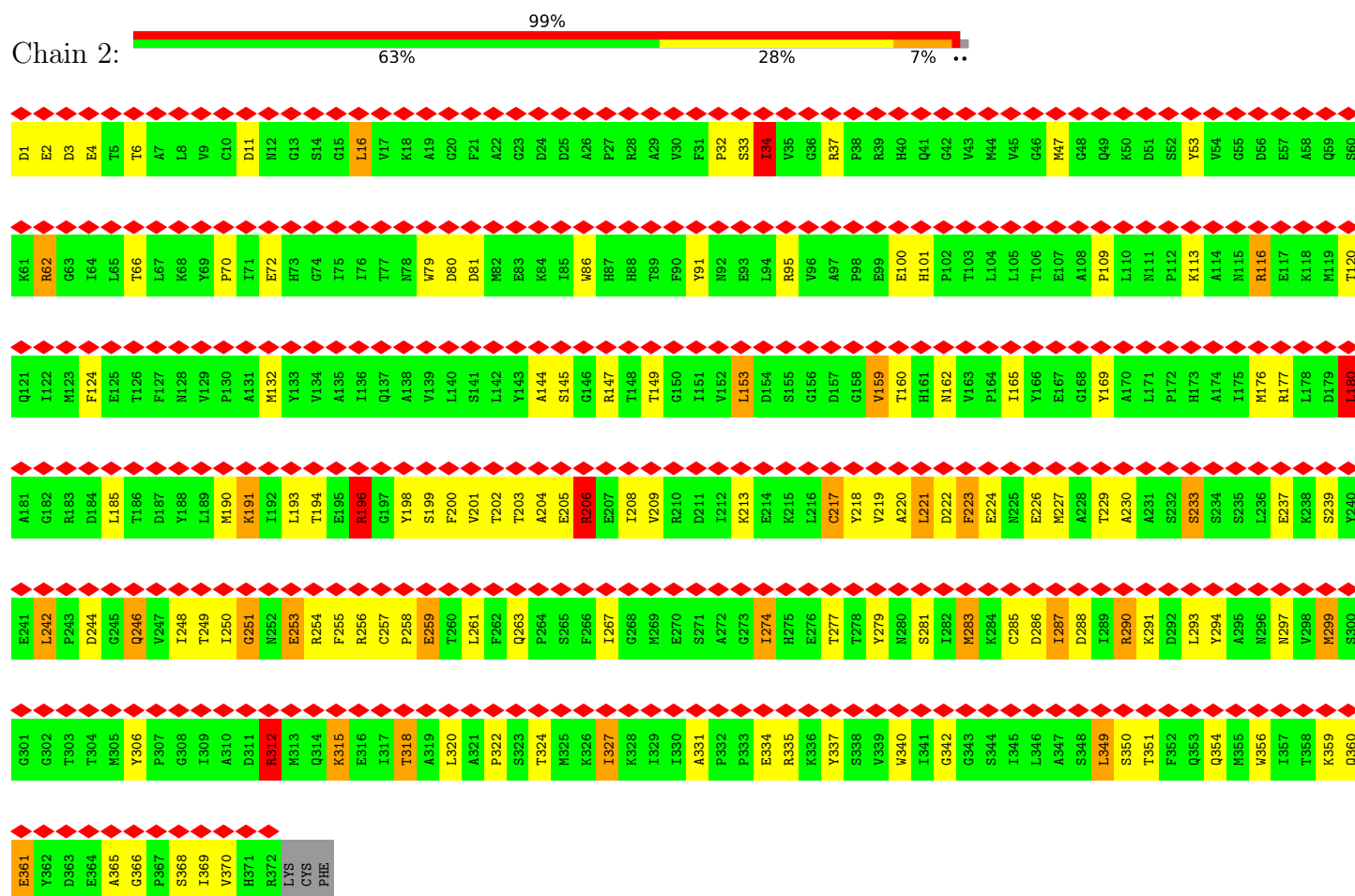




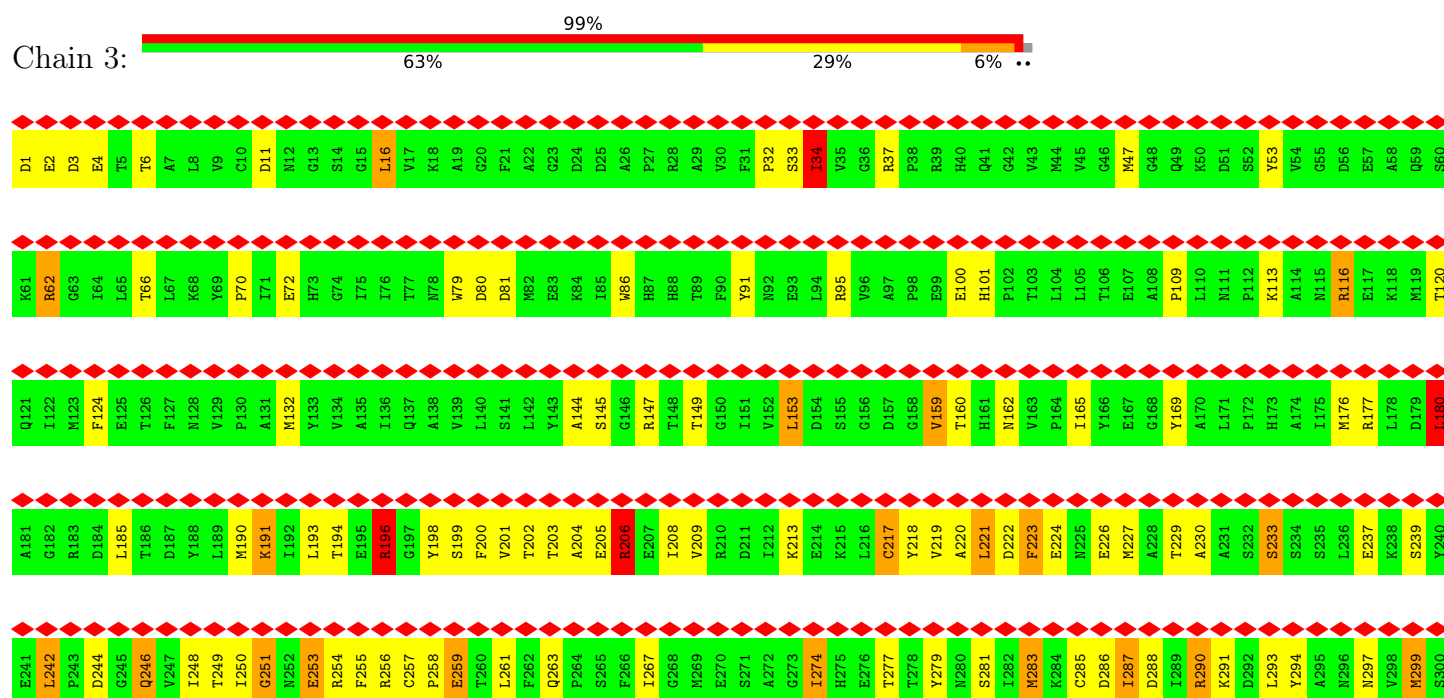
• Molecule 4: SKELETAL MUSCLE ACTIN



● Molecule 4: SKELETAL MUSCLE ACTIN

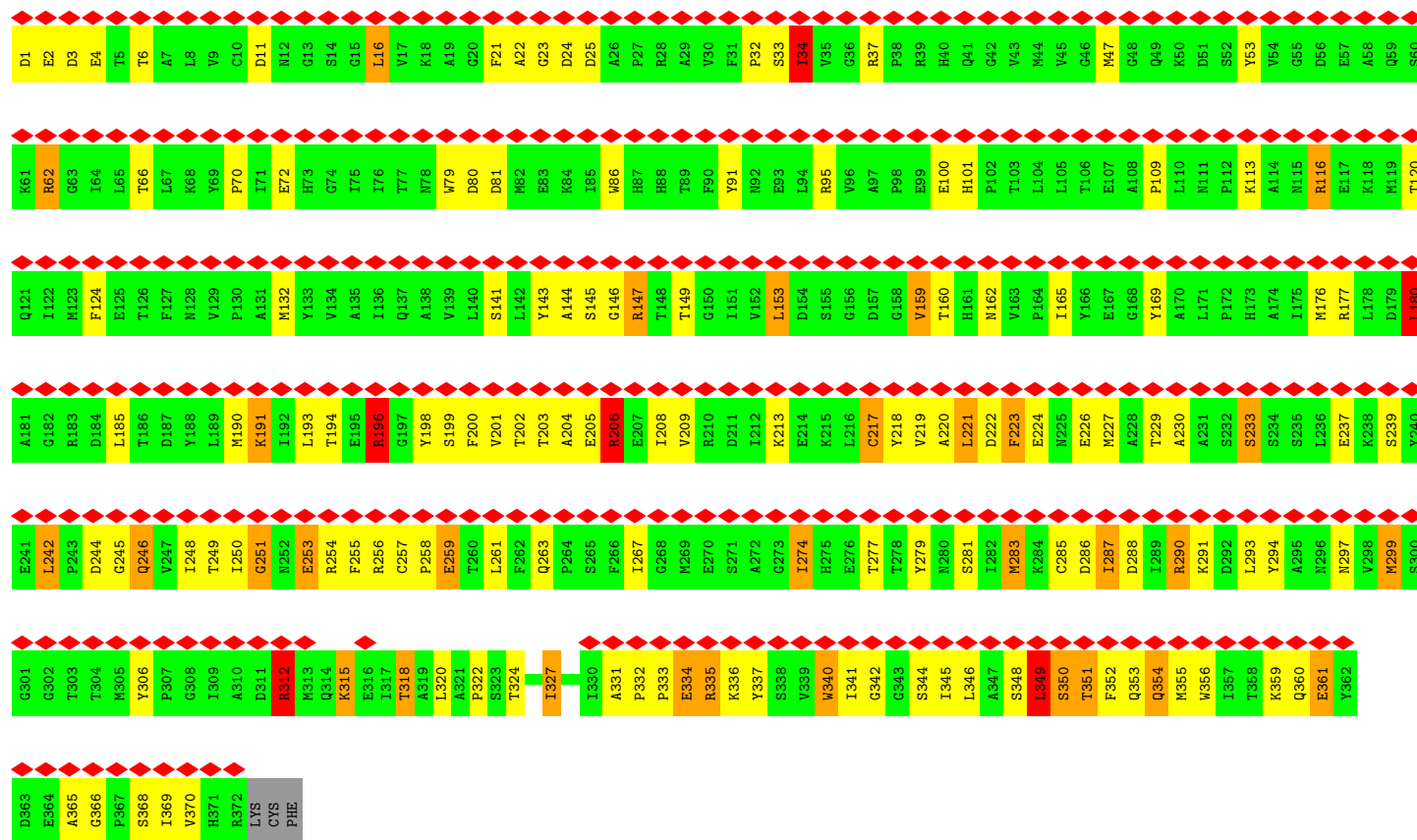
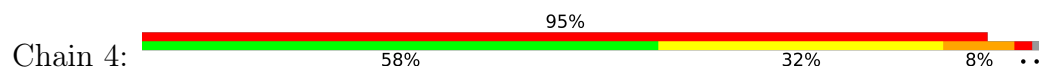


● Molecule 4: SKELETAL MUSCLE ACTIN

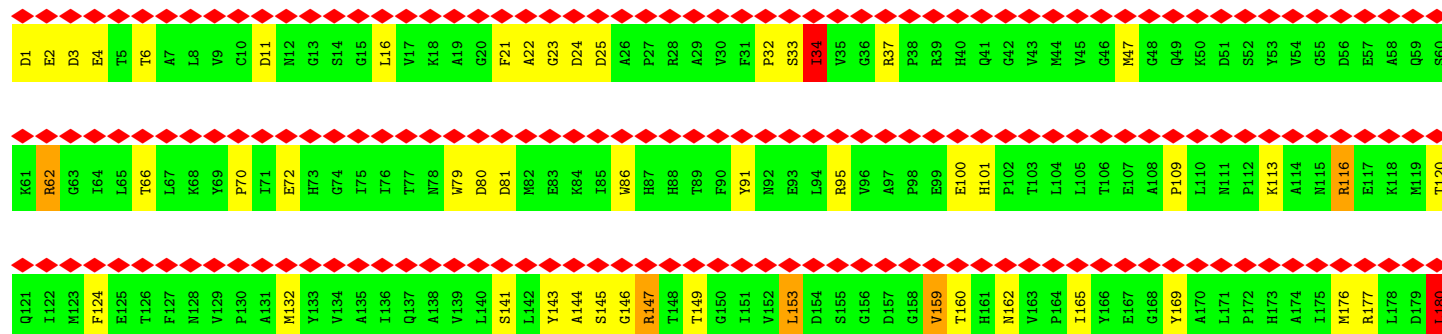




• Molecule 4: SKELETAL MUSCLE ACTIN

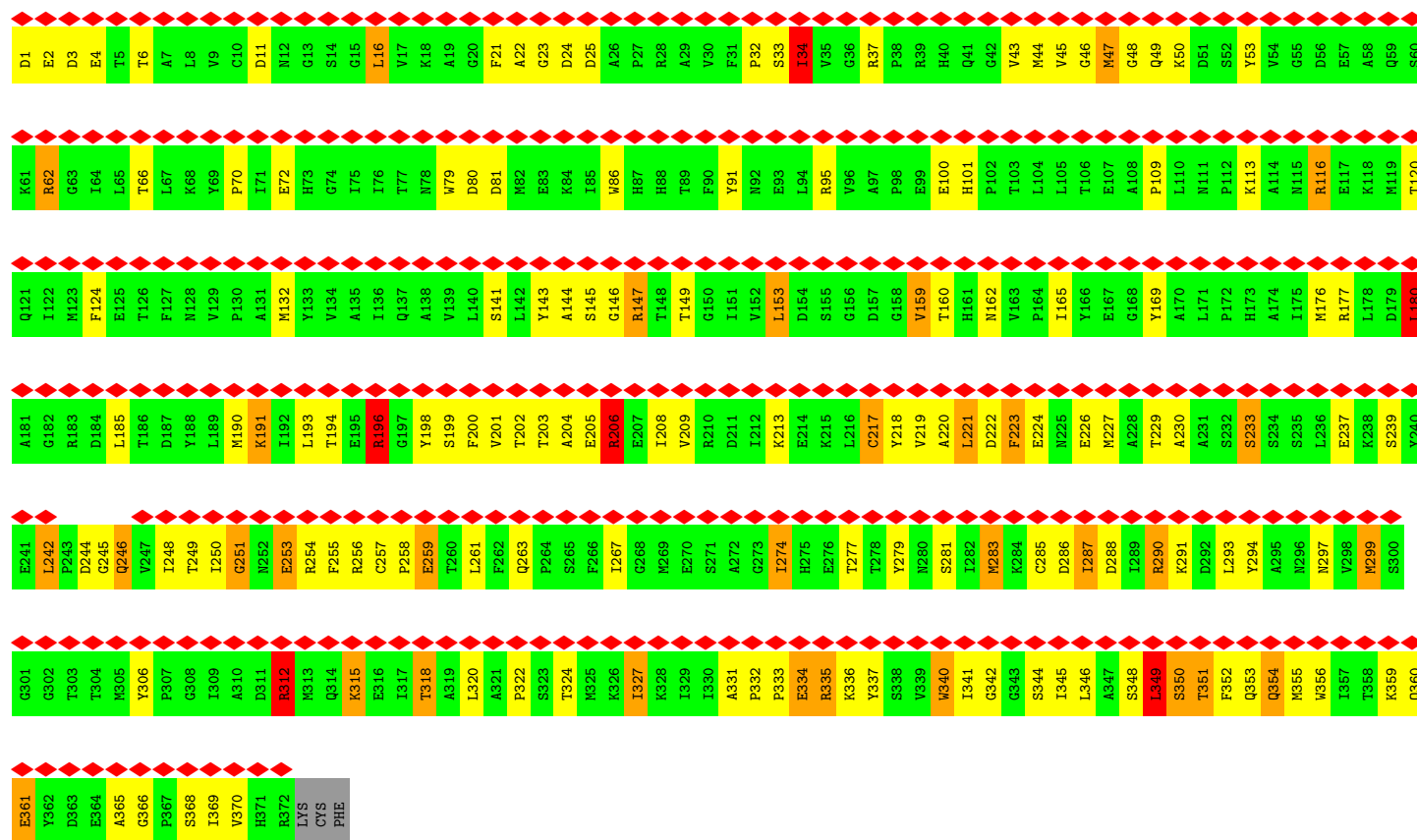


• Molecule 4: SKELETAL MUSCLE ACTIN

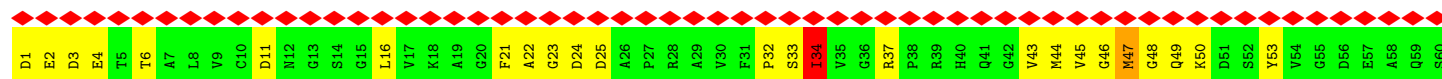


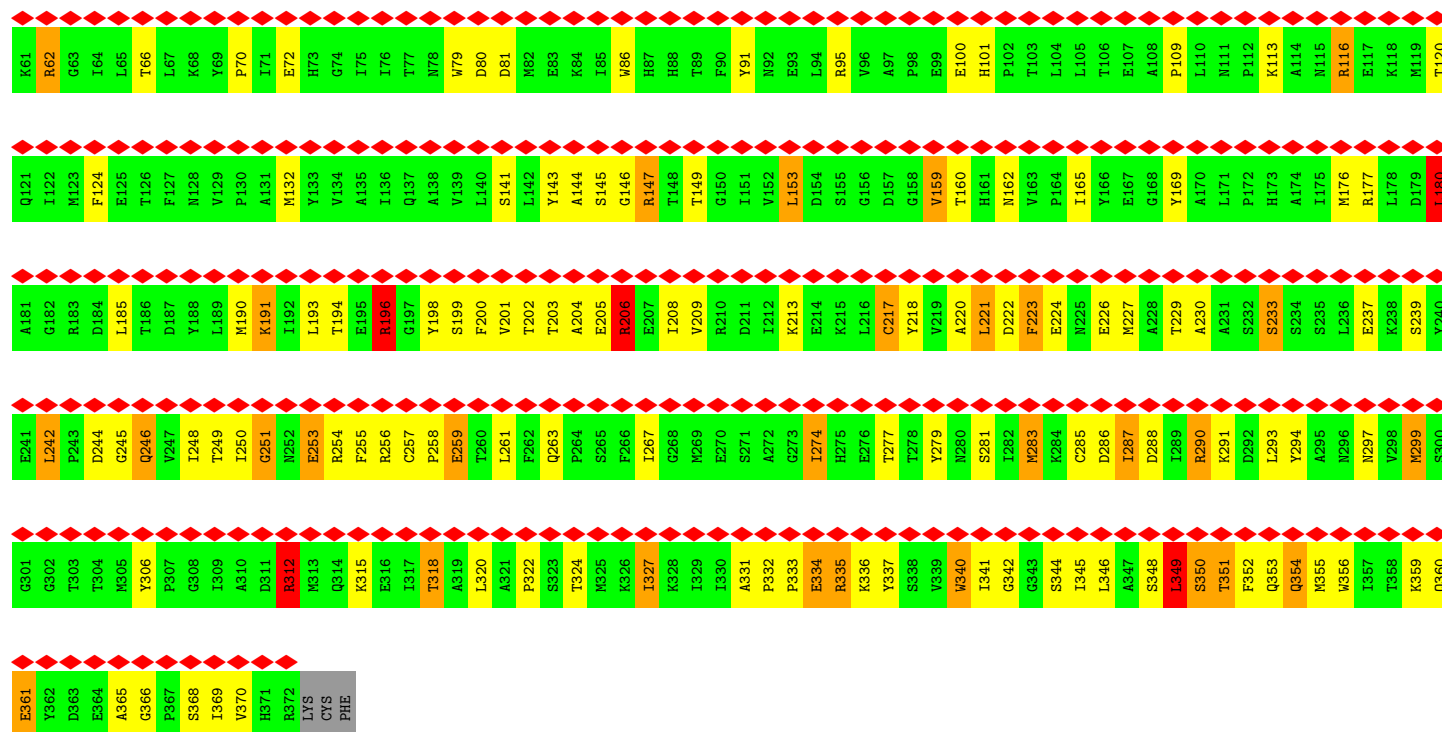


• Molecule 4: SKELETAL MUSCLE ACTIN

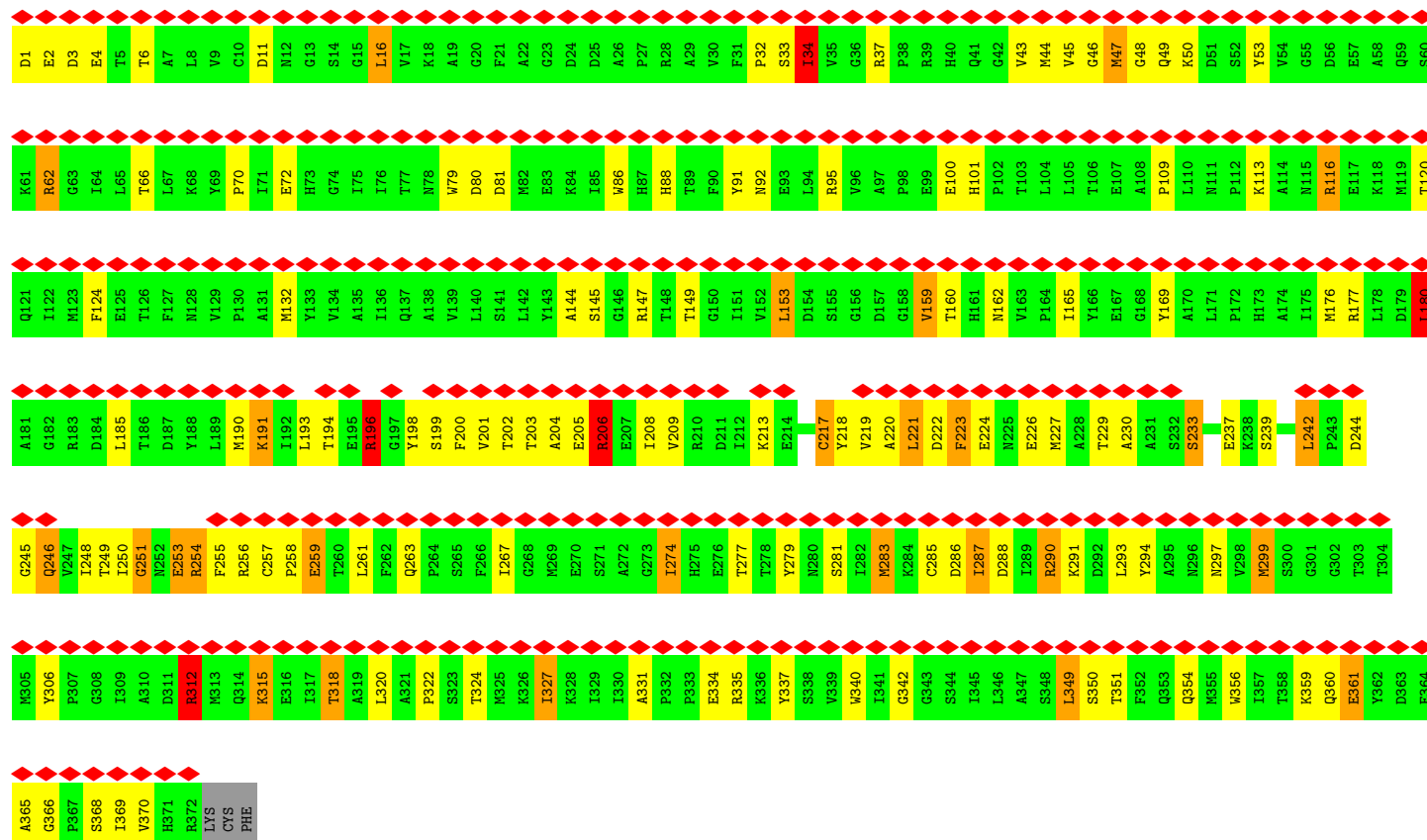
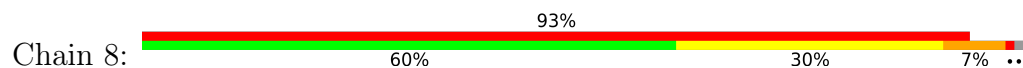


• Molecule 4: SKELETAL MUSCLE ACTIN

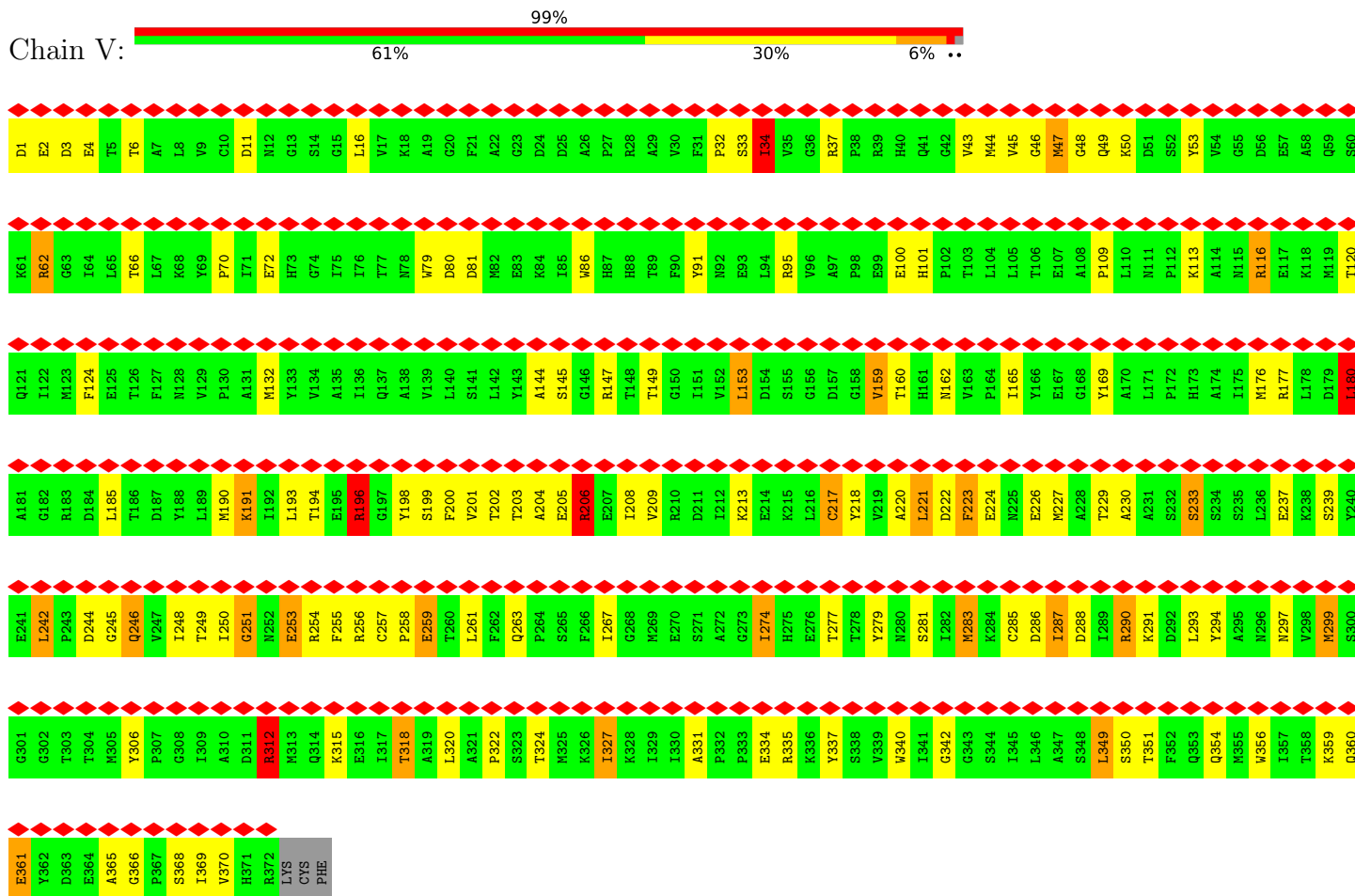




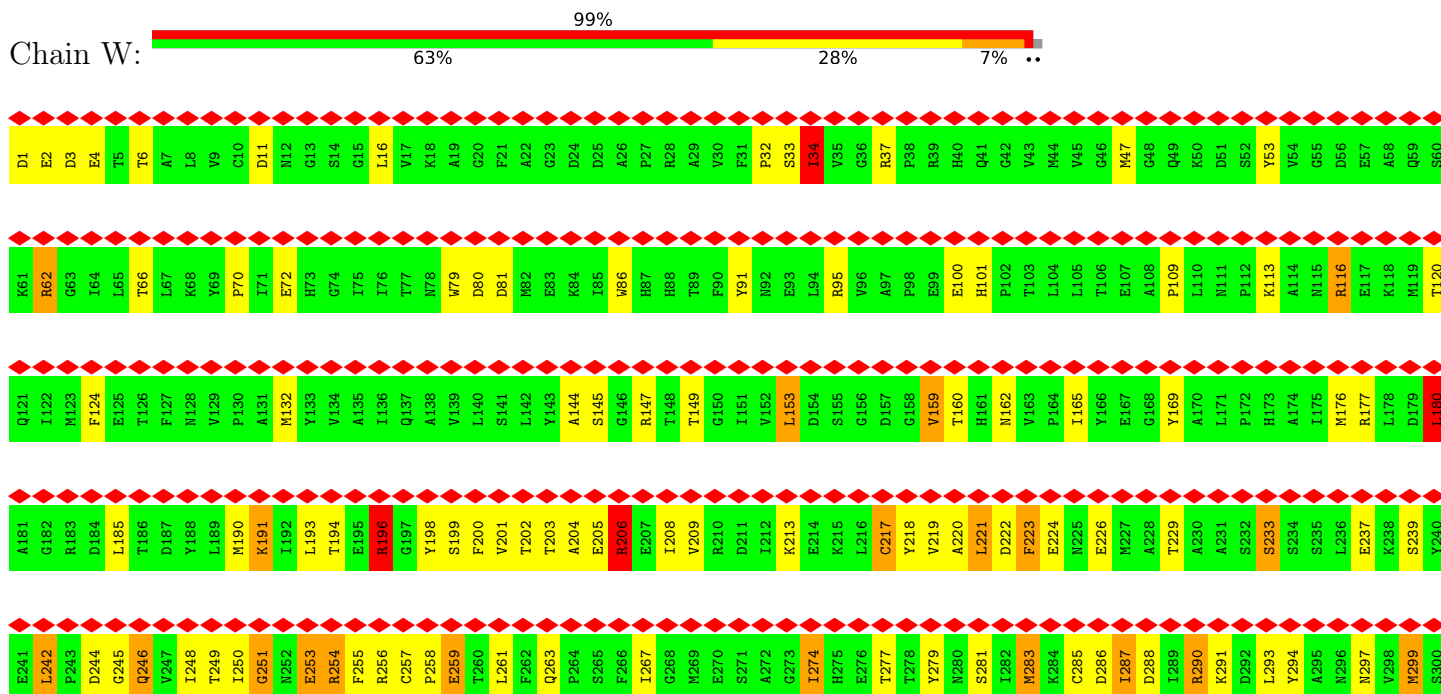
• Molecule 4: SKELETAL MUSCLE ACTIN

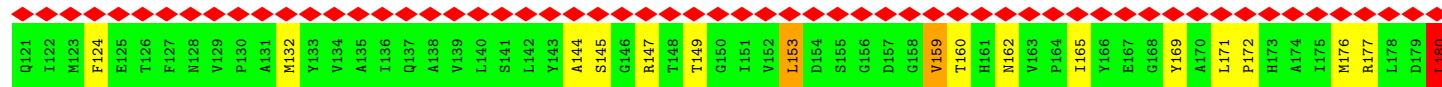


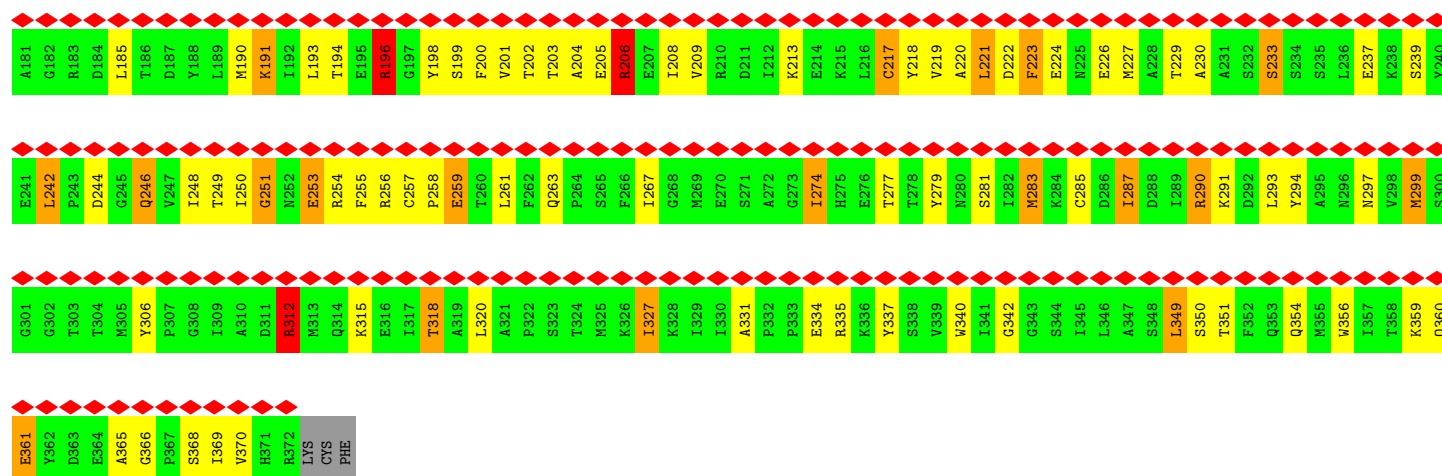
Chain V:



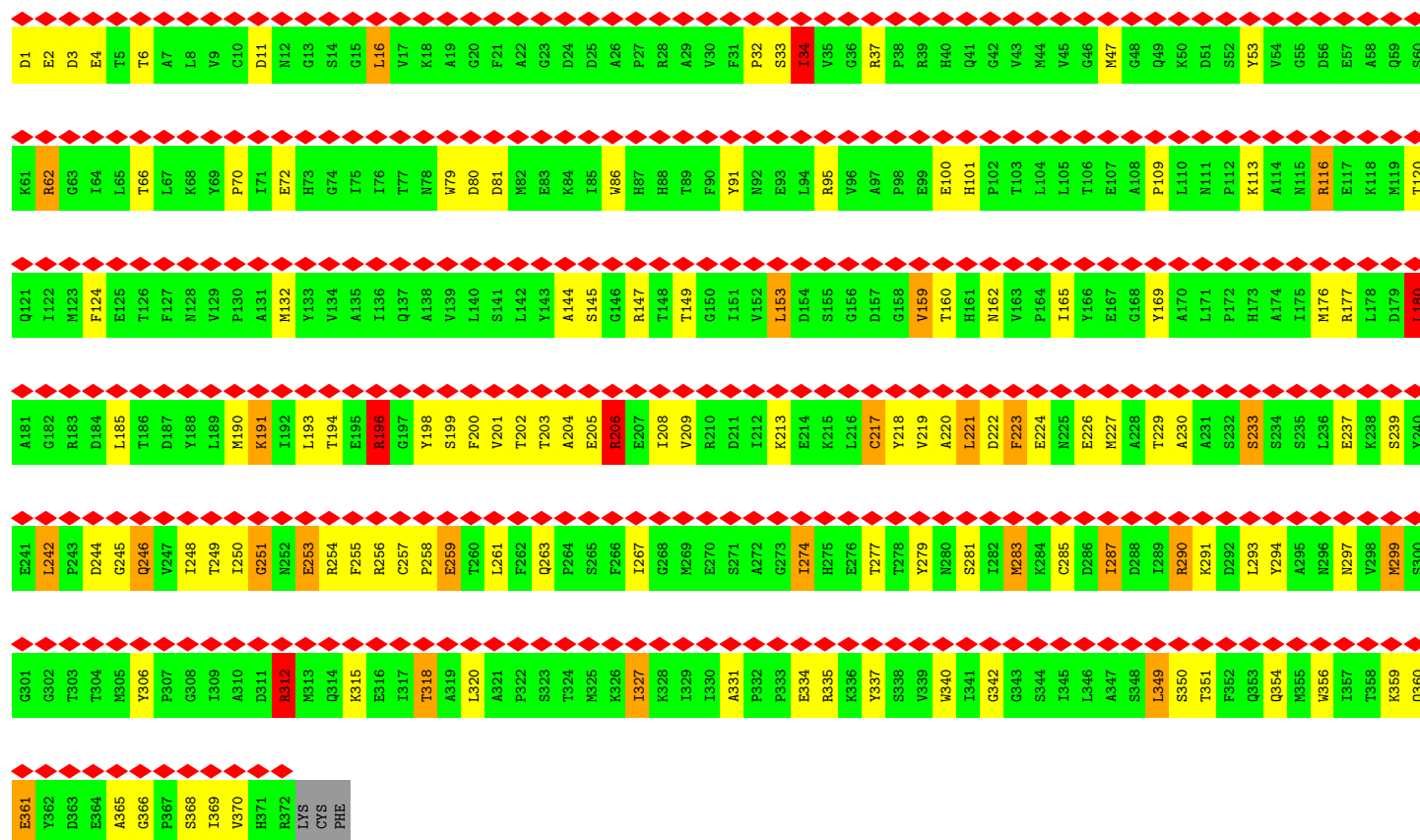
Chain W:







• Molecule 4: SKELETAL MUSCLE ACTIN



4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI/PHILIPS EM400	Depositor
Voltage (kV)	100	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	17000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum voxel value	366.680	Depositor
Minimum voxel value	-417.992	Depositor
Average voxel value	1.860	Depositor
Voxel value standard deviation	47.792	Depositor
Recommended contour level	81.2	Depositor
Tomogram size (\AA)	9280, 9280, 464	wwPDB
Tomogram dimensions	600, 600, 30	wwPDB
Tomogram angles ($^\circ$)	90, 90, 90	wwPDB
Grid spacing (\AA)	15.4667, 15.4667, 15.4667	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.77	67/6448 (1.0%)	1.82	114/8729 (1.3%)
1	D	1.77	65/6448 (1.0%)	1.82	114/8729 (1.3%)
1	G	1.77	67/6448 (1.0%)	1.82	116/8729 (1.3%)
1	J	1.90	68/6449 (1.1%)	1.84	118/8732 (1.4%)
2	B	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	E	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
2	H	1.22	10/1148 (0.9%)	1.62	16/1548 (1.0%)
2	K	1.22	10/1148 (0.9%)	1.61	16/1548 (1.0%)
3	C	0.80	0/1136	0.95	4/1525 (0.3%)
3	F	0.80	0/1136	0.95	4/1525 (0.3%)
3	I	0.80	0/1136	0.95	4/1525 (0.3%)
3	L	0.79	0/1136	0.94	4/1525 (0.3%)
4	0	0.89	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	1	0.89	2/2968 (0.1%)	1.64	50/4023 (1.2%)
4	2	0.89	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	3	0.89	1/2968 (0.0%)	1.64	51/4023 (1.3%)
4	4	0.89	1/2968 (0.0%)	1.64	51/4023 (1.3%)
4	5	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	6	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	7	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
4	8	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	V	0.89	1/2968 (0.0%)	1.64	52/4023 (1.3%)
4	W	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	X	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	Y	0.89	2/2968 (0.1%)	1.64	51/4023 (1.3%)
4	Z	0.89	2/2968 (0.1%)	1.64	52/4023 (1.3%)
All	All	1.29	330/76481 (0.4%)	1.67	1261/103533 (1.2%)

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	1	4
1	D	1	4
1	G	2	4
1	J	1	6
2	B	0	3
2	E	0	3
2	H	0	3
2	K	0	3
3	C	0	2
3	F	0	2
3	I	0	2
3	L	0	2
4	0	0	1
4	1	0	1
4	2	0	1
4	3	0	1
4	4	0	1
4	5	0	1
4	6	0	1
4	7	0	1
4	8	0	1
4	V	0	1
4	W	0	1
4	X	0	1
4	Y	0	1
4	Z	0	1
All	All	5	52

All (330) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	709	LYS	C-N	-55.36	0.33	1.33
1	J	649	VAL	CB-CG1	53.26	2.64	1.52
1	G	649	VAL	CB-CG1	53.23	2.64	1.52
1	D	649	VAL	CB-CG1	53.18	2.64	1.52
1	A	649	VAL	CB-CG1	53.16	2.64	1.52
1	D	623	PHE	CB-CG	48.14	2.33	1.51
1	J	623	PHE	CB-CG	48.11	2.33	1.51
1	A	623	PHE	CB-CG	48.09	2.33	1.51
1	G	623	PHE	CB-CG	48.09	2.33	1.51
1	A	649	VAL	CB-CG2	46.26	2.50	1.52
1	G	649	VAL	CB-CG2	46.20	2.49	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	649	VAL	CB-CG2	46.17	2.49	1.52
1	D	649	VAL	CB-CG2	46.13	2.49	1.52
1	A	648	THR	CB-OG1	34.37	2.12	1.43
1	G	648	THR	CB-OG1	34.36	2.12	1.43
1	D	648	THR	CB-OG1	34.34	2.12	1.43
1	J	648	THR	CB-OG1	34.31	2.11	1.43
1	A	648	THR	CB-CG2	-30.69	0.51	1.52
1	G	648	THR	CB-CG2	-30.68	0.51	1.52
1	J	648	THR	CB-CG2	-30.67	0.51	1.52
1	D	648	THR	CB-CG2	-30.67	0.51	1.52
1	D	637	LYS	C-N	-15.07	1.05	1.33
1	J	637	LYS	C-N	-15.00	1.06	1.33
1	G	637	LYS	C-N	-14.83	1.06	1.33
1	A	637	LYS	C-N	-14.80	1.06	1.33
1	A	649	VAL	C-N	-13.51	1.02	1.34
1	G	649	VAL	C-N	-13.49	1.03	1.34
1	D	649	VAL	C-N	-13.43	1.03	1.34
1	J	649	VAL	C-N	-13.42	1.03	1.34
2	H	150	TYR	CB-CG	-13.39	1.31	1.51
2	B	150	TYR	CB-CG	-13.36	1.31	1.51
2	E	150	TYR	CB-CG	-13.31	1.31	1.51
2	K	150	TYR	CB-CG	-13.30	1.31	1.51
2	B	140	PHE	C-N	-12.96	1.09	1.34
2	E	140	PHE	C-N	-12.96	1.09	1.34
2	K	140	PHE	C-N	-12.92	1.09	1.34
2	H	140	PHE	C-N	-12.82	1.09	1.34
2	B	150	TYR	CG-CD2	-11.36	1.24	1.39
2	K	150	TYR	CG-CD2	-11.20	1.24	1.39
2	H	150	TYR	CG-CD2	-11.18	1.24	1.39
2	E	150	TYR	CG-CD2	-11.14	1.24	1.39
2	K	141	PRO	N-CD	-10.60	1.33	1.47
2	B	141	PRO	N-CD	-10.50	1.33	1.47
2	E	141	PRO	N-CD	-10.45	1.33	1.47
2	H	141	PRO	N-CD	-10.40	1.33	1.47
1	J	476	GLU	CD-OE1	8.88	1.35	1.25
1	D	476	GLU	CD-OE1	8.81	1.35	1.25
1	G	476	GLU	CD-OE1	8.76	1.35	1.25
1	J	785	GLU	C-N	8.71	1.54	1.34
1	A	622	LEU	C-N	8.68	1.54	1.34
1	A	476	GLU	CD-OE1	8.66	1.35	1.25
1	J	622	LEU	C-N	8.65	1.53	1.34
1	G	622	LEU	C-N	8.64	1.53	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	622	LEU	C-N	8.63	1.53	1.34
1	J	411	GLU	CD-OE1	8.32	1.34	1.25
1	G	411	GLU	CD-OE1	8.30	1.34	1.25
2	K	150	TYR	CA-CB	-8.26	1.35	1.53
1	J	745	GLU	CD-OE2	8.25	1.34	1.25
1	D	745	GLU	CD-OE2	8.25	1.34	1.25
2	B	150	TYR	CA-CB	-8.23	1.35	1.53
1	A	745	GLU	CD-OE2	8.15	1.34	1.25
1	D	411	GLU	CD-OE1	8.11	1.34	1.25
2	H	150	TYR	CA-CB	-8.11	1.36	1.53
1	G	745	GLU	CD-OE2	8.10	1.34	1.25
2	E	150	TYR	CA-CB	-8.08	1.36	1.53
1	A	411	GLU	CD-OE1	8.06	1.34	1.25
1	A	381	GLU	CD-OE1	8.04	1.34	1.25
1	G	108	GLU	CD-OE1	7.96	1.34	1.25
1	A	108	GLU	CD-OE1	7.94	1.34	1.25
1	J	108	GLU	CD-OE1	7.91	1.34	1.25
1	G	381	GLU	CD-OE1	7.89	1.34	1.25
1	J	202	SER	CB-OG	7.84	1.52	1.42
1	J	381	GLU	CD-OE1	7.83	1.34	1.25
1	D	381	GLU	CD-OE1	7.81	1.34	1.25
1	D	202	SER	CB-OG	7.74	1.52	1.42
1	G	202	SER	CB-OG	7.72	1.52	1.42
1	D	108	GLU	CD-OE1	7.65	1.34	1.25
1	A	202	SER	CB-OG	7.64	1.52	1.42
1	D	689	GLU	CD-OE2	7.53	1.33	1.25
1	A	689	GLU	CD-OE2	7.51	1.33	1.25
1	J	689	GLU	CD-OE2	7.45	1.33	1.25
1	G	689	GLU	CD-OE2	7.42	1.33	1.25
1	D	23	GLU	CD-OE1	7.31	1.33	1.25
1	D	347	GLU	CD-OE1	7.27	1.33	1.25
1	J	23	GLU	CD-OE1	7.23	1.33	1.25
1	A	347	GLU	CD-OE1	7.21	1.33	1.25
1	J	511	GLU	CD-OE1	7.19	1.33	1.25
1	G	347	GLU	CD-OE1	7.18	1.33	1.25
1	G	23	GLU	CD-OE1	7.17	1.33	1.25
1	A	23	GLU	CD-OE1	7.17	1.33	1.25
1	J	347	GLU	CD-OE1	7.17	1.33	1.25
1	G	26	GLU	CD-OE1	7.08	1.33	1.25
1	D	68	GLU	CD-OE2	7.05	1.33	1.25
1	J	524	GLU	CD-OE1	7.05	1.33	1.25
1	G	330	GLU	CD-OE1	7.04	1.33	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	68	GLU	CD-OE2	7.04	1.33	1.25
1	D	524	GLU	CD-OE1	7.03	1.33	1.25
1	A	511	GLU	CD-OE1	7.02	1.33	1.25
1	J	330	GLU	CD-OE1	6.99	1.33	1.25
1	D	376	GLU	CD-OE1	6.95	1.33	1.25
1	G	376	GLU	CD-OE1	6.94	1.33	1.25
1	A	376	GLU	CD-OE1	6.93	1.33	1.25
1	J	811	GLU	CD-OE1	6.92	1.33	1.25
1	D	511	GLU	CD-OE1	6.91	1.33	1.25
1	A	330	GLU	CD-OE1	6.90	1.33	1.25
1	G	524	GLU	CD-OE1	6.88	1.33	1.25
1	J	68	GLU	CD-OE2	6.88	1.33	1.25
1	A	68	GLU	CD-OE2	6.87	1.33	1.25
1	A	524	GLU	CD-OE1	6.87	1.33	1.25
1	D	26	GLU	CD-OE1	6.85	1.33	1.25
1	J	376	GLU	CD-OE1	6.85	1.33	1.25
1	G	511	GLU	CD-OE1	6.82	1.33	1.25
1	J	26	GLU	CD-OE1	6.81	1.33	1.25
1	D	811	GLU	CD-OE1	6.81	1.33	1.25
1	A	655	GLU	CD-OE1	6.80	1.33	1.25
1	D	330	GLU	CD-OE1	6.78	1.33	1.25
1	A	26	GLU	CD-OE1	6.76	1.33	1.25
1	A	811	GLU	CD-OE1	6.75	1.33	1.25
1	J	538	GLU	CD-OE1	6.69	1.33	1.25
1	J	655	GLU	CD-OE1	6.67	1.32	1.25
1	J	319	GLU	CD-OE1	6.62	1.32	1.25
2	E	150	TYR	CD2-CE2	-6.60	1.29	1.39
1	A	538	GLU	CD-OE1	6.60	1.32	1.25
1	G	319	GLU	CD-OE1	6.59	1.32	1.25
1	G	811	GLU	CD-OE1	6.59	1.32	1.25
1	G	538	GLU	CD-OE1	6.58	1.32	1.25
1	J	266	GLU	CD-OE2	6.56	1.32	1.25
1	D	655	GLU	CD-OE1	6.55	1.32	1.25
1	G	785	GLU	C-N	6.55	1.49	1.34
1	G	89	GLU	CD-OE1	6.55	1.32	1.25
1	G	655	GLU	CD-OE1	6.55	1.32	1.25
1	A	319	GLU	CD-OE1	6.54	1.32	1.25
1	A	266	GLU	CD-OE2	6.52	1.32	1.25
2	B	150	TYR	CD2-CE2	-6.52	1.29	1.39
1	D	538	GLU	CD-OE1	6.50	1.32	1.25
1	G	99	GLU	CD-OE2	6.48	1.32	1.25
1	D	538	GLU	CD-OE2	-6.46	1.18	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	266	GLU	CD-OE2	6.46	1.32	1.25
1	A	538	GLU	CD-OE2	-6.45	1.18	1.25
1	D	319	GLU	CD-OE1	6.44	1.32	1.25
1	J	89	GLU	CD-OE1	6.44	1.32	1.25
1	D	99	GLU	CD-OE2	6.43	1.32	1.25
1	A	89	GLU	CD-OE1	6.43	1.32	1.25
2	K	150	TYR	CD2-CE2	-6.42	1.29	1.39
1	D	89	GLU	CD-OE1	6.41	1.32	1.25
1	G	502	GLU	CD-OE2	6.41	1.32	1.25
1	A	605	GLU	CD-OE1	6.40	1.32	1.25
1	G	266	GLU	CD-OE2	6.38	1.32	1.25
1	J	538	GLU	CD-OE2	-6.38	1.18	1.25
2	H	150	TYR	CD2-CE2	-6.37	1.29	1.39
1	G	802	GLU	CD-OE1	6.37	1.32	1.25
1	J	808	GLU	CD-OE1	6.37	1.32	1.25
1	J	99	GLU	CD-OE2	6.36	1.32	1.25
1	G	808	GLU	CD-OE1	6.34	1.32	1.25
2	B	150	TYR	N-CA	-6.33	1.33	1.46
1	J	6	GLU	CD-OE1	6.32	1.32	1.25
1	G	605	GLU	CD-OE1	6.32	1.32	1.25
1	G	538	GLU	CD-OE2	-6.31	1.18	1.25
1	D	808	GLU	CD-OE1	6.31	1.32	1.25
1	A	808	GLU	CD-OE1	6.30	1.32	1.25
4	7	259	GLU	CG-CD	6.30	1.61	1.51
4	4	259	GLU	CG-CD	6.29	1.61	1.51
1	D	502	GLU	CD-OE2	6.27	1.32	1.25
1	J	502	GLU	CD-OE2	6.27	1.32	1.25
4	X	259	GLU	CG-CD	6.27	1.61	1.51
1	A	6	GLU	CD-OE1	6.27	1.32	1.25
4	V	259	GLU	CG-CD	6.27	1.61	1.51
4	6	259	GLU	CG-CD	6.26	1.61	1.51
4	W	259	GLU	CG-CD	6.25	1.61	1.51
1	J	802	GLU	CD-OE1	6.25	1.32	1.25
4	5	259	GLU	CG-CD	6.24	1.61	1.51
4	Y	259	GLU	CG-CD	6.24	1.61	1.51
2	K	150	TYR	N-CA	-6.24	1.33	1.46
1	A	502	GLU	CD-OE2	6.24	1.32	1.25
1	G	6	GLU	CD-OE1	6.23	1.32	1.25
4	2	259	GLU	CG-CD	6.23	1.61	1.51
4	8	259	GLU	CG-CD	6.23	1.61	1.51
2	E	150	TYR	N-CA	-6.22	1.33	1.46
4	1	259	GLU	CG-CD	6.22	1.61	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	6	GLU	CD-OE1	6.22	1.32	1.25
4	0	259	GLU	CG-CD	6.22	1.61	1.51
4	Z	259	GLU	CG-CD	6.21	1.61	1.51
1	D	605	GLU	CD-OE1	6.20	1.32	1.25
1	J	605	GLU	CD-OE1	6.20	1.32	1.25
1	A	99	GLU	CD-OE2	6.18	1.32	1.25
4	3	259	GLU	CG-CD	6.18	1.61	1.51
2	H	150	TYR	N-CA	-6.17	1.34	1.46
1	D	509	GLU	CD-OE1	6.16	1.32	1.25
1	D	802	GLU	CD-OE1	6.14	1.32	1.25
1	J	509	GLU	CD-OE1	6.13	1.32	1.25
1	G	509	GLU	CD-OE1	6.11	1.32	1.25
1	A	417	GLU	CD-OE1	6.11	1.32	1.25
1	J	329	GLU	CD-OE1	6.05	1.32	1.25
1	D	417	GLU	CD-OE1	6.01	1.32	1.25
1	G	476	GLU	CD-OE2	-6.01	1.19	1.25
1	A	509	GLU	CD-OE1	6.00	1.32	1.25
1	G	540	CYS	CB-SG	-5.98	1.72	1.81
1	A	329	GLU	CD-OE1	5.97	1.32	1.25
1	G	329	GLU	CD-OE1	5.96	1.32	1.25
1	A	802	GLU	CD-OE1	5.96	1.32	1.25
1	D	329	GLU	CD-OE1	5.91	1.32	1.25
1	J	417	GLU	CD-OE1	5.89	1.32	1.25
1	D	230	GLU	CD-OE2	5.88	1.32	1.25
1	G	417	GLU	CD-OE1	5.88	1.32	1.25
1	G	230	GLU	CD-OE2	5.86	1.32	1.25
1	J	540	CYS	CB-SG	-5.86	1.72	1.81
1	D	468	GLU	CD-OE1	5.85	1.32	1.25
1	J	230	GLU	CD-OE2	5.83	1.32	1.25
1	J	476	GLU	CD-OE2	-5.80	1.19	1.25
1	G	597	GLU	CD-OE1	5.80	1.32	1.25
1	J	527	GLU	CD-OE1	5.80	1.32	1.25
1	D	476	GLU	CD-OE2	-5.79	1.19	1.25
1	G	218	LEU	CB-CG	5.79	1.69	1.52
1	A	468	GLU	CD-OE1	5.79	1.32	1.25
1	J	421	GLU	CD-OE2	5.77	1.32	1.25
1	J	499	GLU	CD-OE2	5.77	1.31	1.25
1	A	540	CYS	CB-SG	-5.76	1.72	1.81
1	D	540	CYS	CB-SG	-5.76	1.72	1.81
1	A	476	GLU	CD-OE2	-5.76	1.19	1.25
1	J	468	GLU	CD-OE1	5.75	1.31	1.25
1	A	625	THR	CB-CG2	5.74	1.71	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	785	GLU	CD-OE2	5.73	1.31	1.25
1	A	230	GLU	CD-OE2	5.73	1.31	1.25
1	G	527	GLU	CD-OE1	5.71	1.31	1.25
1	A	785	GLU	CD-OE2	5.70	1.31	1.25
1	G	625	THR	CB-CG2	5.70	1.71	1.52
1	A	597	GLU	CD-OE1	5.69	1.31	1.25
1	J	625	THR	CB-CG2	5.69	1.71	1.52
1	A	74	GLU	CD-OE2	5.67	1.31	1.25
1	J	74	GLU	CD-OE2	5.67	1.31	1.25
1	D	597	GLU	CD-OE1	5.67	1.31	1.25
1	D	625	THR	CB-CG2	5.67	1.71	1.52
1	J	785	GLU	CD-OE2	5.66	1.31	1.25
1	J	218	LEU	CB-CG	5.66	1.69	1.52
1	A	218	LEU	CB-CG	5.65	1.69	1.52
1	G	785	GLU	CD-OE2	5.65	1.31	1.25
1	D	218	LEU	CB-CG	5.63	1.68	1.52
1	D	499	GLU	CD-OE2	5.62	1.31	1.25
1	G	74	GLU	CD-OE2	5.61	1.31	1.25
1	A	527	GLU	CD-OE1	5.61	1.31	1.25
1	D	687	GLU	CD-OE1	5.60	1.31	1.25
1	D	74	GLU	CD-OE2	5.58	1.31	1.25
1	J	687	GLU	CD-OE1	5.56	1.31	1.25
1	J	373	GLU	CD-OE1	5.56	1.31	1.25
1	A	421	GLU	CD-OE2	5.54	1.31	1.25
1	A	687	GLU	CD-OE1	5.54	1.31	1.25
1	G	421	GLU	CD-OE2	5.54	1.31	1.25
1	G	468	GLU	CD-OE1	5.53	1.31	1.25
1	J	597	GLU	CD-OE1	5.52	1.31	1.25
1	G	687	GLU	CD-OE1	5.51	1.31	1.25
2	H	150	TYR	CE1-CZ	5.51	1.45	1.38
1	A	499	GLU	CD-OE2	5.50	1.31	1.25
1	A	777	GLU	CD-OE2	5.50	1.31	1.25
1	D	373	GLU	CD-OE1	5.50	1.31	1.25
1	G	373	GLU	CD-OE1	5.49	1.31	1.25
2	E	150	TYR	CE1-CZ	5.48	1.45	1.38
1	A	506	GLU	CD-OE2	5.48	1.31	1.25
1	G	499	GLU	CD-OE2	5.48	1.31	1.25
1	D	527	GLU	CD-OE1	5.47	1.31	1.25
1	D	777	GLU	CD-OE2	5.47	1.31	1.25
2	K	150	TYR	CE1-CZ	5.46	1.45	1.38
1	G	479	CYS	CB-SG	-5.45	1.73	1.81
1	A	373	GLU	CD-OE1	5.44	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	298	GLU	CD-OE2	5.44	1.31	1.25
1	J	479	CYS	CB-SG	-5.44	1.73	1.81
1	G	777	GLU	CD-OE2	5.43	1.31	1.25
2	K	131	GLU	N-CA	5.42	1.57	1.46
2	E	131	GLU	N-CA	5.41	1.57	1.46
2	H	131	GLU	N-CA	5.41	1.57	1.46
1	A	479	CYS	CB-SG	-5.40	1.73	1.81
1	J	777	GLU	CD-OE2	5.39	1.31	1.25
1	G	506	GLU	CD-OE2	5.39	1.31	1.25
2	B	150	TYR	CE1-CZ	5.38	1.45	1.38
1	D	218	LEU	C-N	-5.37	1.21	1.34
1	A	218	LEU	C-N	-5.36	1.21	1.34
1	G	679	GLU	CD-OE2	5.36	1.31	1.25
1	D	421	GLU	CD-OE2	5.35	1.31	1.25
1	J	218	LEU	C-N	-5.34	1.21	1.34
1	D	298	GLU	CD-OE2	5.34	1.31	1.25
1	J	298	GLU	CD-OE2	5.34	1.31	1.25
1	A	65	GLU	CD-OE1	5.32	1.31	1.25
1	A	298	GLU	CD-OE2	5.31	1.31	1.25
1	G	218	LEU	C-N	-5.30	1.21	1.34
2	B	131	GLU	N-CA	5.29	1.56	1.46
1	D	65	GLU	CD-OE1	5.29	1.31	1.25
1	D	479	CYS	CB-SG	-5.28	1.73	1.81
1	J	679	GLU	CD-OE2	5.28	1.31	1.25
1	J	527	GLU	CD-OE2	-5.27	1.19	1.25
1	D	679	GLU	CD-OE2	5.24	1.31	1.25
1	J	65	GLU	CD-OE1	5.21	1.31	1.25
1	D	282	GLU	CD-OE1	5.20	1.31	1.25
2	K	149	ASP	CB-CG	5.19	1.62	1.51
1	J	12	GLU	CD-OE2	5.18	1.31	1.25
1	J	506	GLU	CD-OE2	5.18	1.31	1.25
1	D	702	GLU	CD-OE2	5.16	1.31	1.25
2	E	149	ASP	CB-CG	5.16	1.62	1.51
1	A	679	GLU	CD-OE2	5.15	1.31	1.25
1	G	12	GLU	CD-OE2	5.15	1.31	1.25
1	A	527	GLU	CD-OE2	-5.14	1.20	1.25
1	A	697	CYS	CB-SG	5.14	1.91	1.82
1	A	539	GLU	CD-OE1	5.13	1.31	1.25
1	G	21	GLU	CD-OE2	5.13	1.31	1.25
2	B	149	ASP	CB-CG	5.12	1.62	1.51
1	A	702	GLU	CD-OE2	5.11	1.31	1.25
1	D	506	GLU	CD-OE2	5.11	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	65	GLU	CD-OE1	5.11	1.31	1.25
1	A	21	GLU	CD-OE2	5.11	1.31	1.25
1	G	702	GLU	CD-OE2	5.10	1.31	1.25
1	J	702	GLU	CD-OE2	5.09	1.31	1.25
1	A	282	GLU	CD-OE1	5.09	1.31	1.25
1	J	282	GLU	CD-OE1	5.09	1.31	1.25
1	A	150	GLU	CD-OE1	5.08	1.31	1.25
1	G	527	GLU	CD-OE2	-5.06	1.20	1.25
1	G	697	CYS	CB-SG	5.05	1.90	1.82
4	Y	259	GLU	CB-CG	5.05	1.61	1.52
2	H	149	ASP	CB-CG	5.05	1.62	1.51
4	1	259	GLU	CB-CG	5.05	1.61	1.52
4	8	259	GLU	CB-CG	5.05	1.61	1.52
1	J	21	GLU	CD-OE2	5.05	1.31	1.25
4	5	259	GLU	CB-CG	5.04	1.61	1.52
1	D	539	GLU	CD-OE1	5.04	1.31	1.25
1	D	21	GLU	CD-OE2	5.03	1.31	1.25
4	6	259	GLU	CB-CG	5.03	1.61	1.52
4	Z	259	GLU	CB-CG	5.03	1.61	1.52
1	G	150	GLU	CD-OE1	5.02	1.31	1.25
4	7	259	GLU	CB-CG	5.02	1.61	1.52
1	J	697	CYS	CB-SG	5.01	1.90	1.82
4	W	259	GLU	CB-CG	5.01	1.61	1.52
4	X	259	GLU	CB-CG	5.01	1.61	1.52
1	D	12	GLU	CD-OE2	5.00	1.31	1.25

All (1261) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	637	LYS	O-C-N	-58.53	23.69	123.20
1	J	637	LYS	O-C-N	-58.47	23.80	123.20
1	D	637	LYS	O-C-N	-58.47	23.81	123.20
1	A	637	LYS	O-C-N	-58.45	23.83	123.20
1	J	649	VAL	CG1-CB-CG2	-34.02	56.47	110.90
1	D	649	VAL	CG1-CB-CG2	-34.00	56.50	110.90
1	A	649	VAL	CG1-CB-CG2	-33.99	56.51	110.90
1	G	649	VAL	CG1-CB-CG2	-33.98	56.53	110.90
1	J	648	THR	CA-CB-OG1	-31.72	42.38	109.00
1	A	648	THR	CA-CB-OG1	-31.70	42.43	109.00
1	D	648	THR	CA-CB-OG1	-31.70	42.43	109.00
1	G	648	THR	CA-CB-OG1	-31.68	42.48	109.00
2	H	150	TYR	CB-CG-CD2	-28.73	103.76	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	150	TYR	CB-CG-CD2	-28.64	103.81	121.00
2	K	150	TYR	CB-CG-CD2	-28.60	103.84	121.00
2	B	150	TYR	CB-CG-CD2	-28.58	103.85	121.00
1	G	649	VAL	CA-CB-CG1	-28.52	68.11	110.90
1	J	649	VAL	CA-CB-CG1	-28.49	68.16	110.90
1	D	649	VAL	CA-CB-CG1	-28.47	68.19	110.90
1	A	649	VAL	CA-CB-CG1	-28.45	68.23	110.90
1	J	649	VAL	CA-CB-CG2	-28.18	68.62	110.90
1	G	649	VAL	CA-CB-CG2	-28.17	68.64	110.90
1	A	649	VAL	CA-CB-CG2	-28.17	68.64	110.90
1	D	649	VAL	CA-CB-CG2	-28.16	68.66	110.90
1	D	648	THR	CA-CB-CG2	-25.60	76.56	112.40
1	J	648	THR	CA-CB-CG2	-25.56	76.61	112.40
1	A	648	THR	CA-CB-CG2	-25.45	76.78	112.40
1	G	648	THR	CA-CB-CG2	-25.36	76.90	112.40
1	J	709	LYS	O-C-N	-21.06	87.39	123.20
2	H	150	TYR	CG-CD2-CE2	-20.84	104.63	121.30
2	K	150	TYR	CG-CD2-CE2	-20.66	104.78	121.30
2	E	150	TYR	CG-CD2-CE2	-20.54	104.86	121.30
2	B	150	TYR	CG-CD2-CE2	-20.43	104.95	121.30
2	K	150	TYR	CD1-CG-CD2	19.49	139.34	117.90
2	H	150	TYR	CD1-CG-CD2	19.45	139.29	117.90
2	E	150	TYR	CD1-CG-CD2	19.40	139.24	117.90
2	B	150	TYR	CD1-CG-CD2	19.38	139.22	117.90
2	H	150	TYR	CG-CD1-CE1	-18.44	106.55	121.30
2	K	150	TYR	CG-CD1-CE1	-18.44	106.55	121.30
2	B	150	TYR	CG-CD1-CE1	-18.39	106.59	121.30
2	E	150	TYR	CG-CD1-CE1	-18.38	106.59	121.30
1	J	800	ARG	NE-CZ-NH2	-16.61	112.00	120.30
1	D	800	ARG	NE-CZ-NH2	-16.48	112.06	120.30
1	G	800	ARG	NE-CZ-NH2	-16.31	112.14	120.30
1	A	800	ARG	NE-CZ-NH2	-16.29	112.16	120.30
1	G	623	PHE	CB-CG-CD2	-13.78	111.16	120.80
1	J	623	PHE	CB-CG-CD2	-13.67	111.23	120.80
1	A	623	PHE	CB-CG-CD2	-13.64	111.25	120.80
1	D	623	PHE	CB-CG-CD2	-13.64	111.25	120.80
1	A	623	PHE	CB-CG-CD1	12.37	129.46	120.80
1	G	623	PHE	CB-CG-CD1	12.35	129.45	120.80
1	J	623	PHE	CB-CG-CD1	12.33	129.43	120.80
1	J	623	PHE	CA-CB-CG	-12.27	84.47	113.90
1	A	623	PHE	CA-CB-CG	-12.26	84.48	113.90
1	D	623	PHE	CA-CB-CG	-12.23	84.54	113.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	623	PHE	CA-CB-CG	-12.21	84.59	113.90
1	D	623	PHE	CB-CG-CD1	12.03	129.22	120.80
1	J	98	HIS	CB-CA-C	-11.57	87.27	110.40
1	A	98	HIS	CB-CA-C	-11.56	87.29	110.40
1	G	98	HIS	CB-CA-C	-11.55	87.29	110.40
1	D	98	HIS	CB-CA-C	-11.54	87.33	110.40
1	G	568	PRO	O-C-N	10.71	139.83	122.70
1	A	568	PRO	O-C-N	10.67	139.78	122.70
1	D	568	PRO	O-C-N	10.66	139.76	122.70
1	J	568	PRO	O-C-N	10.58	139.63	122.70
1	J	709	LYS	C-N-CA	10.30	143.93	122.30
2	E	141	PRO	CA-N-CD	10.30	126.11	111.70
2	H	141	PRO	CA-N-CD	10.27	126.08	111.70
2	K	141	PRO	CA-N-CD	10.21	125.99	111.70
2	B	141	PRO	CA-N-CD	10.18	125.95	111.70
1	G	625	THR	CA-CB-CG2	-10.10	98.26	112.40
1	A	327	ASP	CB-CG-OD1	-10.06	109.24	118.30
1	G	327	ASP	CB-CG-OD1	-10.05	109.25	118.30
1	J	327	ASP	CB-CG-OD1	-10.04	109.26	118.30
1	A	625	THR	CA-CB-CG2	-10.03	98.35	112.40
1	J	625	THR	CA-CB-CG2	-10.03	98.36	112.40
1	D	625	THR	CA-CB-CG2	-10.02	98.38	112.40
1	D	327	ASP	CB-CG-OD1	-10.00	109.30	118.30
1	A	241	ASP	CB-CG-OD1	-9.85	109.44	118.30
1	G	241	ASP	CB-CG-OD1	-9.80	109.48	118.30
3	C	63	ILE	O-C-N	9.80	138.38	122.70
1	D	728	ASN	O-C-N	9.76	138.32	122.70
1	J	241	ASP	CB-CG-OD1	-9.73	109.54	118.30
1	D	241	ASP	CB-CG-OD1	-9.73	109.55	118.30
3	I	63	ILE	O-C-N	9.72	138.25	122.70
3	F	63	ILE	O-C-N	9.71	138.23	122.70
1	A	728	ASN	O-C-N	9.68	138.19	122.70
1	J	728	ASN	O-C-N	9.67	138.17	122.70
3	L	63	ILE	O-C-N	9.66	138.16	122.70
1	G	728	ASN	O-C-N	9.60	138.06	122.70
1	G	264	ASP	CB-CG-OD2	-9.50	109.75	118.30
1	D	264	ASP	CB-CG-OD2	-9.42	109.82	118.30
1	A	264	ASP	CB-CG-OD2	-9.42	109.82	118.30
1	J	709	LYS	CA-C-N	9.42	135.04	116.20
2	E	150	TYR	N-CA-CB	-9.40	93.68	110.60
1	J	264	ASP	CB-CG-OD2	-9.38	109.86	118.30
2	H	150	TYR	N-CA-CB	-9.36	93.75	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	150	TYR	N-CA-CB	-9.36	93.75	110.60
2	B	150	TYR	N-CA-CB	-9.28	93.90	110.60
4	W	356	TRP	CD1-CG-CD2	9.18	113.64	106.30
4	8	356	TRP	CD1-CG-CD2	9.17	113.64	106.30
4	Y	356	TRP	CD1-CG-CD2	9.17	113.64	106.30
4	3	356	TRP	CD1-CG-CD2	9.17	113.63	106.30
4	2	356	TRP	CD1-CG-CD2	9.16	113.63	106.30
4	5	356	TRP	CD1-CG-CD2	9.16	113.63	106.30
4	0	356	TRP	CD1-CG-CD2	9.14	113.61	106.30
4	6	356	TRP	CD1-CG-CD2	9.11	113.59	106.30
4	4	356	TRP	CD1-CG-CD2	9.10	113.58	106.30
4	V	356	TRP	CD1-CG-CD2	9.10	113.58	106.30
4	7	356	TRP	CD1-CG-CD2	9.10	113.58	106.30
4	X	356	TRP	CD1-CG-CD2	9.06	113.54	106.30
4	Z	356	TRP	CD1-CG-CD2	9.04	113.53	106.30
4	1	356	TRP	CD1-CG-CD2	9.02	113.51	106.30
1	J	378	ASP	CB-CG-OD2	8.98	126.39	118.30
1	J	352	TYR	CB-CG-CD1	8.97	126.38	121.00
1	D	378	ASP	CB-CG-OD2	8.95	126.35	118.30
1	A	378	ASP	CB-CG-OD2	8.92	126.32	118.30
1	G	378	ASP	CB-CG-OD2	8.91	126.32	118.30
1	G	352	TYR	CB-CG-CD1	8.84	126.30	121.00
4	2	177	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	D	352	TYR	CB-CG-CD1	8.77	126.26	121.00
2	K	138	ALA	O-C-N	-8.74	108.72	122.70
2	E	138	ALA	O-C-N	-8.72	108.75	122.70
1	A	352	TYR	CB-CG-CD1	8.72	126.23	121.00
4	4	177	ARG	NE-CZ-NH2	-8.70	115.95	120.30
2	B	138	ALA	O-C-N	-8.70	108.79	122.70
2	H	138	ALA	O-C-N	-8.65	108.86	122.70
4	7	177	ARG	NE-CZ-NH2	-8.64	115.98	120.30
4	W	177	ARG	NE-CZ-NH2	-8.57	116.02	120.30
4	4	86	TRP	CD1-CG-CD2	8.53	113.13	106.30
4	Y	86	TRP	CD1-CG-CD2	8.53	113.12	106.30
1	D	601	ASP	CB-CG-OD1	-8.52	110.63	118.30
4	X	177	ARG	NE-CZ-NH2	-8.52	116.04	120.30
4	X	86	TRP	CD1-CG-CD2	8.52	113.11	106.30
1	G	601	ASP	CB-CG-OD1	-8.51	110.64	118.30
4	8	177	ARG	NE-CZ-NH2	-8.50	116.05	120.30
4	7	86	TRP	CD1-CG-CD2	8.49	113.09	106.30
1	J	601	ASP	CB-CG-OD1	-8.49	110.66	118.30
4	0	177	ARG	NE-CZ-NH2	-8.48	116.06	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	177	ARG	NE-CZ-NH2	-8.47	116.06	120.30
4	V	177	ARG	NE-CZ-NH2	-8.47	116.06	120.30
4	Z	177	ARG	NE-CZ-NH2	-8.47	116.06	120.30
4	5	86	TRP	CD1-CG-CD2	8.47	113.08	106.30
4	6	86	TRP	CD1-CG-CD2	8.46	113.07	106.30
4	Z	86	TRP	CD1-CG-CD2	8.46	113.07	106.30
4	2	86	TRP	CD1-CG-CD2	8.46	113.07	106.30
4	1	177	ARG	NE-CZ-NH2	-8.46	116.07	120.30
4	3	177	ARG	NE-CZ-NH2	-8.46	116.07	120.30
4	6	177	ARG	NE-CZ-NH2	-8.46	116.07	120.30
4	8	86	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	J	33	ASP	CB-CG-OD1	-8.44	110.71	118.30
4	0	86	TRP	CD1-CG-CD2	8.44	113.05	106.30
4	V	86	TRP	CD1-CG-CD2	8.43	113.04	106.30
1	A	601	ASP	CB-CG-OD1	-8.42	110.72	118.30
4	3	86	TRP	CD1-CG-CD2	8.42	113.03	106.30
4	W	86	TRP	CD1-CG-CD2	8.41	113.03	106.30
1	J	352	TYR	CB-CG-CD2	-8.38	115.97	121.00
1	G	33	ASP	CB-CG-OD1	-8.36	110.78	118.30
4	1	86	TRP	CD1-CG-CD2	8.36	112.99	106.30
1	A	352	TYR	CB-CG-CD2	-8.33	116.00	121.00
1	D	33	ASP	CB-CG-OD1	-8.27	110.85	118.30
4	Y	177	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	A	33	ASP	CB-CG-OD1	-8.22	110.90	118.30
1	G	352	TYR	CB-CG-CD2	-8.18	116.09	121.00
1	D	352	TYR	CB-CG-CD2	-8.10	116.14	121.00
1	A	339	ASP	CB-CG-OD1	-8.04	111.06	118.30
4	3	356	TRP	CE2-CD2-CG	-8.04	100.87	107.30
4	Y	356	TRP	CE2-CD2-CG	-8.01	100.89	107.30
4	5	356	TRP	CE2-CD2-CG	-8.00	100.90	107.30
4	V	356	TRP	CE2-CD2-CG	-8.00	100.90	107.30
4	8	356	TRP	CE2-CD2-CG	-7.99	100.91	107.30
4	0	356	TRP	CE2-CD2-CG	-7.99	100.91	107.30
4	7	356	TRP	CE2-CD2-CG	-7.99	100.91	107.30
4	6	356	TRP	CE2-CD2-CG	-7.98	100.92	107.30
4	W	356	TRP	CE2-CD2-CG	-7.97	100.92	107.30
1	D	637	LYS	CA-C-N	7.93	132.06	116.20
4	2	356	TRP	CE2-CD2-CG	-7.92	100.96	107.30
4	X	356	TRP	CE2-CD2-CG	-7.92	100.97	107.30
1	A	637	LYS	CA-C-N	7.91	132.01	116.20
1	G	339	ASP	CB-CG-OD1	-7.91	111.18	118.30
1	J	637	LYS	CA-C-N	7.91	132.01	116.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Z	356	TRP	CE2-CD2-CG	-7.90	100.98	107.30
2	E	150	TYR	CD1-CE1-CZ	-7.90	112.69	119.80
1	G	637	LYS	CA-C-N	7.89	131.97	116.20
1	D	339	ASP	CB-CG-OD1	-7.88	111.21	118.30
4	1	356	TRP	CE2-CD2-CG	-7.87	101.00	107.30
2	H	150	TYR	CD1-CE1-CZ	-7.87	112.72	119.80
4	4	356	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	J	339	ASP	CB-CG-OD1	-7.84	111.24	118.30
1	A	202	SER	CB-CA-C	-7.78	95.31	110.10
2	B	150	TYR	CD1-CE1-CZ	-7.76	112.81	119.80
1	D	202	SER	CB-CA-C	-7.76	95.35	110.10
2	K	150	TYR	CD1-CE1-CZ	-7.74	112.83	119.80
1	J	202	SER	CB-CA-C	-7.73	95.41	110.10
4	0	312	ARG	NE-CZ-NH2	7.73	124.17	120.30
1	G	202	SER	CB-CA-C	-7.72	95.44	110.10
4	1	312	ARG	NE-CZ-NH2	7.69	124.15	120.30
1	G	654	ARG	NE-CZ-NH1	7.68	124.14	120.30
4	X	312	ARG	NE-CZ-NH2	7.68	124.14	120.30
4	5	312	ARG	NE-CZ-NH2	7.68	124.14	120.30
4	3	312	ARG	NE-CZ-NH2	7.66	124.13	120.30
1	J	653	PHE	CB-CG-CD1	-7.66	115.44	120.80
4	Y	312	ARG	NE-CZ-NH2	7.65	124.13	120.30
1	D	653	PHE	CB-CG-CD1	-7.65	115.45	120.80
4	X	86	TRP	CE2-CD2-CG	-7.63	101.19	107.30
4	Z	312	ARG	NE-CZ-NH2	7.63	124.12	120.30
4	4	312	ARG	NE-CZ-NH2	7.63	124.11	120.30
4	8	312	ARG	NE-CZ-NH2	7.62	124.11	120.30
4	2	312	ARG	NE-CZ-NH2	7.60	124.10	120.30
4	8	86	TRP	CE2-CD2-CG	-7.59	101.22	107.30
4	4	86	TRP	CE2-CD2-CG	-7.58	101.24	107.30
4	V	312	ARG	NE-CZ-NH2	7.56	124.08	120.30
4	7	86	TRP	CE2-CD2-CG	-7.56	101.25	107.30
4	0	86	TRP	CE2-CD2-CG	-7.56	101.25	107.30
4	6	312	ARG	NE-CZ-NH2	7.56	124.08	120.30
1	A	654	ARG	NE-CZ-NH1	7.55	124.08	120.30
4	Y	86	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	G	653	PHE	CB-CG-CD1	-7.54	115.52	120.80
4	7	312	ARG	NE-CZ-NH2	7.53	124.06	120.30
2	E	127	ARG	NE-CZ-NH2	7.52	124.06	120.30
4	2	86	TRP	CE2-CD2-CG	-7.52	101.28	107.30
4	V	86	TRP	CE2-CD2-CG	-7.52	101.28	107.30
3	C	63	ILE	CG1-CB-CG2	-7.52	94.86	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	86	TRP	CE2-CD2-CG	-7.51	101.29	107.30
4	W	86	TRP	CE2-CD2-CG	-7.51	101.29	107.30
4	W	312	ARG	NE-CZ-NH2	7.49	124.05	120.30
4	3	86	TRP	CE2-CD2-CG	-7.49	101.31	107.30
3	F	63	ILE	CG1-CB-CG2	-7.48	94.94	111.40
1	G	346	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	J	654	ARG	NE-CZ-NH1	7.47	124.04	120.30
3	L	63	ILE	CG1-CB-CG2	-7.47	94.96	111.40
3	I	63	ILE	CG1-CB-CG2	-7.47	94.97	111.40
4	6	86	TRP	CE2-CD2-CG	-7.46	101.33	107.30
4	Z	86	TRP	CE2-CD2-CG	-7.46	101.33	107.30
4	1	86	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	A	653	PHE	CB-CG-CD1	-7.46	115.58	120.80
1	J	518	ASP	CB-CG-OD1	-7.43	111.61	118.30
1	A	518	ASP	CB-CG-OD1	-7.40	111.64	118.30
4	1	254	ARG	NE-CZ-NH2	-7.40	116.60	120.30
3	I	63	ILE	CA-C-N	-7.39	100.94	117.20
4	W	180	LEU	CA-CB-CG	7.39	132.29	115.30
4	0	233	SER	CA-C-N	-7.38	100.95	117.20
4	W	233	SER	CA-C-N	-7.38	100.96	117.20
4	6	233	SER	CA-C-N	-7.38	100.97	117.20
4	X	233	SER	CA-C-N	-7.37	100.98	117.20
4	1	233	SER	CA-C-N	-7.37	100.98	117.20
2	B	127	ARG	NE-CZ-NH2	7.37	123.98	120.30
1	D	346	ASP	CB-CG-OD2	-7.37	111.67	118.30
1	D	654	ARG	NE-CZ-NH1	7.37	123.98	120.30
4	8	233	SER	CA-C-N	-7.37	101.00	117.20
4	3	233	SER	CA-C-N	-7.36	101.00	117.20
4	5	233	SER	CA-C-N	-7.36	101.00	117.20
1	D	518	ASP	CB-CG-OD1	-7.36	111.68	118.30
4	4	233	SER	CA-C-N	-7.36	101.02	117.20
4	7	233	SER	CA-C-N	-7.36	101.01	117.20
3	C	63	ILE	CA-C-N	-7.36	101.02	117.20
4	V	233	SER	CA-C-N	-7.36	101.02	117.20
4	7	180	LEU	CA-CB-CG	7.35	132.21	115.30
4	1	180	LEU	CA-CB-CG	7.35	132.20	115.30
4	Z	233	SER	CA-C-N	-7.35	101.03	117.20
4	2	233	SER	CA-C-N	-7.35	101.04	117.20
4	6	180	LEU	CA-CB-CG	7.34	132.19	115.30
4	3	180	LEU	CA-CB-CG	7.34	132.19	115.30
4	5	180	LEU	CA-CB-CG	7.34	132.19	115.30
3	L	63	ILE	CA-C-N	-7.34	101.05	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	180	LEU	CA-CB-CG	7.34	132.18	115.30
4	0	180	LEU	CA-CB-CG	7.33	132.17	115.30
4	V	180	LEU	CA-CB-CG	7.33	132.16	115.30
4	Y	233	SER	CA-C-N	-7.33	101.08	117.20
1	A	346	ASP	CB-CG-OD2	-7.33	111.71	118.30
4	4	180	LEU	CA-CB-CG	7.33	132.15	115.30
4	8	180	LEU	CA-CB-CG	7.32	132.14	115.30
3	F	63	ILE	CA-C-N	-7.31	101.11	117.20
4	2	180	LEU	CA-CB-CG	7.31	132.12	115.30
4	Y	180	LEU	CA-CB-CG	7.31	132.10	115.30
4	Z	180	LEU	CA-CB-CG	7.30	132.09	115.30
1	G	104	TYR	CB-CG-CD2	7.30	125.38	121.00
4	2	254	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	J	346	ASP	CB-CG-OD2	-7.29	111.73	118.30
4	W	254	ARG	NE-CZ-NH2	-7.29	116.66	120.30
4	4	254	ARG	NE-CZ-NH2	-7.28	116.66	120.30
4	X	79	TRP	CD1-CG-CD2	7.26	112.11	106.30
1	J	104	TYR	CB-CG-CD2	7.26	125.36	121.00
1	G	518	ASP	CB-CG-OD1	-7.25	111.78	118.30
4	V	254	ARG	NE-CZ-NH2	-7.25	116.68	120.30
4	5	254	ARG	NE-CZ-NH2	-7.23	116.69	120.30
4	1	79	TRP	CD1-CG-CD2	7.22	112.07	106.30
4	V	340	TRP	CE2-CD2-CG	-7.21	101.53	107.30
4	X	254	ARG	NE-CZ-NH2	-7.21	116.69	120.30
4	8	254	ARG	NE-CZ-NH2	-7.21	116.70	120.30
4	5	79	TRP	CD1-CG-CD2	7.21	112.06	106.30
4	6	340	TRP	CE2-CD2-CG	-7.20	101.54	107.30
4	W	340	TRP	CE2-CD2-CG	-7.20	101.54	107.30
4	5	340	TRP	CE2-CD2-CG	-7.20	101.54	107.30
4	2	79	TRP	CD1-CG-CD2	7.19	112.06	106.30
4	V	206	ARG	NE-CZ-NH1	7.19	123.90	120.30
4	3	340	TRP	CE2-CD2-CG	-7.18	101.55	107.30
4	0	79	TRP	CD1-CG-CD2	7.17	112.04	106.30
4	2	340	TRP	CE2-CD2-CG	-7.17	101.56	107.30
4	0	340	TRP	CE2-CD2-CG	-7.16	101.57	107.30
4	3	206	ARG	NE-CZ-NH1	7.16	123.88	120.30
4	8	79	TRP	CD1-CG-CD2	7.16	112.02	106.30
1	A	148	ARG	NE-CZ-NH2	-7.15	116.72	120.30
4	6	79	TRP	CD1-CG-CD2	7.15	112.02	106.30
4	Y	340	TRP	CE2-CD2-CG	-7.15	101.58	107.30
4	Z	340	TRP	CE2-CD2-CG	-7.15	101.58	107.30
4	Y	254	ARG	NE-CZ-NH2	-7.15	116.73	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1	340	TRP	CE2-CD2-CG	-7.15	101.58	107.30
4	Z	79	TRP	CD1-CG-CD2	7.15	112.02	106.30
4	W	206	ARG	NE-CZ-NH1	7.14	123.87	120.30
4	7	340	TRP	CE2-CD2-CG	-7.14	101.59	107.30
4	1	206	ARG	NE-CZ-NH1	7.14	123.87	120.30
4	4	79	TRP	CD1-CG-CD2	7.14	112.01	106.30
4	4	340	TRP	CE2-CD2-CG	-7.14	101.59	107.30
4	V	79	TRP	CD1-CG-CD2	7.14	112.01	106.30
1	G	568	PRO	CA-C-N	-7.13	101.51	117.20
1	A	104	TYR	CB-CG-CD2	7.13	125.28	121.00
4	Y	79	TRP	CD1-CG-CD2	7.13	112.01	106.30
2	K	150	TYR	CB-CG-CD1	-7.12	116.73	121.00
4	7	79	TRP	CD1-CG-CD2	7.12	112.00	106.30
4	W	79	TRP	CD1-CG-CD2	7.12	112.00	106.30
4	X	340	TRP	CE2-CD2-CG	-7.12	101.61	107.30
4	6	254	ARG	NE-CZ-NH2	-7.11	116.75	120.30
4	8	206	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	A	568	PRO	CA-C-N	-7.10	101.57	117.20
2	K	127	ARG	NE-CZ-NH2	7.10	123.85	120.30
4	7	254	ARG	NE-CZ-NH2	-7.10	116.75	120.30
4	X	79	TRP	CE2-CD2-CG	-7.10	101.62	107.30
4	3	340	TRP	CD1-CG-CD2	7.09	111.97	106.30
4	5	206	ARG	NE-CZ-NH1	7.09	123.84	120.30
4	3	79	TRP	CD1-CG-CD2	7.08	111.97	106.30
1	D	568	PRO	CA-C-N	-7.08	101.63	117.20
4	0	254	ARG	NE-CZ-NH2	-7.08	116.76	120.30
4	6	206	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	J	568	PRO	CA-C-N	-7.07	101.64	117.20
4	2	206	ARG	NE-CZ-NH1	7.07	123.84	120.30
4	4	206	ARG	NE-CZ-NH1	7.07	123.83	120.30
2	H	127	ARG	NE-CZ-NH2	7.06	123.83	120.30
4	X	206	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	D	218	LEU	CB-CG-CD1	7.05	122.99	111.00
4	1	47	MET	CA-CB-CG	-7.05	101.31	113.30
1	A	264	ASP	N-CA-CB	-7.04	97.92	110.60
4	6	47	MET	CA-CB-CG	-7.04	101.34	113.30
4	7	206	ARG	NE-CZ-NH1	7.04	123.82	120.30
4	8	47	MET	CA-CB-CG	-7.04	101.34	113.30
4	0	47	MET	CA-CB-CG	-7.03	101.35	113.30
4	Z	254	ARG	NE-CZ-NH2	-7.03	116.78	120.30
4	8	340	TRP	CE2-CD2-CG	-7.02	101.68	107.30
4	Z	47	MET	CA-CB-CG	-7.02	101.36	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	206	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	D	217	THR	N-CA-CB	7.01	123.63	110.30
4	8	79	TRP	CE2-CD2-CG	-7.01	101.69	107.30
4	X	47	MET	CA-CB-CG	-7.01	101.38	113.30
4	0	206	ARG	NE-CZ-NH1	7.01	123.81	120.30
4	3	47	MET	CA-CB-CG	-7.01	101.38	113.30
4	V	47	MET	CA-CB-CG	-7.01	101.38	113.30
4	W	47	MET	CA-CB-CG	-7.01	101.38	113.30
1	J	264	ASP	N-CA-CB	-7.01	97.99	110.60
4	0	79	TRP	CE2-CD2-CG	-7.01	101.69	107.30
4	2	47	MET	CA-CB-CG	-7.01	101.39	113.30
1	D	104	TYR	CB-CG-CD2	7.00	125.20	121.00
1	J	218	LEU	CB-CG-CD1	7.00	122.90	111.00
4	W	79	TRP	CE2-CD2-CG	-7.00	101.70	107.30
4	4	47	MET	CA-CB-CG	-7.00	101.40	113.30
4	5	47	MET	CA-CB-CG	-7.00	101.40	113.30
4	7	47	MET	CA-CB-CG	-7.00	101.41	113.30
4	Z	206	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	D	264	ASP	N-CA-CB	-7.00	98.01	110.60
1	G	217	THR	N-CA-CB	6.99	123.58	110.30
1	G	218	LEU	CB-CG-CD1	6.99	122.89	111.00
4	W	340	TRP	CD1-CG-CD2	6.99	111.89	106.30
4	5	79	TRP	CE2-CD2-CG	-6.98	101.71	107.30
4	1	79	TRP	CE2-CD2-CG	-6.98	101.72	107.30
1	G	264	ASP	N-CA-CB	-6.98	98.04	110.60
4	2	79	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	J	148	ARG	NE-CZ-NH2	-6.97	116.81	120.30
4	Z	79	TRP	CE2-CD2-CG	-6.97	101.72	107.30
4	Z	340	TRP	CD1-CG-CD2	6.97	111.88	106.30
4	Y	47	MET	CA-CB-CG	-6.97	101.45	113.30
1	J	217	THR	N-CA-CB	6.96	123.52	110.30
1	A	218	LEU	CB-CG-CD1	6.96	122.83	111.00
4	7	340	TRP	CD1-CG-CD2	6.96	111.86	106.30
2	B	150	TYR	CB-CG-CD1	-6.95	116.83	121.00
4	2	340	TRP	CD1-CG-CD2	6.95	111.86	106.30
4	Y	340	TRP	CD1-CG-CD2	6.95	111.86	106.30
4	5	340	TRP	CD1-CG-CD2	6.95	111.86	106.30
1	A	217	THR	N-CA-CB	6.94	123.49	110.30
4	6	340	TRP	CD1-CG-CD2	6.94	111.86	106.30
4	V	79	TRP	CE2-CD2-CG	-6.94	101.75	107.30
2	H	150	TYR	CB-CG-CD1	-6.93	116.84	121.00
4	3	254	ARG	NE-CZ-NH2	-6.93	116.83	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	340	TRP	CD1-CG-CD2	6.93	111.85	106.30
4	Y	79	TRP	CE2-CD2-CG	-6.93	101.75	107.30
4	X	340	TRP	CD1-CG-CD2	6.93	111.84	106.30
4	1	340	TRP	CD1-CG-CD2	6.93	111.84	106.30
4	4	79	TRP	CE2-CD2-CG	-6.92	101.76	107.30
4	0	340	TRP	CD1-CG-CD2	6.92	111.84	106.30
4	7	79	TRP	CE2-CD2-CG	-6.92	101.76	107.30
4	3	79	TRP	CE2-CD2-CG	-6.92	101.76	107.30
4	V	340	TRP	CD1-CG-CD2	6.92	111.83	106.30
2	E	150	TYR	CB-CG-CD1	-6.91	116.85	121.00
4	6	79	TRP	CE2-CD2-CG	-6.91	101.77	107.30
1	A	75	ASP	N-CA-CB	6.91	123.03	110.60
1	D	728	ASN	CA-C-N	-6.90	102.02	117.20
1	G	75	ASP	N-CA-CB	6.90	123.02	110.60
4	8	340	TRP	CD1-CG-CD2	6.89	111.81	106.30
1	G	148	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	J	75	ASP	N-CA-CB	6.86	122.94	110.60
1	J	728	ASN	CA-C-N	-6.85	102.13	117.20
1	G	728	ASN	CA-C-N	-6.85	102.14	117.20
1	G	450	ASP	CB-CG-OD2	6.85	124.46	118.30
1	A	728	ASN	CA-C-N	-6.84	102.14	117.20
1	D	450	ASP	CB-CG-OD2	6.83	124.45	118.30
1	J	450	ASP	CB-CG-OD2	6.83	124.45	118.30
1	D	148	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	A	450	ASP	CB-CG-OD2	6.79	124.41	118.30
1	D	75	ASP	N-CA-CB	6.76	122.77	110.60
1	D	781	ASP	CB-CG-OD1	-6.73	112.24	118.30
1	J	75	ASP	CB-CG-OD2	6.70	124.33	118.30
1	J	219	GLU	N-CA-C	-6.69	92.94	111.00
1	G	756	THR	N-CA-CB	-6.68	97.61	110.30
1	D	756	THR	N-CA-CB	-6.66	97.64	110.30
1	J	756	THR	N-CA-CB	-6.66	97.64	110.30
4	V	169	TYR	CB-CG-CD2	-6.65	117.01	121.00
1	G	219	GLU	N-CA-C	-6.65	93.04	111.00
1	A	343	PHE	CB-CG-CD1	6.65	125.45	120.80
1	G	781	ASP	CB-CG-OD1	-6.64	112.32	118.30
1	G	555	TYR	CB-CG-CD2	-6.64	117.01	121.00
1	J	555	TYR	CB-CG-CD2	-6.64	117.02	121.00
1	A	75	ASP	CB-CG-OD2	6.63	124.27	118.30
1	A	756	THR	N-CA-CB	-6.63	97.70	110.30
4	2	169	TYR	CB-CG-CD2	-6.63	117.02	121.00
4	5	196	ARG	NE-CZ-NH1	6.62	123.61	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	781	ASP	CB-CG-OD1	-6.62	112.34	118.30
1	A	781	ASP	CB-CG-OD1	-6.60	112.36	118.30
1	D	555	TYR	CB-CG-CD2	-6.60	117.04	121.00
1	A	219	GLU	N-CA-C	-6.60	93.19	111.00
4	4	169	TYR	CB-CG-CD2	-6.57	117.06	121.00
1	D	75	ASP	CB-CG-OD2	6.57	124.21	118.30
4	X	169	TYR	CB-CG-CD2	-6.57	117.06	121.00
1	A	332	MET	CG-SD-CE	-6.56	89.70	100.20
1	D	219	GLU	N-CA-C	-6.56	93.28	111.00
1	A	555	TYR	CB-CG-CD2	-6.56	117.06	121.00
4	7	169	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	G	169	ASP	CB-CG-OD1	-6.55	112.40	118.30
1	D	332	MET	CG-SD-CE	-6.55	89.72	100.20
4	W	283	MET	CG-SD-CE	6.54	110.67	100.20
1	J	332	MET	CG-SD-CE	-6.54	89.73	100.20
4	4	283	MET	CG-SD-CE	6.54	110.67	100.20
4	6	283	MET	CG-SD-CE	6.54	110.67	100.20
4	Y	169	TYR	CB-CG-CD2	-6.54	117.08	121.00
4	5	283	MET	CG-SD-CE	6.54	110.66	100.20
4	W	196	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	G	332	MET	CG-SD-CE	-6.54	89.74	100.20
4	X	283	MET	CG-SD-CE	6.53	110.65	100.20
4	3	169	TYR	CB-CG-CD2	-6.53	117.08	121.00
4	1	283	MET	CG-SD-CE	6.53	110.65	100.20
4	6	196	ARG	NE-CZ-NH1	6.53	123.56	120.30
4	8	169	TYR	CB-CG-CD2	-6.52	117.09	121.00
4	0	283	MET	CG-SD-CE	6.52	110.63	100.20
4	2	283	MET	CG-SD-CE	6.52	110.63	100.20
4	Z	169	TYR	CB-CG-CD2	-6.52	117.09	121.00
4	5	169	TYR	CB-CG-CD2	-6.52	117.09	121.00
4	8	283	MET	CG-SD-CE	6.52	110.63	100.20
1	J	141	LEU	CB-CA-C	-6.51	97.82	110.20
4	1	169	TYR	CB-CG-CD2	-6.51	117.09	121.00
4	3	283	MET	CG-SD-CE	6.51	110.62	100.20
4	7	283	MET	CG-SD-CE	6.51	110.62	100.20
4	Y	283	MET	CG-SD-CE	6.51	110.61	100.20
4	3	159	VAL	CB-CA-C	-6.51	99.04	111.40
4	8	196	ARG	NE-CZ-NH1	6.51	123.55	120.30
4	V	283	MET	CG-SD-CE	6.51	110.61	100.20
1	J	334	THR	CA-CB-CG2	-6.50	103.30	112.40
1	G	590	TYR	CB-CG-CD2	6.50	124.90	121.00
1	D	334	THR	CA-CB-CG2	-6.50	103.31	112.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	141	LEU	CB-CA-C	-6.50	97.86	110.20
4	V	196	ARG	NE-CZ-NH1	6.50	123.55	120.30
4	Z	159	VAL	CB-CA-C	-6.49	99.07	111.40
4	Z	283	MET	CG-SD-CE	6.49	110.59	100.20
1	A	169	ASP	CB-CG-OD1	-6.49	112.46	118.30
4	0	169	TYR	CB-CG-CD2	-6.49	117.11	121.00
2	E	141	PRO	N-CD-CG	-6.49	93.47	103.20
4	2	159	VAL	CB-CA-C	-6.49	99.08	111.40
4	V	159	VAL	CB-CA-C	-6.49	99.08	111.40
1	J	169	ASP	CB-CG-OD1	-6.48	112.47	118.30
4	5	159	VAL	CB-CA-C	-6.48	99.09	111.40
4	Y	196	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	G	334	THR	CA-CB-CG2	-6.48	103.33	112.40
4	0	159	VAL	CB-CA-C	-6.48	99.09	111.40
4	1	159	VAL	CB-CA-C	-6.48	99.09	111.40
4	6	159	VAL	CB-CA-C	-6.47	99.10	111.40
4	8	159	VAL	CB-CA-C	-6.47	99.10	111.40
4	0	196	ARG	NE-CZ-NH1	6.47	123.54	120.30
4	7	196	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	D	141	LEU	CB-CA-C	-6.47	97.91	110.20
2	H	141	PRO	N-CD-CG	-6.47	93.50	103.20
4	4	159	VAL	CB-CA-C	-6.47	99.11	111.40
4	X	159	VAL	CB-CA-C	-6.47	99.11	111.40
4	6	169	TYR	CB-CG-CD2	-6.46	117.12	121.00
4	W	159	VAL	CB-CA-C	-6.46	99.12	111.40
4	1	196	ARG	NE-CZ-NH1	6.46	123.53	120.30
4	Y	159	VAL	CB-CA-C	-6.46	99.13	111.40
1	D	169	ASP	CB-CG-OD1	-6.46	112.49	118.30
4	7	159	VAL	CB-CA-C	-6.46	99.13	111.40
4	W	169	TYR	CB-CG-CD2	-6.46	117.13	121.00
4	Z	196	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	334	THR	CA-CB-CG2	-6.45	103.37	112.40
4	2	196	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	141	LEU	CB-CA-C	-6.44	97.96	110.20
1	D	343	PHE	CB-CG-CD1	6.44	125.31	120.80
4	0	34	ILE	CA-CB-CG2	-6.44	98.03	110.90
1	G	589	ASP	CB-CG-OD1	-6.43	112.51	118.30
1	G	343	PHE	CB-CG-CD1	6.42	125.30	120.80
1	G	75	ASP	CB-CG-OD2	6.41	124.07	118.30
4	W	34	ILE	CA-CB-CG2	-6.41	98.07	110.90
1	J	589	ASP	CB-CG-OD1	-6.41	112.53	118.30
4	7	34	ILE	CA-CB-CG2	-6.41	98.08	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	6	34	ILE	CA-CB-CG2	-6.41	98.09	110.90
1	A	589	ASP	CB-CG-OD1	-6.41	112.54	118.30
4	4	34	ILE	CA-CB-CG2	-6.41	98.09	110.90
4	8	34	ILE	CA-CB-CG2	-6.41	98.09	110.90
4	X	34	ILE	CA-CB-CG2	-6.41	98.09	110.90
4	Z	34	ILE	CA-CB-CG2	-6.40	98.09	110.90
4	2	34	ILE	CA-CB-CG2	-6.40	98.10	110.90
4	3	34	ILE	CA-CB-CG2	-6.39	98.11	110.90
4	3	196	ARG	NE-CZ-NH1	6.39	123.50	120.30
4	1	34	ILE	CA-CB-CG2	-6.39	98.13	110.90
1	J	810	ARG	NE-CZ-NH1	6.38	123.49	120.30
4	4	196	ARG	NE-CZ-NH1	6.38	123.49	120.30
2	K	141	PRO	N-CD-CG	-6.37	93.64	103.20
4	5	34	ILE	CA-CB-CG2	-6.37	98.15	110.90
4	V	34	ILE	CA-CB-CG2	-6.37	98.15	110.90
1	D	129	TYR	CB-CG-CD2	-6.37	117.18	121.00
1	J	327	ASP	CB-CG-OD2	6.37	124.03	118.30
4	Y	34	ILE	CA-CB-CG2	-6.36	98.17	110.90
4	X	196	ARG	NE-CZ-NH1	6.36	123.48	120.30
2	B	141	PRO	N-CD-CG	-6.35	93.68	103.20
1	D	589	ASP	CB-CG-OD1	-6.35	112.59	118.30
1	G	578	HIS	N-CA-CB	6.33	122.00	110.60
1	J	129	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	A	341	LEU	CB-CA-C	6.33	122.23	110.20
1	G	341	LEU	CB-CA-C	6.33	122.22	110.20
1	J	341	LEU	CB-CA-C	6.32	122.20	110.20
4	Z	217	CYS	CA-CB-SG	-6.31	102.64	114.00
1	J	779	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	G	129	TYR	CB-CG-CD2	-6.30	117.22	121.00
4	3	217	CYS	CA-CB-SG	-6.30	102.67	114.00
4	7	217	CYS	CA-CB-SG	-6.30	102.67	114.00
1	A	578	HIS	N-CA-CB	6.29	121.93	110.60
4	5	217	CYS	CA-CB-SG	-6.29	102.67	114.00
4	2	217	CYS	CA-CB-SG	-6.29	102.67	114.00
4	4	217	CYS	CA-CB-SG	-6.29	102.68	114.00
4	0	217	CYS	CA-CB-SG	-6.28	102.69	114.00
4	Y	217	CYS	CA-CB-SG	-6.28	102.69	114.00
1	J	343	PHE	CB-CG-CD1	6.28	125.19	120.80
1	J	578	HIS	N-CA-CB	6.28	121.90	110.60
4	8	217	CYS	CA-CB-SG	-6.28	102.70	114.00
4	W	217	CYS	CA-CB-SG	-6.27	102.71	114.00
4	V	217	CYS	CA-CB-SG	-6.27	102.72	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1	217	CYS	CA-CB-SG	-6.27	102.72	114.00
1	D	341	LEU	CB-CA-C	6.27	122.11	110.20
4	X	217	CYS	CA-CB-SG	-6.27	102.72	114.00
4	6	217	CYS	CA-CB-SG	-6.26	102.73	114.00
1	A	129	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	D	578	HIS	N-CA-CB	6.24	121.83	110.60
1	J	760	PHE	CB-CG-CD2	-6.22	116.45	120.80
2	K	129	THR	CB-CA-C	-6.22	94.81	111.60
1	A	780	ASP	CB-CG-OD2	6.21	123.89	118.30
1	D	760	PHE	CB-CG-CD2	-6.21	116.45	120.80
1	A	463	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	327	ASP	CB-CG-OD2	6.20	123.88	118.30
2	B	129	THR	CB-CA-C	-6.19	94.88	111.60
1	D	327	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	698	ASN	CB-CA-C	-6.19	98.02	110.40
2	H	129	THR	CB-CA-C	-6.19	94.89	111.60
1	J	214	MET	CG-SD-CE	6.18	110.10	100.20
2	E	129	THR	CB-CA-C	-6.17	94.94	111.60
1	D	214	MET	CG-SD-CE	6.17	110.07	100.20
2	K	141	PRO	N-CA-CB	-6.17	95.82	102.60
1	G	214	MET	CG-SD-CE	6.16	110.06	100.20
1	G	327	ASP	CB-CG-OD2	6.16	123.84	118.30
1	J	463	ASP	CB-CG-OD2	-6.16	112.76	118.30
2	H	141	PRO	N-CA-CB	-6.15	95.84	102.60
1	A	214	MET	CG-SD-CE	6.14	110.03	100.20
4	4	259	GLU	CA-CB-CG	6.14	126.92	113.40
1	D	590	TYR	CB-CG-CD2	6.14	124.69	121.00
3	F	58	MET	CG-SD-CE	6.14	110.02	100.20
4	X	259	GLU	CA-CB-CG	6.14	126.91	113.40
1	G	104	TYR	CB-CG-CD1	-6.13	117.32	121.00
4	1	259	GLU	CA-CB-CG	6.13	126.90	113.40
4	Y	259	GLU	CA-CB-CG	6.13	126.89	113.40
4	2	259	GLU	CA-CB-CG	6.13	126.89	113.40
4	3	259	GLU	CA-CB-CG	6.13	126.89	113.40
4	Z	259	GLU	CA-CB-CG	6.13	126.89	113.40
1	A	760	PHE	CB-CG-CD2	-6.13	116.51	120.80
1	D	698	ASN	CB-CA-C	-6.13	98.14	110.40
4	W	259	GLU	CA-CB-CG	6.13	126.88	113.40
4	V	259	GLU	CA-CB-CG	6.13	126.88	113.40
4	0	259	GLU	CA-CB-CG	6.12	126.87	113.40
2	E	129	THR	CA-CB-CG2	6.12	120.96	112.40
4	6	259	GLU	CA-CB-CG	6.12	126.86	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	590	TYR	CB-CG-CD2	6.12	124.67	121.00
1	D	104	TYR	CB-CG-CD1	-6.12	117.33	121.00
4	5	259	GLU	CA-CB-CG	6.12	126.85	113.40
2	E	141	PRO	N-CA-CB	-6.11	95.87	102.60
4	7	259	GLU	CA-CB-CG	6.11	126.85	113.40
4	8	259	GLU	CA-CB-CG	6.11	126.85	113.40
1	J	752	ASP	CB-CG-OD2	6.11	123.80	118.30
1	J	104	TYR	CB-CG-CD1	-6.11	117.33	121.00
1	J	698	ASN	CB-CA-C	-6.11	98.18	110.40
3	L	58	MET	CG-SD-CE	6.10	109.97	100.20
1	G	779	ARG	NE-CZ-NH1	6.10	123.35	120.30
4	5	335	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	G	810	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	J	682	THR	CA-CB-CG2	-6.09	103.87	112.40
1	G	698	ASN	CB-CA-C	-6.09	98.23	110.40
1	G	346	ASP	CB-CG-OD1	6.08	123.78	118.30
4	W	349	LEU	CA-C-N	-6.08	103.82	117.20
1	G	463	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	G	625	THR	CA-CB-OG1	6.07	121.75	109.00
1	D	346	ASP	CB-CG-OD1	6.07	123.76	118.30
2	H	129	THR	CA-CB-CG2	6.07	120.89	112.40
4	3	349	LEU	CA-C-N	-6.07	103.86	117.20
3	I	58	MET	CG-SD-CE	6.06	109.90	100.20
4	2	349	LEU	CA-C-N	-6.06	103.87	117.20
2	B	141	PRO	N-CA-CB	-6.06	95.94	102.60
1	G	682	THR	CA-CB-CG2	-6.06	103.92	112.40
1	J	625	THR	CA-CB-OG1	6.06	121.72	109.00
1	J	590	TYR	CB-CG-CD2	6.05	124.63	121.00
4	0	349	LEU	CA-C-N	-6.05	103.89	117.20
4	7	16	LEU	CA-CB-CG	6.05	129.21	115.30
1	D	810	ARG	NE-CZ-NH1	6.05	123.32	120.30
4	0	16	LEU	CA-CB-CG	6.05	129.21	115.30
4	4	349	LEU	CA-C-N	-6.05	103.89	117.20
4	4	16	LEU	CA-CB-CG	6.05	129.21	115.30
4	V	16	LEU	CA-CB-CG	6.05	129.21	115.30
3	C	58	MET	CG-SD-CE	6.04	109.87	100.20
4	2	16	LEU	CA-CB-CG	6.04	129.20	115.30
1	D	463	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	J	450	ASP	CB-CG-OD1	-6.04	112.86	118.30
4	Y	349	LEU	CA-C-N	-6.04	103.90	117.20
2	K	129	THR	CA-CB-CG2	6.04	120.86	112.40
4	1	349	LEU	CA-C-N	-6.04	103.91	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	6	349	LEU	CA-C-N	-6.04	103.91	117.20
4	5	16	LEU	CA-CB-CG	6.04	129.19	115.30
4	8	16	LEU	CA-CB-CG	6.04	129.19	115.30
4	X	16	LEU	CA-CB-CG	6.04	129.19	115.30
4	Y	16	LEU	CA-CB-CG	6.04	129.18	115.30
4	3	16	LEU	CA-CB-CG	6.03	129.17	115.30
4	8	349	LEU	CA-C-N	-6.03	103.93	117.20
4	W	16	LEU	CA-CB-CG	6.03	129.17	115.30
1	J	192	VAL	CA-CB-CG1	-6.03	101.85	110.90
4	1	16	LEU	CA-CB-CG	6.03	129.17	115.30
1	G	760	PHE	CB-CG-CD2	-6.03	116.58	120.80
4	5	349	LEU	CA-C-N	-6.03	103.94	117.20
4	6	16	LEU	CA-CB-CG	6.03	129.16	115.30
4	Z	349	LEU	CA-C-N	-6.03	103.94	117.20
4	Z	16	LEU	CA-CB-CG	6.02	129.16	115.30
1	A	682	THR	CA-CB-CG2	-6.02	103.97	112.40
1	J	665	ARG	NE-CZ-NH2	-6.02	117.29	120.30
4	7	349	LEU	CA-C-N	-6.02	103.95	117.20
1	A	779	ARG	NE-CZ-NH1	6.02	123.31	120.30
2	B	129	THR	CA-CB-CG2	6.02	120.82	112.40
1	D	378	ASP	CB-CG-OD1	-6.01	112.89	118.30
4	6	335	ARG	NE-CZ-NH2	-6.01	117.29	120.30
4	X	349	LEU	CA-C-N	-6.01	103.97	117.20
1	A	625	THR	CA-CB-OG1	6.01	121.62	109.00
1	D	192	VAL	CA-CB-CG1	-6.01	101.89	110.90
1	D	447	GLN	N-CA-CB	6.01	121.42	110.60
1	D	682	THR	CA-CB-CG2	-6.01	103.99	112.40
4	V	349	LEU	CA-C-N	-6.01	103.98	117.20
1	A	810	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	A	447	GLN	N-CA-CB	6.00	121.41	110.60
1	G	447	GLN	N-CA-CB	6.00	121.41	110.60
1	D	625	THR	CA-CB-OG1	6.00	121.59	109.00
1	G	192	VAL	CA-CB-CG1	-5.99	101.91	110.90
1	J	447	GLN	N-CA-CB	5.99	121.38	110.60
4	Z	116	ARG	NE-CZ-NH1	5.99	123.30	120.30
4	6	116	ARG	NE-CZ-NH1	5.99	123.29	120.30
4	1	79	TRP	CG-CD2-CE3	5.98	139.28	133.90
1	D	450	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	D	780	ASP	CB-CG-OD2	5.97	123.67	118.30
1	G	780	ASP	CB-CG-OD2	5.96	123.67	118.30
1	D	754	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	G	752	ASP	CB-CG-OD2	5.96	123.66	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	116	ARG	NE-CZ-NH1	5.96	123.28	120.30
4	X	79	TRP	CG-CD2-CE3	5.95	139.26	133.90
1	G	378	ASP	CB-CG-OD1	-5.95	112.94	118.30
4	Z	335	ARG	NE-CZ-NH2	-5.95	117.33	120.30
4	3	335	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	665	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	J	378	ASP	CB-CG-OD1	-5.94	112.95	118.30
1	G	754	ASP	CB-CG-OD2	-5.94	112.96	118.30
4	Y	335	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	192	VAL	CA-CB-CG1	-5.93	102.00	110.90
4	3	116	ARG	NE-CZ-NH1	5.93	123.27	120.30
4	4	335	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	D	556	ASP	CB-CG-OD1	-5.93	112.97	118.30
4	8	79	TRP	CG-CD2-CE3	5.92	139.23	133.90
1	A	815	CYS	CA-CB-SG	-5.92	103.34	114.00
1	A	104	TYR	CB-CG-CD1	-5.92	117.45	121.00
1	D	665	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	G	450	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	J	780	ASP	CB-CG-OD2	5.91	123.62	118.30
4	V	335	ARG	NE-CZ-NH2	-5.91	117.35	120.30
4	W	335	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	D	339	ASP	CB-CG-OD2	5.90	123.61	118.30
1	G	665	ARG	NE-CZ-NH2	-5.90	117.35	120.30
4	5	254	ARG	NE-CZ-NH1	5.90	123.25	120.30
4	5	116	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	D	471	ASP	CB-CG-OD1	-5.89	113.00	118.30
4	X	335	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	G	339	ASP	CB-CG-OD2	5.89	123.60	118.30
1	J	754	ASP	CB-CG-OD2	-5.88	113.00	118.30
4	1	200	PHE	CA-C-N	-5.88	104.25	117.20
4	5	200	PHE	CA-C-N	-5.88	104.26	117.20
1	D	779	ARG	NE-CZ-NH1	5.88	123.24	120.30
4	4	200	PHE	CA-C-N	-5.88	104.26	117.20
4	7	200	PHE	CA-C-N	-5.88	104.26	117.20
4	X	200	PHE	CA-C-N	-5.88	104.26	117.20
4	5	79	TRP	CG-CD2-CE3	5.88	139.19	133.90
4	W	116	ARG	NE-CZ-NH1	5.88	123.24	120.30
4	6	200	PHE	CA-C-N	-5.88	104.28	117.20
4	W	200	PHE	CA-C-N	-5.88	104.28	117.20
1	A	450	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	A	752	ASP	CB-CG-OD2	5.87	123.58	118.30
4	Y	200	PHE	CA-C-N	-5.87	104.29	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	738	MET	CG-SD-CE	5.86	109.58	100.20
1	J	471	ASP	CB-CG-OD1	-5.86	113.02	118.30
4	8	116	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	754	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	G	738	MET	CG-SD-CE	5.86	109.58	100.20
4	0	79	TRP	CG-CD2-CE3	5.86	139.17	133.90
4	3	200	PHE	CA-C-N	-5.86	104.31	117.20
1	G	809	ARG	NE-CZ-NH2	-5.86	117.37	120.30
4	8	254	ARG	NE-CZ-NH1	5.86	123.23	120.30
4	2	335	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	D	738	MET	CG-SD-CE	5.86	109.57	100.20
1	J	738	MET	CG-SD-CE	5.86	109.57	100.20
4	2	200	PHE	CA-C-N	-5.85	104.32	117.20
1	A	378	ASP	CB-CG-OD1	-5.85	113.03	118.30
4	0	200	PHE	CA-C-N	-5.85	104.33	117.20
4	V	200	PHE	CA-C-N	-5.85	104.33	117.20
4	Z	200	PHE	CA-C-N	-5.85	104.33	117.20
1	J	346	ASP	CB-CG-OD1	5.85	123.56	118.30
4	2	116	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	G	780	ASP	CB-CG-OD1	-5.84	113.04	118.30
1	D	752	ASP	CB-CG-OD2	5.84	123.56	118.30
1	J	556	ASP	CB-CG-OD1	-5.84	113.04	118.30
4	8	200	PHE	CA-C-N	-5.84	104.36	117.20
4	4	79	TRP	CG-CD2-CE3	5.83	139.15	133.90
4	V	254	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	J	815	CYS	CA-CB-SG	-5.83	103.51	114.00
4	2	79	TRP	CG-CD2-CE3	5.82	139.14	133.90
4	Y	116	ARG	NE-CZ-NH1	5.82	123.21	120.30
4	Y	254	ARG	NE-CZ-NH1	5.82	123.21	120.30
4	8	95	ARG	CA-CB-CG	5.82	126.20	113.40
1	D	809	ARG	NE-CZ-NH2	-5.82	117.39	120.30
4	6	79	TRP	CG-CD2-CE3	5.82	139.13	133.90
4	Z	79	TRP	CG-CD2-CE3	5.82	139.13	133.90
4	1	335	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	G	471	ASP	CB-CG-OD1	-5.81	113.07	118.30
4	1	95	ARG	CA-CB-CG	5.81	126.19	113.40
1	A	780	ASP	CB-CG-OD1	-5.81	113.07	118.30
4	V	95	ARG	CA-CB-CG	5.81	126.18	113.40
4	Z	95	ARG	CA-CB-CG	5.81	126.17	113.40
4	3	79	TRP	CG-CD2-CE3	5.80	139.12	133.90
4	7	95	ARG	CA-CB-CG	5.80	126.16	113.40
4	X	95	ARG	CA-CB-CG	5.80	126.16	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	79	TRP	CG-CD2-CE3	5.80	139.12	133.90
4	4	254	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	D	815	CYS	CA-CB-SG	-5.79	103.57	114.00
4	1	254	ARG	NE-CZ-NH1	5.79	123.20	120.30
4	W	79	TRP	CG-CD2-CE3	5.79	139.11	133.90
4	8	335	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	346	ASP	CB-CG-OD1	5.79	123.51	118.30
4	7	79	TRP	CG-CD2-CE3	5.79	139.11	133.90
1	G	556	ASP	CB-CG-OD1	-5.78	113.09	118.30
4	4	95	ARG	CA-CB-CG	5.78	126.12	113.40
4	6	95	ARG	CA-CB-CG	5.78	126.12	113.40
4	Y	95	ARG	CA-CB-CG	5.78	126.12	113.40
1	A	4	ASP	CB-CG-OD2	5.78	123.50	118.30
1	J	339	ASP	CB-CG-OD2	5.78	123.50	118.30
1	J	809	ARG	NE-CZ-NH2	-5.78	117.41	120.30
4	0	95	ARG	CA-CB-CG	5.78	126.11	113.40
1	A	556	ASP	CB-CG-OD1	-5.77	113.10	118.30
1	A	471	ASP	CB-CG-OD1	-5.77	113.11	118.30
4	0	254	ARG	NE-CZ-NH1	5.77	123.19	120.30
4	0	335	ARG	NE-CZ-NH2	-5.77	117.42	120.30
4	2	95	ARG	CA-CB-CG	5.77	126.09	113.40
4	W	95	ARG	CA-CB-CG	5.77	126.09	113.40
4	7	335	ARG	NE-CZ-NH2	-5.76	117.42	120.30
4	V	79	TRP	CG-CD2-CE3	5.76	139.09	133.90
4	Z	254	ARG	NE-CZ-NH1	5.76	123.18	120.30
4	0	116	ARG	NE-CZ-NH1	5.76	123.18	120.30
4	5	95	ARG	CA-CB-CG	5.76	126.07	113.40
4	1	116	ARG	NE-CZ-NH1	5.76	123.18	120.30
4	3	95	ARG	CA-CB-CG	5.75	126.06	113.40
1	D	352	TYR	N-CA-CB	5.75	120.94	110.60
1	A	809	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	D	781	ASP	CB-CG-OD2	5.74	123.47	118.30
2	B	149	ASP	N-CA-CB	5.74	120.93	110.60
1	D	4	ASP	CB-CG-OD2	5.74	123.46	118.30
1	A	339	ASP	CB-CG-OD2	5.73	123.46	118.30
2	H	149	ASP	N-CA-CB	5.73	120.91	110.60
1	J	165	PHE	N-CA-CB	-5.73	100.29	110.60
4	W	254	ARG	NE-CZ-NH1	5.73	123.16	120.30
2	K	149	ASP	N-CA-CB	5.72	120.90	110.60
4	0	335	ARG	CA-CB-CG	5.72	125.99	113.40
4	X	254	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	165	PHE	N-CA-CB	-5.72	100.31	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	6	254	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	G	815	CYS	CA-CB-SG	-5.72	103.71	114.00
4	7	335	ARG	CA-CB-CG	5.72	125.98	113.40
4	V	335	ARG	CA-CB-CG	5.72	125.98	113.40
1	J	4	ASP	CB-CG-OD2	5.71	123.44	118.30
4	1	335	ARG	CA-CB-CG	5.71	125.96	113.40
4	2	335	ARG	CA-CB-CG	5.71	125.96	113.40
1	G	4	ASP	CB-CG-OD2	5.71	123.44	118.30
4	5	335	ARG	CA-CB-CG	5.71	125.95	113.40
4	7	254	ARG	NE-CZ-NH1	5.71	123.15	120.30
4	3	335	ARG	CA-CB-CG	5.71	125.95	113.40
4	4	335	ARG	CA-CB-CG	5.70	125.94	113.40
4	X	335	ARG	CA-CB-CG	5.70	125.94	113.40
1	G	165	PHE	N-CA-CB	-5.70	100.35	110.60
4	6	335	ARG	CA-CB-CG	5.70	125.93	113.40
4	8	335	ARG	CA-CB-CG	5.70	125.93	113.40
4	W	335	ARG	CA-CB-CG	5.69	125.92	113.40
4	4	116	ARG	NE-CZ-NH1	5.68	123.14	120.30
4	Z	335	ARG	CA-CB-CG	5.68	125.90	113.40
4	Y	335	ARG	CA-CB-CG	5.68	125.89	113.40
4	2	254	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	D	780	ASP	CB-CG-OD1	-5.67	113.20	118.30
1	G	352	TYR	N-CA-CB	5.66	120.79	110.60
1	D	165	PHE	N-CA-CB	-5.66	100.42	110.60
2	E	149	ASP	N-CA-CB	5.65	120.77	110.60
1	G	693	HIS	CA-CB-CG	-5.63	104.02	113.60
4	7	116	ARG	NE-CZ-NH1	5.63	123.11	120.30
4	Z	294	TYR	CB-CG-CD2	-5.63	117.62	121.00
4	X	294	TYR	CB-CG-CD2	-5.62	117.63	121.00
4	X	116	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	J	693	HIS	CA-CB-CG	-5.62	104.05	113.60
4	3	113	LYS	CA-CB-CG	5.62	125.76	113.40
1	G	785	GLU	O-C-N	5.62	131.69	122.70
1	J	780	ASP	CB-CG-OD1	-5.61	113.25	118.30
1	A	781	ASP	CB-CG-OD2	5.61	123.35	118.30
1	J	352	TYR	N-CA-CB	5.61	120.69	110.60
4	0	113	LYS	CA-CB-CG	5.61	125.74	113.40
4	3	356	TRP	CG-CD2-CE3	5.61	138.95	133.90
4	8	356	TRP	CG-CD2-CE3	5.61	138.94	133.90
1	A	352	TYR	N-CA-CB	5.60	120.68	110.60
1	D	693	HIS	CA-CB-CG	-5.60	104.08	113.60
4	5	113	LYS	CA-CB-CG	5.59	125.71	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2	113	LYS	CA-CB-CG	5.59	125.70	113.40
4	5	356	TRP	CG-CD2-CE3	5.59	138.93	133.90
4	5	294	TYR	CB-CG-CD2	-5.59	117.65	121.00
4	V	113	LYS	CA-CB-CG	5.59	125.69	113.40
4	2	356	TRP	CG-CD2-CE3	5.59	138.93	133.90
4	8	113	LYS	CA-CB-CG	5.58	125.69	113.40
4	X	113	LYS	CA-CB-CG	5.58	125.68	113.40
4	1	113	LYS	CA-CB-CG	5.58	125.68	113.40
4	6	294	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	G	320	ILE	CB-CA-C	-5.57	100.45	111.60
4	Y	294	TYR	CB-CG-CD2	-5.57	117.66	121.00
4	Z	113	LYS	CA-CB-CG	5.57	125.66	113.40
4	Y	356	TRP	CG-CD2-CE3	5.57	138.91	133.90
4	1	279	TYR	CB-CG-CD2	-5.57	117.66	121.00
4	W	356	TRP	CG-CD2-CE3	5.57	138.91	133.90
4	7	294	TYR	CB-CG-CD2	-5.57	117.66	121.00
4	8	279	TYR	CB-CG-CD2	-5.57	117.66	121.00
4	W	113	LYS	CA-CB-CG	5.57	125.65	113.40
1	J	33	ASP	CB-CG-OD2	5.57	123.31	118.30
1	G	781	ASP	CB-CG-OD2	5.56	123.31	118.30
4	0	11	ASP	CB-CG-OD1	5.56	123.31	118.30
4	4	294	TYR	CB-CG-CD2	-5.56	117.66	121.00
4	6	113	LYS	CA-CB-CG	5.56	125.63	113.40
4	7	113	LYS	CA-CB-CG	5.56	125.63	113.40
4	Y	113	LYS	CA-CB-CG	5.56	125.63	113.40
4	W	294	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	J	686	MET	N-CA-CB	-5.55	100.61	110.60
1	J	384	ASP	CB-CG-OD1	-5.55	113.30	118.30
4	0	254	ARG	N-CA-CB	-5.55	100.61	110.60
4	6	356	TRP	CG-CD2-CE3	5.55	138.89	133.90
4	4	113	LYS	CA-CB-CG	5.55	125.61	113.40
4	7	254	ARG	N-CA-CB	-5.55	100.61	110.60
1	J	781	ASP	CB-CG-OD2	5.55	123.29	118.30
4	3	254	ARG	N-CA-CB	-5.55	100.62	110.60
1	D	384	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	G	686	MET	N-CA-CB	-5.54	100.62	110.60
4	0	356	TRP	CG-CD2-CE3	5.54	138.89	133.90
4	Y	279	TYR	CB-CG-CD2	-5.54	117.67	121.00
4	Z	254	ARG	N-CA-CB	-5.54	100.62	110.60
1	D	686	MET	N-CA-CB	-5.54	100.63	110.60
1	A	693	HIS	CA-CB-CG	-5.54	104.19	113.60
4	3	279	TYR	CB-CG-CD2	-5.54	117.68	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	0	294	TYR	CB-CG-CD2	-5.54	117.68	121.00
1	D	752	ASP	CB-CA-C	5.54	121.47	110.40
4	V	294	TYR	CB-CG-CD2	-5.54	117.68	121.00
4	W	254	ARG	N-CA-CB	-5.54	100.64	110.60
4	7	279	TYR	CB-CG-CD2	-5.53	117.68	121.00
4	6	254	ARG	N-CA-CB	-5.53	100.65	110.60
1	D	306	THR	CA-CB-CG2	-5.53	104.66	112.40
4	4	254	ARG	N-CA-CB	-5.53	100.65	110.60
1	G	306	THR	CA-CB-CG2	-5.53	104.67	112.40
4	3	294	TYR	CB-CG-CD2	-5.53	117.69	121.00
4	5	254	ARG	N-CA-CB	-5.53	100.66	110.60
4	8	254	ARG	N-CA-CB	-5.52	100.66	110.60
4	8	11	ASP	CB-CG-OD1	5.52	123.27	118.30
4	4	279	TYR	CB-CG-CD2	-5.52	117.69	121.00
4	1	294	TYR	CB-CG-CD2	-5.52	117.69	121.00
4	X	254	ARG	N-CA-CB	-5.52	100.66	110.60
4	1	254	ARG	N-CA-CB	-5.52	100.67	110.60
4	Y	254	ARG	N-CA-CB	-5.52	100.67	110.60
4	2	254	ARG	N-CA-CB	-5.51	100.67	110.60
4	V	254	ARG	N-CA-CB	-5.51	100.67	110.60
1	J	343	PHE	CB-CG-CD2	-5.51	116.94	120.80
1	J	752	ASP	CB-CA-C	5.51	121.42	110.40
1	A	752	ASP	CB-CA-C	5.51	121.41	110.40
4	7	356	TRP	CG-CD2-CE3	5.51	138.86	133.90
1	A	686	MET	N-CA-CB	-5.50	100.69	110.60
4	4	11	ASP	CB-CG-OD1	5.50	123.25	118.30
1	G	752	ASP	CB-CA-C	5.50	121.40	110.40
4	2	294	TYR	CB-CG-CD2	-5.50	117.70	121.00
4	V	11	ASP	CB-CG-OD1	5.49	123.24	118.30
4	4	356	TRP	CG-CD2-CE3	5.49	138.84	133.90
4	6	147	ARG	NE-CZ-NH2	-5.49	117.56	120.30
4	6	279	TYR	CB-CG-CD2	-5.49	117.71	121.00
4	Z	279	TYR	CB-CG-CD2	-5.49	117.71	121.00
4	3	254	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	J	320	ILE	CB-CA-C	-5.48	100.63	111.60
1	D	723	ARG	NE-CZ-NH1	5.48	123.04	120.30
4	0	279	TYR	CB-CG-CD2	-5.48	117.71	121.00
4	1	356	TRP	CG-CD2-CE3	5.48	138.83	133.90
4	2	79	TRP	CB-CG-CD1	-5.48	119.88	127.00
4	3	11	ASP	CB-CG-OD1	5.48	123.23	118.30
4	8	294	TYR	CB-CG-CD2	-5.48	117.71	121.00
4	Z	11	ASP	CB-CG-OD1	5.48	123.23	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	33	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	33	ASP	CB-CG-OD2	5.47	123.22	118.30
4	X	279	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	A	241	ASP	CB-CG-OD2	5.47	123.22	118.30
4	5	11	ASP	CB-CG-OD1	5.47	123.22	118.30
4	Y	11	ASP	CB-CG-OD1	5.47	123.22	118.30
4	W	11	ASP	CB-CG-OD1	5.47	123.22	118.30
4	X	356	TRP	CG-CD2-CE3	5.47	138.82	133.90
4	Z	356	TRP	CG-CD2-CE3	5.47	138.82	133.90
1	D	320	ILE	CB-CA-C	-5.46	100.68	111.60
4	V	279	TYR	CB-CG-CD2	-5.46	117.72	121.00
4	2	279	TYR	CB-CG-CD2	-5.46	117.73	121.00
4	W	356	TRP	CB-CG-CD1	-5.46	119.91	127.00
1	A	306	THR	CA-CB-CG2	-5.45	104.77	112.40
4	V	356	TRP	CG-CD2-CE3	5.45	138.81	133.90
1	A	320	ILE	CB-CA-C	-5.45	100.70	111.60
4	7	79	TRP	CB-CG-CD1	-5.45	119.92	127.00
1	J	547	ASP	CB-CG-OD2	5.45	123.20	118.30
4	2	147	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	D	326	ASP	CB-CG-OD2	5.44	123.20	118.30
4	2	11	ASP	CB-CG-OD1	5.44	123.20	118.30
4	4	356	TRP	CB-CG-CD1	-5.44	119.93	127.00
4	5	279	TYR	CB-CG-CD2	-5.44	117.74	121.00
4	W	279	TYR	CB-CG-CD2	-5.44	117.74	121.00
1	J	326	ASP	CB-CG-OD2	5.43	123.19	118.30
4	X	335	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	D	547	ASP	CB-CG-OD2	5.43	123.19	118.30
1	J	306	THR	CA-CB-CG2	-5.43	104.80	112.40
4	4	356	TRP	CG-CD1-NE1	-5.43	104.67	110.10
1	A	343	PHE	CB-CG-CD2	-5.43	117.00	120.80
4	1	79	TRP	CB-CG-CD1	-5.43	119.94	127.00
4	3	79	TRP	CB-CG-CD1	-5.43	119.94	127.00
1	J	218	LEU	O-C-N	5.43	131.38	122.70
4	6	356	TRP	CB-CG-CD1	-5.43	119.95	127.00
4	W	356	TRP	CG-CD1-NE1	-5.43	104.67	110.10
4	W	147	ARG	NE-CZ-NH2	-5.42	117.59	120.30
4	7	11	ASP	CB-CG-OD1	5.42	123.18	118.30
4	1	11	ASP	CB-CG-OD1	5.42	123.18	118.30
4	3	356	TRP	CB-CG-CD1	-5.42	119.95	127.00
1	A	723	ARG	NE-CZ-NH1	5.42	123.01	120.30
4	2	356	TRP	CB-CG-CD1	-5.42	119.96	127.00
4	7	356	TRP	CB-CG-CD1	-5.42	119.96	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2	356	TRP	CG-CD1-NE1	-5.42	104.69	110.10
4	Z	356	TRP	CB-CG-CD1	-5.42	119.96	127.00
4	8	356	TRP	CG-CD1-NE1	-5.41	104.69	110.10
4	Z	79	TRP	CB-CG-CD1	-5.41	119.96	127.00
4	4	79	TRP	CB-CG-CD1	-5.41	119.97	127.00
4	5	79	TRP	CB-CG-CD1	-5.41	119.97	127.00
4	6	356	TRP	CG-CD1-NE1	-5.41	104.69	110.10
4	V	79	TRP	CB-CG-CD1	-5.41	119.97	127.00
4	Y	356	TRP	CG-CD1-NE1	-5.41	104.69	110.10
4	W	79	TRP	CB-CG-CD1	-5.41	119.97	127.00
4	Y	356	TRP	CB-CG-CD1	-5.41	119.97	127.00
1	A	326	ASP	CB-CG-OD2	5.40	123.16	118.30
4	6	11	ASP	CB-CG-OD1	5.40	123.16	118.30
4	V	356	TRP	CB-CG-CD1	-5.40	119.98	127.00
4	X	11	ASP	CB-CG-OD1	5.40	123.16	118.30
4	X	79	TRP	CB-CG-CD1	-5.40	119.98	127.00
4	1	356	TRP	CB-CG-CD1	-5.40	119.98	127.00
4	Y	79	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	A	601	ASP	CB-CG-OD2	5.39	123.16	118.30
4	6	79	TRP	CB-CG-CD1	-5.39	119.99	127.00
4	6	335	ARG	NE-CZ-NH1	5.39	123.00	120.30
4	X	356	TRP	CB-CG-CD1	-5.39	120.00	127.00
1	G	33	ASP	CB-CG-OD2	5.39	123.15	118.30
4	0	79	TRP	CB-CG-CD1	-5.39	120.00	127.00
4	5	335	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	A	384	ASP	CB-CG-OD1	-5.38	113.45	118.30
4	0	356	TRP	CB-CG-CD1	-5.38	120.00	127.00
4	5	356	TRP	CB-CG-CD1	-5.38	120.00	127.00
4	8	356	TRP	CB-CG-CD1	-5.38	120.00	127.00
1	A	686	MET	CG-SD-CE	-5.38	91.60	100.20
4	1	356	TRP	CG-CD1-NE1	-5.38	104.72	110.10
4	5	356	TRP	CG-CD1-NE1	-5.38	104.72	110.10
4	5	251	GLY	CA-C-N	-5.38	105.38	117.20
1	J	241	ASP	CB-CG-OD2	5.37	123.14	118.30
4	V	251	GLY	CA-C-N	-5.37	105.38	117.20
4	Z	356	TRP	CG-CD1-NE1	-5.37	104.73	110.10
4	X	251	GLY	CA-C-N	-5.37	105.40	117.20
1	G	686	MET	CG-SD-CE	-5.36	91.62	100.20
1	G	218	LEU	O-C-N	5.36	131.28	122.70
4	Z	147	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	J	686	MET	CG-SD-CE	-5.36	91.63	100.20
4	8	79	TRP	CB-CG-CD1	-5.36	120.04	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	0	356	TRP	CG-CD1-NE1	-5.35	104.75	110.10
4	7	356	TRP	CG-CD1-NE1	-5.35	104.75	110.10
4	V	147	ARG	NE-CZ-NH2	-5.35	117.62	120.30
4	4	251	GLY	CA-C-N	-5.35	105.43	117.20
1	G	326	ASP	CB-CG-OD2	5.35	123.11	118.30
2	K	136	MET	CG-SD-CE	5.35	108.76	100.20
4	0	251	GLY	CA-C-N	-5.35	105.43	117.20
4	2	251	GLY	CA-C-N	-5.35	105.43	117.20
4	X	356	TRP	CG-CD1-NE1	-5.35	104.75	110.10
4	3	251	GLY	CA-C-N	-5.35	105.44	117.20
4	7	251	GLY	CA-C-N	-5.35	105.44	117.20
1	G	800	ARG	NH1-CZ-NH2	5.34	125.28	119.40
2	B	136	MET	CG-SD-CE	5.34	108.75	100.20
1	D	601	ASP	CB-CG-OD2	5.34	123.11	118.30
4	5	147	ARG	NE-CZ-NH2	-5.34	117.63	120.30
4	W	251	GLY	CA-C-N	-5.34	105.46	117.20
4	4	335	ARG	NE-CZ-NH1	5.34	122.97	120.30
4	7	147	ARG	NE-CZ-NH2	-5.34	117.63	120.30
4	8	251	GLY	CA-C-N	-5.34	105.46	117.20
1	D	241	ASP	CB-CG-OD2	5.33	123.10	118.30
1	D	800	ARG	NH1-CZ-NH2	5.33	125.27	119.40
4	6	251	GLY	CA-C-N	-5.33	105.47	117.20
4	1	251	GLY	CA-C-N	-5.33	105.47	117.20
1	J	601	ASP	CB-CG-OD2	5.33	123.09	118.30
1	J	723	ARG	NE-CZ-NH1	5.33	122.96	120.30
4	W	176	MET	CG-SD-CE	5.33	108.72	100.20
4	Z	251	GLY	CA-C-N	-5.33	105.48	117.20
1	G	241	ASP	CB-CG-OD2	5.32	123.09	118.30
4	Y	251	GLY	CA-C-N	-5.32	105.49	117.20
1	A	125	THR	CA-CB-CG2	-5.32	104.95	112.40
1	G	125	THR	CA-CB-CG2	-5.32	104.95	112.40
1	G	601	ASP	CB-CG-OD2	5.32	123.09	118.30
4	6	176	MET	CG-SD-CE	5.32	108.71	100.20
4	6	337	TYR	CB-CG-CD1	-5.32	117.81	121.00
4	Y	147	ARG	NE-CZ-NH2	-5.32	117.64	120.30
4	V	356	TRP	CG-CD1-NE1	-5.31	104.79	110.10
4	Z	176	MET	CG-SD-CE	5.31	108.70	100.20
4	4	176	MET	CG-SD-CE	5.31	108.70	100.20
1	D	343	PHE	CB-CG-CD2	-5.31	117.08	120.80
4	V	176	MET	CG-SD-CE	5.31	108.69	100.20
4	X	176	MET	CG-SD-CE	5.31	108.69	100.20
1	D	354	LEU	CB-CG-CD2	-5.30	101.98	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	660	LEU	CB-CG-CD2	5.30	120.02	111.00
4	3	356	TRP	CG-CD1-NE1	-5.30	104.80	110.10
4	3	147	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	660	LEU	CB-CG-CD2	5.30	120.01	111.00
1	G	723	ARG	NE-CZ-NH1	5.30	122.95	120.30
4	2	176	MET	CG-SD-CE	5.30	108.67	100.20
4	7	176	MET	CG-SD-CE	5.30	108.67	100.20
1	D	760	PHE	CB-CG-CD1	5.29	124.50	120.80
4	3	176	MET	CG-SD-CE	5.29	108.67	100.20
4	4	147	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	G	384	ASP	CB-CG-OD1	-5.29	113.54	118.30
4	Y	176	MET	CG-SD-CE	5.29	108.66	100.20
4	1	176	MET	CG-SD-CE	5.29	108.66	100.20
2	E	136	MET	CG-SD-CE	5.29	108.66	100.20
1	J	170	ARG	NE-CZ-NH1	5.29	122.94	120.30
4	0	176	MET	CG-SD-CE	5.28	108.65	100.20
4	X	147	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	D	125	THR	CA-CB-CG2	-5.28	105.01	112.40
1	D	660	LEU	CB-CG-CD2	5.28	119.97	111.00
2	H	136	MET	CG-SD-CE	5.28	108.65	100.20
1	J	125	THR	CA-CB-CG2	-5.28	105.01	112.40
1	A	354	LEU	CB-CG-CD2	-5.28	102.03	111.00
1	J	800	ARG	NH1-CZ-NH2	5.28	125.20	119.40
4	0	147	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	D	686	MET	CG-SD-CE	-5.27	91.76	100.20
4	Z	62	ARG	NE-CZ-NH1	5.27	122.94	120.30
4	1	335	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	800	ARG	NH1-CZ-NH2	5.26	125.19	119.40
4	8	62	ARG	NE-CZ-NH1	5.26	122.93	120.30
4	8	176	MET	CG-SD-CE	5.26	108.62	100.20
1	G	354	LEU	CB-CG-CD2	-5.26	102.06	111.00
4	5	176	MET	CG-SD-CE	5.25	108.60	100.20
1	J	660	LEU	CB-CG-CD2	5.25	119.93	111.00
4	Z	335	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	346	ASP	N-CA-CB	-5.24	101.17	110.60
1	G	547	ASP	CB-CG-OD2	5.23	123.00	118.30
1	G	555	TYR	CB-CG-CD1	5.22	124.14	121.00
4	V	62	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	218	LEU	O-C-N	5.22	131.06	122.70
1	D	218	LEU	O-C-N	5.22	131.05	122.70
4	1	62	ARG	NE-CZ-NH1	5.22	122.91	120.30
4	8	147	ARG	NE-CZ-NH2	-5.22	117.69	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	W	335	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	760	PHE	CB-CG-CD1	5.21	124.45	120.80
1	J	346	ASP	N-CA-CB	-5.21	101.22	110.60
1	D	346	ASP	N-CA-CB	-5.21	101.22	110.60
1	J	354	LEU	CB-CG-CD2	-5.21	102.14	111.00
4	3	337	TYR	CB-CG-CD1	-5.21	117.87	121.00
1	A	547	ASP	CB-CG-OD2	5.21	122.99	118.30
1	G	343	PHE	CB-CG-CD2	-5.20	117.16	120.80
1	J	760	PHE	CB-CG-CD1	5.20	124.44	120.80
4	3	62	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	D	4	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	J	4	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	A	90	ASP	CB-CG-OD1	-5.19	113.63	118.30
4	8	335	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	G	4	ASP	CB-CG-OD1	-5.19	113.63	118.30
4	0	337	TYR	CB-CG-CD1	-5.19	117.89	121.00
4	0	62	ARG	NE-CZ-NH1	5.18	122.89	120.30
4	V	290	ARG	CA-C-N	5.17	128.59	117.20
4	1	147	ARG	NE-CZ-NH2	-5.17	117.72	120.30
4	V	335	ARG	NE-CZ-NH1	5.17	122.89	120.30
4	X	337	TYR	CB-CG-CD1	-5.17	117.90	121.00
4	4	290	ARG	CA-C-N	5.17	128.56	117.20
4	5	290	ARG	CA-C-N	5.17	128.56	117.20
4	6	290	ARG	CA-C-N	5.16	128.56	117.20
4	X	290	ARG	CA-C-N	5.16	128.56	117.20
4	Y	290	ARG	CA-C-N	5.16	128.56	117.20
4	2	62	ARG	NE-CZ-NH1	5.16	122.88	120.30
4	7	335	ARG	NE-CZ-NH1	5.16	122.88	120.30
4	0	290	ARG	CA-C-N	5.16	128.55	117.20
4	8	290	ARG	CA-C-N	5.16	128.55	117.20
4	3	290	ARG	CA-C-N	5.16	128.54	117.20
4	2	290	ARG	CA-C-N	5.16	128.54	117.20
4	3	335	ARG	NE-CZ-NH1	5.16	122.88	120.30
4	1	290	ARG	CA-C-N	5.15	128.54	117.20
4	V	53	TYR	CB-CG-CD1	-5.15	117.91	121.00
4	Z	290	ARG	CA-C-N	5.15	128.54	117.20
1	A	4	ASP	CB-CG-OD1	-5.15	113.67	118.30
4	2	337	TYR	CB-CG-CD1	-5.15	117.91	121.00
4	6	53	TYR	CB-CG-CD1	-5.15	117.91	121.00
4	7	290	ARG	CA-C-N	5.15	128.53	117.20
4	W	290	ARG	CA-C-N	5.15	128.52	117.20
4	6	62	ARG	NE-CZ-NH1	5.14	122.87	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	335	ARG	NE-CZ-NH1	5.14	122.87	120.30
4	W	91	TYR	CB-CG-CD2	-5.14	117.92	121.00
4	Z	53	TYR	CB-CG-CD1	-5.14	117.92	121.00
4	0	335	ARG	NE-CZ-NH1	5.14	122.87	120.30
4	W	337	TYR	CB-CG-CD1	-5.13	117.92	121.00
4	Y	62	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	G	346	ASP	N-CA-CB	-5.13	101.36	110.60
4	1	91	TYR	CB-CG-CD2	-5.13	117.92	121.00
4	7	62	ARG	NE-CZ-NH1	5.13	122.86	120.30
4	8	91	TYR	CB-CG-CD2	-5.12	117.92	121.00
4	Y	86	TRP	CG-CD1-NE1	-5.12	104.97	110.10
1	A	160	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	D	576	GLU	CA-CB-CG	-5.12	102.13	113.40
1	J	576	GLU	CA-CB-CG	-5.12	102.13	113.40
4	2	335	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	576	GLU	CA-CB-CG	-5.12	102.14	113.40
4	Z	62	ARG	CA-CB-CG	5.12	124.66	113.40
1	G	760	PHE	CB-CG-CD1	5.11	124.38	120.80
1	G	160	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	G	576	GLU	CA-CB-CG	-5.11	102.16	113.40
4	0	53	TYR	CB-CG-CD1	-5.11	117.93	121.00
4	5	337	TYR	CB-CG-CD1	-5.11	117.93	121.00
4	7	86	TRP	CG-CD1-NE1	-5.11	104.99	110.10
4	Y	337	TYR	CB-CG-CD1	-5.11	117.93	121.00
1	J	628	GLY	O-C-N	-5.11	114.53	122.70
1	D	628	GLY	O-C-N	-5.11	114.53	122.70
1	J	301	ASP	CB-CG-OD2	5.11	122.90	118.30
4	5	62	ARG	CA-CB-CG	5.11	124.64	113.40
4	8	62	ARG	CA-CB-CG	5.11	124.63	113.40
4	Z	86	TRP	CG-CD1-NE1	-5.10	105.00	110.10
4	7	53	TYR	CB-CG-CD1	-5.10	117.94	121.00
4	1	53	TYR	CB-CG-CD1	-5.10	117.94	121.00
4	8	337	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	G	90	ASP	CB-CG-OD1	-5.10	113.71	118.30
4	6	62	ARG	CA-CB-CG	5.10	124.62	113.40
4	W	62	ARG	CA-CB-CG	5.10	124.61	113.40
4	7	337	TYR	CB-CG-CD1	-5.10	117.94	121.00
4	5	86	TRP	CG-CD1-NE1	-5.09	105.00	110.10
1	A	218	LEU	CA-CB-CG	5.09	127.01	115.30
4	W	62	ARG	NE-CZ-NH1	5.09	122.85	120.30
4	4	62	ARG	CA-CB-CG	5.09	124.59	113.40
4	8	53	TYR	CB-CG-CD1	-5.09	117.95	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Z	337	TYR	CB-CG-CD1	-5.09	117.95	121.00
4	1	62	ARG	CA-CB-CG	5.09	124.59	113.40
4	2	62	ARG	CA-CB-CG	5.09	124.59	113.40
4	Y	62	ARG	CA-CB-CG	5.08	124.59	113.40
1	D	82	PRO	N-CA-CB	5.08	109.40	103.30
1	D	218	LEU	CA-CB-CG	5.08	126.99	115.30
4	7	62	ARG	CA-CB-CG	5.08	124.58	113.40
1	D	621	LEU	CA-CB-CG	-5.08	103.61	115.30
1	J	555	TYR	CB-CG-CD1	5.08	124.05	121.00
4	4	337	TYR	CB-CG-CD1	-5.08	117.95	121.00
4	X	62	ARG	CA-CB-CG	5.08	124.58	113.40
4	X	91	TYR	CB-CG-CD2	-5.08	117.95	121.00
4	4	191	LYS	CA-C-N	5.08	128.38	117.20
4	V	62	ARG	CA-CB-CG	5.08	124.58	113.40
4	V	91	TYR	CB-CG-CD2	-5.08	117.95	121.00
4	0	91	TYR	CB-CG-CD2	-5.08	117.95	121.00
4	3	53	TYR	CB-CG-CD1	-5.08	117.95	121.00
4	5	191	LYS	CA-C-N	5.08	128.37	117.20
4	Y	191	LYS	CA-C-N	5.08	128.37	117.20
1	G	621	LEU	CA-CB-CG	-5.08	103.62	115.30
4	0	62	ARG	CA-CB-CG	5.08	124.57	113.40
4	3	62	ARG	CA-CB-CG	5.07	124.56	113.40
1	G	170	ARG	NE-CZ-NH1	5.07	122.84	120.30
4	5	91	TYR	CB-CG-CD2	-5.07	117.96	121.00
4	W	191	LYS	CA-C-N	5.07	128.35	117.20
4	X	191	LYS	CA-C-N	5.07	128.35	117.20
1	J	160	ASP	CB-CG-OD2	-5.07	113.74	118.30
4	X	86	TRP	CG-CD1-NE1	-5.07	105.03	110.10
1	A	621	LEU	CA-CB-CG	-5.06	103.66	115.30
4	0	191	LYS	CA-C-N	5.06	128.34	117.20
4	X	62	ARG	NE-CZ-NH1	5.06	122.83	120.30
4	3	191	LYS	CA-C-N	5.06	128.33	117.20
4	6	86	TRP	CG-CD1-NE1	-5.06	105.04	110.10
1	J	621	LEU	CA-CB-CG	-5.06	103.67	115.30
4	8	191	LYS	CA-C-N	5.06	128.33	117.20
4	4	86	TRP	CG-CD1-NE1	-5.05	105.05	110.10
4	V	337	TYR	CB-CG-CD1	-5.05	117.97	121.00
4	Y	53	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	A	628	GLY	O-C-N	-5.05	114.62	122.70
1	D	160	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	J	218	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	739	ASP	CA-CB-CG	-5.05	102.29	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	PRO	N-CA-CB	5.05	109.36	103.30
4	4	91	TYR	CB-CG-CD2	-5.05	117.97	121.00
4	Z	191	LYS	CA-C-N	5.05	128.30	117.20
4	2	86	TRP	CG-CD1-NE1	-5.04	105.06	110.10
4	1	191	LYS	CA-C-N	5.04	128.29	117.20
4	4	53	TYR	CB-CG-CD1	-5.04	117.97	121.00
4	6	91	TYR	CB-CG-CD2	-5.04	117.97	121.00
4	7	191	LYS	CA-C-N	5.04	128.29	117.20
1	J	82	PRO	N-CA-CB	5.04	109.35	103.30
4	2	191	LYS	CA-C-N	5.04	128.28	117.20
1	A	235	ALA	N-CA-CB	-5.04	103.05	110.10
4	2	91	TYR	CB-CG-CD2	-5.04	117.98	121.00
4	5	62	ARG	NE-CZ-NH1	5.04	122.82	120.30
4	W	53	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	G	218	LEU	CA-CB-CG	5.03	126.87	115.30
4	2	53	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	J	739	ASP	N-CA-CB	5.03	119.65	110.60
1	G	739	ASP	N-CA-CB	5.03	119.64	110.60
1	D	739	ASP	N-CA-CB	5.02	119.64	110.60
1	G	628	GLY	O-C-N	-5.02	114.66	122.70
4	7	91	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	D	90	ASP	CB-CG-OD1	-5.02	113.78	118.30
4	V	191	LYS	CA-C-N	5.02	128.25	117.20
4	6	191	LYS	CA-C-N	5.02	128.24	117.20
4	V	86	TRP	CG-CD1-NE1	-5.02	105.08	110.10
4	0	86	TRP	CG-CD1-NE1	-5.01	105.09	110.10
4	3	91	TYR	CB-CG-CD2	-5.01	117.99	121.00
4	Z	91	TYR	CB-CG-CD2	-5.01	117.99	121.00
1	G	82	PRO	N-CA-CB	5.01	109.32	103.30
1	D	235	ALA	N-CA-CB	-5.01	103.09	110.10

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	648	THR	CB
1	D	648	THR	CB
1	G	75	ASP	CA
1	G	648	THR	CB
1	J	648	THR	CB

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	0	62	ARG	Sidechain
4	1	62	ARG	Sidechain
4	2	62	ARG	Sidechain
4	3	62	ARG	Sidechain
4	4	62	ARG	Sidechain
4	5	62	ARG	Sidechain
4	6	62	ARG	Sidechain
4	7	62	ARG	Sidechain
4	8	62	ARG	Sidechain
1	A	623	PHE	Sidechain
1	A	637	LYS	Mainchain
1	A	649	VAL	Mainchain
1	A	98	HIS	Mainchain
2	B	150	TYR	Sidechain
2	B	155	TYR	Mainchain
2	B	22	THR	Mainchain
3	C	75	ALA	Mainchain
3	C	85	GLU	Mainchain
1	D	623	PHE	Sidechain
1	D	637	LYS	Mainchain
1	D	649	VAL	Mainchain
1	D	98	HIS	Mainchain
2	E	150	TYR	Sidechain
2	E	155	TYR	Mainchain
2	E	22	THR	Mainchain
3	F	75	ALA	Mainchain
3	F	85	GLU	Mainchain
1	G	623	PHE	Sidechain
1	G	637	LYS	Mainchain
1	G	649	VAL	Mainchain
1	G	98	HIS	Mainchain
2	H	150	TYR	Sidechain
2	H	155	TYR	Mainchain
2	H	22	THR	Mainchain
3	I	75	ALA	Mainchain
3	I	85	GLU	Mainchain
1	J	623	PHE	Sidechain
1	J	637	LYS	Mainchain
1	J	649	VAL	Mainchain
1	J	709	LYS	Mainchain,Peptide
1	J	98	HIS	Mainchain
2	K	150	TYR	Sidechain
2	K	155	TYR	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	K	22	THR	Mainchain
3	L	75	ALA	Mainchain
3	L	85	GLU	Mainchain
4	V	62	ARG	Sidechain
4	W	62	ARG	Sidechain
4	X	62	ARG	Sidechain
4	Y	62	ARG	Sidechain
4	Z	62	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6797	0	6752	1414	0
1	D	6797	0	6761	1431	0
1	G	6797	0	6754	1380	0
1	J	6797	0	6760	1429	0
2	B	1127	0	1086	252	0
2	E	1127	0	1087	320	0
2	H	1127	0	1087	228	0
2	K	1127	0	1087	227	0
3	C	1123	0	1084	181	0
3	F	1123	0	1082	139	0
3	I	1123	0	1084	169	0
3	L	1123	0	1084	165	0
4	0	2906	0	2866	75	0
4	1	2906	0	2866	77	0
4	2	2906	0	2864	102	0
4	3	2906	0	2864	100	0
4	4	2906	0	2855	345	0
4	5	2906	0	2855	340	0
4	6	2906	0	2852	382	0
4	7	2906	0	2852	377	0
4	8	2906	0	2861	150	0
4	V	2906	0	2861	142	0
4	W	2906	0	2864	107	0
4	X	2906	0	2864	105	0
4	Y	2906	0	2865	78	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Z	2906	0	2865	78	0
All	All	76872	0	75762	7444	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 49.

All (7444) 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:G:797:PHE:CD1	3:I:149:VAL:HG11	1.20	1.68
2:E:144:VAL:HG13	2:E:153:ILE:CD1	1.22	1.66
1:G:798:LEU:CD1	3:I:126:LEU:HD21	1.20	1.65
1:A:725:ARG:HE	1:A:733:PRO:CB	1.09	1.64
1:D:725:ARG:HE	1:D:733:PRO:CB	1.09	1.64
1:A:757:GLN:CB	1:A:771:LEU:HD11	1.19	1.64
1:J:831:TRP:CZ3	2:K:34:ILE:HD13	1.21	1.64
2:B:144:VAL:HG13	2:B:153:ILE:CG1	1.17	1.64
2:H:144:VAL:HG13	2:H:153:ILE:CD1	1.22	1.62
2:K:144:VAL:HG13	2:K:153:ILE:CG1	1.17	1.62
1:D:831:TRP:HZ2	2:E:47:LEU:CA	1.09	1.61
1:J:510:TRP:CH2	1:J:768:MLY:HH11	1.34	1.61
1:A:206:LYS:CD	1:A:217:THR:HG23	1.28	1.61
1:A:757:GLN:HB3	1:A:771:LEU:CD1	1.26	1.61
2:E:144:VAL:HG13	2:E:153:ILE:CG1	1.17	1.59
1:G:831:TRP:HH2	2:H:47:LEU:CD2	1.06	1.59
1:G:838:ILE:HD11	2:H:54:MET:CE	1.26	1.59
1:G:206:LYS:CD	1:G:217:THR:HG23	1.28	1.59
1:J:84:MLY:CH1	1:J:715:VAL:HG13	1.22	1.59
1:J:206:LYS:CD	1:J:217:THR:HG23	1.28	1.59
1:J:538:GLU:CA	4:7:349:LEU:CD1	1.79	1.59
2:B:144:VAL:HG13	2:B:153:ILE:CD1	1.22	1.59
1:G:769:ALA:CB	1:G:770:GLY:HA2	1.20	1.58
2:K:144:VAL:HG13	2:K:153:ILE:CD1	1.22	1.58
1:A:799:MET:SD	3:C:32:ASP:HB3	1.43	1.58
1:G:725:ARG:HE	1:G:733:PRO:CB	1.09	1.58
1:J:725:ARG:HE	1:J:733:PRO:CB	1.09	1.58
1:D:831:TRP:CZ2	2:E:47:LEU:HA	1.11	1.58
1:D:538:GLU:CA	4:5:349:LEU:CD1	1.78	1.58
1:G:93:MET:CE	1:G:763:THR:HB	1.22	1.57
1:G:538:GLU:CA	4:6:349:LEU:CD1	1.79	1.57
1:G:797:PHE:HD1	3:I:149:VAL:CG1	1.17	1.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:144:VAL:HG13	2:H:153:ILE:CG1	1.17	1.57
1:A:798:LEU:CD1	3:C:126:LEU:HD21	1.27	1.56
1:D:206:LYS:CD	1:D:217:THR:HG23	1.28	1.56
1:J:530:MET:HG2	4:7:354:GLN:CB	1.36	1.56
1:A:736:GLN:HA	1:A:743:ALA:CB	1.35	1.55
1:G:831:TRP:CH2	2:H:47:LEU:HD22	1.39	1.55
1:A:530:MET:HG2	4:4:354:GLN:CB	1.35	1.55
1:D:830:PRO:CG	2:E:67:MET:CE	1.82	1.55
1:G:530:MET:HG2	4:6:354:GLN:CB	1.35	1.54
1:A:836:PHE:CZ	2:B:160:GLY:N	1.71	1.54
1:A:538:GLU:CA	4:4:349:LEU:CD1	1.78	1.54
1:D:530:MET:HG2	4:5:354:GLN:CB	1.35	1.54
1:D:641:LYS:HG3	1:D:647:GLN:CG	1.36	1.53
1:J:768:MLY:CH2	1:J:772:LEU:HD22	1.37	1.53
1:J:641:LYS:HG3	1:J:647:GLN:CG	1.37	1.53
1:J:800:ARG:CD	3:L:149:VAL:CG2	1.81	1.53
1:J:829:TRP:HZ3	2:K:84:PHE:CZ	1.27	1.52
1:D:736:GLN:HA	1:D:743:ALA:CB	1.35	1.52
1:J:829:TRP:CZ3	2:K:84:PHE:CZ	1.96	1.52
1:A:641:LYS:HG3	1:A:647:GLN:CG	1.37	1.52
1:D:799:MET:SD	3:F:32:ASP:HB3	1.48	1.52
1:D:834:LEU:CG	2:E:54:MET:HG3	1.38	1.51
1:G:206:LYS:HD3	1:G:217:THR:CG2	1.40	1.51
1:J:84:MLY:CE	1:J:719:ASP:HB3	1.08	1.51
1:J:757:GLN:CG	1:J:776:GLU:HG3	1.34	1.51
1:G:736:GLN:HA	1:G:743:ALA:CB	1.35	1.51
1:G:641:LYS:HG3	1:G:647:GLN:CG	1.37	1.51
1:J:736:GLN:HA	1:J:743:ALA:CB	1.35	1.51
1:G:93:MET:HE1	1:G:763:THR:CB	1.38	1.50
2:K:117:LEU:HD12	2:K:147:ASN:CB	1.41	1.50
1:J:800:ARG:CD	3:L:149:VAL:HG22	1.39	1.49
1:D:831:TRP:CH2	2:E:47:LEU:HA	1.41	1.49
1:J:768:MLY:HH12	1:J:772:LEU:CD2	1.41	1.49
1:D:206:LYS:HD3	1:D:217:THR:CG2	1.40	1.49
1:A:813:ILE:CG2	2:B:127:ARG:HD2	1.39	1.49
1:G:84:MLY:CH1	1:G:715:VAL:HG13	1.35	1.49
2:E:117:LEU:HD12	2:E:147:ASN:CB	1.41	1.48
1:J:206:LYS:HD3	1:J:217:THR:CG2	1.40	1.48
2:E:111:SER:HB2	2:E:148:VAL:C	1.23	1.48
2:K:111:SER:HB2	2:K:148:VAL:C	1.23	1.48
2:B:117:LEU:HD12	2:B:147:ASN:CB	1.42	1.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:831:TRP:CZ2	2:E:47:LEU:CA	1.82	1.48
1:J:508:ILE:HD11	1:J:759:ALA:CB	1.41	1.48
1:A:206:LYS:HD3	1:A:217:THR:CG2	1.40	1.47
2:E:117:LEU:HD12	2:E:147:ASN:CG	1.30	1.47
2:B:111:SER:HB2	2:B:148:VAL:C	1.23	1.47
1:D:830:PRO:CG	2:E:67:MET:HE3	1.38	1.47
1:J:795:ARG:CD	3:L:35:ARG:HH22	1.28	1.47
1:G:641:LYS:CG	1:G:647:GLN:NE2	1.76	1.47
1:J:768:MLY:HH23	1:J:772:LEU:CD2	1.44	1.47
1:D:831:TRP:CZ3	2:E:34:ILE:HG23	1.48	1.47
2:K:117:LEU:HD12	2:K:147:ASN:CG	1.29	1.47
1:J:800:ARG:HD2	3:L:149:VAL:CG2	1.03	1.46
2:H:117:LEU:HD12	2:H:147:ASN:CB	1.42	1.46
1:J:795:ARG:HD2	3:L:35:ARG:NH2	1.23	1.46
1:A:641:LYS:CG	1:A:647:GLN:NE2	1.76	1.46
1:J:538:GLU:C	4:7:349:LEU:CD1	1.84	1.46
1:J:641:LYS:CG	1:J:647:GLN:NE2	1.77	1.46
1:G:538:GLU:C	4:6:349:LEU:CD1	1.84	1.46
2:H:111:SER:HB2	2:H:148:VAL:C	1.23	1.46
1:A:641:LYS:CD	1:A:647:GLN:CD	1.85	1.45
2:B:117:LEU:HD12	2:B:147:ASN:CG	1.30	1.45
1:J:641:LYS:CD	1:J:647:GLN:CD	1.85	1.45
1:D:830:PRO:HG2	2:E:67:MET:CE	0.99	1.45
1:A:800:ARG:HB3	3:C:149:VAL:CG2	1.44	1.45
1:D:538:GLU:C	4:5:349:LEU:CD1	1.84	1.45
1:G:641:LYS:CD	1:G:647:GLN:CD	1.85	1.45
1:A:836:PHE:CE1	2:B:160:GLY:N	1.82	1.45
1:G:798:LEU:CD1	3:I:126:LEU:CD2	1.93	1.45
1:J:769:ALA:HB3	1:J:770:GLY:CA	1.45	1.45
2:H:117:LEU:HD12	2:H:147:ASN:CG	1.30	1.44
1:D:641:LYS:CG	1:D:647:GLN:NE2	1.76	1.44
1:J:93:MET:CG	1:J:764:MLY:HD3	1.43	1.44
1:A:538:GLU:C	4:4:349:LEU:CD1	1.84	1.44
1:D:814:PHE:CD1	2:E:127:ARG:NH2	1.78	1.44
1:J:721:LYS:HG3	1:J:736:GLN:CG	1.15	1.43
1:D:641:LYS:CD	1:D:647:GLN:CD	1.85	1.42
1:D:768:MLY:C	1:D:771:LEU:HD13	1.34	1.42
1:G:93:MET:CE	1:G:763:THR:CB	1.89	1.42
1:G:721:LYS:HG3	1:G:736:GLN:CG	1.15	1.42
1:G:800:ARG:NH1	3:I:149:VAL:HG22	1.33	1.42
1:A:733:PRO:O	1:A:737:PHE:CD1	1.73	1.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:736:GLN:N	1:D:743:ALA:HB1	1.34	1.42
1:G:733:PRO:O	1:G:737:PHE:CD1	1.74	1.41
1:G:736:GLN:N	1:G:743:ALA:HB1	1.34	1.41
2:H:144:VAL:CG1	2:H:153:ILE:CD1	1.99	1.41
1:A:530:MET:CG	4:4:354:GLN:HB2	1.50	1.41
2:B:144:VAL:CG1	2:B:153:ILE:CD1	1.99	1.41
1:D:530:MET:CG	4:5:354:GLN:HB2	1.50	1.41
1:J:202:SER:HA	1:J:207:LYS:CE	1.51	1.40
1:J:218:LEU:CB	1:J:221:GLN:HG3	1.52	1.40
1:G:730:SER:OG	3:I:109:HIS:CD2	1.72	1.40
1:J:768:MLY:HH23	1:J:772:LEU:CG	1.51	1.40
1:A:202:SER:HA	1:A:207:LYS:CE	1.51	1.40
1:D:218:LEU:CB	1:D:221:GLN:HG3	1.52	1.40
1:D:736:GLN:CA	1:D:743:ALA:CB	2.00	1.39
1:A:149:GLN:CB	1:A:719:ASP:OD1	1.71	1.39
1:A:537:GLU:O	4:4:349:LEU:CD1	1.70	1.39
1:D:537:GLU:O	4:5:349:LEU:CD1	1.70	1.39
2:E:144:VAL:CG1	2:E:153:ILE:CD1	1.99	1.39
1:J:733:PRO:O	1:J:737:PHE:CD1	1.73	1.39
1:D:202:SER:HA	1:D:207:LYS:CE	1.51	1.39
1:G:202:SER:HA	1:G:207:LYS:CE	1.51	1.39
1:G:821:ARG:NH2	2:H:127:ARG:HG2	1.07	1.39
1:D:733:PRO:O	1:D:737:PHE:CD1	1.74	1.39
2:K:144:VAL:CG1	2:K:153:ILE:CD1	1.99	1.39
1:G:819:ASN:CA	2:H:90:GLY:O	1.67	1.38
1:J:530:MET:CG	4:7:354:GLN:HB2	1.51	1.38
1:A:800:ARG:CD	3:C:149:VAL:HG22	1.53	1.38
1:A:831:TRP:NE1	2:B:51:PHE:CZ	1.91	1.38
1:D:831:TRP:HZ2	2:E:47:LEU:CB	1.36	1.38
1:J:736:GLN:CA	1:J:743:ALA:CB	2.00	1.38
1:A:218:LEU:CB	1:A:221:GLN:HG3	1.52	1.38
1:G:795:ARG:CD	3:I:35:ARG:HH22	1.34	1.38
1:G:831:TRP:CH2	2:H:47:LEU:CD2	1.98	1.38
1:J:537:GLU:O	4:7:349:LEU:CD1	1.70	1.38
1:A:736:GLN:CA	1:A:743:ALA:CB	2.00	1.37
1:D:736:GLN:CA	1:D:743:ALA:HB1	1.53	1.38
2:E:144:VAL:CG1	2:E:153:ILE:HG12	1.54	1.37
1:G:534:SER:O	4:6:351:THR:CG2	1.64	1.37
1:J:768:MLY:CH1	1:J:772:LEU:HD22	1.52	1.37
1:A:736:GLN:N	1:A:743:ALA:HB1	1.35	1.37
1:G:218:LEU:CB	1:G:221:GLN:HG3	1.52	1.37

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:GLN:CA	1:A:743:ALA:HB1	1.53	1.37
1:D:721:LYS:CG	1:D:736:GLN:CG	1.97	1.37
1:D:641:LYS:CG	1:D:647:GLN:CD	1.93	1.37
1:D:642:LYS:HG3	4:5:23:GLY:N	1.40	1.37
2:H:144:VAL:CG1	2:H:153:ILE:HG12	1.54	1.37
1:J:736:GLN:CA	1:J:743:ALA:HB1	1.53	1.37
2:K:144:VAL:CG1	2:K:153:ILE:CG1	2.03	1.37
1:A:641:LYS:HG3	1:A:647:GLN:CD	1.46	1.36
2:B:117:LEU:HB2	2:B:147:ASN:ND2	1.39	1.36
1:A:721:LYS:HG3	1:A:736:GLN:CG	1.15	1.36
1:G:530:MET:CG	4:6:354:GLN:HB2	1.51	1.36
1:G:537:GLU:O	4:6:349:LEU:CD1	1.71	1.36
2:H:117:LEU:HB2	2:H:147:ASN:ND2	1.40	1.36
1:A:649:VAL:O	1:A:649:VAL:CG1	1.74	1.36
2:B:144:VAL:CG1	2:B:153:ILE:HG12	1.54	1.36
1:J:642:LYS:HG3	4:7:23:GLY:N	1.40	1.36
1:J:641:LYS:CG	1:J:647:GLN:CD	1.93	1.36
1:J:831:TRP:HZ3	2:K:34:ILE:CD1	1.36	1.36
2:K:144:VAL:CG1	2:K:153:ILE:HG12	1.54	1.36
1:G:649:VAL:O	1:G:649:VAL:CG1	1.74	1.36
2:B:117:LEU:CD1	2:B:147:ASN:OD1	1.74	1.35
1:D:800:ARG:HB3	3:F:149:VAL:CG2	1.56	1.35
1:G:538:GLU:CA	4:6:349:LEU:HD12	0.88	1.35
1:D:831:TRP:CE2	2:E:47:LEU:HD22	1.61	1.35
1:G:642:LYS:HG3	4:6:23:GLY:N	1.39	1.35
1:G:736:GLN:CA	1:G:743:ALA:CB	2.00	1.35
1:J:736:GLN:N	1:J:743:ALA:HB1	1.35	1.35
2:K:117:LEU:HB2	2:K:147:ASN:ND2	1.39	1.35
2:B:144:VAL:CG1	2:B:153:ILE:CG1	2.03	1.35
1:G:736:GLN:CA	1:G:743:ALA:HB1	1.53	1.35
1:A:530:MET:HA	4:4:354:GLN:CG	1.56	1.35
1:A:534:SER:O	4:4:351:THR:CG2	1.64	1.35
1:D:721:LYS:HG3	1:D:736:GLN:CG	1.15	1.35
1:G:721:LYS:CG	1:G:736:GLN:CG	1.97	1.35
2:H:144:VAL:CG1	2:H:153:ILE:CG1	2.03	1.35
1:D:534:SER:O	4:5:351:THR:CG2	1.64	1.34
1:J:538:GLU:CA	4:7:349:LEU:HD12	0.88	1.34
1:G:641:LYS:CG	1:G:647:GLN:CD	1.93	1.34
1:G:834:LEU:HD13	2:H:51:PHE:CE1	1.61	1.34
1:D:649:VAL:O	1:D:649:VAL:CG1	1.73	1.34
2:E:144:VAL:CG1	2:E:153:ILE:CG1	2.03	1.34

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:117:LEU:CD1	2:K:147:ASN:OD1	1.74	1.34
1:A:538:GLU:CA	4:4:349:LEU:HD12	0.87	1.34
1:A:641:LYS:CG	1:A:647:GLN:CD	1.93	1.34
1:A:642:LYS:HG3	4:4:23:GLY:N	1.40	1.34
2:E:117:LEU:CD1	2:E:147:ASN:OD1	1.74	1.33
2:H:114:LYS:CA	2:H:146:GLY:O	1.76	1.33
2:H:117:LEU:CD1	2:H:147:ASN:OD1	1.74	1.33
1:D:538:GLU:CA	4:5:349:LEU:HD12	0.87	1.33
1:J:629:GLU:HA	1:J:643:GLY:O	1.17	1.33
1:J:641:LYS:HG3	1:J:647:GLN:CD	1.46	1.33
1:J:795:ARG:HD2	3:L:35:ARG:CZ	1.57	1.33
1:J:821:ARG:NH2	2:K:127:ARG:HG2	1.42	1.33
1:D:530:MET:HA	4:5:354:GLN:CG	1.56	1.33
1:D:635:GLY:CA	4:5:334:GLU:HG2	1.59	1.33
2:E:117:LEU:HB2	2:E:147:ASN:ND2	1.40	1.33
1:J:530:MET:HA	4:7:354:GLN:CG	1.56	1.33
1:J:649:VAL:O	1:J:649:VAL:CG1	1.74	1.33
1:A:813:ILE:CG2	2:B:127:ARG:CD	2.07	1.33
1:G:831:TRP:HE1	2:H:67:MET:CG	1.41	1.33
1:J:635:GLY:CA	4:7:334:GLU:HG2	1.59	1.33
1:J:735:GLY:O	1:J:743:ALA:HB2	1.29	1.33
1:D:629:GLU:HA	1:D:643:GLY:O	1.17	1.32
1:G:530:MET:HA	4:6:354:GLN:CG	1.57	1.32
1:J:534:SER:O	4:7:351:THR:CG2	1.64	1.32
1:J:792:ALA:CB	3:L:40:ASN:HB3	1.59	1.32
1:D:799:MET:SD	3:F:32:ASP:CB	2.18	1.32
1:D:831:TRP:CZ2	2:E:47:LEU:HD23	1.64	1.32
1:J:721:LYS:CG	1:J:736:GLN:CD	1.98	1.32
1:A:725:ARG:NE	1:A:733:PRO:HB3	0.99	1.32
1:G:769:ALA:CB	1:G:770:GLY:CA	2.07	1.32
1:D:831:TRP:NE1	2:E:47:LEU:HD22	1.44	1.32
2:E:114:LYS:CA	2:E:146:GLY:O	1.76	1.32
1:G:757:GLN:OE1	1:G:772:LEU:HB3	1.30	1.32
1:A:538:GLU:O	4:4:349:LEU:CD1	1.78	1.31
1:A:813:ILE:HG22	2:B:127:ARG:CD	1.58	1.31
1:J:831:TRP:CZ3	2:K:34:ILE:CD1	2.11	1.31
2:K:114:LYS:CA	2:K:146:GLY:O	1.76	1.31
2:K:121:LEU:O	2:K:128:PHE:CB	1.78	1.31
1:A:629:GLU:HA	1:A:643:GLY:O	1.17	1.31
2:B:114:LYS:CA	2:B:146:GLY:O	1.76	1.31
1:G:629:GLU:HA	1:G:643:GLY:O	1.17	1.31

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:721:LYS:HG2	1:D:736:GLN:OE1	1.28	1.31
1:D:831:TRP:CE2	2:E:47:LEU:CD2	2.13	1.31
1:J:725:ARG:NE	1:J:733:PRO:HB3	1.00	1.31
1:A:721:LYS:CG	1:A:736:GLN:CD	1.98	1.31
1:G:635:GLY:CA	4:6:334:GLU:HG2	1.59	1.31
1:G:798:LEU:HD11	3:I:126:LEU:CD2	1.55	1.31
1:A:635:GLY:CA	4:4:334:GLU:HG2	1.59	1.30
1:D:599:ASN:HA	1:D:649:VAL:CB	1.60	1.30
1:D:839:MLY:CH1	2:E:159:HIS:CD2	2.15	1.30
1:A:819:ASN:OD1	2:B:91:ALA:CA	1.79	1.30
1:A:834:LEU:HD11	2:B:54:MET:CB	1.60	1.30
1:D:721:LYS:CG	1:D:736:GLN:CD	1.98	1.30
1:D:725:ARG:NE	1:D:733:PRO:HB3	1.00	1.30
2:E:121:LEU:O	2:E:128:PHE:CB	1.79	1.30
1:G:641:LYS:HG3	1:G:647:GLN:CD	1.45	1.30
1:G:789:ALA:HB2	3:I:81:GLN:NE2	1.43	1.30
1:G:538:GLU:O	4:6:349:LEU:CD1	1.78	1.30
1:G:725:ARG:NE	1:G:733:PRO:HB3	0.99	1.30
1:J:599:ASN:HA	1:J:649:VAL:CB	1.60	1.30
1:A:831:TRP:CE2	2:B:51:PHE:CZ	2.20	1.30
1:G:721:LYS:CG	1:G:736:GLN:CD	1.98	1.30
1:D:723:ARG:O	1:D:782:MLY:HD3	1.30	1.29
1:D:735:GLY:C	1:D:743:ALA:CB	2.01	1.29
1:G:800:ARG:HH11	3:I:149:VAL:CG2	1.42	1.29
1:A:735:GLY:O	1:A:743:ALA:HB2	1.29	1.29
2:B:121:LEU:O	2:B:128:PHE:CB	1.79	1.29
1:G:735:GLY:C	1:G:743:ALA:CB	2.01	1.29
1:A:599:ASN:HA	1:A:649:VAL:CB	1.60	1.29
1:D:215:GLN:N	1:D:340:ILE:HG12	1.20	1.29
1:D:641:LYS:HG3	1:D:647:GLN:CD	1.45	1.29
1:G:599:ASN:HA	1:G:649:VAL:CB	1.60	1.29
1:J:537:GLU:C	4:7:349:LEU:HD13	1.52	1.29
1:J:735:GLY:C	1:J:743:ALA:CB	2.01	1.29
1:J:768:MLY:CH1	1:J:772:LEU:CD2	2.10	1.29
1:A:836:PHE:HB2	2:B:161:GLU:OE1	1.32	1.28
1:G:537:GLU:C	4:6:349:LEU:HD13	1.53	1.28
1:J:800:ARG:CB	3:L:149:VAL:HG21	1.62	1.28
1:J:215:GLN:N	1:J:340:ILE:HG12	1.19	1.28
1:G:721:LYS:HG2	1:G:736:GLN:OE1	1.29	1.28
1:G:795:ARG:HD2	3:I:35:ARG:NH2	1.47	1.28
1:J:721:LYS:HG2	1:J:736:GLN:OE1	1.29	1.28

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:819:ASN:HA	2:K:90:GLY:O	1.19	1.28
1:G:752:ASP:O	1:G:779:ARG:NH1	1.66	1.28
2:H:121:LEU:O	2:H:128:PHE:CB	1.78	1.28
1:D:831:TRP:CZ2	2:E:47:LEU:CD2	2.17	1.27
1:G:836:PHE:CE1	2:H:159:HIS:HA	1.67	1.27
1:A:537:GLU:C	4:4:349:LEU:HD13	1.52	1.27
1:A:735:GLY:C	1:A:743:ALA:CB	2.01	1.27
1:J:538:GLU:O	4:7:349:LEU:CD1	1.78	1.27
1:A:534:SER:O	4:4:351:THR:CA	1.81	1.27
1:D:721:LYS:CG	1:D:736:GLN:OE1	1.82	1.27
1:J:733:PRO:O	1:J:737:PHE:HD1	0.93	1.26
1:D:534:SER:O	4:5:351:THR:CA	1.82	1.26
1:J:534:SER:O	4:7:351:THR:CA	1.82	1.26
1:A:836:PHE:CB	2:B:161:GLU:OE1	1.81	1.26
1:D:735:GLY:O	1:D:743:ALA:HB2	1.29	1.26
1:G:721:LYS:CG	1:G:736:GLN:OE1	1.83	1.26
1:J:768:MLY:HH23	1:J:772:LEU:CB	1.65	1.26
1:A:813:ILE:HG22	2:B:127:ARG:NE	1.45	1.26
1:D:537:GLU:C	4:5:349:LEU:HD13	1.52	1.26
1:D:721:LYS:HG3	1:D:736:GLN:CD	1.53	1.26
1:G:790:THR:OG1	3:I:87:PHE:CE2	1.89	1.26
1:A:149:GLN:HB3	1:A:719:ASP:OD1	1.12	1.26
1:A:733:PRO:O	1:A:737:PHE:HD1	0.92	1.25
1:D:538:GLU:O	4:5:349:LEU:CD1	1.78	1.25
1:G:508:ILE:HD11	1:G:759:ALA:CB	1.62	1.25
1:G:821:ARG:NH2	2:H:127:ARG:CG	1.99	1.25
1:J:768:MLY:CH2	1:J:772:LEU:HB2	1.66	1.25
1:A:797:PHE:CD1	3:C:149:VAL:HG11	1.71	1.25
1:G:735:GLY:O	1:G:743:ALA:HB2	1.29	1.25
1:G:721:LYS:HG3	1:G:736:GLN:CD	1.53	1.25
1:J:508:ILE:CD1	1:J:759:ALA:HB2	1.63	1.25
1:J:630:ALA:O	4:7:25:ASP:OD2	1.52	1.25
1:D:641:LYS:CG	1:D:647:GLN:CG	2.15	1.24
1:G:534:SER:O	4:6:351:THR:CA	1.83	1.24
1:G:93:MET:SD	1:G:716:LEU:HD12	1.75	1.24
1:J:641:LYS:CD	1:J:647:GLN:NE2	1.99	1.24
4:5:322:PRO:CB	4:7:244:ASP:OD2	1.86	1.24
1:A:721:LYS:CG	1:A:736:GLN:CG	1.97	1.24
1:G:508:ILE:CD1	1:G:759:ALA:HB2	1.67	1.24
1:G:646:PHE:CE2	1:G:652:LEU:HD11	1.73	1.24
1:G:733:PRO:O	1:G:737:PHE:HD1	0.93	1.24

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:721:LYS:HG3	1:J:736:GLN:CD	1.54	1.24
1:J:792:ALA:HB1	3:L:40:ASN:CB	1.67	1.24
2:K:117:LEU:CD1	2:K:147:ASN:CG	2.05	1.24
4:7:322:PRO:CB	4:V:244:ASP:OD2	1.86	1.24
1:A:795:ARG:HD2	3:C:35:ARG:NH1	1.49	1.24
1:D:646:PHE:CE2	1:D:652:LEU:HD11	1.73	1.24
1:A:646:PHE:CE2	1:A:652:LEU:HD11	1.73	1.24
1:A:834:LEU:HD11	2:B:54:MET:CG	1.67	1.24
1:D:836:PHE:HB3	2:E:161:GLU:OE1	1.35	1.24
1:J:641:LYS:CG	1:J:647:GLN:CG	2.16	1.24
1:A:721:LYS:HG2	1:A:736:GLN:OE1	1.29	1.23
1:J:721:LYS:CG	1:J:736:GLN:OE1	1.83	1.23
1:J:795:ARG:CD	3:L:35:ARG:NH2	1.90	1.23
2:K:117:LEU:HD12	2:K:147:ASN:OD1	1.32	1.23
4:3:322:PRO:CB	4:5:244:ASP:OD2	1.86	1.23
2:B:117:LEU:CD1	2:B:147:ASN:CG	2.05	1.23
1:D:795:ARG:NH2	3:F:116:GLU:OE2	1.67	1.23
4:4:322:PRO:CB	4:6:244:ASP:OD2	1.86	1.23
4:8:322:PRO:CB	4:W:244:ASP:OD2	1.86	1.23
1:A:538:GLU:O	4:4:349:LEU:HD11	1.35	1.23
1:A:630:ALA:O	4:4:25:ASP:OD2	1.53	1.23
1:A:800:ARG:HD2	3:C:149:VAL:CG2	1.68	1.23
2:E:121:LEU:C	2:E:128:PHE:CB	2.07	1.23
4:V:322:PRO:CB	4:X:244:ASP:OD2	1.86	1.23
1:A:629:GLU:CA	1:A:643:GLY:O	1.87	1.23
1:A:721:LYS:CG	1:A:736:GLN:OE1	1.82	1.23
1:A:795:ARG:NH2	3:C:116:GLU:OE2	1.69	1.23
1:A:800:ARG:CB	3:C:149:VAL:CG2	2.17	1.23
1:D:834:LEU:HD11	2:E:54:MET:CG	1.66	1.23
1:J:646:PHE:CE2	1:J:652:LEU:HD11	1.73	1.23
1:A:506:GLU:OE2	1:A:717:TYR:OH	1.57	1.23
1:G:783:LEU:O	1:G:787:ILE:N	1.71	1.23
4:2:322:PRO:CB	4:4:244:ASP:OD2	1.86	1.23
4:W:322:PRO:CB	4:Y:244:ASP:OD2	1.86	1.23
1:D:538:GLU:C	4:5:349:LEU:HD12	1.48	1.22
1:G:538:GLU:C	4:6:349:LEU:HD12	1.48	1.22
1:G:838:ILE:CD1	2:H:54:MET:HE3	1.69	1.22
4:0:322:PRO:CB	4:2:244:ASP:OD2	1.86	1.22
4:X:322:PRO:CB	4:Z:244:ASP:OD2	1.86	1.22
1:A:215:GLN:N	1:A:340:ILE:CG1	2.02	1.22
1:A:534:SER:O	4:4:351:THR:CB	1.87	1.22

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:641:LYS:CD	1:G:647:GLN:NE2	1.99	1.22
1:A:641:LYS:CG	1:A:647:GLN:CG	2.16	1.22
1:A:836:PHE:CZ	2:B:160:GLY:CA	2.20	1.22
2:B:121:LEU:C	2:B:128:PHE:CB	2.07	1.22
1:D:630:ALA:O	4:5:25:ASP:OD2	1.52	1.22
1:D:641:LYS:CD	1:D:647:GLN:NE2	1.99	1.22
1:D:733:PRO:O	1:D:737:PHE:HD1	0.93	1.22
1:G:553:MLY:CE	4:8:45:VAL:HA	1.52	1.22
1:G:757:GLN:OE1	1:G:772:LEU:CB	1.86	1.22
1:J:215:GLN:N	1:J:340:ILE:CG1	2.02	1.22
4:1:322:PRO:CB	4:3:244:ASP:OD2	1.86	1.22
1:D:799:MET:SD	3:F:32:ASP:O	1.97	1.22
2:E:117:LEU:CD1	2:E:147:ASN:CG	2.05	1.22
1:G:215:GLN:N	1:G:340:ILE:CG1	2.02	1.22
2:H:144:VAL:CG1	2:H:153:ILE:HD11	1.64	1.22
1:A:798:LEU:CD1	3:C:126:LEU:CD2	2.16	1.21
1:D:534:SER:O	4:5:351:THR:CB	1.87	1.21
1:D:799:MET:SD	3:F:32:ASP:C	2.18	1.21
1:G:538:GLU:O	4:6:349:LEU:HD11	1.34	1.21
1:G:707:CYS:HB3	1:G:714:ARG:NH1	1.54	1.21
1:J:534:SER:O	4:7:351:THR:CB	1.87	1.21
1:A:641:LYS:CG	1:A:647:GLN:HG3	1.71	1.21
2:B:144:VAL:CG1	2:B:153:ILE:HD11	1.65	1.21
1:D:629:GLU:CA	1:D:643:GLY:O	1.87	1.21
1:G:629:GLU:CA	1:G:643:GLY:O	1.87	1.21
2:H:121:LEU:C	2:H:128:PHE:CB	2.07	1.21
4:6:322:PRO:CB	4:8:244:ASP:OD2	1.86	1.21
1:A:641:LYS:CD	1:A:647:GLN:NE2	1.99	1.21
1:D:215:GLN:N	1:D:340:ILE:CG1	2.02	1.21
1:D:822:SER:OG	2:E:88:LEU:HD23	1.06	1.21
1:J:629:GLU:CA	1:J:643:GLY:O	1.87	1.21
2:K:121:LEU:C	2:K:128:PHE:CB	2.07	1.21
1:D:641:LYS:CG	1:D:647:GLN:HG3	1.71	1.21
2:E:144:VAL:CG1	2:E:153:ILE:HD11	1.65	1.21
1:A:795:ARG:HB3	3:C:35:ARG:NH2	1.56	1.20
1:G:641:LYS:CG	1:G:647:GLN:HG3	1.71	1.20
2:B:117:LEU:CD1	2:B:147:ASN:CB	2.19	1.20
1:G:215:GLN:N	1:G:340:ILE:HG12	1.19	1.20
2:H:117:LEU:CD1	2:H:147:ASN:CB	2.19	1.20
1:J:93:MET:SD	1:J:716:LEU:HD12	1.82	1.20
1:A:797:PHE:HD1	3:C:149:VAL:CG1	1.54	1.20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:826:VAL:HG21	2:K:88:LEU:HD21	1.21	1.20
4:0:322:PRO:HB2	4:2:244:ASP:OD2	1.39	1.20
1:A:757:GLN:CG	1:A:771:LEU:HD11	1.71	1.20
1:D:553:MLY:CE	4:7:45:VAL:HA	1.52	1.20
4:5:322:PRO:HB2	4:7:244:ASP:OD2	1.39	1.20
1:A:721:LYS:HG3	1:A:736:GLN:CD	1.53	1.19
1:G:534:SER:O	4:6:351:THR:CB	1.88	1.19
4:2:322:PRO:HB2	4:4:244:ASP:OD2	1.39	1.19
1:A:538:GLU:OE2	4:4:355:MET:CE	1.91	1.19
1:G:538:GLU:OE2	4:6:355:MET:CE	1.90	1.19
1:G:769:ALA:HB3	1:G:770:GLY:CA	1.65	1.19
2:H:117:LEU:CD1	2:H:147:ASN:CG	2.05	1.19
1:A:822:SER:OG	2:B:88:LEU:HD23	1.04	1.19
1:G:834:LEU:CD1	2:H:51:PHE:HE1	1.56	1.19
1:G:838:ILE:CD1	2:H:54:MET:CE	2.20	1.19
1:J:538:GLU:OE2	4:7:355:MET:CE	1.90	1.19
1:J:557:GLU:H	4:V:48:GLY:CA	1.56	1.19
1:A:538:GLU:C	4:4:349:LEU:HD11	1.54	1.19
1:A:538:GLU:C	4:4:349:LEU:HD12	1.48	1.19
1:D:538:GLU:OE2	4:5:355:MET:CE	1.90	1.19
1:J:800:ARG:CD	3:L:149:VAL:HG23	1.57	1.19
4:1:322:PRO:HB2	4:3:244:ASP:OD2	1.39	1.19
1:D:735:GLY:O	1:D:743:ALA:CB	1.91	1.19
1:J:90:ASP:CG	1:J:764:MLY:HH11	1.61	1.19
1:A:557:GLU:H	4:6:48:GLY:CA	1.56	1.18
4:4:322:PRO:HB2	4:6:244:ASP:OD2	1.39	1.18
1:D:834:LEU:HG	2:E:54:MET:HG3	1.21	1.18
1:G:510:TRP:CZ3	1:G:768:MLY:HH11	1.77	1.18
1:G:641:LYS:CB	1:G:647:GLN:NE2	2.07	1.18
1:D:557:GLU:H	4:7:48:GLY:CA	1.56	1.18
1:J:641:LYS:CG	1:J:647:GLN:HG3	1.71	1.18
2:K:117:LEU:CD1	2:K:147:ASN:CB	2.19	1.18
1:A:735:GLY:O	1:A:743:ALA:CB	1.91	1.18
1:G:795:ARG:CB	3:I:35:ARG:NH2	2.07	1.18
1:J:721:LYS:HG3	1:J:736:GLN:HG2	1.25	1.18
1:J:817:GLN:CD	2:K:127:ARG:HD2	1.64	1.18
1:G:721:LYS:HA	1:G:736:GLN:NE2	1.58	1.18
1:J:538:GLU:C	4:7:349:LEU:HD12	1.48	1.18
1:J:641:LYS:CB	1:J:647:GLN:NE2	2.07	1.18
4:7:322:PRO:HB2	4:V:244:ASP:OD2	1.39	1.18
2:E:117:LEU:CD1	2:E:147:ASN:CB	2.19	1.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:557:GLU:H	4:8:48:GLY:CA	1.56	1.17
1:J:538:GLU:HA	4:7:349:LEU:CD1	1.55	1.17
1:J:768:MLY:HD3	1:J:772:LEU:CB	1.72	1.17
1:J:798:LEU:CD2	3:L:126:LEU:HD11	1.73	1.17
1:J:829:TRP:HZ3	2:K:84:PHE:CE2	1.62	1.17
4:X:322:PRO:HB2	4:Z:244:ASP:OD2	1.39	1.17
1:A:215:GLN:N	1:A:340:ILE:HG12	1.20	1.17
1:A:502:GLU:HG3	1:A:761:GLY:CA	1.75	1.17
1:A:721:LYS:HA	1:A:736:GLN:NE2	1.58	1.17
1:D:725:ARG:N	1:D:782:MLY:HH21	1.57	1.17
1:D:769:ALA:HA	1:D:771:LEU:CA	1.73	1.17
1:G:754:ASP:HB2	1:G:776:GLU:OE2	1.41	1.17
1:G:817:GLN:CG	2:H:127:ARG:HD2	1.72	1.17
4:W:290:ARG:NH2	4:Y:202:THR:HG23	1.59	1.17
1:D:829:TRP:NE1	2:E:67:MET:HG2	1.56	1.17
1:G:201:ALA:O	1:G:202:SER:HB3	1.35	1.17
1:J:530:MET:HE2	4:7:354:GLN:HG2	1.24	1.17
4:4:290:ARG:NH2	4:6:202:THR:HG23	1.59	1.17
1:G:735:GLY:O	1:G:743:ALA:CB	1.91	1.17
1:J:735:GLY:O	1:J:743:ALA:CB	1.91	1.17
1:J:800:ARG:CB	3:L:149:VAL:CG2	2.20	1.17
1:J:829:TRP:CH2	2:K:84:PHE:CE1	2.33	1.17
1:J:829:TRP:HH2	2:K:84:PHE:CE1	1.60	1.17
4:3:322:PRO:HB2	4:5:244:ASP:OD2	1.39	1.17
4:8:322:PRO:HB2	4:W:244:ASP:OD2	1.39	1.17
1:D:538:GLU:HA	4:5:349:LEU:CD1	1.55	1.17
1:D:641:LYS:CE	4:5:348:SER:O	1.93	1.17
1:D:641:LYS:CB	1:D:647:GLN:NE2	2.07	1.17
1:D:830:PRO:HB2	2:E:51:PHE:CZ	1.78	1.17
2:E:117:LEU:CD1	2:E:147:ASN:HB3	1.75	1.17
1:J:641:LYS:CE	4:7:348:SER:O	1.93	1.17
4:6:290:ARG:NH2	4:8:202:THR:HG23	1.59	1.17
4:7:290:ARG:NH2	4:V:202:THR:HG23	1.59	1.17
1:A:553:MLY:CE	4:6:45:VAL:HA	1.52	1.16
1:A:641:LYS:CB	1:A:647:GLN:NE2	2.07	1.16
1:G:201:ALA:O	1:G:202:SER:CB	1.92	1.16
1:A:831:TRP:CD1	2:B:51:PHE:HZ	1.62	1.16
1:D:538:GLU:OE2	4:5:355:MET:HE1	1.44	1.16
4:5:290:ARG:NH2	4:7:202:THR:HG23	1.59	1.16
4:8:290:ARG:NH2	4:W:202:THR:HG23	1.59	1.16
1:A:201:ALA:O	1:A:202:SER:HB3	1.35	1.16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:822:SER:OG	2:E:88:LEU:CD2	1.92	1.16
1:J:721:LYS:CG	1:J:736:GLN:CG	1.97	1.16
4:V:290:ARG:NH2	4:X:202:THR:HG23	1.59	1.16
1:D:726:VAL:HB	1:D:782:MLY:CH1	1.75	1.16
1:G:215:GLN:HA	1:G:340:ILE:CG2	1.75	1.16
1:G:739:ASP:HB3	1:G:742:LYS:HB3	1.21	1.16
1:J:215:GLN:HA	1:J:340:ILE:CG2	1.75	1.16
1:J:510:TRP:CH2	1:J:768:MLY:CH1	2.28	1.16
1:J:800:ARG:NH1	3:L:149:VAL:HG13	1.59	1.16
1:A:639:GLY:CA	4:4:345:ILE:HA	1.74	1.16
1:D:769:ALA:HB1	1:D:770:GLY:CA	1.74	1.16
1:G:642:LYS:CG	4:6:23:GLY:N	2.08	1.16
1:J:201:ALA:O	1:J:202:SER:CB	1.92	1.16
1:J:510:TRP:CZ2	1:J:768:MLY:HH11	1.80	1.16
1:J:538:GLU:C	4:7:349:LEU:HD11	1.54	1.16
1:J:641:LYS:HD2	1:J:647:GLN:NE2	1.58	1.16
2:K:117:LEU:CD1	2:K:147:ASN:HB3	1.76	1.16
2:K:144:VAL:CG1	2:K:153:ILE:HD11	1.65	1.16
4:3:290:ARG:NH2	4:5:202:THR:HG23	1.59	1.16
4:W:322:PRO:HB2	4:Y:244:ASP:OD2	1.39	1.16
1:A:553:MLY:HB3	4:6:46:GLY:CA	1.51	1.15
1:A:641:LYS:HD2	1:A:647:GLN:NE2	1.59	1.15
1:A:641:LYS:CE	4:4:348:SER:O	1.93	1.15
1:G:93:MET:CE	1:G:763:THR:CG2	2.25	1.15
1:G:93:MET:HE1	1:G:763:THR:CA	1.76	1.15
1:G:553:MLY:HB3	4:8:46:GLY:CA	1.51	1.15
1:G:640:LYS:HB3	1:G:645:SER:OG	1.46	1.15
2:H:117:LEU:CD1	2:H:147:ASN:HB3	1.75	1.15
1:J:538:GLU:OE2	4:7:355:MET:HE1	1.44	1.15
1:D:649:VAL:HA	1:D:649:VAL:CG2	1.76	1.15
1:D:839:MLY:HH11	2:E:159:HIS:CD2	1.79	1.15
2:H:111:SER:CA	2:H:148:VAL:O	1.95	1.15
1:J:640:LYS:HB3	1:J:645:SER:OG	1.45	1.15
4:1:290:ARG:NH2	4:3:202:THR:HG23	1.59	1.15
4:X:290:ARG:NH2	4:Z:202:THR:HG23	1.59	1.15
1:J:749:GLY:O	3:L:114:LEU:HD21	1.45	1.15
4:0:290:ARG:NH2	4:2:202:THR:HG23	1.59	1.15
4:2:290:ARG:NH2	4:4:202:THR:HG23	1.59	1.15
1:A:639:GLY:HA3	4:4:344:SER:O	1.47	1.15
1:D:215:GLN:HA	1:D:340:ILE:CG2	1.75	1.15
1:D:538:GLU:C	4:5:349:LEU:HD11	1.54	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:542:PHE:HA	4:5:143:TYR:CE1	1.82	1.15
1:D:641:LYS:HD2	1:D:647:GLN:NE2	1.59	1.15
1:D:721:LYS:HA	1:D:736:GLN:NE2	1.58	1.15
1:G:641:LYS:HD2	1:G:647:GLN:NE2	1.59	1.15
1:J:635:GLY:HA2	4:7:334:GLU:HG2	1.16	1.15
1:J:642:LYS:CG	4:7:23:GLY:N	2.08	1.15
1:J:721:LYS:HA	1:J:736:GLN:NE2	1.58	1.15
1:A:215:GLN:HA	1:A:340:ILE:CG2	1.76	1.15
1:A:542:PHE:HA	4:4:143:TYR:CE1	1.82	1.15
1:D:642:LYS:CG	4:5:23:GLY:N	2.08	1.15
2:E:111:SER:CB	2:E:148:VAL:C	1.93	1.15
2:H:121:LEU:CA	2:H:128:PHE:HB3	1.77	1.15
1:J:542:PHE:HA	4:7:143:TYR:CE1	1.82	1.15
1:A:642:LYS:CG	4:4:23:GLY:N	2.09	1.14
1:A:649:VAL:HG13	1:A:649:VAL:HG22	1.21	1.14
2:B:117:LEU:CD1	2:B:147:ASN:HB3	1.76	1.14
1:D:639:GLY:CA	4:5:345:ILE:HA	1.73	1.14
1:D:640:LYS:HB3	1:D:645:SER:OG	1.46	1.14
1:G:639:GLY:HA3	4:6:344:SER:O	1.46	1.14
1:G:639:GLY:HA2	4:6:345:ILE:HA	1.26	1.14
1:J:649:VAL:HA	1:J:649:VAL:CG2	1.76	1.14
1:J:739:ASP:HB3	1:J:742:LYS:HB3	1.21	1.14
1:J:757:GLN:CG	1:J:776:GLU:CG	2.23	1.14
4:1:287:ILE:HG21	4:3:205:GLU:HG2	1.17	1.14
4:3:287:ILE:HG21	4:5:205:GLU:HG2	1.17	1.14
1:A:813:ILE:HG22	2:B:127:ARG:CZ	1.77	1.14
1:D:726:VAL:HG23	1:D:782:MLY:HH22	1.16	1.14
2:E:111:SER:CA	2:E:148:VAL:O	1.95	1.14
1:G:542:PHE:HA	4:6:143:TYR:CE1	1.82	1.14
1:A:149:GLN:CG	1:A:719:ASP:OD1	1.96	1.14
1:A:795:ARG:HE	3:C:118:MET:HE1	1.04	1.14
1:A:836:PHE:CE2	2:B:160:GLY:HA3	1.81	1.14
1:D:201:ALA:O	1:D:202:SER:HB3	1.36	1.14
1:D:641:LYS:NZ	4:5:348:SER:O	1.80	1.14
1:D:839:MLY:HH13	2:E:159:HIS:CD2	1.82	1.14
2:E:121:LEU:CA	2:E:128:PHE:HB3	1.77	1.14
1:G:649:VAL:HA	1:G:649:VAL:CG2	1.76	1.14
1:J:639:GLY:HA3	4:7:344:SER:O	1.46	1.14
1:J:768:MLY:NZ	1:J:772:LEU:HD22	1.62	1.14
1:J:797:PHE:HD1	3:L:149:VAL:CG1	1.59	1.14
2:K:111:SER:CA	2:K:148:VAL:O	1.95	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:121:LEU:C	2:K:128:PHE:HB2	1.67	1.14
1:A:501:GLU:HG2	1:A:762:HIS:ND1	1.62	1.14
1:A:640:LYS:HB3	1:A:645:SER:OG	1.46	1.14
2:B:111:SER:CA	2:B:148:VAL:O	1.95	1.14
2:B:121:LEU:CA	2:B:128:PHE:HB3	1.78	1.14
1:D:635:GLY:HA2	4:5:334:GLU:HG2	1.16	1.14
1:D:736:GLN:N	1:D:743:ALA:CB	2.05	1.14
2:E:117:LEU:HD12	2:E:147:ASN:OD1	1.32	1.14
1:G:641:LYS:CE	4:6:348:SER:O	1.93	1.14
2:K:121:LEU:CA	2:K:128:PHE:HB3	1.77	1.14
4:6:322:PRO:HB2	4:8:244:ASP:OD2	1.39	1.14
1:A:649:VAL:HA	1:A:649:VAL:CG2	1.76	1.14
2:B:117:LEU:HD12	2:B:147:ASN:OD1	1.32	1.14
1:G:599:ASN:OD1	1:G:649:VAL:CB	1.96	1.14
1:G:831:TRP:NE1	2:H:67:MET:HG2	1.63	1.14
1:J:757:GLN:HG2	1:J:776:GLU:CG	1.76	1.14
4:5:287:ILE:HG21	4:7:205:GLU:HG2	1.17	1.14
1:D:641:LYS:HG3	1:D:647:GLN:HG3	1.20	1.13
1:D:739:ASP:HB3	1:D:742:LYS:HB3	1.21	1.13
1:G:649:VAL:HG22	1:G:649:VAL:HG13	1.21	1.13
2:H:117:LEU:HD12	2:H:147:ASN:OD1	1.32	1.13
2:K:112:ILE:O	2:K:147:ASN:O	1.65	1.13
2:B:121:LEU:C	2:B:128:PHE:HB2	1.67	1.13
1:D:639:GLY:HA3	4:5:344:SER:O	1.46	1.13
1:D:830:PRO:CG	2:E:67:MET:HE1	1.77	1.13
1:G:84:MLY:HH11	1:G:715:VAL:CG1	1.76	1.13
1:G:93:MET:HE1	1:G:763:THR:C	1.67	1.13
1:G:768:MLY:HD3	1:G:772:LEU:HD22	1.19	1.13
1:J:541:MET:C	4:7:143:TYR:OH	1.87	1.13
1:A:599:ASN:OD1	1:A:649:VAL:CB	1.96	1.13
1:A:641:LYS:CE	1:A:647:GLN:OE1	1.97	1.13
1:D:599:ASN:OD1	1:D:649:VAL:CB	1.96	1.13
1:D:834:LEU:CD1	2:E:54:MET:HG3	1.78	1.13
1:G:538:GLU:C	4:6:349:LEU:HD11	1.54	1.13
2:H:112:ILE:O	2:H:147:ASN:O	1.65	1.13
1:A:768:MLY:HB3	1:A:771:LEU:HD13	1.31	1.13
1:A:795:ARG:HH21	3:C:116:GLU:HB3	1.01	1.13
1:G:768:MLY:HD3	1:G:772:LEU:CD2	1.79	1.13
1:J:599:ASN:OD1	1:J:649:VAL:CB	1.96	1.13
1:J:641:LYS:CE	1:J:647:GLN:OE1	1.97	1.13
1:J:831:TRP:HZ2	2:K:47:LEU:HD22	1.08	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:ARG:NH1	3:C:149:VAL:HG13	1.61	1.13
1:A:831:TRP:NE1	2:B:51:PHE:HZ	1.32	1.13
1:A:541:MET:C	4:4:143:TYR:OH	1.87	1.12
1:D:201:ALA:O	1:D:202:SER:CB	1.92	1.12
1:D:541:MET:C	4:5:143:TYR:OH	1.87	1.12
1:D:726:VAL:CB	1:D:782:MLY:HH13	1.77	1.13
1:G:541:MET:C	4:6:143:TYR:OH	1.87	1.12
1:G:639:GLY:CA	4:6:345:ILE:HA	1.73	1.12
1:J:510:TRP:CZ3	1:J:768:MLY:HH11	1.83	1.12
4:W:287:ILE:HG21	4:Y:205:GLU:HG2	1.17	1.12
1:A:641:LYS:NZ	4:4:348:SER:O	1.80	1.12
1:A:839:MLY:HH21	2:B:158:THR:HG22	1.30	1.12
2:B:112:ILE:O	2:B:147:ASN:O	1.65	1.12
1:D:641:LYS:CE	1:D:647:GLN:OE1	1.97	1.12
1:D:724:TYR:CE1	1:D:778:MET:HB3	1.85	1.12
1:D:831:TRP:CZ3	2:E:34:ILE:CG2	2.32	1.12
1:G:641:LYS:NZ	4:6:348:SER:O	1.80	1.12
1:G:834:LEU:CD1	2:H:51:PHE:CE1	2.30	1.12
1:A:201:ALA:O	1:A:202:SER:CB	1.92	1.12
1:D:507:GLY:O	1:D:761:GLY:CA	1.97	1.12
1:D:538:GLU:O	4:5:349:LEU:HD11	1.35	1.12
1:G:641:LYS:CE	1:G:647:GLN:OE1	1.97	1.12
1:G:819:ASN:CG	2:H:92:ASP:HB2	1.62	1.12
2:K:111:SER:HB3	2:K:148:VAL:O	1.50	1.12
4:7:287:ILE:HG21	4:V:205:GLU:HG2	1.17	1.12
1:A:707:CYS:HA	1:A:714:ARG:HH12	1.11	1.12
2:B:121:LEU:O	2:B:128:PHE:HB2	0.94	1.12
1:J:92:ALA:O	1:J:714:ARG:HD2	1.49	1.12
1:J:623:PHE:CG	1:J:623:PHE:CB	2.33	1.12
1:J:821:ARG:NH2	2:K:127:ARG:CG	2.13	1.12
1:J:829:TRP:CH2	2:K:84:PHE:CZ	2.38	1.12
1:A:530:MET:HE2	4:4:354:GLN:HG2	1.30	1.12
1:A:707:CYS:HA	1:A:714:ARG:NH1	1.64	1.12
3:C:48:LYS:C	3:C:52:ASN:ND2	2.03	1.12
2:E:112:ILE:O	2:E:147:ASN:O	1.65	1.12
1:G:538:GLU:OE2	4:6:355:MET:HE1	1.50	1.12
1:J:795:ARG:NH2	3:L:116:GLU:OE2	1.83	1.12
3:I:48:LYS:C	3:I:52:ASN:ND2	2.03	1.11
1:G:649:VAL:O	1:G:649:VAL:HG12	0.94	1.11
1:G:788:THR:C	3:I:42:THR:HG22	1.56	1.11
1:J:641:LYS:NZ	4:7:348:SER:O	1.80	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:LEU:HD11	3:C:126:LEU:HD21	1.29	1.11
2:B:117:LEU:HB2	2:B:147:ASN:CG	1.70	1.11
1:G:819:ASN:CG	2:H:90:GLY:O	1.88	1.11
3:L:24:LYS:CB	3:L:63:ILE:O	1.99	1.11
4:5:290:ARG:CZ	4:7:202:THR:HG21	1.81	1.11
4:7:290:ARG:CZ	4:V:202:THR:HG21	1.81	1.11
4:8:287:ILE:HG21	4:W:205:GLU:HG2	1.17	1.11
4:8:290:ARG:CZ	4:W:202:THR:HG21	1.81	1.11
4:V:322:PRO:HB2	4:X:244:ASP:OD2	1.39	1.11
1:A:649:VAL:O	1:A:649:VAL:HG12	0.94	1.11
1:A:814:PHE:CD1	2:B:127:ARG:NH2	2.16	1.11
3:C:24:LYS:CB	3:C:63:ILE:O	1.99	1.11
1:D:623:PHE:CB	1:D:623:PHE:CG	2.33	1.11
1:D:641:LYS:CE	1:D:647:GLN:CD	2.18	1.11
1:G:736:GLN:N	1:G:743:ALA:CB	2.04	1.11
2:H:111:SER:CB	2:H:148:VAL:C	1.93	1.11
2:H:117:LEU:HB2	2:H:147:ASN:CG	1.70	1.11
4:0:290:ARG:CZ	4:2:202:THR:HG21	1.81	1.11
1:A:623:PHE:CB	1:A:623:PHE:CG	2.33	1.11
1:D:834:LEU:CD1	2:E:54:MET:CG	2.28	1.11
3:F:48:LYS:C	3:F:52:ASN:ND2	2.03	1.11
1:G:798:LEU:HD13	3:I:126:LEU:CD2	1.67	1.11
1:G:817:GLN:CD	2:H:127:ARG:HD2	1.68	1.11
1:J:641:LYS:CE	1:J:647:GLN:CD	2.18	1.11
1:J:798:LEU:HD22	3:L:126:LEU:CD1	1.79	1.11
4:6:290:ARG:CZ	4:8:202:THR:HG21	1.81	1.11
1:D:530:MET:CE	4:5:354:GLN:HG2	1.80	1.10
1:D:530:MET:HE2	4:5:354:GLN:HG2	1.22	1.10
1:D:799:MET:SD	3:F:32:ASP:CA	2.38	1.10
1:G:93:MET:SD	1:G:716:LEU:CD1	2.39	1.10
1:D:798:LEU:HD11	3:F:126:LEU:HD21	1.27	1.10
2:E:117:LEU:HB2	2:E:147:ASN:CG	1.70	1.10
2:E:121:LEU:O	2:E:128:PHE:HB2	0.94	1.10
1:G:623:PHE:CB	1:G:623:PHE:CG	2.33	1.10
1:G:641:LYS:HG3	1:G:647:GLN:HG3	1.21	1.10
1:G:641:LYS:CE	1:G:647:GLN:CD	2.18	1.10
1:J:84:MLY:HH11	1:J:715:VAL:CG1	1.70	1.10
1:J:530:MET:CE	4:7:354:GLN:HG2	1.80	1.10
1:J:538:GLU:O	4:7:349:LEU:HD11	1.35	1.10
4:W:290:ARG:CZ	4:Y:202:THR:HG21	1.81	1.10
1:A:641:LYS:CE	1:A:647:GLN:CD	2.18	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:649:VAL:HG22	1:D:649:VAL:HG13	1.21	1.10
1:G:730:SER:OG	3:I:109:HIS:CG	2.05	1.10
1:G:838:ILE:HD11	2:H:54:MET:HE1	1.19	1.10
1:J:218:LEU:HB2	1:J:221:GLN:HG3	1.17	1.10
3:L:48:LYS:C	3:L:52:ASN:ND2	2.03	1.10
4:2:290:ARG:CZ	4:4:202:THR:HG21	1.81	1.10
4:V:287:ILE:HG21	4:X:205:GLU:HG2	1.17	1.10
4:V:290:ARG:CZ	4:X:202:THR:HG21	1.81	1.10
1:A:202:SER:CA	1:A:207:LYS:HE2	1.82	1.10
1:A:218:LEU:HB2	1:A:221:GLN:HG3	1.17	1.10
2:H:121:LEU:O	2:H:128:PHE:HB2	0.94	1.10
1:J:553:MLY:CE	4:V:45:VAL:HA	1.52	1.10
1:J:797:PHE:CD1	3:L:149:VAL:CG1	2.34	1.10
1:J:800:ARG:NE	3:L:149:VAL:HG22	1.65	1.10
4:3:290:ARG:CZ	4:5:202:THR:HG21	1.81	1.10
1:A:641:LYS:HE3	1:A:647:GLN:OE1	1.50	1.10
1:A:822:SER:OG	2:B:88:LEU:CD2	2.00	1.10
1:D:817:GLN:CD	2:E:127:ARG:NE	2.04	1.10
1:D:822:SER:CB	2:E:88:LEU:HD23	1.82	1.10
1:D:831:TRP:CZ2	2:E:47:LEU:CB	2.23	1.10
1:D:831:TRP:CD1	2:E:67:MET:SD	2.45	1.10
1:G:202:SER:CA	1:G:207:LYS:HE2	1.82	1.10
1:J:641:LYS:HE3	1:J:647:GLN:OE1	1.50	1.10
1:A:721:LYS:HA	1:A:736:GLN:CD	1.73	1.09
1:A:739:ASP:HB3	1:A:742:LYS:HB3	1.21	1.09
1:A:799:MET:SD	3:C:32:ASP:CB	2.38	1.09
1:D:639:GLY:HA2	4:5:345:ILE:HA	1.26	1.09
1:D:734:GLU:O	1:D:738:MET:HG2	1.51	1.09
1:D:817:GLN:HE21	2:E:127:ARG:HG2	1.12	1.09
3:I:24:LYS:CB	3:I:63:ILE:O	1.99	1.09
1:J:641:LYS:HD2	1:J:647:GLN:CD	1.70	1.09
1:J:768:MLY:HD3	1:J:772:LEU:HB3	1.30	1.09
4:6:287:ILE:HG21	4:8:205:GLU:HG2	1.17	1.09
1:A:530:MET:CE	4:4:354:GLN:HG2	1.80	1.09
1:A:538:GLU:HA	4:4:349:LEU:CD1	1.54	1.09
1:D:218:LEU:HB2	1:D:221:GLN:HG3	1.17	1.09
1:D:768:MLY:O	1:D:771:LEU:HD11	1.29	1.09
2:E:121:LEU:C	2:E:128:PHE:HB2	1.67	1.09
1:G:530:MET:CE	4:6:354:GLN:HG2	1.80	1.09
1:J:571:ALA:O	1:J:572:LYS:HG3	1.52	1.09
1:J:649:VAL:O	1:J:649:VAL:HG12	0.94	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:290:ARG:CZ	4:6:202:THR:HG21	1.81	1.09
1:D:571:ALA:O	1:D:572:LYS:HG3	1.52	1.09
3:F:24:LYS:CB	3:F:63:ILE:O	1.99	1.09
1:G:218:LEU:HB2	1:G:221:GLN:HG3	1.17	1.09
1:J:93:MET:O	1:J:714:ARG:O	1.71	1.09
1:J:641:LYS:HG3	1:J:647:GLN:HG3	1.20	1.09
1:J:721:LYS:HA	1:J:736:GLN:CD	1.73	1.09
1:J:754:ASP:OD2	1:J:776:GLU:CA	1.99	1.09
2:K:121:LEU:O	2:K:128:PHE:HB2	0.94	1.09
4:X:290:ARG:CZ	4:Z:202:THR:HG21	1.81	1.09
1:D:641:LYS:HE3	1:D:647:GLN:OE1	1.50	1.09
1:D:649:VAL:O	1:D:649:VAL:HG12	0.94	1.09
1:D:809:ARG:NH1	2:E:124:GLY:HA2	1.68	1.09
1:G:84:MLY:HH12	1:G:715:VAL:HG13	1.32	1.09
1:G:707:CYS:CB	1:G:714:ARG:HH12	1.65	1.09
1:G:831:TRP:HE1	2:H:67:MET:HG2	0.92	1.09
1:G:831:TRP:NE1	2:H:67:MET:CG	2.13	1.09
2:H:121:LEU:C	2:H:128:PHE:HB2	1.67	1.09
1:J:201:ALA:O	1:J:202:SER:HB3	1.36	1.09
1:J:649:VAL:HG22	1:J:649:VAL:HG13	1.21	1.09
1:J:734:GLU:O	1:J:738:MET:HG2	1.51	1.09
2:K:121:LEU:C	2:K:128:PHE:HB3	1.71	1.09
4:0:287:ILE:HG21	4:2:205:GLU:HG2	1.17	1.09
4:1:290:ARG:CZ	4:3:202:THR:HG21	1.81	1.09
1:A:734:GLU:O	1:A:738:MET:HG2	1.51	1.09
1:D:202:SER:CA	1:D:207:LYS:HE2	1.82	1.09
1:G:84:MLY:HH13	1:G:715:VAL:HG13	1.17	1.09
1:G:791:GLN:OE1	3:I:116:GLU:HB2	1.52	1.09
1:G:821:ARG:HH22	2:H:127:ARG:CG	1.63	1.09
2:H:111:SER:OG	2:H:148:VAL:O	1.71	1.09
1:J:643:GLY:O	1:J:644:SER:OG	1.70	1.09
2:K:117:LEU:HB2	2:K:147:ASN:CG	1.70	1.09
1:A:798:LEU:HD13	3:C:126:LEU:HD21	1.09	1.08
1:D:530:MET:HE2	4:5:354:GLN:CG	1.82	1.08
1:D:721:LYS:HA	1:D:736:GLN:CD	1.73	1.08
1:D:829:TRP:HE1	2:E:67:MET:CG	1.64	1.08
1:G:538:GLU:HA	4:6:349:LEU:CD1	1.55	1.08
2:K:111:SER:OG	2:K:148:VAL:O	1.71	1.08
4:X:287:ILE:HG21	4:Z:205:GLU:HG2	1.17	1.08
2:B:111:SER:CB	2:B:148:VAL:C	1.93	1.08
1:D:721:LYS:HG3	1:D:736:GLN:HG2	1.25	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:800:ARG:CB	3:F:149:VAL:HG22	1.83	1.08
1:J:95:THR:OG1	1:J:713:SER:HB3	1.50	1.08
1:J:769:ALA:CB	1:J:770:GLY:CA	2.31	1.08
1:A:635:GLY:HA2	4:4:334:GLU:HG2	1.16	1.08
1:D:834:LEU:CD2	2:E:54:MET:HG3	1.82	1.08
1:J:84:MLY:HH13	1:J:715:VAL:HG13	1.28	1.08
1:J:639:GLY:CA	4:7:345:ILE:HA	1.73	1.08
1:J:797:PHE:CD1	3:L:149:VAL:HG11	1.88	1.08
4:4:287:ILE:HG21	4:6:205:GLU:HG2	1.17	1.08
1:A:639:GLY:HA2	4:4:345:ILE:HA	1.26	1.08
2:E:111:SER:HB3	2:E:148:VAL:O	1.50	1.08
1:G:530:MET:HE2	4:6:354:GLN:HG2	1.27	1.08
1:G:734:GLU:O	1:G:738:MET:HG2	1.51	1.08
1:J:202:SER:CA	1:J:207:LYS:HE2	1.82	1.08
1:J:736:GLN:HA	1:J:743:ALA:HB3	1.35	1.08
1:A:798:LEU:HD11	3:C:126:LEU:CD2	1.79	1.08
2:E:111:SER:OG	2:E:148:VAL:O	1.71	1.08
1:J:639:GLY:HA2	4:7:345:ILE:HA	1.26	1.08
2:B:111:SER:CB	2:B:148:VAL:O	0.78	1.07
2:B:121:LEU:C	2:B:128:PHE:HB3	1.72	1.07
1:D:643:GLY:O	1:D:644:SER:OG	1.70	1.07
2:E:111:SER:CB	2:E:148:VAL:O	0.78	1.07
2:E:121:LEU:C	2:E:128:PHE:HB3	1.72	1.07
1:G:641:LYS:HE3	1:G:647:GLN:OE1	1.50	1.07
1:G:643:GLY:O	1:G:644:SER:OG	1.70	1.07
1:G:721:LYS:HG3	1:G:736:GLN:HG2	1.25	1.07
1:J:529:PRO:HB3	4:7:353:GLN:OE1	1.53	1.07
1:J:768:MLY:HH22	1:J:772:LEU:HB2	1.36	1.07
4:2:287:ILE:HG21	4:4:205:GLU:HG2	1.17	1.07
1:A:409:GLY:N	1:A:636:LYS:HG3	1.69	1.07
1:A:501:GLU:O	1:A:762:HIS:NE2	1.87	1.07
1:D:409:GLY:N	1:D:636:LYS:HG3	1.69	1.07
1:D:529:PRO:HB3	4:5:353:GLN:OE1	1.53	1.07
1:D:638:GLY:CA	4:5:341:ILE:O	2.01	1.07
1:G:721:LYS:HA	1:G:736:GLN:CD	1.73	1.07
2:H:111:SER:CB	2:H:148:VAL:O	0.77	1.07
1:J:530:MET:HE2	4:7:354:GLN:CG	1.84	1.07
1:D:769:ALA:HB1	1:D:770:GLY:C	1.72	1.07
1:G:72:VAL:HG13	1:G:76:GLN:HB3	1.36	1.07
1:G:529:PRO:HB3	4:6:353:GLN:OE1	1.53	1.07
1:G:641:LYS:CG	1:G:647:GLN:CG	2.16	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:641:LYS:HB2	1:G:647:GLN:NE2	1.68	1.07
1:J:831:TRP:CZ2	2:K:47:LEU:HD22	1.88	1.07
2:K:111:SER:CB	2:K:148:VAL:O	0.78	1.07
1:A:529:PRO:HB3	4:4:353:GLN:OE1	1.53	1.07
1:A:641:LYS:HB2	1:A:647:GLN:NE2	1.68	1.07
1:A:839:MLY:HD2	2:B:159:HIS:CG	1.88	1.07
1:D:541:MET:SD	4:5:345:ILE:O	2.12	1.07
1:G:409:GLY:N	1:G:636:LYS:HG3	1.69	1.07
1:J:541:MET:SD	4:7:345:ILE:O	2.13	1.07
1:J:638:GLY:CA	4:7:341:ILE:O	2.01	1.07
2:K:111:SER:CB	2:K:148:VAL:C	1.93	1.07
1:A:541:MET:SD	4:4:345:ILE:O	2.12	1.07
1:A:638:GLY:CA	4:4:341:ILE:O	2.01	1.07
1:G:638:GLY:CA	4:6:341:ILE:O	2.02	1.07
1:J:793:ARG:HE	3:L:147:MET:HA	0.93	1.07
1:J:795:ARG:HD3	3:L:35:ARG:HH22	1.14	1.07
1:A:502:GLU:HG3	1:A:761:GLY:HA3	1.34	1.06
1:D:834:LEU:CG	2:E:54:MET:CG	2.32	1.06
1:J:409:GLY:N	1:J:636:LYS:HG3	1.69	1.06
1:A:643:GLY:O	1:A:644:SER:OG	1.69	1.06
1:G:635:GLY:HA2	4:6:334:GLU:HG2	1.16	1.06
1:G:831:TRP:HH2	2:H:47:LEU:HD21	1.13	1.06
1:J:768:MLY:CH2	1:J:772:LEU:CD2	2.12	1.06
1:A:72:VAL:HG13	1:A:76:GLN:HB3	1.36	1.06
1:A:571:ALA:O	1:A:572:LYS:HG3	1.52	1.06
1:D:542:PHE:CG	4:5:143:TYR:HE1	1.73	1.06
1:D:736:GLN:HA	1:D:743:ALA:HB3	1.34	1.06
2:E:114:LYS:HA	2:E:146:GLY:O	0.89	1.06
1:G:541:MET:SD	4:6:345:ILE:O	2.13	1.06
2:H:111:SER:HB3	2:H:148:VAL:O	1.49	1.06
2:K:114:LYS:HA	2:K:146:GLY:O	0.89	1.06
1:D:576:GLU:HG2	1:D:577:ALA:N	1.66	1.06
1:G:797:PHE:CD1	3:I:149:VAL:CG1	2.03	1.06
1:J:510:TRP:CZ3	1:J:768:MLY:CH1	2.39	1.06
1:A:736:GLN:HA	1:A:743:ALA:HB3	1.35	1.06
1:A:793:ARG:NE	3:C:147:MET:HG2	1.70	1.06
1:A:795:ARG:CD	3:C:35:ARG:HH22	1.68	1.06
2:B:111:SER:OG	2:B:148:VAL:O	1.71	1.06
2:B:114:LYS:HA	2:B:146:GLY:O	0.89	1.06
1:D:641:LYS:HE3	4:5:348:SER:O	1.55	1.06
1:D:768:MLY:O	1:D:771:LEU:CD1	0.76	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:571:ALA:O	1:G:572:LYS:HG3	1.52	1.06
1:A:800:ARG:NH1	3:C:149:VAL:C	2.08	1.05
1:D:641:LYS:HB2	1:D:647:GLN:NE2	1.68	1.05
2:E:140:PHE:O	2:E:141:PRO:O	1.74	1.05
1:G:635:GLY:HA3	4:6:341:ILE:HD13	1.36	1.05
1:J:769:ALA:CB	1:J:770:GLY:HA2	1.86	1.05
2:K:140:PHE:O	2:K:141:PRO:O	1.75	1.05
1:A:530:MET:CA	4:4:354:GLN:HG3	1.86	1.05
1:A:721:LYS:HG3	1:A:736:GLN:HG2	1.25	1.05
1:D:831:TRP:CH2	2:E:34:ILE:HG23	1.89	1.05
1:J:530:MET:CA	4:7:354:GLN:HG3	1.87	1.05
4:1:3:ASP:HA	4:1:6:THR:HB	1.36	1.05
1:A:542:PHE:CG	4:4:143:TYR:HE1	1.73	1.05
1:D:72:VAL:HG13	1:D:76:GLN:HB3	1.36	1.05
1:D:795:ARG:HH21	3:F:116:GLU:CD	1.59	1.05
1:G:819:ASN:HA	2:H:90:GLY:O	0.87	1.05
1:J:638:GLY:HA2	4:7:341:ILE:O	1.57	1.05
1:J:641:LYS:HE3	4:7:348:SER:O	1.55	1.05
1:J:641:LYS:HB2	1:J:647:GLN:NE2	1.68	1.05
4:Y:3:ASP:HA	4:Y:6:THR:HB	1.36	1.05
1:A:797:PHE:CD1	3:C:149:VAL:CG1	2.33	1.05
1:G:542:PHE:CG	4:6:143:TYR:HE1	1.74	1.05
1:J:793:ARG:NE	3:L:147:MET:HA	1.71	1.05
1:J:795:ARG:HD2	3:L:35:ARG:NH1	1.72	1.05
1:J:797:PHE:HD1	3:L:149:VAL:HG12	1.21	1.05
1:J:819:ASN:CA	2:K:90:GLY:O	2.04	1.05
1:A:800:ARG:CB	3:C:149:VAL:HG22	1.83	1.05
1:J:72:VAL:HG13	1:J:76:GLN:HB3	1.36	1.05
1:J:641:LYS:HE3	1:J:647:GLN:CD	1.77	1.05
1:J:800:ARG:HB3	3:L:149:VAL:HG21	1.35	1.05
1:A:505:MLY:CB	1:A:762:HIS:H	1.68	1.04
1:A:635:GLY:HA3	4:4:341:ILE:HD13	1.37	1.04
1:D:530:MET:CA	4:5:354:GLN:HG3	1.87	1.04
1:D:829:TRP:HE1	2:E:67:MET:HG2	0.88	1.04
1:G:829:TRP:CH2	2:H:87:LYS:HE2	1.91	1.04
2:H:114:LYS:HA	2:H:146:GLY:O	0.88	1.04
1:A:599:ASN:HA	1:A:649:VAL:HB	1.06	1.04
1:A:641:LYS:HE3	1:A:647:GLN:CD	1.77	1.04
1:A:834:LEU:CD1	2:B:54:MET:HG3	1.86	1.04
3:C:49:ILE:CA	3:C:52:ASN:HD22	1.70	1.04
1:D:638:GLY:HA2	4:5:341:ILE:O	1.57	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:830:PRO:CD	2:E:67:MET:HE1	1.86	1.04
1:G:530:MET:HE2	4:6:354:GLN:CG	1.87	1.04
1:J:542:PHE:CG	4:7:143:TYR:HE1	1.73	1.04
1:J:576:GLU:HG2	1:J:577:ALA:N	1.66	1.04
1:J:736:GLN:N	1:J:743:ALA:CB	2.05	1.04
1:J:800:ARG:CZ	3:L:149:VAL:HG22	1.86	1.04
1:A:641:LYS:HD2	1:A:647:GLN:CD	1.70	1.04
1:G:641:LYS:HE3	1:G:647:GLN:CD	1.77	1.04
1:G:757:GLN:OE1	1:G:772:LEU:CG	2.03	1.04
1:G:769:ALA:HB1	1:G:770:GLY:HA2	1.37	1.04
1:G:817:GLN:HB3	2:H:127:ARG:CD	1.86	1.04
1:J:795:ARG:NH1	3:L:35:ARG:HH12	1.56	1.04
4:O:290:ARG:CZ	4:2:202:THR:CG2	2.36	1.04
4:W:3:ASP:HA	4:W:6:THR:HB	1.36	1.04
1:A:529:PRO:C	4:4:354:GLN:HB3	1.78	1.04
1:A:757:GLN:HB3	1:A:771:LEU:HD13	1.32	1.04
1:A:795:ARG:NH2	3:C:116:GLU:HB3	1.70	1.04
2:B:111:SER:HB3	2:B:148:VAL:O	1.49	1.04
1:G:93:MET:O	1:G:714:ARG:O	1.76	1.04
1:G:789:ALA:CB	3:I:81:GLN:HE21	1.68	1.04
4:2:3:ASP:HA	4:2:6:THR:HB	1.36	1.04
4:8:290:ARG:CZ	4:W:202:THR:CG2	2.36	1.04
1:J:56:GLU:HB2	1:J:59:MLY:HB3	1.40	1.04
1:A:538:GLU:OE2	4:4:355:MET:HE1	1.55	1.03
1:D:202:SER:CA	1:D:207:LYS:CE	2.36	1.03
1:D:641:LYS:HE3	1:D:647:GLN:CD	1.77	1.03
1:G:639:GLY:N	4:6:345:ILE:N	1.94	1.03
1:G:641:LYS:HD2	1:G:647:GLN:CD	1.70	1.03
2:K:149:ASP:OD2	2:K:150:TYR:N	1.91	1.03
4:2:290:ARG:CZ	4:4:202:THR:CG2	2.36	1.03
4:V:290:ARG:CZ	4:X:202:THR:CG2	2.36	1.03
1:A:502:GLU:OE1	1:A:763:THR:N	1.89	1.03
1:A:795:ARG:HH21	3:C:116:GLU:CB	1.71	1.03
1:A:800:ARG:HH11	3:C:149:VAL:C	1.61	1.03
1:G:56:GLU:HB2	1:G:59:MLY:HB3	1.40	1.03
1:G:599:ASN:HA	1:G:649:VAL:HB	1.05	1.03
4:4:3:ASP:HA	4:4:6:THR:HB	1.36	1.03
4:6:290:ARG:CZ	4:8:202:THR:CG2	2.36	1.03
4:W:290:ARG:CZ	4:Y:202:THR:CG2	2.36	1.03
4:X:290:ARG:CZ	4:Z:202:THR:CG2	2.36	1.03
1:A:642:LYS:HG3	4:4:23:GLY:H	0.87	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:49:ILE:CA	3:F:52:ASN:HD22	1.70	1.03
1:G:639:GLY:HA3	4:6:344:SER:C	1.78	1.03
3:L:49:ILE:CA	3:L:52:ASN:HD22	1.71	1.03
1:A:639:GLY:HA3	4:4:344:SER:C	1.78	1.03
1:A:795:ARG:HD2	3:C:35:ARG:HH12	0.88	1.03
1:A:836:PHE:CE2	2:B:160:GLY:CA	2.40	1.03
2:B:140:PHE:O	2:B:141:PRO:O	1.75	1.03
1:D:553:MLY:CB	4:7:46:GLY:CA	2.32	1.03
2:H:149:ASP:OD2	2:H:150:TYR:N	1.91	1.03
3:I:49:ILE:CA	3:I:52:ASN:HD22	1.70	1.03
1:J:202:SER:CA	1:J:207:LYS:CE	2.36	1.03
1:J:553:MLY:HB3	4:V:46:GLY:CA	1.51	1.03
4:3:3:ASP:HA	4:3:6:THR:HB	1.36	1.03
1:A:638:GLY:HA2	4:4:341:ILE:O	1.56	1.03
1:G:93:MET:HE3	1:G:763:THR:HB	1.03	1.03
1:G:557:GLU:N	4:8:48:GLY:CA	2.12	1.03
1:J:93:MET:HG3	1:J:764:MLY:NZ	1.72	1.03
1:J:795:ARG:HE	3:L:118:MET:HE1	1.16	1.03
4:4:290:ARG:CZ	4:6:202:THR:CG2	2.36	1.03
4:7:290:ARG:CZ	4:V:202:THR:CG2	2.36	1.03
4:V:3:ASP:HA	4:V:6:THR:HB	1.36	1.03
4:X:3:ASP:HA	4:X:6:THR:HB	1.36	1.03
1:A:202:SER:CA	1:A:207:LYS:CE	2.36	1.02
1:A:501:GLU:O	1:A:762:HIS:CD2	2.12	1.02
1:A:502:GLU:O	1:A:761:GLY:HA2	1.58	1.02
1:A:541:MET:HB3	4:4:143:TYR:OH	1.60	1.02
1:A:641:LYS:HG3	1:A:647:GLN:HG3	1.21	1.02
1:A:641:LYS:HE3	4:4:348:SER:O	1.56	1.02
1:A:646:PHE:HE2	1:A:652:LEU:HD21	1.24	1.02
1:A:813:ILE:HG23	2:B:127:ARG:HD2	1.05	1.02
1:A:834:LEU:HD11	2:B:54:MET:HB3	1.32	1.02
2:E:144:VAL:HG13	2:E:153:ILE:HD11	1.21	1.02
1:G:529:PRO:C	4:6:354:GLN:HB3	1.79	1.02
1:G:642:LYS:HG3	4:6:23:GLY:H	0.85	1.02
1:G:817:GLN:CB	2:H:127:ARG:HD2	1.89	1.02
1:G:836:PHE:CE2	2:H:160:GLY:N	2.26	1.02
2:H:140:PHE:O	2:H:141:PRO:O	1.75	1.02
1:J:541:MET:HB3	4:7:143:TYR:OH	1.59	1.02
4:0:3:ASP:HA	4:0:6:THR:HB	1.36	1.02
4:8:3:ASP:HA	4:8:6:THR:HB	1.36	1.02
1:D:642:LYS:HG3	4:5:23:GLY:H	0.86	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:150:TYR:O	2:E:151:LYS:CB	2.06	1.02
1:G:530:MET:CA	4:6:354:GLN:HG3	1.88	1.02
1:G:638:GLY:HA2	4:6:341:ILE:O	1.58	1.02
4:5:290:ARG:CZ	4:7:202:THR:CG2	2.36	1.02
4:6:3:ASP:HA	4:6:6:THR:HB	1.36	1.02
1:A:800:ARG:CG	3:C:149:VAL:HG22	1.88	1.02
2:B:149:ASP:OD2	2:B:150:TYR:N	1.91	1.02
1:D:639:GLY:HA3	4:5:344:SER:C	1.78	1.02
1:D:817:GLN:NE2	2:E:127:ARG:HG2	1.74	1.02
1:J:553:MLY:CB	4:V:46:GLY:CA	2.33	1.02
1:J:599:ASN:CA	1:J:649:VAL:HB	1.89	1.02
1:J:639:GLY:HA3	4:7:344:SER:C	1.78	1.02
1:J:800:ARG:HB2	3:L:149:VAL:HG21	1.36	1.02
2:K:144:VAL:HG13	2:K:153:ILE:HD11	1.21	1.02
2:K:144:VAL:HG11	2:K:153:ILE:HG12	1.37	1.02
3:L:24:LYS:CG	3:L:63:ILE:O	2.08	1.02
4:3:290:ARG:CZ	4:5:202:THR:CG2	2.36	1.02
1:A:800:ARG:HB3	3:C:149:VAL:HG21	1.05	1.02
1:D:800:ARG:HD2	3:F:149:VAL:C	1.79	1.02
1:D:839:MLY:HH13	2:E:159:HIS:CG	1.94	1.02
3:F:24:LYS:HG2	3:F:63:ILE:O	1.59	1.02
4:1:290:ARG:CZ	4:3:202:THR:CG2	2.36	1.02
4:6:287:ILE:HB	4:8:204:ALA:H	1.25	1.02
4:7:3:ASP:HA	4:7:6:THR:HB	1.36	1.02
4:Z:3:ASP:HA	4:Z:6:THR:HB	1.36	1.02
1:A:642:LYS:HD3	4:4:340:TRP:CH2	1.95	1.02
1:A:642:LYS:HD3	4:4:340:TRP:CZ3	1.95	1.02
2:B:121:LEU:HG	2:B:128:PHE:CA	1.59	1.02
1:D:507:GLY:HA3	1:D:762:HIS:CG	1.95	1.02
1:G:736:GLN:HA	1:G:743:ALA:HB3	1.35	1.02
1:J:754:ASP:HB2	1:J:776:GLU:HB3	1.38	1.02
3:C:24:LYS:HG2	3:C:63:ILE:O	1.59	1.01
1:D:557:GLU:N	4:7:48:GLY:CA	2.12	1.01
1:D:814:PHE:CE1	2:E:127:ARG:NH2	2.26	1.01
1:G:576:GLU:HG2	1:G:577:ALA:H	0.85	1.01
3:I:24:LYS:CG	3:I:63:ILE:O	2.08	1.01
1:J:98:HIS:HB3	1:J:100:PRO:HD2	1.42	1.01
4:1:290:ARG:NH2	4:3:202:THR:CG2	2.23	1.01
4:3:290:ARG:NH2	4:5:202:THR:CG2	2.23	1.01
4:8:290:ARG:NH2	4:W:202:THR:CG2	2.23	1.01
4:W:290:ARG:NH2	4:Y:202:THR:CG2	2.23	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:599:ASN:CA	1:D:649:VAL:HB	1.89	1.01
1:D:830:PRO:CD	2:E:67:MET:CE	2.37	1.01
1:G:751:GLY:HA2	3:I:114:LEU:HD13	1.40	1.01
2:H:144:VAL:HG13	2:H:153:ILE:HD11	1.21	1.01
3:I:49:ILE:HA	3:I:52:ASN:HD22	1.22	1.01
1:J:757:GLN:NE2	1:J:776:GLU:HG2	1.75	1.01
4:1:287:ILE:HB	4:3:204:ALA:H	1.25	1.01
4:2:287:ILE:HB	4:4:204:ALA:H	1.25	1.01
4:6:290:ARG:NH2	4:8:202:THR:CG2	2.23	1.01
1:A:599:ASN:CA	1:A:649:VAL:HB	1.89	1.01
1:A:639:GLY:N	4:4:345:ILE:N	1.94	1.01
1:A:822:SER:CB	2:B:88:LEU:HD23	1.91	1.01
2:B:144:VAL:HG11	2:B:153:ILE:HG12	1.38	1.01
2:E:144:VAL:HG11	2:E:153:ILE:HG12	1.38	1.01
2:E:149:ASP:OD2	2:E:150:TYR:N	1.91	1.01
1:G:797:PHE:CG	3:I:149:VAL:HG11	1.95	1.01
1:J:599:ASN:HA	1:J:649:VAL:HB	1.05	1.01
1:J:635:GLY:HA3	4:7:341:ILE:HD13	1.36	1.01
4:5:290:ARG:NH2	4:7:202:THR:CG2	2.23	1.01
4:W:287:ILE:HB	4:Y:204:ALA:H	1.26	1.01
2:B:150:TYR:O	2:B:151:LYS:CB	2.07	1.01
1:D:541:MET:HB3	4:5:143:TYR:OH	1.60	1.01
1:D:553:MLY:HG2	4:7:44:MET:O	1.59	1.01
1:G:202:SER:CA	1:G:207:LYS:CE	2.36	1.01
1:G:641:LYS:HE3	1:G:647:GLN:HB2	1.42	1.01
2:H:144:VAL:HG11	2:H:153:ILE:HG12	1.38	1.01
1:A:793:ARG:HE	3:C:147:MET:HG2	1.24	1.01
3:C:48:LYS:O	3:C:52:ASN:ND2	1.94	1.01
1:D:635:GLY:HA3	4:5:341:ILE:HD13	1.37	1.01
1:D:788:THR:HG23	3:F:42:THR:HG21	1.42	1.01
2:E:163:ALA:O	2:K:22:THR:N	1.94	1.01
1:G:84:MLY:HH12	1:G:715:VAL:CG1	1.83	1.01
1:G:553:MLY:HG2	4:8:44:MET:O	1.60	1.01
3:I:48:LYS:O	3:I:52:ASN:ND2	1.94	1.01
1:J:641:LYS:HE3	1:J:647:GLN:HB2	1.43	1.01
1:J:642:LYS:HG3	4:7:23:GLY:H	0.86	1.01
2:K:121:LEU:CB	2:K:128:PHE:HB3	1.69	1.01
3:L:48:LYS:O	3:L:52:ASN:ND2	1.94	1.01
4:4:290:ARG:NH2	4:6:202:THR:CG2	2.23	1.01
4:7:290:ARG:NH2	4:V:202:THR:CG2	2.23	1.01
1:A:502:GLU:CA	1:A:761:GLY:HA3	1.91	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:LYS:HD2	1:D:217:THR:HG23	1.41	1.00
1:D:553:MLY:HB3	4:7:46:GLY:CA	1.51	1.00
1:G:599:ASN:CA	1:G:649:VAL:HB	1.89	1.00
1:G:646:PHE:HE2	1:G:652:LEU:HD21	1.24	1.00
3:I:24:LYS:HG2	3:I:63:ILE:O	1.59	1.00
1:J:84:MLY:HH12	1:J:715:VAL:HG13	1.03	1.00
1:J:553:MLY:HG2	4:V:44:MET:O	1.59	1.00
1:J:557:GLU:N	4:V:48:GLY:CA	2.12	1.00
1:J:642:LYS:HD3	4:7:340:TRP:CH2	1.96	1.00
1:J:646:PHE:HE2	1:J:652:LEU:HD21	1.24	1.00
1:J:707:CYS:SG	1:J:714:ARG:NH1	2.31	1.00
4:5:3:ASP:HA	4:5:6:THR:HB	1.36	1.00
1:A:149:GLN:HG2	1:A:719:ASP:OD1	1.57	1.00
1:A:206:LYS:HD2	1:A:217:THR:HG23	1.41	1.00
1:A:501:GLU:O	1:A:762:HIS:CE1	2.14	1.00
1:A:530:MET:HE2	4:4:354:GLN:CG	1.91	1.00
1:A:534:SER:O	4:4:351:THR:HA	1.60	1.00
1:A:800:ARG:HD2	3:C:149:VAL:C	1.81	1.00
1:D:599:ASN:HA	1:D:649:VAL:HB	1.05	1.00
1:D:769:ALA:HA	1:D:771:LEU:HA	1.42	1.00
1:D:800:ARG:HB3	3:F:149:VAL:HG22	1.38	1.00
1:G:93:MET:HE1	1:G:763:THR:CG2	1.86	1.00
1:G:642:LYS:HD3	4:6:340:TRP:CH2	1.96	1.00
1:G:800:ARG:HD2	3:I:149:VAL:CG2	1.90	1.00
1:J:800:ARG:CG	3:L:149:VAL:CG2	2.38	1.00
3:L:24:LYS:HG2	3:L:63:ILE:O	1.59	1.00
4:5:287:ILE:HB	4:7:204:ALA:H	1.25	1.00
4:X:287:ILE:HB	4:Z:204:ALA:H	1.25	1.00
1:A:576:GLU:HG2	1:A:577:ALA:H	0.85	1.00
1:A:641:LYS:HE3	1:A:647:GLN:CB	1.91	1.00
1:D:174:SER:HB3	1:D:667:THR:HG21	1.44	1.00
1:D:809:ARG:NH1	2:E:124:GLY:CA	2.23	1.00
3:F:24:LYS:CG	3:F:63:ILE:O	2.08	1.00
3:F:49:ILE:HA	3:F:52:ASN:HD22	1.22	1.00
1:G:215:GLN:CA	1:G:340:ILE:HG23	1.92	1.00
1:G:534:SER:O	4:6:351:THR:HA	1.60	1.00
1:G:534:SER:C	4:6:351:THR:HA	1.82	1.00
1:J:90:ASP:CB	1:J:764:MLY:HH21	1.89	1.00
1:J:529:PRO:C	4:7:354:GLN:HB3	1.77	1.00
1:J:534:SER:C	4:7:351:THR:HA	1.81	1.00
4:2:290:ARG:NH2	4:4:202:THR:CG2	2.23	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:GLN:N	1:A:743:ALA:CB	2.05	1.00
3:C:24:LYS:CG	3:C:63:ILE:O	2.08	1.00
1:D:642:LYS:HD3	4:5:340:TRP:CZ3	1.95	1.00
1:G:576:GLU:CG	1:G:577:ALA:H	1.75	1.00
1:G:641:LYS:HE3	1:G:647:GLN:CB	1.91	1.00
1:G:642:LYS:HD3	4:6:340:TRP:CZ3	1.96	1.00
2:H:150:TYR:O	2:H:151:LYS:CB	2.06	1.00
1:J:174:SER:HB3	1:J:667:THR:HG21	1.44	1.00
1:J:642:LYS:HD3	4:7:340:TRP:CZ3	1.96	1.00
4:0:286:ASP:OD1	4:2:203:THR:HG22	1.62	1.00
1:A:641:LYS:HE3	1:A:647:GLN:HB2	1.42	1.00
1:D:218:LEU:CA	1:D:221:GLN:HG3	1.91	1.00
1:D:534:SER:O	4:5:351:THR:HA	1.60	1.00
1:D:641:LYS:HE3	1:D:647:GLN:HB2	1.42	1.00
1:D:809:ARG:HH12	2:E:124:GLY:HA2	1.27	1.00
1:G:541:MET:HB3	4:6:143:TYR:OH	1.59	1.00
1:J:93:MET:HG2	1:J:764:MLY:CD	1.78	1.00
1:J:757:GLN:OE1	1:J:772:LEU:C	2.00	1.00
1:A:56:GLU:HB2	1:A:59:MLY:HB3	1.40	1.00
1:D:642:LYS:HD3	4:5:340:TRP:CH2	1.95	1.00
1:D:831:TRP:HD1	2:E:67:MET:SD	1.81	1.00
1:G:206:LYS:HD2	1:G:217:THR:HG23	1.41	1.00
1:A:576:GLU:CG	1:A:577:ALA:H	1.75	1.00
1:G:98:HIS:HB3	1:G:100:PRO:HD2	1.42	1.00
4:6:286:ASP:OD1	4:8:203:THR:HG22	1.62	1.00
4:7:286:ASP:OD1	4:V:203:THR:HG22	1.62	1.00
4:V:290:ARG:NH2	4:X:202:THR:CG2	2.24	1.00
4:W:286:ASP:OD1	4:Y:203:THR:HG22	1.62	1.00
1:D:98:HIS:HB3	1:D:100:PRO:HD2	1.42	0.99
1:A:576:GLU:HG2	1:A:577:ALA:N	1.66	0.99
1:A:795:ARG:HD3	3:C:35:ARG:HH22	1.25	0.99
1:J:206:LYS:HD2	1:J:217:THR:HG23	1.41	0.99
2:K:141:PRO:HB2	2:K:142:PRO:HD2	1.44	0.99
4:0:290:ARG:NH2	4:2:202:THR:CG2	2.23	0.99
4:V:286:ASP:OD1	4:X:203:THR:HG22	1.62	0.99
1:A:501:GLU:CG	1:A:762:HIS:HD1	1.74	0.99
1:A:612:GLN:HE22	1:A:627:GLY:CA	1.75	0.99
2:B:139:ALA:O	2:B:141:PRO:HD3	1.62	0.99
1:D:56:GLU:HB2	1:D:59:MLY:HB3	1.40	0.99
1:D:800:ARG:CB	3:F:149:VAL:CG2	2.37	0.99
3:F:48:LYS:O	3:F:52:ASN:ND2	1.94	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:218:LEU:CA	1:J:221:GLN:HG3	1.91	0.99
4:2:322:PRO:HB3	4:4:244:ASP:OD2	1.62	0.99
4:V:287:ILE:HB	4:X:204:ALA:H	1.25	0.99
4:X:290:ARG:NH2	4:Z:202:THR:CG2	2.23	0.99
1:A:797:PHE:HD1	3:C:149:VAL:HG12	1.27	0.99
4:4:286:ASP:OD1	4:6:203:THR:HG22	1.62	0.99
4:4:322:PRO:HB3	4:6:244:ASP:OD2	1.62	0.99
1:A:502:GLU:CG	1:A:761:GLY:HA3	1.92	0.99
1:A:534:SER:C	4:4:351:THR:HA	1.81	0.99
1:D:534:SER:C	4:5:351:THR:HA	1.81	0.99
1:D:639:GLY:CA	4:5:345:ILE:CA	2.41	0.99
1:D:792:ALA:HB1	3:F:40:ASN:CB	1.92	0.99
2:E:139:ALA:O	2:E:141:PRO:HD3	1.62	0.99
1:G:649:VAL:CG1	1:G:649:VAL:HG22	1.92	0.99
2:H:121:LEU:HG	2:H:128:PHE:CA	1.59	0.99
1:J:641:LYS:HE3	1:J:647:GLN:CB	1.91	0.99
2:K:149:ASP:OD2	2:K:150:TYR:O	1.80	0.99
1:A:553:MLY:HG2	4:6:44:MET:O	1.59	0.99
1:A:834:LEU:HD11	2:B:54:MET:HG3	1.35	0.99
1:D:612:GLN:HE22	1:D:627:GLY:CA	1.75	0.99
4:1:286:ASP:OD1	4:3:203:THR:HG22	1.62	0.99
4:6:322:PRO:HB3	4:8:244:ASP:OD2	1.62	0.99
1:D:834:LEU:HD11	2:E:54:MET:CB	1.92	0.99
1:J:639:GLY:CA	4:7:345:ILE:CA	2.40	0.99
4:5:286:ASP:OD1	4:7:203:THR:HG22	1.62	0.99
4:8:287:ILE:HB	4:W:204:ALA:H	1.25	0.99
1:A:836:PHE:HB3	2:B:161:GLU:CD	1.83	0.99
1:D:529:PRO:C	4:5:354:GLN:HB3	1.78	0.99
2:E:149:ASP:OD2	2:E:150:TYR:O	1.80	0.99
1:G:218:LEU:CA	1:G:221:GLN:HG3	1.91	0.99
1:J:215:GLN:CA	1:J:340:ILE:HG23	1.91	0.99
1:J:798:LEU:CD2	3:L:126:LEU:CD1	2.36	0.99
1:A:98:HIS:HB3	1:A:100:PRO:HD2	1.42	0.99
1:A:215:GLN:CA	1:A:340:ILE:HG23	1.92	0.99
1:A:218:LEU:CA	1:A:221:GLN:HG3	1.91	0.99
1:A:797:PHE:CE2	3:C:126:LEU:CD2	2.45	0.99
1:D:576:GLU:HG2	1:D:577:ALA:H	0.85	0.99
1:D:639:GLY:N	4:5:345:ILE:N	1.94	0.99
1:J:534:SER:O	4:7:351:THR:HG23	1.13	0.99
4:0:322:PRO:HB3	4:2:244:ASP:OD2	1.62	0.99
4:X:286:ASP:OD1	4:Z:203:THR:HG22	1.62	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:797:PHE:HE2	3:C:126:LEU:HD23	1.26	0.99
2:B:149:ASP:OD2	2:B:150:TYR:O	1.80	0.99
1:D:641:LYS:CG	4:5:348:SER:HB2	1.87	0.99
1:G:530:MET:CE	4:6:354:GLN:CG	2.39	0.99
1:D:768:MLY:C	1:D:771:LEU:HD12	1.61	0.98
1:G:831:TRP:CZ2	2:H:67:MET:SD	2.56	0.98
2:K:121:LEU:HG	2:K:128:PHE:CA	1.60	0.98
4:3:287:ILE:HB	4:5:204:ALA:H	1.26	0.98
4:8:322:PRO:HB3	4:W:244:ASP:OD2	1.62	0.98
1:A:639:GLY:CA	4:4:345:ILE:CA	2.41	0.98
1:D:649:VAL:CG1	1:D:649:VAL:HG22	1.92	0.98
2:E:112:ILE:O	2:E:147:ASN:C	2.01	0.98
1:G:798:LEU:HD23	3:I:122:GLU:HB3	1.45	0.98
1:J:508:ILE:CD1	1:J:759:ALA:CB	2.31	0.98
1:J:649:VAL:CG1	1:J:649:VAL:HG22	1.92	0.98
1:J:831:TRP:CZ2	2:K:47:LEU:CD2	2.47	0.98
4:1:322:PRO:HB3	4:3:244:ASP:OD2	1.62	0.98
4:W:322:PRO:HB3	4:Y:244:ASP:OD2	1.62	0.98
1:A:649:VAL:CG1	1:A:649:VAL:HG22	1.92	0.98
1:A:819:ASN:H	2:B:90:GLY:HA3	1.28	0.98
2:B:141:PRO:HB2	2:B:142:PRO:HD2	1.44	0.98
1:G:639:GLY:CA	4:6:345:ILE:CA	2.40	0.98
1:G:788:THR:O	3:I:42:THR:HG22	1.62	0.98
1:J:757:GLN:CD	1:J:776:GLU:CG	2.32	0.98
1:A:530:MET:CE	4:4:354:GLN:CG	2.41	0.98
2:B:112:ILE:O	2:B:147:ASN:C	2.01	0.98
1:D:215:GLN:CA	1:D:340:ILE:HG23	1.92	0.98
1:G:641:LYS:HE3	4:6:348:SER:O	1.56	0.98
2:K:150:TYR:O	2:K:151:LYS:CB	2.06	0.98
4:2:286:ASP:OD1	4:4:203:THR:HG22	1.62	0.98
1:A:836:PHE:HB3	2:B:161:GLU:OE1	1.60	0.98
3:C:52:ASN:HB2	3:C:53:PRO:HD3	1.45	0.98
1:D:530:MET:CE	4:5:354:GLN:CG	2.40	0.98
1:D:641:LYS:HE3	1:D:647:GLN:CB	1.91	0.98
1:G:612:GLN:HE22	1:G:627:GLY:CA	1.75	0.98
2:H:112:ILE:O	2:H:147:ASN:C	2.01	0.98
1:J:641:LYS:HG3	1:J:647:GLN:NE2	1.59	0.98
1:J:800:ARG:NH1	3:L:149:VAL:CG1	2.17	0.98
1:A:206:LYS:CD	1:A:217:THR:CG2	2.16	0.98
2:E:121:LEU:HG	2:E:128:PHE:CA	1.59	0.98
1:G:817:GLN:HG2	2:H:127:ARG:HB2	1.40	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:121:LEU:C	2:H:128:PHE:HB3	1.71	0.98
2:K:112:ILE:O	2:K:147:ASN:C	2.02	0.98
1:A:505:MLY:HB2	1:A:762:HIS:N	1.76	0.98
1:A:641:LYS:CG	4:4:348:SER:HB2	1.87	0.98
2:B:117:LEU:CB	2:B:147:ASN:CG	2.32	0.98
1:D:576:GLU:CG	1:D:577:ALA:H	1.75	0.98
1:D:642:LYS:HD2	4:5:24:ASP:O	1.64	0.98
1:D:646:PHE:HE2	1:D:652:LEU:HD21	1.24	0.98
2:E:130:PRO:O	2:E:133:ILE:N	1.96	0.98
1:G:576:GLU:HG2	1:G:577:ALA:N	1.66	0.98
1:J:534:SER:O	4:7:351:THR:HA	1.60	0.98
3:C:49:ILE:HA	3:C:52:ASN:HD22	1.22	0.98
2:E:117:LEU:CB	2:E:147:ASN:CG	2.32	0.98
2:E:150:TYR:C	2:E:151:LYS:HG3	1.83	0.98
4:4:287:ILE:HB	4:6:204:ALA:H	1.25	0.98
2:E:141:PRO:HB2	2:E:142:PRO:HD2	1.44	0.98
2:H:141:PRO:HB2	2:H:142:PRO:HD2	1.44	0.98
1:J:612:GLN:HE22	1:J:627:GLY:CA	1.76	0.98
3:L:52:ASN:HB2	3:L:53:PRO:HD3	1.46	0.98
1:A:831:TRP:HH2	2:B:50:THR:HB	1.25	0.97
2:K:139:ALA:O	2:K:141:PRO:HD3	1.62	0.97
3:L:49:ILE:HA	3:L:52:ASN:HD22	1.23	0.97
4:3:322:PRO:HB3	4:5:244:ASP:OD2	1.62	0.97
2:B:130:PRO:O	2:B:133:ILE:N	1.96	0.97
1:D:218:LEU:CA	1:D:221:GLN:CG	2.42	0.97
1:D:795:ARG:HB3	3:F:35:ARG:NE	1.35	0.97
2:H:149:ASP:OD2	2:H:150:TYR:O	1.80	0.97
1:J:576:GLU:HG2	1:J:577:ALA:H	0.85	0.97
1:A:174:SER:HB3	1:A:667:THR:HG21	1.44	0.97
2:B:150:TYR:C	2:B:151:LYS:HG3	1.83	0.97
3:F:46:ILE:O	3:F:50:LEU:HG	1.65	0.97
2:H:117:LEU:CB	2:H:147:ASN:CG	2.32	0.97
4:3:286:ASP:OD1	4:5:203:THR:HG22	1.62	0.97
4:X:322:PRO:HB3	4:Z:244:ASP:OD2	1.62	0.97
1:A:795:ARG:CD	3:C:35:ARG:HH12	1.77	0.97
4:8:286:ASP:OD1	4:W:203:THR:HG22	1.62	0.97
1:A:215:GLN:H	1:A:340:ILE:CG1	1.73	0.97
1:A:218:LEU:CA	1:A:221:GLN:CG	2.42	0.97
1:A:542:PHE:CG	4:4:143:TYR:CE1	2.52	0.97
1:A:642:LYS:HG2	4:4:21:PHE:O	1.65	0.97
1:G:829:TRP:CZ3	2:H:87:LYS:NZ	2.30	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:139:ALA:O	2:H:141:PRO:HD3	1.62	0.97
1:J:642:LYS:HG2	4:7:21:PHE:O	1.65	0.97
2:K:130:PRO:O	2:K:133:ILE:N	1.96	0.97
4:7:287:ILE:HB	4:V:204:ALA:H	1.25	0.97
1:A:502:GLU:C	1:A:761:GLY:HA3	1.84	0.97
2:H:121:LEU:HG	2:H:128:PHE:HA	1.46	0.97
2:K:117:LEU:CB	2:K:147:ASN:CG	2.32	0.97
4:0:287:ILE:HB	4:2:204:ALA:H	1.25	0.97
1:G:174:SER:HB3	1:G:667:THR:HG21	1.44	0.97
1:G:784:ALA:O	1:G:788:THR:N	1.96	0.97
1:J:639:GLY:N	4:7:345:ILE:N	1.94	0.97
1:J:754:ASP:OD2	1:J:776:GLU:C	2.03	0.97
2:K:150:TYR:C	2:K:151:LYS:HG3	1.83	0.97
2:E:121:LEU:HG	2:E:128:PHE:HA	1.46	0.97
1:G:736:GLN:CA	1:G:743:ALA:HB2	1.95	0.97
1:J:649:VAL:CG2	1:J:649:VAL:CA	2.42	0.97
1:D:724:TYR:HE1	1:D:778:MET:HB3	1.24	0.97
1:G:642:LYS:HG2	4:6:21:PHE:O	1.65	0.97
1:J:218:LEU:CA	1:J:221:GLN:CG	2.42	0.97
1:J:576:GLU:CG	1:J:577:ALA:H	1.75	0.97
1:J:797:PHE:CB	3:L:149:VAL:HG11	1.94	0.97
1:D:542:PHE:CG	4:5:143:TYR:CE1	2.52	0.97
1:G:218:LEU:CA	1:G:221:GLN:CG	2.42	0.97
2:H:130:PRO:O	2:H:133:ILE:N	1.96	0.97
1:A:501:GLU:HG2	1:A:762:HIS:HD1	0.83	0.96
1:A:502:GLU:O	1:A:761:GLY:CA	2.13	0.96
1:A:795:ARG:NH2	3:C:116:GLU:CD	2.18	0.96
1:D:724:TYR:C	1:D:782:MLY:HH21	1.85	0.96
1:G:819:ASN:HA	2:H:90:GLY:C	1.85	0.96
3:L:46:ILE:O	3:L:50:LEU:HG	1.64	0.96
2:E:150:TYR:O	2:E:151:LYS:HG3	1.65	0.96
1:J:642:LYS:HD2	4:7:24:ASP:O	1.64	0.96
1:J:768:MLY:HH12	1:J:772:LEU:HD23	1.44	0.96
1:A:534:SER:O	4:4:351:THR:HG23	1.13	0.96
1:A:795:ARG:NE	3:C:118:MET:HE1	1.80	0.96
1:D:215:GLN:H	1:D:340:ILE:CG1	1.73	0.96
1:D:553:MLY:HB3	4:7:46:GLY:HA2	1.47	0.96
1:G:637:LYS:NZ	4:6:141:SER:O	1.99	0.96
4:V:322:PRO:HB3	4:X:244:ASP:OD2	1.62	0.96
2:B:144:VAL:HG13	2:B:153:ILE:HD11	1.22	0.96
1:D:649:VAL:CG2	1:D:649:VAL:CA	2.42	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:736:GLN:CA	1:D:743:ALA:HB2	1.95	0.96
2:H:117:LEU:HD13	2:H:147:ASN:OD1	1.64	0.96
1:A:642:LYS:HD2	4:4:24:ASP:O	1.64	0.96
2:B:150:TYR:O	2:B:151:LYS:HG3	1.65	0.96
1:A:538:GLU:N	4:4:349:LEU:CD1	2.28	0.96
1:A:649:VAL:CG1	1:A:649:VAL:CG2	2.43	0.96
1:G:635:GLY:HA3	4:6:334:GLU:HG2	1.47	0.96
1:G:649:VAL:CG2	1:G:649:VAL:CA	2.42	0.96
1:J:821:ARG:HH21	2:K:127:ARG:HG2	1.21	0.96
1:A:649:VAL:CG2	1:A:649:VAL:CA	2.43	0.96
1:D:642:LYS:HG2	4:5:21:PHE:O	1.65	0.96
1:G:642:LYS:HD2	4:6:24:ASP:O	1.64	0.96
1:J:543:PRO:CG	4:7:143:TYR:O	2.14	0.96
1:J:793:ARG:HE	3:L:147:MET:CA	1.77	0.96
4:5:322:PRO:HB3	4:7:244:ASP:OD2	1.62	0.96
4:V:288:ASP:HA	4:X:204:ALA:HB2	1.48	0.96
4:W:288:ASP:HA	4:Y:204:ALA:HB2	1.48	0.96
1:D:206:LYS:CD	1:D:217:THR:CG2	2.16	0.96
4:6:288:ASP:HA	4:8:204:ALA:HB2	1.48	0.96
4:7:288:ASP:HA	4:V:204:ALA:HB2	1.48	0.96
4:8:288:ASP:HA	4:W:204:ALA:HB2	1.48	0.96
1:G:641:LYS:HG3	1:G:647:GLN:NE2	1.58	0.96
1:G:735:GLY:C	1:G:743:ALA:CA	2.34	0.96
3:I:46:ILE:O	3:I:50:LEU:HG	1.64	0.96
1:J:542:PHE:CG	4:7:143:TYR:CE1	2.53	0.96
4:X:288:ASP:HA	4:Z:204:ALA:HB2	1.48	0.96
1:A:795:ARG:HH22	3:C:116:GLU:CD	1.69	0.96
2:B:121:LEU:HG	2:B:128:PHE:HA	1.47	0.96
3:C:46:ILE:O	3:C:50:LEU:HG	1.65	0.96
2:H:150:TYR:C	2:H:151:LYS:HG3	1.83	0.96
2:K:121:LEU:HG	2:K:128:PHE:HA	1.47	0.96
4:4:288:ASP:HA	4:6:204:ALA:HB2	1.48	0.96
4:5:288:ASP:HA	4:7:204:ALA:HB2	1.48	0.96
1:D:538:GLU:N	4:5:349:LEU:CD1	2.28	0.95
1:D:735:GLY:C	1:D:743:ALA:CA	2.34	0.95
1:D:792:ALA:C	3:F:40:ASN:HB3	1.85	0.95
1:G:206:LYS:CD	1:G:217:THR:CG2	2.16	0.95
4:0:288:ASP:HA	4:2:204:ALA:HB2	1.48	0.95
4:2:288:ASP:HA	4:4:204:ALA:HB2	1.48	0.95
1:D:726:VAL:CG2	1:D:782:MLY:HH22	1.96	0.95
1:J:649:VAL:CG1	1:J:649:VAL:CG2	2.43	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:736:GLN:CA	1:J:743:ALA:HB2	1.95	0.95
1:D:649:VAL:CG1	1:D:649:VAL:CG2	2.43	0.95
1:G:538:GLU:HG3	4:6:352:PHE:N	1.81	0.95
1:G:754:ASP:CB	1:G:776:GLU:OE2	2.14	0.95
1:J:817:GLN:CG	2:K:127:ARG:HD2	1.95	0.95
1:A:635:GLY:HA3	4:4:334:GLU:HG2	1.47	0.95
1:A:721:LYS:CA	1:A:736:GLN:CD	2.34	0.95
1:A:735:GLY:C	1:A:743:ALA:CA	2.34	0.95
1:D:839:MLY:HH11	2:E:159:HIS:HD2	1.18	0.95
1:G:530:MET:HA	4:6:354:GLN:HG3	0.97	0.95
1:G:649:VAL:CG1	1:G:649:VAL:CG2	2.44	0.95
1:G:790:THR:OG1	3:I:87:PHE:CD2	2.18	0.95
1:J:84:MLY:HE2	1:J:719:ASP:HB3	0.99	0.95
1:J:735:GLY:C	1:J:743:ALA:CA	2.34	0.95
4:3:288:ASP:HA	4:5:204:ALA:HB2	1.48	0.95
1:A:505:MLY:HG3	1:A:741:LYS:NZ	1.81	0.95
1:A:834:LEU:CD1	2:B:54:MET:CB	2.45	0.95
1:D:721:LYS:CA	1:D:736:GLN:CD	2.34	0.95
1:G:542:PHE:CG	4:6:143:TYR:CE1	2.53	0.95
1:J:553:MLY:HB3	4:V:46:GLY:HA2	1.48	0.95
4:1:288:ASP:HA	4:3:204:ALA:HB2	1.48	0.95
1:A:637:LYS:NZ	4:4:141:SER:O	1.99	0.95
1:D:641:LYS:HD2	1:D:647:GLN:CD	1.70	0.95
1:G:538:GLU:N	4:6:349:LEU:CD1	2.29	0.95
2:H:150:TYR:O	2:H:151:LYS:HB2	1.67	0.95
4:7:322:PRO:HB3	4:V:244:ASP:OD2	1.62	0.95
1:A:541:MET:N	4:4:349:LEU:HD21	1.80	0.95
1:D:724:TYR:HA	1:D:782:MLY:NZ	1.81	0.95
1:G:546:THR:HG22	1:G:548:THR:H	1.32	0.95
2:K:117:LEU:HD13	2:K:147:ASN:OD1	1.64	0.95
1:A:502:GLU:CD	1:A:764:MLY:N	2.20	0.95
2:B:117:LEU:HD13	2:B:147:ASN:OD1	1.64	0.95
1:D:543:PRO:CG	4:5:143:TYR:O	2.14	0.95
1:D:818:TYR:HB2	2:E:90:GLY:N	1.81	0.95
2:H:150:TYR:O	2:H:151:LYS:HG3	1.65	0.95
1:J:538:GLU:N	4:7:349:LEU:CD1	2.28	0.95
1:J:795:ARG:NH1	3:L:35:ARG:NH1	2.15	0.95
2:K:150:TYR:O	2:K:151:LYS:HG3	1.65	0.95
1:A:813:ILE:CG2	2:B:127:ARG:NE	2.26	0.95
1:A:819:ASN:N	2:B:90:GLY:HA3	1.81	0.95
2:E:150:TYR:O	2:E:151:LYS:CG	2.15	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:93:MET:CG	1:J:764:MLY:NZ	2.22	0.95
1:J:637:LYS:NZ	4:7:141:SER:O	1.98	0.95
1:A:543:PRO:CG	4:4:143:TYR:O	2.14	0.95
1:A:768:MLY:C	1:A:771:LEU:HB2	1.96	0.95
2:B:121:LEU:CB	2:B:128:PHE:HB3	1.69	0.95
1:D:215:GLN:HA	1:D:340:ILE:HG23	0.95	0.95
1:D:537:GLU:C	4:5:349:LEU:CD1	2.20	0.95
1:D:635:GLY:HA3	4:5:334:GLU:HG2	1.47	0.95
3:F:52:ASN:HB2	3:F:53:PRO:HD3	1.45	0.95
1:G:721:LYS:CA	1:G:736:GLN:CD	2.34	0.95
1:A:530:MET:HA	4:4:354:GLN:HG3	0.96	0.94
1:A:538:GLU:HG3	4:4:352:PHE:N	1.82	0.94
1:A:800:ARG:HH11	3:C:149:VAL:HG13	1.21	0.94
1:J:721:LYS:CA	1:J:736:GLN:CD	2.34	0.94
1:J:749:GLY:O	3:L:114:LEU:CD2	2.14	0.94
1:J:783:LEU:O	1:J:787:ILE:N	1.99	0.94
1:A:709:LYS:C	1:A:710:GLY:HA3	1.88	0.94
1:A:757:GLN:CB	1:A:771:LEU:CD1	2.05	0.94
1:D:637:LYS:NZ	4:5:141:SER:O	1.99	0.94
2:H:121:LEU:CB	2:H:128:PHE:HB3	1.69	0.94
1:A:530:MET:CA	4:4:354:GLN:CG	2.44	0.94
1:A:768:MLY:HB3	1:A:771:LEU:HB2	1.46	0.94
1:D:541:MET:N	4:5:349:LEU:HD21	1.80	0.94
1:J:538:GLU:HG3	4:7:352:PHE:N	1.82	0.94
1:J:635:GLY:HA3	4:7:334:GLU:HG2	1.47	0.94
2:K:150:TYR:O	2:K:151:LYS:CG	2.15	0.94
2:B:150:TYR:O	2:B:151:LYS:HB2	1.67	0.94
2:E:150:TYR:O	2:E:151:LYS:HB2	1.67	0.94
1:J:795:ARG:HH11	3:L:35:ARG:NH1	1.65	0.94
1:A:800:ARG:CD	3:C:149:VAL:C	2.35	0.94
1:G:84:MLY:CH2	1:G:716:LEU:O	2.14	0.94
1:G:642:LYS:CG	4:6:23:GLY:H	1.76	0.94
2:H:150:TYR:O	2:H:151:LYS:CG	2.15	0.94
1:A:502:GLU:CG	1:A:761:GLY:CA	2.45	0.94
1:D:538:GLU:HG3	4:5:352:PHE:N	1.82	0.94
1:G:93:MET:HE2	1:G:764:MLY:HG3	1.49	0.94
1:G:218:LEU:CB	1:G:221:GLN:CG	2.46	0.94
1:G:831:TRP:CE2	2:H:67:MET:SD	2.60	0.94
2:H:144:VAL:HG13	2:H:153:ILE:HG12	1.14	0.94
1:A:553:MLY:HB3	4:6:46:GLY:HA2	1.47	0.94
1:A:612:GLN:NE2	1:A:627:GLY:HA3	1.83	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:LYS:CG	4:4:23:GLY:H	1.77	0.94
1:D:530:MET:HA	4:5:354:GLN:HG3	0.96	0.94
1:D:546:THR:HG22	1:D:548:THR:H	1.32	0.94
1:D:839:MLY:NZ	2:E:159:HIS:HB3	1.83	0.94
1:G:834:LEU:HD13	2:H:51:PHE:HE1	0.79	0.94
3:I:52:ASN:HB2	3:I:53:PRO:HD3	1.46	0.94
1:J:530:MET:HA	4:7:354:GLN:HG3	0.96	0.94
1:J:612:GLN:NE2	1:J:627:GLY:CA	2.31	0.94
1:J:797:PHE:CA	3:L:149:VAL:HG11	1.98	0.94
1:J:823:PHE:CE1	2:K:156:VAL:O	2.21	0.94
1:A:218:LEU:CB	1:A:221:GLN:CG	2.46	0.94
1:A:736:GLN:CA	1:A:743:ALA:HB2	1.95	0.94
2:E:163:ALA:C	2:K:22:THR:H	1.69	0.94
1:A:768:MLY:HB3	1:A:771:LEU:CD1	1.97	0.93
1:D:218:LEU:CB	1:D:221:GLN:CG	2.46	0.93
1:J:798:LEU:HD22	3:L:126:LEU:HD11	0.94	0.93
1:J:800:ARG:NH1	3:L:149:VAL:HG22	1.84	0.93
2:B:150:TYR:O	2:B:151:LYS:CG	2.15	0.93
1:G:541:MET:N	4:6:349:LEU:HD21	1.80	0.93
1:G:543:PRO:CG	4:6:143:TYR:O	2.14	0.93
1:G:612:GLN:NE2	1:G:627:GLY:HA3	1.83	0.93
1:G:817:GLN:HG2	2:H:127:ARG:CB	1.97	0.93
1:D:507:GLY:O	1:D:761:GLY:HA3	1.69	0.93
1:D:798:LEU:CD1	3:F:126:LEU:HD21	1.97	0.93
1:D:839:MLY:CH1	2:E:159:HIS:HB3	1.97	0.93
1:G:707:CYS:C	1:G:714:ARG:HH22	1.70	0.93
1:J:557:GLU:H	4:V:48:GLY:HA2	1.32	0.93
1:D:817:GLN:HG3	2:E:127:ARG:HD3	1.49	0.93
1:D:830:PRO:HG2	2:E:67:MET:HE2	1.46	0.93
2:E:117:LEU:HD13	2:E:147:ASN:OD1	1.64	0.93
1:J:530:MET:CE	4:7:354:GLN:CG	2.40	0.93
1:J:537:GLU:C	4:7:349:LEU:CD1	2.20	0.93
1:J:612:GLN:NE2	1:J:627:GLY:HA3	1.83	0.93
1:A:557:GLU:N	4:6:48:GLY:CA	2.12	0.93
1:A:836:PHE:CE1	2:B:159:HIS:C	2.42	0.93
1:D:834:LEU:CD1	2:E:54:MET:HB2	1.98	0.93
1:J:508:ILE:HD11	1:J:759:ALA:HB1	1.48	0.93
1:J:530:MET:CA	4:7:354:GLN:CG	2.44	0.93
1:A:836:PHE:CZ	2:B:160:GLY:HA3	1.94	0.93
1:G:553:MLY:HB3	4:8:46:GLY:HA2	1.48	0.93
1:J:786:ILE:HG12	3:L:86:ASP:HB3	1.51	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:612:GLN:NE2	1:D:627:GLY:CA	2.31	0.93
1:J:538:GLU:N	4:7:351:THR:H	1.67	0.93
1:A:502:GLU:HG3	1:A:761:GLY:N	1.84	0.93
1:A:629:GLU:CB	1:A:643:GLY:O	2.17	0.93
1:A:753:VAL:HA	1:A:778:MET:SD	2.09	0.93
1:G:789:ALA:HB2	3:I:81:GLN:HE21	0.77	0.93
1:G:798:LEU:HD11	3:I:126:LEU:HD23	1.49	0.93
1:A:648:THR:HG21	1:A:651:ALA:HB2	1.50	0.93
1:D:831:TRP:CE2	2:E:47:LEU:HD23	1.94	0.93
1:G:612:GLN:NE2	1:G:627:GLY:CA	2.31	0.93
1:G:819:ASN:CB	2:H:90:GLY:O	2.16	0.93
1:J:206:LYS:CD	1:J:217:THR:CG2	2.16	0.93
1:J:739:ASP:HB3	1:J:742:LYS:CB	1.98	0.93
1:A:549:SER:C	4:6:46:GLY:HA3	1.90	0.92
1:A:215:GLN:HA	1:A:340:ILE:HG23	0.96	0.92
1:A:505:MLY:NZ	1:A:762:HIS:C	2.16	0.92
1:A:612:GLN:NE2	1:A:627:GLY:CA	2.31	0.92
1:A:793:ARG:HH21	3:C:147:MET:HB3	1.33	0.92
1:G:215:GLN:HA	1:G:340:ILE:HG23	0.95	0.92
1:G:530:MET:CA	4:6:354:GLN:CG	2.45	0.92
1:G:795:ARG:HB3	3:I:35:ARG:NH2	1.82	0.92
1:J:90:ASP:CG	1:J:764:MLY:CH1	2.37	0.92
1:J:215:GLN:HA	1:J:340:ILE:HG23	0.95	0.92
1:J:768:MLY:HD3	1:J:772:LEU:HB2	1.49	0.92
1:D:549:SER:C	4:7:46:GLY:HA3	1.90	0.92
1:G:642:LYS:CB	4:6:21:PHE:O	2.17	0.92
1:J:541:MET:N	4:7:349:LEU:HD21	1.80	0.92
1:J:549:SER:C	4:V:46:GLY:HA3	1.90	0.92
1:J:648:THR:HG21	1:J:651:ALA:HB2	1.50	0.92
1:J:768:MLY:HH12	1:J:772:LEU:HD21	1.49	0.92
1:A:641:LYS:HE3	1:A:647:GLN:CG	2.00	0.92
1:D:213:LYS:HA	1:D:220:ASP:CG	1.90	0.92
1:D:530:MET:CA	4:5:354:GLN:CG	2.44	0.92
1:D:834:LEU:CD1	2:E:54:MET:CB	2.47	0.92
1:G:537:GLU:C	4:6:349:LEU:CD1	2.21	0.92
1:A:739:ASP:HB3	1:A:742:LYS:CB	1.98	0.92
1:A:800:ARG:CB	3:C:149:VAL:HG21	1.89	0.92
1:D:557:GLU:H	4:7:48:GLY:HA2	1.32	0.92
1:J:546:THR:HG22	1:J:548:THR:H	1.32	0.92
1:J:636:LYS:HD2	4:7:332:PRO:HB3	1.52	0.92
1:J:818:TYR:HB3	2:K:90:GLY:HA3	1.51	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:821:ARG:HH22	2:K:127:ARG:HG2	1.31	0.92
1:A:642:LYS:CB	4:4:21:PHE:O	2.17	0.92
1:D:550:PHE:HA	4:7:46:GLY:CA	2.00	0.92
1:D:612:GLN:NE2	1:D:627:GLY:HA3	1.83	0.92
1:D:629:GLU:CB	1:D:643:GLY:O	2.17	0.92
1:D:790:THR:HA	3:F:87:PHE:CE2	2.04	0.92
1:J:213:LYS:HA	1:J:220:ASP:CG	1.90	0.92
1:J:629:GLU:CB	1:J:643:GLY:O	2.17	0.92
1:D:278:GLN:HG2	1:D:317:GLU:HB2	1.52	0.92
1:D:790:THR:N	3:F:87:PHE:HE2	1.67	0.92
1:G:629:GLU:CB	1:G:643:GLY:O	2.17	0.92
1:G:783:LEU:O	1:G:787:ILE:HB	1.70	0.92
1:A:795:ARG:HD2	3:C:35:ARG:CZ	1.99	0.92
1:A:546:THR:HG22	1:A:548:THR:H	1.32	0.92
1:A:636:LYS:HD2	4:4:332:PRO:HB3	1.51	0.92
1:D:790:THR:CA	3:F:87:PHE:CE2	2.47	0.92
1:G:648:THR:HG21	1:G:651:ALA:HB2	1.51	0.92
1:J:92:ALA:O	1:J:714:ARG:CD	2.18	0.92
1:A:831:TRP:CE2	2:B:51:PHE:CE1	2.58	0.92
1:D:537:GLU:O	4:5:349:LEU:HD13	0.74	0.92
1:G:641:LYS:HE3	1:G:647:GLN:CG	2.00	0.92
1:G:757:GLN:OE1	1:G:772:LEU:HG	1.70	0.92
1:G:831:TRP:CH2	2:H:47:LEU:HD21	1.93	0.92
1:J:550:PHE:HA	4:V:46:GLY:CA	2.00	0.92
1:D:636:LYS:HD2	4:5:332:PRO:HB3	1.52	0.91
1:D:648:THR:HG21	1:D:651:ALA:HB2	1.50	0.91
1:D:739:ASP:HB3	1:D:742:LYS:CB	1.98	0.91
1:G:549:SER:C	4:8:46:GLY:HA3	1.90	0.91
1:G:795:ARG:CG	3:I:35:ARG:HH22	1.82	0.91
1:J:537:GLU:O	4:7:349:LEU:HD13	0.73	0.91
1:J:642:LYS:CB	4:7:21:PHE:O	2.17	0.91
1:A:735:GLY:C	1:A:743:ALA:HA	1.90	0.91
1:D:642:LYS:CB	4:5:21:PHE:O	2.17	0.91
1:G:795:ARG:HB3	3:I:35:ARG:HH21	1.33	0.91
1:G:821:ARG:HH21	2:H:127:ARG:HG2	1.34	0.91
1:J:538:GLU:N	4:7:349:LEU:HD12	1.86	0.91
1:J:797:PHE:CG	3:L:149:VAL:HG11	2.05	0.91
1:A:218:LEU:HA	1:A:221:GLN:CG	2.01	0.91
1:G:537:GLU:O	4:6:349:LEU:HD13	0.74	0.91
1:J:641:LYS:HE3	1:J:647:GLN:CG	2.00	0.91
1:A:649:VAL:CG1	1:A:649:VAL:C	2.38	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:538:GLU:N	4:5:351:THR:H	1.68	0.91
1:G:550:PHE:HA	4:8:46:GLY:CA	2.00	0.91
1:G:838:ILE:HD11	2:H:54:MET:HE3	0.92	0.91
1:J:278:GLN:HG2	1:J:317:GLU:HB2	1.52	0.91
1:A:544:LYS:HD2	4:4:147:ARG:HB3	1.53	0.91
1:D:834:LEU:HD11	2:E:54:MET:HG2	1.53	0.91
1:G:218:LEU:HA	1:G:221:GLN:CG	2.01	0.91
1:J:218:LEU:CB	1:J:221:GLN:CG	2.46	0.91
1:J:735:GLY:C	1:J:743:ALA:HA	1.90	0.91
1:A:557:GLU:H	4:6:48:GLY:HA2	1.32	0.91
3:F:62:ALA:O	3:F:63:ILE:CG1	2.19	0.91
1:G:544:LYS:HD2	4:6:147:ARG:HB3	1.53	0.91
1:J:736:GLN:HA	1:J:743:ALA:HB2	1.50	0.91
1:D:649:VAL:CG1	1:D:649:VAL:C	2.38	0.91
1:G:410:ASN:OD1	4:6:334:GLU:C	2.10	0.91
1:G:557:GLU:H	4:8:48:GLY:HA2	1.33	0.91
1:A:819:ASN:ND2	2:B:91:ALA:C	2.23	0.91
2:B:149:ASP:CG	2:B:150:TYR:H	1.73	0.91
3:C:62:ALA:O	3:C:63:ILE:CG1	2.19	0.91
1:D:735:GLY:C	1:D:743:ALA:HA	1.91	0.91
3:F:62:ALA:O	3:F:63:ILE:HG12	1.71	0.91
1:G:538:GLU:N	4:6:351:THR:H	1.68	0.91
1:G:768:MLY:HH23	1:G:772:LEU:HD22	1.53	0.91
1:J:93:MET:HG2	1:J:764:MLY:HD3	0.92	0.91
1:A:537:GLU:O	4:4:349:LEU:HD13	0.74	0.91
1:A:537:GLU:C	4:4:349:LEU:CD1	2.20	0.91
1:A:550:PHE:HA	4:6:46:GLY:CA	2.00	0.91
1:D:724:TYR:CE1	1:D:778:MET:SD	2.64	0.91
1:G:638:GLY:HA3	4:6:341:ILE:O	1.70	0.91
1:G:739:ASP:HB3	1:G:742:LYS:CB	1.99	0.91
3:I:62:ALA:O	3:I:63:ILE:HG12	1.71	0.91
1:A:538:GLU:N	4:4:349:LEU:HD12	1.86	0.90
1:A:836:PHE:HB3	2:B:161:GLU:CG	2.01	0.90
1:D:553:MLY:HE2	4:7:45:VAL:HA	1.53	0.90
1:D:735:GLY:O	1:D:743:ALA:CA	2.19	0.90
1:D:790:THR:N	3:F:87:PHE:CE2	2.39	0.90
1:G:649:VAL:CG1	1:G:649:VAL:C	2.38	0.90
1:J:800:ARG:HB3	3:L:149:VAL:CG2	1.94	0.90
1:A:538:GLU:N	4:4:351:THR:H	1.68	0.90
1:A:649:VAL:CB	1:A:649:VAL:CG2	2.50	0.90
1:G:213:LYS:HA	1:G:220:ASP:CG	1.90	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:636:LYS:HD2	4:6:332:PRO:HB3	1.52	0.90
1:G:649:VAL:CB	1:G:649:VAL:CG2	2.49	0.90
2:H:149:ASP:CG	2:H:150:TYR:H	1.73	0.90
1:J:544:LYS:HD2	4:7:147:ARG:HB3	1.53	0.90
1:A:638:GLY:HA3	4:4:341:ILE:O	1.70	0.90
1:A:768:MLY:CB	1:A:771:LEU:HB2	2.00	0.90
1:D:649:VAL:CG2	1:D:649:VAL:HG13	2.02	0.90
1:G:278:GLN:HG2	1:G:317:GLU:HB2	1.52	0.90
1:J:649:VAL:CG1	1:J:649:VAL:C	2.38	0.90
1:J:798:LEU:HD21	3:L:126:LEU:HG	1.51	0.90
2:K:150:TYR:O	2:K:151:LYS:HB2	1.67	0.90
1:A:213:LYS:HA	1:A:220:ASP:CG	1.90	0.90
1:A:505:MLY:CH2	1:A:762:HIS:O	2.19	0.90
1:A:757:GLN:CG	1:A:771:LEU:CD1	2.44	0.90
1:D:218:LEU:HA	1:D:221:GLN:CG	2.01	0.90
1:D:538:GLU:O	4:5:349:LEU:CG	2.20	0.90
1:D:641:LYS:HE3	1:D:647:GLN:CG	2.00	0.90
1:D:796:GLY:HA3	3:F:40:ASN:OD1	1.71	0.90
1:G:538:GLU:N	4:6:349:LEU:HD12	1.87	0.90
1:G:721:LYS:CB	1:G:736:GLN:OE1	2.20	0.90
1:G:735:GLY:C	1:G:743:ALA:HA	1.90	0.90
1:J:553:MLY:HE2	4:V:45:VAL:HA	1.53	0.90
1:J:649:VAL:CG2	1:J:649:VAL:HG13	2.02	0.90
1:D:544:LYS:HD2	4:5:147:ARG:HB3	1.53	0.90
1:G:557:GLU:H	4:8:48:GLY:HA3	1.28	0.90
1:G:754:ASP:OD2	1:G:776:GLU:OE2	1.89	0.90
3:I:62:ALA:O	3:I:63:ILE:CG1	2.19	0.90
1:J:735:GLY:O	1:J:743:ALA:CA	2.19	0.90
1:D:534:SER:O	4:5:351:THR:HG23	1.13	0.90
1:D:839:MLY:CH1	2:E:159:HIS:CG	2.50	0.90
2:E:121:LEU:CB	2:E:128:PHE:HB3	1.69	0.90
1:J:553:MLY:CG	4:V:44:MET:O	2.20	0.90
2:H:137:TRP:HA	2:H:145:ALA:HB2	1.54	0.90
1:J:818:TYR:HB3	2:K:90:GLY:CA	2.01	0.90
1:A:278:GLN:HG2	1:A:317:GLU:HB2	1.52	0.90
1:D:550:PHE:CA	4:7:46:GLY:HA3	2.02	0.90
2:E:137:TRP:HA	2:E:145:ALA:HB2	1.53	0.90
1:J:757:GLN:CD	1:J:776:GLU:HG2	1.90	0.90
1:A:410:ASN:OD1	4:4:334:GLU:C	2.10	0.90
1:A:629:GLU:HG2	1:A:643:GLY:O	1.72	0.90
1:D:538:GLU:N	4:5:349:LEU:HD12	1.86	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:795:ARG:CB	3:F:35:ARG:NE	2.26	0.90
1:D:836:PHE:CB	2:E:161:GLU:OE1	2.20	0.90
2:E:163:ALA:C	2:K:22:THR:OG1	2.10	0.90
1:G:629:GLU:HG2	1:G:643:GLY:O	1.72	0.90
1:J:218:LEU:HA	1:J:221:GLN:CG	2.01	0.90
1:J:410:ASN:OD1	4:7:334:GLU:C	2.10	0.90
1:J:530:MET:N	4:7:354:GLN:HB3	1.87	0.90
1:A:817:GLN:HB2	2:B:127:ARG:CZ	2.02	0.90
1:G:215:GLN:H	1:G:340:ILE:CG1	1.72	0.90
1:G:817:GLN:OE1	2:H:127:ARG:HD2	1.71	0.90
1:J:538:GLU:O	4:7:349:LEU:CG	2.20	0.90
1:J:550:PHE:CA	4:V:46:GLY:HA3	2.02	0.90
1:A:735:GLY:O	1:A:743:ALA:CA	2.19	0.89
1:D:799:MET:CE	3:F:32:ASP:HB3	2.02	0.89
2:E:163:ALA:C	2:K:22:THR:N	2.24	0.89
1:J:635:GLY:CA	4:7:341:ILE:HD13	2.02	0.89
1:D:638:GLY:HA3	4:5:341:ILE:O	1.70	0.89
1:G:735:GLY:O	1:G:743:ALA:CA	2.19	0.89
1:J:84:MLY:HE2	1:J:719:ASP:CG	1.92	0.89
1:J:821:ARG:NH2	2:K:127:ARG:CD	2.35	0.89
3:C:24:LYS:HB3	3:C:63:ILE:O	1.72	0.89
3:C:62:ALA:O	3:C:63:ILE:HG12	1.71	0.89
1:D:553:MLY:CG	4:7:44:MET:O	2.20	0.89
1:D:649:VAL:CB	1:D:649:VAL:CG2	2.49	0.89
1:A:795:ARG:CZ	3:C:116:GLU:OE2	2.19	0.89
1:A:800:ARG:HD2	3:C:149:VAL:HG22	0.92	0.89
1:D:815:CYS:O	2:E:90:GLY:O	1.89	0.89
1:G:599:ASN:OD1	1:G:649:VAL:HB	1.72	0.89
1:J:534:SER:HA	4:7:350:SER:O	1.71	0.89
3:L:62:ALA:O	3:L:63:ILE:CG1	2.19	0.89
1:A:530:MET:N	4:4:354:GLN:HB3	1.87	0.89
1:D:629:GLU:HG2	1:D:643:GLY:O	1.72	0.89
1:D:721:LYS:CB	1:D:736:GLN:OE1	2.20	0.89
1:J:557:GLU:H	4:V:48:GLY:HA3	1.28	0.89
1:J:649:VAL:CB	1:J:649:VAL:CG2	2.49	0.89
1:J:721:LYS:CB	1:J:736:GLN:OE1	2.20	0.89
1:D:410:ASN:OD1	4:5:334:GLU:C	2.10	0.89
1:D:630:ALA:O	4:5:25:ASP:CG	2.09	0.89
1:D:635:GLY:CA	4:5:341:ILE:HD13	2.03	0.89
1:G:538:GLU:O	4:6:349:LEU:CG	2.20	0.89
1:J:630:ALA:O	4:7:25:ASP:CG	2.09	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:137:TRP:HA	2:K:145:ALA:HB2	1.53	0.89
1:D:534:SER:HA	4:5:350:SER:O	1.71	0.89
1:J:503:TYR:OH	1:J:711:PHE:HD2	1.55	0.89
1:A:553:MLY:CG	4:6:44:MET:O	2.20	0.89
1:A:721:LYS:CB	1:A:736:GLN:OE1	2.20	0.89
1:D:507:GLY:CA	1:D:762:HIS:CG	2.56	0.89
1:D:530:MET:N	4:5:354:GLN:HB3	1.87	0.89
1:D:641:LYS:HD2	4:5:348:SER:CB	2.02	0.89
1:G:93:MET:HE3	1:G:763:THR:CB	1.74	0.89
1:J:215:GLN:H	1:J:340:ILE:CG1	1.72	0.89
1:G:816:ILE:HD11	2:H:100:ALA:CB	2.02	0.89
1:A:505:MLY:HG3	1:A:741:LYS:HZ3	1.37	0.89
1:A:538:GLU:O	4:4:349:LEU:CG	2.20	0.89
1:A:630:ALA:O	4:4:25:ASP:CG	2.10	0.89
1:J:638:GLY:HA3	4:7:341:ILE:O	1.70	0.89
1:J:641:LYS:HD2	4:7:348:SER:CB	2.02	0.89
1:J:826:VAL:HG21	2:K:88:LEU:CD2	2.03	0.89
1:A:534:SER:HA	4:4:350:SER:O	1.71	0.88
1:A:769:ALA:C	1:A:772:LEU:H	1.76	0.88
1:A:795:ARG:CD	3:C:35:ARG:NH2	2.36	0.88
1:G:534:SER:HA	4:6:350:SER:O	1.71	0.88
1:G:838:ILE:CD1	2:H:54:MET:HE1	1.96	0.88
2:H:121:LEU:CA	2:H:128:PHE:CB	2.46	0.88
1:A:550:PHE:CA	4:6:46:GLY:HA3	2.02	0.88
1:G:530:MET:N	4:6:354:GLN:HB3	1.88	0.88
1:J:829:TRP:CZ3	2:K:84:PHE:HZ	1.85	0.88
1:D:541:MET:CB	4:5:143:TYR:OH	2.21	0.88
1:D:800:ARG:HD2	3:F:149:VAL:HG22	1.53	0.88
2:E:137:TRP:HA	2:E:145:ALA:CB	2.03	0.88
1:J:769:ALA:HB3	1:J:770:GLY:HA2	0.90	0.88
3:L:62:ALA:O	3:L:63:ILE:HG12	1.71	0.88
4:X:322:PRO:HB2	4:Z:244:ASP:CG	1.94	0.88
1:A:836:PHE:HE1	2:B:159:HIS:HA	1.37	0.88
1:D:215:GLN:H	1:D:340:ILE:HG12	1.06	0.88
1:D:641:LYS:CD	1:D:647:GLN:OE1	2.17	0.88
1:G:541:MET:CB	4:6:143:TYR:OH	2.21	0.88
1:G:795:ARG:CG	3:I:35:ARG:NH2	2.35	0.88
1:D:599:ASN:OD1	1:D:649:VAL:HB	1.73	0.88
1:G:553:MLY:HE2	4:8:45:VAL:HA	1.53	0.88
1:J:629:GLU:HG2	1:J:643:GLY:O	1.72	0.88
1:J:757:GLN:OE1	1:J:772:LEU:O	1.92	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:818:TYR:CE1	2:K:127:ARG:NH2	2.42	0.88
1:A:541:MET:CB	4:4:143:TYR:OH	2.20	0.88
1:G:553:MLY:CG	4:8:44:MET:O	2.20	0.88
1:G:641:LYS:CD	1:G:647:GLN:OE1	2.17	0.88
1:G:728:ASN:HD21	3:I:110:VAL:HA	1.38	0.88
1:J:215:GLN:H	1:J:340:ILE:HG12	1.05	0.88
1:J:642:LYS:HG2	4:7:22:ALA:CA	2.03	0.88
1:J:838:ILE:HD11	2:K:54:MET:CE	2.04	0.88
3:L:24:LYS:HB3	3:L:63:ILE:O	1.72	0.88
4:0:322:PRO:HB2	4:2:244:ASP:CG	1.94	0.88
1:A:642:LYS:HG2	4:4:22:ALA:CA	2.04	0.88
1:A:707:CYS:SG	1:A:714:ARG:NH1	2.47	0.88
1:G:93:MET:CB	1:G:764:MLY:NZ	2.27	0.88
1:G:642:LYS:HG2	4:6:22:ALA:CA	2.03	0.88
1:J:831:TRP:HZ2	2:K:47:LEU:CD2	1.83	0.88
1:A:641:LYS:HD2	4:4:348:SER:CB	2.02	0.88
1:A:795:ARG:HB3	3:C:35:ARG:CZ	2.04	0.88
1:J:642:LYS:CG	4:7:21:PHE:O	2.22	0.88
1:A:553:MLY:HE2	4:6:45:VAL:HA	1.53	0.88
2:B:137:TRP:HA	2:B:145:ALA:HB2	1.54	0.88
1:D:635:GLY:HA2	4:5:334:GLU:CG	2.03	0.88
3:F:139:TYR:HA	3:F:142:PHE:HB3	1.56	0.88
1:G:510:TRP:CZ3	1:G:768:MLY:CH1	2.57	0.88
1:G:542:PHE:HA	4:6:143:TYR:HE1	1.34	0.88
1:G:642:LYS:CG	4:6:21:PHE:O	2.22	0.88
4:2:322:PRO:HB2	4:4:244:ASP:CG	1.94	0.88
4:V:322:PRO:HB2	4:X:244:ASP:CG	1.94	0.88
1:A:789:ALA:HB1	3:C:87:PHE:HE2	1.39	0.88
1:A:817:GLN:OE1	2:B:127:ARG:NH2	1.81	0.88
1:A:839:MLY:NZ	2:B:159:HIS:HB3	1.89	0.88
1:D:646:PHE:CE2	1:D:652:LEU:CD1	2.57	0.88
1:G:550:PHE:CA	4:8:46:GLY:HA3	2.03	0.88
1:G:707:CYS:O	1:G:714:ARG:NH2	2.06	0.88
3:C:139:TYR:HA	3:C:142:PHE:HB3	1.56	0.87
1:G:646:PHE:CE2	1:G:652:LEU:CD1	2.58	0.87
1:G:649:VAL:CG2	1:G:649:VAL:HG13	2.02	0.87
1:G:817:GLN:HB3	2:H:127:ARG:HH11	1.39	0.87
1:J:541:MET:CB	4:7:143:TYR:OH	2.20	0.87
1:J:795:ARG:HE	3:L:118:MET:CE	1.87	0.87
1:D:795:ARG:HB3	3:F:35:ARG:CD	2.04	0.87
1:G:817:GLN:CG	2:H:127:ARG:CD	2.52	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:84:MLY:HE2	1:J:719:ASP:OD2	1.73	0.87
1:J:735:GLY:C	1:J:743:ALA:HB2	1.82	0.87
1:J:754:ASP:CB	1:J:776:GLU:HB3	2.03	0.87
1:A:72:VAL:CG1	1:A:76:GLN:HB3	2.05	0.87
1:A:641:LYS:HG3	1:A:647:GLN:NE2	1.58	0.87
2:B:137:TRP:HA	2:B:145:ALA:CB	2.04	0.87
1:J:92:ALA:O	1:J:714:ARG:HG3	1.74	0.87
4:8:322:PRO:HB2	4:W:244:ASP:CG	1.94	0.87
1:D:642:LYS:CG	4:5:21:PHE:O	2.22	0.87
1:G:534:SER:O	4:6:351:THR:HG23	1.12	0.87
1:G:635:GLY:CA	4:6:341:ILE:HD13	2.02	0.87
3:I:24:LYS:HB3	3:I:63:ILE:O	1.72	0.87
1:J:768:MLY:CH2	1:J:772:LEU:CG	2.45	0.87
3:L:139:TYR:HA	3:L:142:PHE:HB3	1.56	0.87
1:A:642:LYS:CG	4:4:21:PHE:O	2.22	0.87
1:G:752:ASP:OD2	1:G:783:LEU:CB	2.22	0.87
1:G:816:ILE:HD11	2:H:100:ALA:HB1	1.56	0.87
4:4:322:PRO:HB2	4:6:244:ASP:CG	1.94	0.87
4:5:322:PRO:HB2	4:7:244:ASP:CG	1.94	0.87
1:A:635:GLY:CA	4:4:341:ILE:HD13	2.02	0.87
1:D:636:LYS:H	4:5:334:GLU:CD	1.77	0.87
1:D:792:ALA:HB1	3:F:40:ASN:O	1.74	0.87
1:D:795:ARG:NH2	3:F:116:GLU:CD	2.20	0.87
1:G:649:VAL:CG1	1:G:649:VAL:CA	2.53	0.87
1:J:635:GLY:HA2	4:7:334:GLU:CG	2.03	0.87
1:J:646:PHE:CE2	1:J:652:LEU:CD1	2.58	0.87
1:A:649:VAL:HG13	1:A:649:VAL:CG2	2.02	0.87
1:D:642:LYS:HG2	4:5:22:ALA:CA	2.04	0.87
2:K:149:ASP:CG	2:K:150:TYR:H	1.73	0.87
1:A:215:GLN:H	1:A:340:ILE:HG12	1.06	0.87
1:A:649:VAL:CG1	1:A:649:VAL:CA	2.53	0.87
1:A:819:ASN:OD1	2:B:91:ALA:HA	0.87	0.87
1:D:649:VAL:CG1	1:D:649:VAL:CA	2.53	0.87
1:G:93:MET:CE	1:G:763:THR:HG22	2.03	0.87
1:G:823:PHE:CE1	2:H:156:VAL:O	2.28	0.87
1:J:93:MET:HG3	1:J:764:MLY:CH1	2.04	0.87
1:J:754:ASP:OD2	1:J:776:GLU:O	1.91	0.87
4:3:322:PRO:HB2	4:5:244:ASP:CG	1.94	0.87
4:W:322:PRO:HB2	4:Y:244:ASP:CG	1.94	0.87
1:A:831:TRP:CH2	2:B:50:THR:HB	2.08	0.87
1:J:636:LYS:H	4:7:334:GLU:CD	1.78	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:641:LYS:CD	1:J:647:GLN:OE1	2.18	0.87
1:J:649:VAL:CG1	1:J:649:VAL:CA	2.53	0.87
1:A:798:LEU:CD2	3:C:122:GLU:HB3	2.05	0.86
1:G:72:VAL:CG1	1:G:76:GLN:HB3	2.05	0.86
1:G:795:ARG:HD2	3:I:35:ARG:HH22	0.71	0.86
1:G:831:TRP:HE1	2:H:67:MET:CB	1.87	0.86
1:J:84:MLY:HH12	1:J:715:VAL:CG1	1.75	0.86
4:7:322:PRO:HB2	4:V:244:ASP:CG	1.94	0.86
1:D:755:HIS:HA	1:D:758:TYR:CE1	2.10	0.86
1:G:817:GLN:HB3	2:H:127:ARG:HD3	1.56	0.86
4:0:287:ILE:CG2	4:2:205:GLU:HG2	2.05	0.86
4:1:322:PRO:HB2	4:3:244:ASP:CG	1.94	0.86
1:A:530:MET:HG2	4:4:354:GLN:CG	2.05	0.86
1:D:646:PHE:CD2	1:D:652:LEU:HD11	2.09	0.86
1:G:636:LYS:H	4:6:334:GLU:CD	1.78	0.86
1:G:641:LYS:HD2	4:6:348:SER:CB	2.03	0.86
2:H:137:TRP:HA	2:H:145:ALA:CB	2.04	0.86
1:J:508:ILE:HD11	1:J:759:ALA:HB2	0.87	0.86
1:J:757:GLN:CD	1:J:776:GLU:HG3	1.93	0.86
1:J:797:PHE:CD1	3:L:149:VAL:HG12	2.06	0.86
1:A:95:THR:OG1	1:A:769:ALA:HA	1.74	0.86
1:D:310:TYR:CZ	1:D:320:ILE:HD11	2.11	0.86
1:D:735:GLY:C	1:D:743:ALA:HB2	1.82	0.86
1:D:800:ARG:HB3	3:F:149:VAL:HG21	1.57	0.86
1:G:646:PHE:CD2	1:G:652:LEU:HD11	2.09	0.86
2:K:137:TRP:HA	2:K:145:ALA:CB	2.04	0.86
1:A:542:PHE:HA	4:4:143:TYR:HE1	1.34	0.86
1:D:530:MET:HG2	4:5:354:GLN:CG	2.05	0.86
1:G:107:MLY:HB3	1:G:686:MET:HE2	1.58	0.86
1:J:72:VAL:CG1	1:J:76:GLN:HB3	2.05	0.86
1:J:599:ASN:OD1	1:J:649:VAL:HB	1.73	0.86
1:A:502:GLU:HA	1:A:762:HIS:N	1.90	0.86
1:A:636:LYS:H	4:4:334:GLU:CD	1.77	0.86
2:E:149:ASP:CG	2:E:150:TYR:H	1.73	0.86
3:F:24:LYS:HB3	3:F:63:ILE:O	1.72	0.86
1:G:530:MET:HG2	4:6:354:GLN:CG	2.05	0.86
1:J:310:TYR:CZ	1:J:320:ILE:HD11	2.11	0.86
1:J:530:MET:HG2	4:7:354:GLN:CG	2.06	0.86
1:D:72:VAL:CG1	1:D:76:GLN:HB3	2.05	0.86
1:D:206:LYS:HD3	1:D:217:THR:CB	2.06	0.86
1:D:769:ALA:C	1:D:770:GLY:O	2.14	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:287:ILE:CG2	4:6:205:GLU:HG2	2.05	0.86
4:6:322:PRO:HB2	4:8:244:ASP:CG	1.94	0.86
1:G:84:MLY:CH1	1:G:715:VAL:HG12	2.05	0.86
1:G:206:LYS:HD3	1:G:217:THR:CB	2.06	0.86
1:G:755:HIS:HA	1:G:758:TYR:CE1	2.10	0.86
4:V:287:ILE:CG2	4:X:205:GLU:HG2	2.05	0.86
1:D:814:PHE:HD1	2:E:127:ARG:NH2	1.70	0.86
1:A:538:GLU:N	4:4:351:THR:N	2.24	0.86
1:A:793:ARG:HG3	3:C:146:ILE:HG22	1.58	0.86
1:D:724:TYR:HE1	1:D:778:MET:CB	1.89	0.86
1:J:755:HIS:HA	1:J:758:TYR:CE1	2.10	0.86
1:A:538:GLU:OE2	4:4:355:MET:HE3	1.73	0.85
1:A:641:LYS:CD	1:A:647:GLN:OE1	2.17	0.85
1:A:755:HIS:HA	1:A:758:TYR:CE1	2.10	0.85
2:E:163:ALA:HA	2:K:21:GLU:HB3	1.55	0.85
1:G:798:LEU:HD11	3:I:126:LEU:CG	2.06	0.85
1:J:206:LYS:HD3	1:J:217:THR:CB	2.06	0.85
1:A:599:ASN:OD1	1:A:649:VAL:CA	2.25	0.85
2:B:117:LEU:CG	2:B:147:ASN:CG	2.44	0.85
1:G:215:GLN:H	1:G:340:ILE:HG12	1.06	0.85
1:J:410:ASN:OD1	4:7:334:GLU:CA	2.24	0.85
1:A:97:LEU:HD22	1:A:712:PRO:HB3	1.58	0.85
1:A:831:TRP:CD1	2:B:51:PHE:CZ	2.49	0.85
2:E:117:LEU:CG	2:E:147:ASN:CG	2.44	0.85
1:G:204:GLU:H	1:G:207:LYS:HE3	1.42	0.85
2:H:117:LEU:CG	2:H:147:ASN:CG	2.45	0.85
1:J:646:PHE:CD2	1:J:652:LEU:HD11	2.09	0.85
1:J:797:PHE:HA	3:L:149:VAL:HG11	1.58	0.85
3:I:139:TYR:HA	3:I:142:PHE:HB3	1.56	0.85
1:J:630:ALA:C	4:7:25:ASP:OD2	2.15	0.85
1:D:507:GLY:O	1:D:761:GLY:HA2	1.75	0.85
1:D:732:ILE:HG23	1:D:747:LEU:HB2	1.57	0.85
1:G:202:SER:HA	1:G:207:LYS:HE2	0.85	0.85
1:G:599:ASN:OD1	1:G:649:VAL:CA	2.25	0.85
1:G:725:ARG:CZ	1:G:733:PRO:HB3	2.05	0.85
4:7:287:ILE:CG2	4:V:205:GLU:HG2	2.05	0.85
1:A:204:GLU:H	1:A:207:LYS:HE3	1.42	0.85
4:6:287:ILE:CG2	4:8:205:GLU:HG2	2.05	0.85
1:A:206:LYS:HD3	1:A:217:THR:CB	2.06	0.85
1:A:410:ASN:OD1	4:4:334:GLU:CA	2.25	0.85
1:G:752:ASP:OD2	1:G:783:LEU:HB2	1.77	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:640:LYS:CB	1:J:645:SER:OG	2.25	0.85
2:K:117:LEU:CG	2:K:147:ASN:CG	2.44	0.85
4:X:287:ILE:CG2	4:Z:205:GLU:HG2	2.05	0.85
1:A:202:SER:HA	1:A:207:LYS:HE2	0.85	0.85
1:A:800:ARG:HH11	3:C:149:VAL:CG1	1.90	0.85
1:D:599:ASN:OD1	1:D:649:VAL:CA	2.25	0.85
1:D:630:ALA:C	4:5:25:ASP:OD2	2.15	0.85
1:G:310:TYR:CZ	1:G:320:ILE:HD11	2.11	0.85
1:G:707:CYS:HB3	1:G:714:ARG:HH12	0.75	0.85
1:A:630:ALA:C	4:4:25:ASP:OD2	2.15	0.85
1:A:646:PHE:CD2	1:A:652:LEU:HD11	2.09	0.85
1:A:797:PHE:CD2	3:C:126:LEU:CD2	2.59	0.85
1:D:204:GLU:H	1:D:207:LYS:HE3	1.42	0.85
1:D:418:THR:HB	1:D:421:GLU:HG3	1.59	0.85
1:D:769:ALA:CB	1:D:770:GLY:C	2.45	0.85
1:G:410:ASN:OD1	4:6:334:GLU:CA	2.24	0.85
1:J:797:PHE:CB	3:L:149:VAL:CG1	2.54	0.85
1:A:725:ARG:CD	1:A:733:PRO:HB3	2.07	0.85
1:D:410:ASN:OD1	4:5:334:GLU:CA	2.24	0.85
1:D:792:ALA:HB1	3:F:40:ASN:HB2	1.55	0.85
1:J:725:ARG:CZ	1:J:733:PRO:HB3	2.06	0.85
4:2:287:ILE:CG2	4:4:205:GLU:HG2	2.05	0.85
1:A:530:MET:HE1	4:4:355:MET:SD	2.17	0.84
1:A:640:LYS:C	4:4:23:GLY:O	2.15	0.84
1:G:725:ARG:CD	1:G:733:PRO:HB3	2.07	0.84
1:G:732:ILE:HG23	1:G:747:LEU:HB2	1.57	0.84
1:J:410:ASN:ND2	4:7:336:LYS:HG2	1.92	0.84
1:J:529:PRO:CB	4:7:353:GLN:OE1	2.25	0.84
2:K:121:LEU:CA	2:K:128:PHE:CB	2.46	0.84
4:5:287:ILE:CG2	4:7:205:GLU:HG2	2.05	0.84
4:8:287:ILE:CG2	4:W:205:GLU:HG2	2.05	0.84
1:A:836:PHE:HB3	2:B:161:GLU:HG2	1.57	0.84
1:D:202:SER:HA	1:D:207:LYS:HE2	0.85	0.84
1:J:543:PRO:HG3	4:7:143:TYR:O	1.77	0.84
1:J:800:ARG:HD2	3:L:149:VAL:HG23	0.85	0.84
1:J:821:ARG:HH22	2:K:127:ARG:CD	1.89	0.84
1:A:795:ARG:NH2	3:C:116:GLU:CB	2.36	0.84
1:A:822:SER:OG	2:B:88:LEU:HA	1.77	0.84
1:G:410:ASN:ND2	4:6:336:LYS:HG2	1.92	0.84
1:G:538:GLU:N	4:6:351:THR:N	2.24	0.84
1:G:553:MLY:HG2	4:8:47:MET:H	1.43	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:418:THR:HB	1:J:421:GLU:HG3	1.60	0.84
1:J:510:TRP:CZ3	1:J:772:LEU:HD21	2.11	0.84
1:J:757:GLN:NE2	1:J:776:GLU:CG	2.39	0.84
4:3:287:ILE:CG2	4:5:205:GLU:HG2	2.05	0.84
2:B:121:LEU:CA	2:B:128:PHE:CB	2.46	0.84
1:J:202:SER:HA	1:J:207:LYS:HE2	0.85	0.84
1:J:640:LYS:C	4:7:23:GLY:O	2.15	0.84
1:J:732:ILE:HG23	1:J:747:LEU:CB	1.85	0.84
1:A:635:GLY:HA2	4:4:334:GLU:CG	2.03	0.84
1:A:800:ARG:NH1	3:C:149:VAL:O	2.10	0.84
1:D:732:ILE:HG21	1:D:747:LEU:HD13	0.91	0.84
1:D:769:ALA:HA	1:D:771:LEU:CB	2.07	0.84
1:D:817:GLN:NE2	2:E:127:ARG:CG	2.40	0.84
1:G:730:SER:OG	3:I:109:HIS:NE2	2.09	0.84
1:G:735:GLY:C	1:G:743:ALA:HB2	1.82	0.84
1:G:768:MLY:CD	1:G:772:LEU:HD22	2.06	0.84
1:J:732:ILE:HG23	1:J:747:LEU:HB2	1.57	0.84
1:J:754:ASP:OD2	1:J:776:GLU:HA	1.77	0.84
1:A:310:TYR:CZ	1:A:320:ILE:HD11	2.11	0.84
1:A:732:ILE:HG23	1:A:747:LEU:HB2	1.57	0.84
1:D:529:PRO:CB	4:5:353:GLN:OE1	2.25	0.84
1:D:557:GLU:H	4:7:48:GLY:HA3	1.28	0.84
1:D:640:LYS:C	4:5:23:GLY:O	2.15	0.84
1:J:735:GLY:C	1:J:743:ALA:HB1	1.84	0.84
4:W:287:ILE:CG2	4:Y:205:GLU:HG2	2.05	0.84
1:J:649:VAL:HG12	1:J:649:VAL:C	1.98	0.84
1:A:814:PHE:HA	2:B:127:ARG:NH2	1.93	0.84
1:D:641:LYS:HG3	1:D:647:GLN:NE2	1.59	0.84
1:D:649:VAL:HG12	1:D:649:VAL:C	1.98	0.84
1:G:557:GLU:N	4:8:48:GLY:HA2	1.91	0.84
1:G:648:THR:CG2	1:G:651:ALA:HB2	2.08	0.84
1:J:204:GLU:H	1:J:207:LYS:HE3	1.41	0.84
1:J:753:VAL:HA	1:J:780:ASP:OD2	1.78	0.84
4:5:237:GLU:HA	4:5:251:GLY:HA2	1.60	0.84
1:A:410:ASN:ND2	4:4:336:LYS:HG2	1.93	0.84
1:D:629:GLU:CG	1:D:643:GLY:O	2.26	0.84
1:D:640:LYS:CB	1:D:645:SER:OG	2.25	0.84
1:G:788:THR:C	3:I:42:THR:CG2	2.34	0.84
1:J:629:GLU:CG	1:J:643:GLY:O	2.26	0.84
4:3:237:GLU:HA	4:3:251:GLY:HA2	1.60	0.84
4:7:237:GLU:HA	4:7:251:GLY:HA2	1.60	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:286:ASP:OD1	4:Z:203:THR:CG2	2.26	0.84
1:A:542:PHE:CA	4:4:143:TYR:CE1	2.61	0.84
2:H:141:PRO:CB	2:H:142:PRO:CD	2.56	0.84
4:0:286:ASP:OD1	4:2:203:THR:CG2	2.26	0.84
4:1:286:ASP:OD1	4:3:203:THR:CG2	2.26	0.84
1:A:797:PHE:CE2	3:C:126:LEU:HD23	2.07	0.83
1:D:538:GLU:N	4:5:351:THR:N	2.25	0.83
1:D:730:SER:O	1:D:734:GLU:HG3	1.78	0.83
1:G:635:GLY:HA2	4:6:334:GLU:CG	2.03	0.83
1:J:95:THR:OG1	1:J:713:SER:CB	2.25	0.83
1:J:599:ASN:OD1	1:J:649:VAL:CA	2.25	0.83
4:1:237:GLU:HA	4:1:251:GLY:HA2	1.60	0.83
1:A:543:PRO:HG3	4:4:143:TYR:O	1.77	0.83
1:A:648:THR:CG2	1:A:651:ALA:HB2	2.08	0.83
1:A:798:LEU:HD13	3:C:126:LEU:CD2	1.95	0.83
1:D:410:ASN:ND2	4:5:336:LYS:HG2	1.92	0.83
1:D:648:THR:CG2	1:D:651:ALA:HB2	2.08	0.83
1:D:725:ARG:CD	1:D:733:PRO:HB3	2.07	0.83
1:J:783:LEU:O	1:J:787:ILE:HB	1.79	0.83
2:K:141:PRO:CB	2:K:142:PRO:CD	2.56	0.83
4:3:286:ASP:OD1	4:5:203:THR:CG2	2.26	0.83
4:V:237:GLU:HA	4:V:251:GLY:HA2	1.60	0.83
1:A:768:MLY:CB	1:A:771:LEU:HD13	2.08	0.83
1:D:724:TYR:CE1	1:D:778:MET:CB	2.61	0.83
1:G:549:SER:O	4:8:46:GLY:HA3	1.78	0.83
1:G:640:LYS:C	4:6:23:GLY:O	2.16	0.83
1:G:736:GLN:HA	1:G:743:ALA:HB2	1.51	0.83
1:G:819:ASN:CG	2:H:92:ASP:CB	2.47	0.83
1:J:542:PHE:CA	4:7:143:TYR:CE1	2.61	0.83
4:V:286:ASP:OD1	4:X:203:THR:CG2	2.26	0.83
1:A:599:ASN:OD1	1:A:649:VAL:HB	1.72	0.83
1:G:529:PRO:CB	4:6:353:GLN:OE1	2.25	0.83
1:G:795:ARG:HB2	3:I:35:ARG:NH2	1.91	0.83
1:D:732:ILE:CG2	1:D:747:LEU:HD13	1.34	0.83
1:G:542:PHE:CA	4:6:143:TYR:CE1	2.61	0.83
1:G:640:LYS:CB	1:G:645:SER:OG	2.25	0.83
1:J:795:ARG:CZ	3:L:35:ARG:HH12	1.92	0.83
4:2:286:ASP:OD1	4:4:203:THR:CG2	2.26	0.83
1:A:549:SER:O	4:6:46:GLY:HA3	1.77	0.83
1:A:553:MLY:HG2	4:6:47:MET:H	1.44	0.83
1:A:646:PHE:CE2	1:A:652:LEU:CD1	2.58	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:TRP:HZ3	2:B:50:THR:HG21	1.44	0.83
1:J:218:LEU:HB3	1:J:221:GLN:HG3	1.60	0.83
1:J:549:SER:O	4:V:46:GLY:HA3	1.78	0.83
1:J:817:GLN:HB3	2:K:127:ARG:HH11	1.44	0.83
4:1:287:ILE:CG2	4:3:205:GLU:HG2	2.05	0.83
4:X:237:GLU:HA	4:X:251:GLY:HA2	1.60	0.83
1:A:629:GLU:CG	1:A:643:GLY:O	2.26	0.83
2:B:141:PRO:CB	2:B:142:PRO:CD	2.56	0.83
1:D:549:SER:O	4:7:46:GLY:HA3	1.77	0.83
1:D:725:ARG:CZ	1:D:733:PRO:HB3	2.05	0.83
1:D:834:LEU:HD11	2:E:54:MET:HB2	1.56	0.83
1:J:730:SER:O	1:J:734:GLU:HG3	1.79	0.83
4:Z:237:GLU:HA	4:Z:251:GLY:HA2	1.60	0.83
1:A:506:GLU:H	1:A:761:GLY:HA2	1.43	0.83
1:A:529:PRO:CB	4:4:353:GLN:OE1	2.25	0.83
2:E:141:PRO:CB	2:E:142:PRO:CD	2.56	0.83
2:H:144:VAL:HG12	2:H:153:ILE:CD1	2.09	0.83
1:J:538:GLU:N	4:7:351:THR:N	2.24	0.83
4:5:286:ASP:OD1	4:7:203:THR:CG2	2.26	0.83
4:6:286:ASP:OD1	4:8:203:THR:CG2	2.26	0.83
1:A:732:ILE:CG2	1:A:747:LEU:HD13	1.34	0.83
1:G:418:THR:HB	1:G:421:GLU:HG3	1.59	0.83
1:G:791:GLN:OE1	3:I:116:GLU:CB	2.27	0.83
1:J:279:LEU:HB2	1:J:282:GLU:HG3	1.60	0.83
1:A:836:PHE:HE1	2:B:159:HIS:CA	1.92	0.83
1:D:279:LEU:HB2	1:D:282:GLU:HG3	1.60	0.83
1:D:553:MLY:HG2	4:7:47:MET:H	1.44	0.83
2:E:121:LEU:CA	2:E:128:PHE:CB	2.46	0.83
4:0:237:GLU:HA	4:0:251:GLY:HA2	1.60	0.83
4:7:286:ASP:OD1	4:V:203:THR:CG2	2.26	0.83
4:8:286:ASP:OD1	4:W:203:THR:CG2	2.26	0.83
4:X:290:ARG:NH1	4:Z:202:THR:HG21	1.94	0.83
1:D:641:LYS:HG2	1:D:647:GLN:HG3	1.61	0.82
1:G:543:PRO:HG3	4:6:143:TYR:O	1.78	0.82
1:J:831:TRP:CH2	2:K:34:ILE:HG21	2.14	0.82
4:0:290:ARG:NH1	4:2:202:THR:HG21	1.94	0.82
1:A:499:GLU:OE1	1:A:766:PHE:HZ	1.61	0.82
1:A:814:PHE:HD1	2:B:127:ARG:HH22	1.14	0.82
1:D:542:PHE:CA	4:5:143:TYR:CE1	2.61	0.82
1:G:538:GLU:OE2	4:6:355:MET:HE3	1.78	0.82
1:J:549:SER:O	4:V:46:GLY:CA	2.27	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:111:SER:OG	2:K:148:VAL:C	2.15	0.82
4:1:290:ARG:NH1	4:3:202:THR:HG21	1.95	0.82
4:2:290:ARG:NH1	4:4:202:THR:HG21	1.94	0.82
4:4:290:ARG:NH1	4:6:202:THR:HG21	1.94	0.82
4:8:290:ARG:NH1	4:W:202:THR:HG21	1.94	0.82
4:W:286:ASP:OD1	4:Y:203:THR:CG2	2.26	0.82
1:A:418:THR:HB	1:A:421:GLU:HG3	1.60	0.82
1:D:831:TRP:HH2	2:E:47:LEU:HA	1.43	0.82
1:J:542:PHE:CA	4:7:143:TYR:HE1	1.92	0.82
1:A:557:GLU:H	4:6:48:GLY:HA3	1.28	0.82
1:A:578:HIS:HB3	1:A:592:ILE:HD12	1.62	0.82
1:A:795:ARG:NH1	3:C:43:ASN:H	1.78	0.82
1:J:641:LYS:HG2	1:J:647:GLN:HG3	1.61	0.82
4:2:237:GLU:HA	4:2:251:GLY:HA2	1.60	0.82
4:6:290:ARG:NH1	4:8:202:THR:HG21	1.94	0.82
1:A:735:GLY:C	1:A:743:ALA:HB2	1.82	0.82
1:G:556:ASP:HA	4:8:49:GLN:O	1.69	0.82
1:G:629:GLU:CG	1:G:643:GLY:O	2.26	0.82
1:G:769:ALA:HB3	1:G:770:GLY:HA2	0.83	0.82
1:J:90:ASP:OD2	1:J:764:MLY:CH1	2.27	0.82
1:J:648:THR:CG2	1:J:651:ALA:HB2	2.08	0.82
4:W:290:ARG:NH1	4:Y:202:THR:HG21	1.94	0.82
1:A:107:MLY:HB3	1:A:686:MET:HE2	1.61	0.82
1:D:218:LEU:HD22	1:D:222:ILE:CG1	2.10	0.82
1:G:218:LEU:HD22	1:G:222:ILE:CG1	2.09	0.82
1:G:549:SER:O	4:8:46:GLY:C	2.18	0.82
1:G:549:SER:O	4:8:46:GLY:CA	2.27	0.82
1:J:127:ASN:HD22	1:J:128:PRO:HD2	1.44	0.82
1:J:218:LEU:HD22	1:J:222:ILE:CG1	2.10	0.82
1:J:549:SER:O	4:V:46:GLY:C	2.18	0.82
4:V:290:ARG:NH1	4:X:202:THR:HG21	1.95	0.82
4:Y:237:GLU:HA	4:Y:251:GLY:HA2	1.60	0.82
1:D:543:PRO:HG3	4:5:143:TYR:O	1.77	0.82
1:D:817:GLN:NE2	2:E:127:ARG:HE	1.77	0.82
1:G:279:LEU:HB2	1:G:282:GLU:HG3	1.60	0.82
1:G:578:HIS:HB3	1:G:592:ILE:HD12	1.62	0.82
1:G:643:GLY:N	4:6:24:ASP:HA	1.94	0.82
1:J:218:LEU:HA	1:J:221:GLN:HG2	1.62	0.82
1:J:643:GLY:N	4:7:24:ASP:HA	1.93	0.82
4:3:290:ARG:NH1	4:5:202:THR:HG21	1.95	0.82
4:4:286:ASP:OD1	4:6:203:THR:CG2	2.26	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ASN:HD22	1:A:128:PRO:HD2	1.45	0.82
1:A:279:LEU:HB2	1:A:282:GLU:HG3	1.60	0.82
1:A:542:PHE:CA	4:4:143:TYR:HE1	1.92	0.82
1:D:817:GLN:OE1	2:E:127:ARG:CZ	2.28	0.82
1:D:834:LEU:HD21	2:E:54:MET:CG	2.09	0.82
1:J:725:ARG:CD	1:J:733:PRO:HB3	2.07	0.82
1:J:816:ILE:HD11	2:K:100:ALA:HB1	1.59	0.82
1:A:641:LYS:HG2	1:A:647:GLN:HG3	1.61	0.82
1:A:768:MLY:C	1:A:771:LEU:CB	2.57	0.82
1:G:95:THR:OG1	1:G:713:SER:HB3	1.79	0.82
1:J:599:ASN:CA	1:J:649:VAL:CB	2.53	0.82
1:J:721:LYS:CA	1:J:736:GLN:NE2	2.43	0.82
1:J:757:GLN:HG2	1:J:776:GLU:HG3	0.82	0.82
1:A:218:LEU:HD22	1:A:222:ILE:CG1	2.10	0.82
1:D:218:LEU:HB3	1:D:221:GLN:HG3	1.60	0.82
1:D:809:ARG:CZ	2:E:124:GLY:HA3	2.10	0.82
1:D:817:GLN:NE2	2:E:127:ARG:NE	2.28	0.82
1:G:730:SER:O	1:G:734:GLU:HG3	1.78	0.82
1:A:639:GLY:CA	4:4:344:SER:C	2.48	0.81
1:D:549:SER:O	4:7:46:GLY:C	2.18	0.81
1:J:734:GLU:O	1:J:738:MET:CG	2.28	0.81
1:J:821:ARG:HH22	2:K:127:ARG:CG	1.84	0.81
1:A:640:LYS:CB	1:A:645:SER:OG	2.25	0.81
1:A:730:SER:O	1:A:734:GLU:HG3	1.78	0.81
1:D:549:SER:O	4:7:46:GLY:CA	2.27	0.81
1:D:734:GLU:O	1:D:738:MET:CG	2.28	0.81
4:4:237:GLU:HA	4:4:251:GLY:HA2	1.60	0.81
4:7:290:ARG:NH1	4:V:202:THR:HG21	1.94	0.81
4:W:237:GLU:HA	4:W:251:GLY:HA2	1.60	0.81
1:A:549:SER:O	4:6:46:GLY:CA	2.28	0.81
1:A:553:MLY:CB	4:6:46:GLY:CA	2.32	0.81
1:A:798:LEU:HD12	3:C:126:LEU:HD21	1.58	0.81
1:A:831:TRP:CZ3	2:B:50:THR:HG21	2.15	0.81
2:B:111:SER:OG	2:B:148:VAL:C	2.15	0.81
1:D:571:ALA:O	1:D:572:LYS:CG	2.28	0.81
1:D:639:GLY:CA	4:5:344:SER:C	2.48	0.81
1:D:643:GLY:N	4:5:24:ASP:HA	1.93	0.81
1:D:830:PRO:HD2	2:E:67:MET:HE1	1.63	0.81
1:D:834:LEU:HD21	2:E:54:MET:HG3	1.62	0.81
1:G:232:PHE:CZ	1:G:287:ILE:HD13	2.16	0.81
1:G:734:GLU:O	1:G:738:MET:CG	2.28	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:480:ILE:HG22	1:J:481:ASN:HD22	1.45	0.81
1:J:578:HIS:HB3	1:J:592:ILE:HD12	1.62	0.81
2:K:121:LEU:CG	2:K:128:PHE:CA	2.48	0.81
4:6:237:GLU:HA	4:6:251:GLY:HA2	1.60	0.81
4:8:237:GLU:HA	4:8:251:GLY:HA2	1.60	0.81
1:A:549:SER:O	4:6:46:GLY:C	2.19	0.81
1:D:127:ASN:HD22	1:D:128:PRO:HD2	1.45	0.81
1:D:557:GLU:N	4:7:48:GLY:HA2	1.90	0.81
1:D:792:ALA:HB1	3:F:40:ASN:HB3	1.62	0.81
1:G:641:LYS:HG2	1:G:647:GLN:HG3	1.61	0.81
1:G:800:ARG:HD2	3:I:149:VAL:HG22	1.61	0.81
1:J:510:TRP:CZ2	1:J:768:MLY:CH1	2.58	0.81
1:J:639:GLY:CA	4:7:344:SER:C	2.48	0.81
1:J:768:MLY:CH2	1:J:772:LEU:CB	2.35	0.81
1:A:218:LEU:HA	1:A:221:GLN:HG2	1.62	0.81
1:A:789:ALA:CB	3:C:87:PHE:HE2	1.94	0.81
1:A:834:LEU:CD1	2:B:54:MET:HB3	2.08	0.81
1:D:550:PHE:CA	4:7:46:GLY:CA	2.59	0.81
1:D:578:HIS:HD2	1:D:591:ASN:HA	1.45	0.81
1:G:127:ASN:HD22	1:G:128:PRO:HD2	1.45	0.81
1:J:550:PHE:CA	4:V:46:GLY:CA	2.59	0.81
1:A:643:GLY:N	4:4:24:ASP:HA	1.93	0.81
1:D:538:GLU:CA	4:5:351:THR:H	1.93	0.81
1:D:542:PHE:CA	4:5:143:TYR:HE1	1.92	0.81
1:J:553:MLY:HG2	4:V:47:MET:H	1.44	0.81
4:5:290:ARG:NH1	4:7:202:THR:HG21	1.94	0.81
1:A:538:GLU:CA	4:4:351:THR:H	1.93	0.81
1:A:721:LYS:CA	1:A:736:GLN:NE2	2.43	0.81
1:D:641:LYS:HD2	4:5:348:SER:CA	2.09	0.81
1:G:480:ILE:HG22	1:G:481:ASN:HD22	1.45	0.81
4:5:223:PHE:HE1	4:5:255:PHE:HB2	1.46	0.81
1:A:793:ARG:HE	3:C:147:MET:CG	1.94	0.81
2:B:121:LEU:CG	2:B:128:PHE:CA	2.48	0.81
1:D:107:MLY:HB3	1:D:686:MET:HE2	1.63	0.81
1:D:218:LEU:CA	1:D:221:GLN:HG2	2.10	0.81
1:D:723:ARG:O	1:D:782:MLY:NZ	2.13	0.81
1:G:530:MET:HE1	4:6:355:MET:SD	2.20	0.81
1:G:721:LYS:CA	1:G:736:GLN:NE2	2.43	0.81
2:K:144:VAL:HG12	2:K:153:ILE:CD1	2.10	0.81
4:2:223:PHE:HE1	4:2:255:PHE:HB2	1.46	0.81
4:4:223:PHE:HE1	4:4:255:PHE:HB2	1.46	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:223:PHE:HE1	4:7:255:PHE:HB2	1.46	0.81
1:A:734:GLU:O	1:A:738:MET:CG	2.28	0.81
1:D:507:GLY:HA2	1:D:762:HIS:CE1	2.16	0.81
1:D:724:TYR:CZ	1:D:778:MET:SD	2.73	0.81
1:D:792:ALA:CB	3:F:40:ASN:O	2.29	0.81
1:D:831:TRP:CZ2	2:E:47:LEU:CG	2.63	0.81
1:G:639:GLY:CA	4:6:344:SER:C	2.48	0.81
1:J:641:LYS:HD2	4:7:348:SER:CA	2.09	0.81
4:3:223:PHE:HE1	4:3:255:PHE:HB2	1.46	0.81
1:A:232:PHE:CZ	1:A:287:ILE:HD13	2.16	0.81
1:A:709:LYS:O	1:A:710:GLY:HA3	1.81	0.81
1:D:218:LEU:HA	1:D:221:GLN:HG2	1.62	0.81
1:D:724:TYR:O	1:D:782:MLY:HH11	1.80	0.81
4:V:223:PHE:HE1	4:V:255:PHE:HB2	1.46	0.81
1:A:646:PHE:CE2	1:A:652:LEU:HD21	2.14	0.80
1:G:641:LYS:HD2	4:6:348:SER:CA	2.10	0.80
1:G:646:PHE:CE2	1:G:652:LEU:HD21	2.14	0.80
1:J:218:LEU:CA	1:J:221:GLN:HG2	2.10	0.80
1:J:538:GLU:CA	4:7:351:THR:H	1.93	0.80
1:J:578:HIS:HD2	1:J:591:ASN:HA	1.45	0.80
4:0:223:PHE:HE1	4:0:255:PHE:HB2	1.46	0.80
4:X:223:PHE:HE1	4:X:255:PHE:HB2	1.46	0.80
1:A:550:PHE:CA	4:6:46:GLY:CA	2.59	0.80
1:A:641:LYS:HD2	4:4:348:SER:CA	2.09	0.80
1:A:725:ARG:CZ	1:A:733:PRO:HB3	2.06	0.80
1:A:813:ILE:HG23	2:B:127:ARG:CD	1.94	0.80
1:D:374:GLN:HG3	1:D:375:ALA:N	1.96	0.80
1:D:721:LYS:CA	1:D:736:GLN:NE2	2.43	0.80
1:G:571:ALA:O	1:G:572:LYS:CG	2.28	0.80
1:G:836:PHE:CZ	2:H:159:HIS:HA	2.15	0.80
1:J:800:ARG:HD2	3:L:149:VAL:CB	2.10	0.80
4:Y:223:PHE:HE1	4:Y:255:PHE:HB2	1.46	0.80
1:D:215:GLN:N	1:D:340:ILE:CD1	2.44	0.80
1:D:723:ARG:O	1:D:782:MLY:CE	2.30	0.80
1:J:798:LEU:CD2	3:L:126:LEU:CG	2.59	0.80
2:K:141:PRO:CB	2:K:142:PRO:HD2	2.11	0.80
2:B:144:VAL:CA	2:B:153:ILE:HD11	2.11	0.80
1:D:818:TYR:CB	2:E:90:GLY:N	2.45	0.80
1:G:93:MET:CE	1:G:763:THR:C	2.48	0.80
1:G:553:MLY:NZ	4:8:45:VAL:HA	1.84	0.80
1:J:215:GLN:N	1:J:340:ILE:CD1	2.44	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:374:GLN:HG3	1:J:375:ALA:N	1.96	0.80
4:Z:223:PHE:HE1	4:Z:255:PHE:HB2	1.46	0.80
2:B:141:PRO:CB	2:B:142:PRO:HD2	2.11	0.80
1:D:732:ILE:HG22	1:D:747:LEU:HD12	0.81	0.80
1:D:797:PHE:HE2	3:F:126:LEU:CD2	1.93	0.80
1:D:831:TRP:HA	2:E:51:PHE:HE1	1.45	0.80
1:G:538:GLU:CA	4:6:351:THR:H	1.93	0.80
1:G:538:GLU:HG3	4:6:351:THR:C	2.02	0.80
1:A:215:GLN:N	1:A:340:ILE:CD1	2.44	0.80
1:A:732:ILE:HG21	1:A:747:LEU:HD13	0.91	0.80
1:D:578:HIS:HB3	1:D:592:ILE:HD12	1.62	0.80
1:D:822:SER:CB	2:E:88:LEU:CD2	2.52	0.80
2:E:111:SER:OG	2:E:148:VAL:C	2.15	0.80
1:G:829:TRP:CH2	2:H:87:LYS:CE	2.63	0.80
2:K:141:PRO:HB2	2:K:142:PRO:CD	2.11	0.80
1:A:480:ILE:HG22	1:A:481:ASN:HD22	1.45	0.80
1:J:93:MET:SD	1:J:716:LEU:CD1	2.67	0.80
1:J:93:MET:HG3	1:J:764:MLY:CD	2.11	0.80
1:G:542:PHE:CA	4:6:143:TYR:HE1	1.93	0.80
1:G:578:HIS:HD2	1:G:591:ASN:HA	1.44	0.80
1:G:599:ASN:CA	1:G:649:VAL:CB	2.53	0.80
1:G:732:ILE:HG22	1:G:747:LEU:HD12	0.81	0.80
3:L:49:ILE:N	3:L:52:ASN:ND2	2.29	0.80
4:6:223:PHE:HE1	4:6:255:PHE:HB2	1.46	0.80
1:A:374:GLN:HG3	1:A:375:ALA:N	1.96	0.80
1:A:578:HIS:HD2	1:A:591:ASN:HA	1.45	0.80
1:D:232:PHE:CZ	1:D:287:ILE:HD13	2.16	0.80
1:G:215:GLN:N	1:G:340:ILE:CD1	2.44	0.80
1:G:798:LEU:CD2	3:I:122:GLU:HB3	2.10	0.80
1:J:571:ALA:O	1:J:572:LYS:CG	2.28	0.80
1:J:797:PHE:HB2	3:L:149:VAL:CG1	2.12	0.80
2:K:144:VAL:CA	2:K:153:ILE:HD11	2.11	0.80
4:1:223:PHE:HE1	4:1:255:PHE:HB2	1.46	0.80
1:G:218:LEU:HA	1:G:221:GLN:HG2	1.62	0.80
1:G:550:PHE:CA	4:8:46:GLY:CA	2.59	0.80
1:G:769:ALA:HB2	1:G:770:GLY:CA	2.12	0.80
1:A:732:ILE:HG22	1:A:747:LEU:HD12	0.81	0.79
1:A:752:ASP:O	1:A:778:MET:SD	2.39	0.79
3:C:49:ILE:N	3:C:52:ASN:ND2	2.29	0.79
1:D:830:PRO:HB2	2:E:51:PHE:CE2	2.16	0.79
3:F:49:ILE:N	3:F:52:ASN:ND2	2.29	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:374:GLN:HG3	1:G:375:ALA:N	1.96	0.79
1:G:553:MLY:CB	4:8:46:GLY:CA	2.33	0.79
1:J:232:PHE:CZ	1:J:287:ILE:HD13	2.16	0.79
1:J:732:ILE:HG22	1:J:747:LEU:HD12	0.81	0.79
1:J:820:VAL:HG11	2:K:136:MET:HE3	1.64	0.79
1:J:838:ILE:CD1	2:K:54:MET:CE	2.61	0.79
1:D:480:ILE:HG22	1:D:481:ASN:HD22	1.45	0.79
1:J:84:MLY:HE2	1:J:719:ASP:CB	1.63	0.79
1:J:784:ALA:O	1:J:788:THR:N	2.14	0.79
1:A:571:ALA:O	1:A:572:LYS:CG	2.28	0.79
1:D:736:GLN:HA	1:D:743:ALA:HB2	1.51	0.79
2:E:144:VAL:HG12	2:E:153:ILE:CD1	2.10	0.79
1:G:752:ASP:C	1:G:779:ARG:NH1	2.34	0.79
1:J:732:ILE:CG2	1:J:747:LEU:HD13	1.34	0.79
1:J:732:ILE:HG21	1:J:747:LEU:HD13	0.90	0.79
4:6:287:ILE:HB	4:8:204:ALA:N	1.97	0.79
1:A:599:ASN:CA	1:A:649:VAL:CB	2.54	0.79
1:A:732:ILE:HG23	1:A:747:LEU:CB	1.85	0.79
1:D:769:ALA:HA	1:D:771:LEU:N	1.97	0.79
2:E:144:VAL:CA	2:E:153:ILE:HD11	2.11	0.79
1:G:819:ASN:ND2	2:H:92:ASP:HB2	1.96	0.79
2:H:121:LEU:CG	2:H:128:PHE:CA	2.49	0.79
3:I:49:ILE:N	3:I:52:ASN:ND2	2.29	0.79
4:W:223:PHE:HE1	4:W:255:PHE:HB2	1.46	0.79
1:A:174:SER:CB	1:A:667:THR:HG21	2.13	0.79
1:A:557:GLU:N	4:6:48:GLY:HA2	1.90	0.79
1:A:641:LYS:CE	1:A:647:GLN:CG	2.60	0.79
2:H:144:VAL:CA	2:H:153:ILE:HD11	2.11	0.79
4:4:287:ILE:HB	4:6:204:ALA:N	1.97	0.79
2:E:150:TYR:C	2:E:151:LYS:CG	2.48	0.79
1:G:754:ASP:HB2	1:G:776:GLU:CD	2.02	0.79
1:J:530:MET:HE1	4:7:355:MET:SD	2.23	0.79
1:J:817:GLN:OE1	2:K:127:ARG:HD2	1.82	0.79
1:A:218:LEU:CA	1:A:221:GLN:HG2	2.10	0.79
1:A:538:GLU:HG3	4:4:351:THR:C	2.03	0.79
1:D:830:PRO:HD2	2:E:67:MET:CE	2.11	0.79
2:E:141:PRO:CB	2:E:142:PRO:HD2	2.12	0.79
2:H:141:PRO:CB	2:H:142:PRO:HD2	2.12	0.79
1:A:409:GLY:N	1:A:636:LYS:CG	2.44	0.79
1:A:537:GLU:O	4:4:350:SER:N	2.16	0.79
1:A:550:PHE:N	4:6:46:GLY:HA3	1.97	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:PRO:HB2	2:B:142:PRO:CD	2.11	0.79
1:D:641:LYS:CE	1:D:647:GLN:HB2	2.13	0.79
1:D:768:MLY:CA	1:D:771:LEU:HD13	2.12	0.79
1:G:537:GLU:O	4:6:350:SER:N	2.16	0.79
1:G:550:PHE:N	4:8:46:GLY:HA3	1.97	0.79
1:G:641:LYS:HD2	4:6:348:SER:HB2	1.54	0.79
1:D:407:GLY:HA2	1:D:412:ALA:HA	1.65	0.79
1:D:409:GLY:N	1:D:636:LYS:CG	2.44	0.79
1:D:537:GLU:O	4:5:350:SER:N	2.16	0.79
1:D:550:PHE:HA	4:7:46:GLY:HA2	1.64	0.79
1:D:793:ARG:HA	3:F:40:ASN:ND2	1.96	0.79
2:E:141:PRO:HB2	2:E:142:PRO:CD	2.12	0.79
3:I:50:LEU:C	3:I:53:PRO:HD2	2.03	0.79
1:J:407:GLY:HA2	1:J:412:ALA:HA	1.65	0.79
3:L:50:LEU:C	3:L:53:PRO:HD2	2.03	0.79
4:W:287:ILE:HB	4:Y:204:ALA:N	1.98	0.79
1:A:641:LYS:HD2	4:4:348:SER:HB2	1.54	0.79
1:A:769:ALA:C	1:A:772:LEU:N	2.33	0.79
1:D:792:ALA:CA	3:F:40:ASN:HB3	2.12	0.79
1:D:834:LEU:HG	2:E:54:MET:CG	2.03	0.79
1:G:174:SER:CB	1:G:667:THR:HG21	2.13	0.79
1:G:218:LEU:CA	1:G:221:GLN:HG2	2.10	0.79
1:G:550:PHE:HA	4:8:46:GLY:HA2	1.64	0.79
1:J:92:ALA:O	1:J:714:ARG:CG	2.31	0.79
2:B:144:VAL:HG12	2:B:153:ILE:CD1	2.09	0.78
1:D:732:ILE:HG23	1:D:747:LEU:CB	1.85	0.78
1:J:642:LYS:CG	4:7:23:GLY:H	1.77	0.78
4:1:287:ILE:HB	4:3:204:ALA:N	1.97	0.78
1:A:817:GLN:HB2	2:B:127:ARG:NH1	1.97	0.78
1:D:291:ILE:HA	1:D:331:LEU:HD11	1.64	0.78
3:F:50:LEU:C	3:F:53:PRO:HD2	2.03	0.78
1:G:407:GLY:HA2	1:G:412:ALA:HA	1.65	0.78
1:A:550:PHE:HA	4:6:46:GLY:HA2	1.65	0.78
1:A:553:MLY:NZ	4:6:45:VAL:HA	1.84	0.78
1:J:409:GLY:N	1:J:636:LYS:CG	2.44	0.78
1:J:538:GLU:HG3	4:7:351:THR:C	2.03	0.78
1:J:550:PHE:HA	4:V:46:GLY:HA2	1.64	0.78
1:J:754:ASP:OD2	1:J:776:GLU:CB	2.32	0.78
4:V:287:ILE:HB	4:X:204:ALA:N	1.97	0.78
1:A:51:THR:O	1:A:62:VAL:HG13	1.84	0.78
3:C:50:LEU:C	3:C:53:PRO:HD2	2.03	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:481:ASN:HD22	1:D:481:ASN:N	1.82	0.78
2:E:162:ASP:HB3	2:K:20:ASP:HB2	1.64	0.78
1:J:291:ILE:HA	1:J:331:LEU:HD11	1.64	0.78
1:J:639:GLY:CA	4:7:345:ILE:N	2.47	0.78
1:J:641:LYS:CE	1:J:647:GLN:HB2	2.13	0.78
1:A:642:LYS:HG2	4:4:22:ALA:HA	1.66	0.78
1:D:550:PHE:N	4:7:46:GLY:HA3	1.97	0.78
1:D:815:CYS:SG	2:E:92:ASP:HB2	2.24	0.78
1:G:642:LYS:HG2	4:6:22:ALA:HA	1.65	0.78
1:G:646:PHE:HE2	1:G:652:LEU:CD2	1.97	0.78
4:5:287:ILE:HB	4:7:204:ALA:N	1.97	0.78
1:G:537:GLU:HG3	4:6:350:SER:O	1.79	0.78
1:J:537:GLU:O	4:7:350:SER:N	2.16	0.78
4:3:287:ILE:HB	4:5:204:ALA:N	1.98	0.78
4:8:287:ILE:HB	4:W:204:ALA:N	1.97	0.78
1:A:556:ASP:HA	4:6:49:GLN:O	1.70	0.78
3:C:49:ILE:N	3:C:52:ASN:HD22	1.82	0.78
1:G:51:THR:O	1:G:62:VAL:HG13	1.84	0.78
1:G:93:MET:SD	1:G:763:THR:HG22	2.24	0.78
1:G:291:ILE:HA	1:G:331:LEU:HD11	1.64	0.78
1:J:174:SER:CB	1:J:667:THR:HG21	2.13	0.78
1:J:646:PHE:HE2	1:J:652:LEU:CD2	1.97	0.78
1:J:797:PHE:HA	3:L:149:VAL:CG1	2.12	0.78
1:A:537:GLU:HG3	4:4:350:SER:O	1.79	0.78
2:B:121:LEU:CG	2:B:128:PHE:HA	2.14	0.78
1:D:800:ARG:CD	3:F:149:VAL:C	2.53	0.78
1:G:93:MET:CA	1:G:764:MLY:NZ	2.35	0.78
1:G:732:ILE:HG21	1:G:747:LEU:HD13	0.91	0.78
1:J:51:THR:O	1:J:62:VAL:HG13	1.84	0.78
1:J:530:MET:CG	4:7:354:GLN:CB	2.30	0.78
1:J:550:PHE:N	4:V:46:GLY:HA3	1.97	0.78
1:J:798:LEU:HD21	3:L:126:LEU:CG	2.14	0.78
4:2:287:ILE:HB	4:4:204:ALA:N	1.98	0.78
4:8:223:PHE:HE1	4:8:255:PHE:HB2	1.46	0.78
1:A:496:PHE:CD2	1:A:514:ASP:HA	2.19	0.78
1:D:831:TRP:HA	2:E:51:PHE:CE1	2.19	0.78
1:D:831:TRP:N	2:E:51:PHE:CZ	2.52	0.78
1:J:95:THR:HA	1:J:713:SER:HA	1.66	0.78
1:A:789:ALA:HB1	3:C:87:PHE:CE2	2.18	0.78
2:B:117:LEU:HB2	2:B:147:ASN:HD21	1.47	0.78
1:D:646:PHE:CE2	1:D:652:LEU:HD21	2.14	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:793:ARG:HE	3:F:147:MET:HA	1.47	0.78
1:D:839:MLY:CH1	2:E:159:HIS:CB	2.61	0.78
1:G:219:GLU:O	1:G:223:ILE:HG13	1.84	0.78
1:G:496:PHE:CD2	1:G:514:ASP:HA	2.19	0.78
1:G:639:GLY:CA	4:6:345:ILE:N	2.47	0.78
1:J:84:MLY:HH11	1:J:715:VAL:HG11	1.66	0.78
1:J:107:MLY:HB3	1:J:686:MET:HE2	1.66	0.78
1:J:496:PHE:CD2	1:J:514:ASP:HA	2.19	0.78
1:A:219:GLU:O	1:A:223:ILE:HG13	1.84	0.77
1:A:795:ARG:CB	3:C:35:ARG:NH2	2.43	0.77
1:D:538:GLU:HG3	4:5:351:THR:C	2.03	0.77
1:D:639:GLY:CA	4:5:345:ILE:N	2.47	0.77
1:G:409:GLY:N	1:G:636:LYS:CG	2.44	0.77
1:G:727:LEU:O	3:I:113:THR:OG1	2.02	0.77
1:J:829:TRP:CZ3	2:K:84:PHE:CE2	2.51	0.77
1:A:530:MET:HE3	4:4:354:GLN:HG2	1.65	0.77
1:D:496:PHE:CD2	1:D:514:ASP:HA	2.19	0.77
1:D:724:TYR:C	1:D:782:MLY:HH11	2.04	0.77
1:D:831:TRP:CH2	2:E:34:ILE:CG2	2.65	0.77
2:K:117:LEU:HB2	2:K:147:ASN:HD21	1.47	0.77
4:5:223:PHE:HD2	4:5:312:ARG:HH21	1.32	0.77
4:V:223:PHE:HD2	4:V:312:ARG:HH21	1.33	0.77
4:Z:223:PHE:HD2	4:Z:312:ARG:HH21	1.33	0.77
1:A:407:GLY:HA2	1:A:412:ALA:HA	1.65	0.77
1:A:502:GLU:CG	1:A:764:MLY:O	2.31	0.77
1:D:530:MET:HE1	4:5:355:MET:SD	2.24	0.77
1:D:831:TRP:CH2	2:E:47:LEU:CA	2.37	0.77
1:J:116:TYR:O	1:J:153:PRO:HB2	1.85	0.77
4:X:223:PHE:HD2	4:X:312:ARG:HH21	1.33	0.77
1:A:291:ILE:HA	1:A:331:LEU:HD11	1.64	0.77
1:D:51:THR:O	1:D:62:VAL:HG13	1.84	0.77
1:D:809:ARG:CZ	2:E:124:GLY:CA	2.61	0.77
1:G:93:MET:CE	1:G:764:MLY:HE3	2.14	0.77
1:G:836:PHE:CZ	2:H:160:GLY:N	2.50	0.77
1:A:793:ARG:HH21	3:C:147:MET:CB	1.97	0.77
1:D:831:TRP:HZ3	2:E:34:ILE:HG23	1.42	0.77
3:I:49:ILE:N	3:I:52:ASN:HD22	1.82	0.77
1:J:725:ARG:HG3	1:J:733:PRO:HA	1.67	0.77
1:A:639:GLY:CA	4:4:345:ILE:N	2.47	0.77
1:D:629:GLU:HA	1:D:643:GLY:C	2.05	0.77
1:G:116:TYR:O	1:G:153:PRO:HB2	1.85	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:218:LEU:HD22	1:G:222:ILE:HG12	1.66	0.77
1:G:641:LYS:CE	1:G:647:GLN:HB2	2.13	0.77
1:G:831:TRP:CZ2	2:H:47:LEU:HD22	2.17	0.77
1:J:93:MET:HG3	1:J:764:MLY:HD3	1.60	0.77
4:7:223:PHE:HD2	4:7:312:ARG:HH21	1.33	0.77
1:A:736:GLN:HA	1:A:743:ALA:HB2	1.51	0.77
1:D:116:TYR:O	1:D:153:PRO:HB2	1.85	0.77
1:D:174:SER:CB	1:D:667:THR:HG21	2.13	0.77
1:G:728:ASN:ND2	3:I:113:THR:OG1	2.18	0.77
1:G:732:ILE:CG2	1:G:747:LEU:HD13	1.34	0.77
1:G:736:GLN:HA	1:G:743:ALA:HB1	1.26	0.77
1:D:94:MET:CE	1:D:101:ALA:HB1	2.15	0.77
1:D:646:PHE:HE2	1:D:652:LEU:CD2	1.97	0.77
3:I:3:SER:O	3:I:4:LYS:HB2	1.84	0.77
1:J:629:GLU:HA	1:J:643:GLY:C	2.05	0.77
2:K:121:LEU:CG	2:K:128:PHE:HA	2.14	0.77
4:0:223:PHE:HD2	4:0:312:ARG:HH21	1.33	0.77
1:A:641:LYS:CE	1:A:647:GLN:HB2	2.13	0.77
1:A:646:PHE:HE2	1:A:652:LEU:CD2	1.97	0.77
1:A:725:ARG:HG3	1:A:733:PRO:HA	1.67	0.77
1:A:757:GLN:HB2	1:A:771:LEU:HD11	1.58	0.77
4:1:223:PHE:HD2	4:1:312:ARG:HH21	1.33	0.77
4:3:223:PHE:HD2	4:3:312:ARG:HH21	1.33	0.77
4:4:223:PHE:HD2	4:4:312:ARG:HH21	1.33	0.77
4:X:287:ILE:HB	4:Z:204:ALA:N	1.97	0.77
1:D:508:ILE:HA	1:D:761:GLY:HA3	1.65	0.77
1:D:642:LYS:HG2	4:5:22:ALA:HA	1.65	0.77
1:D:721:LYS:CA	1:D:736:GLN:OE1	2.33	0.77
1:D:818:TYR:CG	2:E:89:LYS:HB2	2.20	0.77
1:G:725:ARG:HG3	1:G:733:PRO:HA	1.67	0.77
1:G:733:PRO:C	1:G:737:PHE:HD1	1.88	0.77
1:G:769:ALA:O	1:G:773:GLY:CA	2.33	0.77
2:H:141:PRO:HB2	2:H:142:PRO:CD	2.11	0.77
1:J:218:LEU:HD22	1:J:222:ILE:HG12	1.67	0.77
1:J:219:GLU:O	1:J:223:ILE:HG13	1.84	0.77
1:J:646:PHE:CE2	1:J:652:LEU:HD21	2.14	0.77
1:A:502:GLU:CB	1:A:761:GLY:HA3	2.16	0.76
1:A:721:LYS:CA	1:A:736:GLN:OE1	2.33	0.76
1:A:793:ARG:NH2	3:C:147:MET:CE	2.48	0.76
1:D:635:GLY:HA3	4:5:341:ILE:CD1	2.14	0.76
1:D:733:PRO:C	1:D:737:PHE:HD1	1.88	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:49:ILE:N	3:F:52:ASN:HD22	1.82	0.76
1:G:732:ILE:N	1:G:733:PRO:HD2	2.00	0.76
1:J:641:LYS:CE	1:J:647:GLN:CG	2.60	0.76
3:L:3:SER:O	3:L:4:LYS:HB2	1.85	0.76
4:2:223:PHE:HD2	4:2:312:ARG:HH21	1.33	0.76
1:A:732:ILE:N	1:A:733:PRO:HD2	2.00	0.76
1:D:599:ASN:CA	1:D:649:VAL:CB	2.53	0.76
1:G:798:LEU:HD22	3:I:126:LEU:HD11	1.66	0.76
1:J:94:MET:CE	1:J:101:ALA:HB1	2.15	0.76
1:J:635:GLY:HA3	4:7:341:ILE:CD1	2.14	0.76
4:0:287:ILE:HB	4:2:204:ALA:N	1.97	0.76
1:A:94:MET:CE	1:A:101:ALA:HB1	2.15	0.76
1:D:219:GLU:O	1:D:223:ILE:HG13	1.84	0.76
1:D:641:LYS:CE	1:D:647:GLN:CG	2.60	0.76
2:E:121:LEU:CG	2:E:128:PHE:HA	2.14	0.76
1:J:721:LYS:CA	1:J:736:GLN:OE1	2.33	0.76
1:A:623:PHE:CG	1:A:623:PHE:CA	2.68	0.76
1:A:629:GLU:HA	1:A:643:GLY:C	2.05	0.76
1:A:795:ARG:NH1	3:C:43:ASN:N	2.31	0.76
1:D:534:SER:O	4:5:351:THR:N	2.19	0.76
1:G:218:LEU:HB2	1:G:221:GLN:CG	2.09	0.76
1:G:530:MET:CG	4:6:354:GLN:CB	2.30	0.76
1:J:721:LYS:HG2	1:J:736:GLN:CD	1.86	0.76
4:7:287:ILE:HB	4:V:204:ALA:N	1.97	0.76
1:A:218:LEU:HD22	1:A:222:ILE:HG12	1.67	0.76
1:D:732:ILE:N	1:D:733:PRO:HD2	2.00	0.76
1:G:629:GLU:HA	1:G:643:GLY:C	2.05	0.76
1:G:641:LYS:HD2	1:G:647:GLN:OE1	1.81	0.76
2:H:121:LEU:CG	2:H:128:PHE:HA	2.14	0.76
2:H:150:TYR:C	2:H:151:LYS:CG	2.48	0.76
1:J:732:ILE:N	1:J:733:PRO:HD2	2.01	0.76
1:J:733:PRO:C	1:J:737:PHE:HD1	1.88	0.76
1:J:831:TRP:CH2	2:K:47:LEU:CD2	2.68	0.76
4:6:290:ARG:HH22	4:8:202:THR:HG23	1.50	0.76
4:Y:223:PHE:HD2	4:Y:312:ARG:HH21	1.33	0.76
1:A:721:LYS:HG2	1:A:736:GLN:CD	1.86	0.76
1:D:529:PRO:C	4:5:354:GLN:CB	2.49	0.76
1:D:831:TRP:CG	2:E:51:PHE:CZ	2.74	0.76
1:G:530:MET:HE3	4:6:354:GLN:HG2	1.66	0.76
1:G:797:PHE:HD1	3:I:149:VAL:CB	1.97	0.76
1:G:817:GLN:HB3	2:H:127:ARG:HD2	1.53	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:481:ASN:HD22	1:J:481:ASN:N	1.82	0.76
1:J:623:PHE:CG	1:J:623:PHE:CA	2.68	0.76
4:6:223:PHE:HD2	4:6:312:ARG:HH21	1.33	0.76
4:8:223:PHE:HD2	4:8:312:ARG:HH21	1.32	0.76
4:8:290:ARG:NH1	4:W:202:THR:CG2	2.49	0.76
4:8:290:ARG:HH22	4:W:202:THR:HG23	1.50	0.76
4:V:290:ARG:NH1	4:X:202:THR:CG2	2.49	0.76
4:W:223:PHE:HD2	4:W:312:ARG:HH21	1.32	0.76
1:J:550:PHE:HA	4:V:46:GLY:HA3	1.66	0.76
4:0:290:ARG:NH1	4:2:202:THR:CG2	2.49	0.76
4:5:290:ARG:NH1	4:7:202:THR:CG2	2.49	0.76
1:D:553:MLY:NZ	4:7:45:VAL:HA	1.84	0.76
1:D:623:PHE:CG	1:D:623:PHE:CA	2.68	0.76
2:E:117:LEU:HB2	2:E:147:ASN:HD21	1.47	0.76
1:A:116:TYR:O	1:A:153:PRO:HB2	1.85	0.76
1:A:218:LEU:HB2	1:A:221:GLN:CG	2.09	0.76
1:D:550:PHE:HA	4:7:46:GLY:HA3	1.66	0.76
1:D:649:VAL:CG1	1:D:649:VAL:CB	2.64	0.76
1:D:664:LEU:O	1:D:667:THR:HB	1.86	0.76
1:G:649:VAL:CG1	1:G:649:VAL:CB	2.64	0.76
1:G:735:GLY:C	1:G:743:ALA:HB1	1.84	0.76
1:J:820:VAL:HG11	2:K:136:MET:CE	2.16	0.76
4:4:290:ARG:NH1	4:6:202:THR:CG2	2.49	0.76
4:X:290:ARG:NH1	4:Z:202:THR:CG2	2.49	0.76
1:A:218:LEU:HB3	1:A:221:GLN:HG3	1.61	0.76
1:D:538:GLU:OE2	4:5:355:MET:HE3	1.86	0.76
1:G:94:MET:CE	1:G:101:ALA:HB1	2.15	0.76
1:A:768:MLY:HB3	1:A:771:LEU:CB	2.16	0.75
1:G:534:SER:O	4:6:351:THR:N	2.20	0.75
1:G:641:LYS:CE	1:G:647:GLN:CG	2.61	0.75
3:L:49:ILE:N	3:L:52:ASN:HD22	1.82	0.75
1:A:502:GLU:CD	1:A:763:THR:H	1.88	0.75
1:D:831:TRP:CZ2	2:E:47:LEU:HB3	2.19	0.75
1:G:798:LEU:CD1	3:I:126:LEU:CG	2.65	0.75
1:J:818:TYR:CZ	2:K:127:ARG:NH2	2.54	0.75
1:A:793:ARG:HE	3:C:147:MET:HA	1.49	0.75
1:G:481:ASN:HD22	1:G:481:ASN:N	1.82	0.75
1:J:90:ASP:HB3	1:J:764:MLY:HH21	1.69	0.75
1:J:95:THR:HG1	1:J:713:SER:HB3	1.47	0.75
1:J:556:ASP:HA	4:V:49:GLN:O	1.69	0.75
1:A:649:VAL:CG1	1:A:649:VAL:CB	2.64	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:LEU:O	1:A:667:THR:HB	1.86	0.75
1:A:831:TRP:HH2	2:B:50:THR:CB	2.00	0.75
1:D:537:GLU:HG3	4:5:350:SER:O	1.79	0.75
1:D:642:LYS:CG	4:5:23:GLY:H	1.77	0.75
1:G:751:GLY:CA	3:I:114:LEU:HD13	2.16	0.75
1:D:166:MET:HE1	1:D:254:PHE:HB2	1.68	0.75
1:J:541:MET:O	4:7:143:TYR:CZ	2.40	0.75
1:G:623:PHE:CG	1:G:623:PHE:CA	2.68	0.75
1:G:721:LYS:CA	1:G:736:GLN:OE1	2.33	0.75
1:J:642:LYS:HG2	4:7:22:ALA:HA	1.65	0.75
1:J:649:VAL:CG1	1:J:649:VAL:CB	2.64	0.75
1:A:502:GLU:CA	1:A:761:GLY:CA	2.65	0.75
4:X:288:ASP:H	4:Z:203:THR:HG22	1.52	0.75
1:A:530:MET:CG	4:4:354:GLN:CB	2.30	0.75
1:A:534:SER:O	4:4:351:THR:N	2.18	0.75
3:C:3:SER:O	3:C:4:LYS:HB2	1.84	0.75
1:D:724:TYR:HA	1:D:782:MLY:CH1	2.16	0.75
1:D:725:ARG:HG3	1:D:733:PRO:HA	1.67	0.75
1:D:818:TYR:HB2	2:E:90:GLY:CA	2.17	0.75
1:D:839:MLY:CH1	2:E:159:HIS:HD2	1.76	0.75
1:G:664:LEU:O	1:G:667:THR:HB	1.86	0.75
1:G:817:GLN:CD	2:H:127:ARG:CD	2.54	0.75
4:O:288:ASP:H	4:2:203:THR:HG22	1.52	0.75
1:A:481:ASN:HD22	1:A:481:ASN:N	1.82	0.75
1:A:636:LYS:O	1:A:637:LYS:HB2	1.86	0.75
1:D:538:GLU:O	4:5:349:LEU:HG	1.86	0.75
1:G:817:GLN:HG3	2:H:128:PHE:CE1	2.22	0.75
1:J:350:ALA:O	1:J:354:LEU:HB2	1.87	0.75
1:J:538:GLU:OE2	4:7:355:MET:HE3	1.87	0.75
1:J:664:LEU:O	1:J:667:THR:HB	1.86	0.75
1:J:823:PHE:CE1	2:K:156:VAL:HG12	2.21	0.75
1:A:350:ALA:O	1:A:354:LEU:HB2	1.87	0.74
1:J:310:TYR:CE2	1:J:320:ILE:HD11	2.22	0.74
1:J:736:GLN:HA	1:J:743:ALA:HB1	1.26	0.74
4:7:290:ARG:NH1	4:V:202:THR:CG2	2.49	0.74
4:W:288:ASP:H	4:Y:203:THR:HG22	1.52	0.74
1:A:793:ARG:NH2	3:C:147:MET:HE3	2.02	0.74
1:A:836:PHE:HZ	2:B:160:GLY:N	1.80	0.74
3:F:3:SER:O	3:F:4:LYS:HB2	1.84	0.74
1:G:783:LEU:O	1:G:787:ILE:CB	2.35	0.74
2:H:117:LEU:HB2	2:H:147:ASN:HD21	1.47	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:90:ASP:OD2	1:J:764:MLY:CH2	2.35	0.74
1:J:93:MET:HG3	1:J:764:MLY:HH12	1.69	0.74
4:5:253:GLU:HA	4:5:256:ARG:HG3	1.69	0.74
4:5:288:ASP:H	4:7:203:THR:HG22	1.52	0.74
4:Y:253:GLU:HA	4:Y:256:ARG:HG3	1.69	0.74
1:A:502:GLU:C	1:A:761:GLY:CA	2.54	0.74
1:D:272:MLY:HH13	1:D:435:GLU:OE1	1.87	0.74
1:D:350:ALA:O	1:D:354:LEU:HB2	1.87	0.74
1:D:732:ILE:N	1:D:733:PRO:CD	2.51	0.74
1:G:541:MET:O	4:6:143:TYR:CZ	2.40	0.74
1:J:636:LYS:O	1:J:637:LYS:HB2	1.86	0.74
4:1:253:GLU:HA	4:1:256:ARG:HG3	1.70	0.74
4:3:288:ASP:H	4:5:203:THR:HG22	1.52	0.74
1:A:215:GLN:NE2	1:A:336:SER:O	2.21	0.74
1:A:541:MET:O	4:4:143:TYR:CZ	2.40	0.74
1:A:732:ILE:N	1:A:733:PRO:CD	2.51	0.74
1:G:350:ALA:O	1:G:354:LEU:HB2	1.87	0.74
1:G:735:GLY:CA	1:G:743:ALA:HA	2.17	0.74
2:H:111:SER:OG	2:H:148:VAL:C	2.15	0.74
4:1:290:ARG:NH1	4:3:202:THR:CG2	2.49	0.74
4:3:290:ARG:HH22	4:5:202:THR:HG23	1.50	0.74
4:7:253:GLU:HA	4:7:256:ARG:HG3	1.69	0.74
4:8:288:ASP:H	4:W:203:THR:HG22	1.52	0.74
1:A:499:GLU:OE1	1:A:766:PHE:CZ	2.40	0.74
1:A:538:GLU:O	4:4:349:LEU:HG	1.86	0.74
1:D:218:LEU:HD22	1:D:222:ILE:HG12	1.67	0.74
1:D:310:TYR:CE2	1:D:320:ILE:HD11	2.22	0.74
1:G:218:LEU:HB3	1:G:221:GLN:HG3	1.60	0.74
1:G:538:GLU:HA	4:6:349:LEU:HD12	0.74	0.74
1:J:538:GLU:HA	4:7:349:LEU:HD12	0.75	0.74
1:J:640:LYS:O	4:7:23:GLY:O	2.06	0.74
1:J:641:LYS:HD2	1:J:647:GLN:OE1	1.81	0.74
4:4:288:ASP:H	4:6:203:THR:HG22	1.52	0.74
4:8:253:GLU:HA	4:8:256:ARG:HG3	1.69	0.74
1:A:436:MLY:HE3	1:A:626:TYR:CE1	2.23	0.74
1:D:215:GLN:NE2	1:D:336:SER:O	2.20	0.74
1:D:541:MET:O	4:5:143:TYR:CZ	2.40	0.74
1:D:636:LYS:O	1:D:637:LYS:HB2	1.86	0.74
1:G:636:LYS:O	1:G:637:LYS:HB2	1.86	0.74
1:G:831:TRP:NE1	2:H:67:MET:SD	2.60	0.74
3:I:4:LYS:N	3:I:5:ALA:O	2.16	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:534:SER:O	4:7:351:THR:N	2.19	0.74
1:J:739:ASP:CB	1:J:742:LYS:HB3	2.12	0.74
4:3:253:GLU:HA	4:3:256:ARG:HG3	1.69	0.74
4:6:288:ASP:H	4:8:203:THR:HG22	1.52	0.74
4:W:253:GLU:HA	4:W:256:ARG:HG3	1.69	0.74
1:A:409:GLY:HA3	4:4:333:PRO:N	2.02	0.74
1:A:640:LYS:O	4:4:23:GLY:O	2.06	0.74
1:J:797:PHE:CA	3:L:149:VAL:CG1	2.65	0.74
1:A:635:GLY:HA3	4:4:341:ILE:CD1	2.14	0.74
1:A:793:ARG:NE	3:C:147:MET:HA	2.03	0.74
1:D:538:GLU:HA	4:5:349:LEU:HD12	0.74	0.74
1:D:769:ALA:CA	1:D:771:LEU:HA	2.17	0.74
1:D:834:LEU:HD13	2:E:51:PHE:HD1	1.53	0.74
1:G:310:TYR:CE2	1:G:320:ILE:HD11	2.22	0.74
1:G:730:SER:CB	3:I:109:HIS:NE2	2.50	0.74
1:J:272:MLY:HH13	1:J:435:GLU:OE1	1.87	0.74
1:J:768:MLY:CD	1:J:772:LEU:HB2	2.18	0.74
4:1:288:ASP:H	4:3:203:THR:HG22	1.52	0.74
4:2:290:ARG:NH1	4:4:202:THR:CG2	2.49	0.74
4:V:253:GLU:HA	4:V:256:ARG:HG3	1.69	0.74
4:V:288:ASP:H	4:X:203:THR:HG22	1.52	0.74
4:V:290:ARG:HH22	4:X:202:THR:HG23	1.50	0.74
1:A:538:GLU:HA	4:4:349:LEU:HD12	0.74	0.74
1:A:538:GLU:CD	4:4:355:MET:HE3	2.08	0.74
1:A:757:GLN:HG3	1:A:771:LEU:HD11	1.70	0.74
1:D:436:MLY:HE3	1:D:626:TYR:CE1	2.23	0.74
1:J:538:GLU:O	4:7:349:LEU:HG	1.86	0.74
1:A:530:MET:CE	4:4:355:MET:SD	2.76	0.74
1:A:733:PRO:C	1:A:737:PHE:HD1	1.88	0.74
1:D:640:LYS:O	4:5:23:GLY:O	2.06	0.74
4:2:288:ASP:H	4:4:203:THR:HG22	1.52	0.74
4:4:290:ARG:HH22	4:6:202:THR:HG23	1.50	0.74
4:W:290:ARG:NH1	4:Y:202:THR:CG2	2.49	0.74
4:X:253:GLU:HA	4:X:256:ARG:HG3	1.69	0.74
1:A:486:MLY:HH13	1:A:527:GLU:OE1	1.88	0.73
1:A:839:MLY:CD	2:B:159:HIS:CB	2.65	0.73
1:D:530:MET:CG	4:5:354:GLN:CB	2.30	0.73
3:I:24:LYS:CA	3:I:63:ILE:O	2.36	0.73
1:J:84:MLY:CH1	1:J:715:VAL:HG12	2.15	0.73
2:K:130:PRO:O	2:K:132:GLU:N	2.21	0.73
1:J:735:GLY:CA	1:J:743:ALA:HA	2.18	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:253:GLU:HA	4:4:256:ARG:HG3	1.69	0.73
4:6:253:GLU:HA	4:6:256:ARG:HG3	1.69	0.73
1:A:542:PHE:CD2	4:4:143:TYR:CE1	2.76	0.73
1:D:409:GLY:HA3	4:5:333:PRO:N	2.03	0.73
1:D:487:LEU:O	1:D:490:PHE:HB3	1.89	0.73
1:G:732:ILE:N	1:G:733:PRO:CD	2.51	0.73
1:G:795:ARG:CD	3:I:35:ARG:NH2	2.17	0.73
1:J:166:MET:HE3	1:J:254:PHE:CD2	2.23	0.73
1:J:529:PRO:C	4:7:354:GLN:CB	2.48	0.73
1:J:557:GLU:N	4:V:48:GLY:HA3	1.90	0.73
1:A:709:LYS:O	1:A:710:GLY:CA	2.37	0.73
1:D:534:SER:CA	4:5:351:THR:HA	2.19	0.73
1:G:215:GLN:NE2	1:G:336:SER:O	2.20	0.73
1:J:93:MET:HA	1:J:714:ARG:HG3	1.70	0.73
1:J:441:MET:O	1:J:445:ILE:HG13	1.88	0.73
1:A:310:TYR:CE2	1:A:320:ILE:HD11	2.22	0.73
1:A:529:PRO:C	4:4:354:GLN:CB	2.49	0.73
1:A:735:GLY:C	1:A:743:ALA:HB1	1.84	0.73
1:D:721:LYS:CB	1:D:736:GLN:CD	2.56	0.73
1:D:726:VAL:H	1:D:782:MLY:CH2	2.01	0.73
1:J:486:MLY:HH13	1:J:527:GLU:OE1	1.88	0.73
1:J:487:LEU:O	1:J:490:PHE:HB3	1.88	0.73
1:J:534:SER:CA	4:7:351:THR:HA	2.19	0.73
1:J:818:TYR:CE1	2:K:127:ARG:NH1	2.57	0.73
4:1:290:ARG:HH22	4:3:202:THR:HG23	1.50	0.73
4:6:290:ARG:NH1	4:8:202:THR:CG2	2.49	0.73
1:A:237:THR:HG22	1:A:239:ARG:H	1.53	0.73
1:A:707:CYS:HA	1:A:714:ARG:CZ	2.18	0.73
1:A:831:TRP:CD2	2:B:51:PHE:CE1	2.77	0.73
1:D:542:PHE:CD2	4:5:143:TYR:CE1	2.77	0.73
2:E:130:PRO:O	2:E:132:GLU:N	2.21	0.73
1:G:93:MET:HE2	1:G:764:MLY:HE3	1.69	0.73
1:G:409:GLY:HA3	4:6:333:PRO:N	2.03	0.73
1:G:486:MLY:HH13	1:G:527:GLU:OE1	1.87	0.73
1:G:487:LEU:O	1:G:490:PHE:HB3	1.89	0.73
1:G:536:LEU:HD13	1:G:550:PHE:CZ	2.24	0.73
2:H:130:PRO:O	2:H:132:GLU:N	2.21	0.73
1:A:131:TRP:C	1:A:132:LEU:HD12	2.09	0.73
2:B:130:PRO:O	2:B:132:GLU:N	2.21	0.73
1:D:530:MET:CE	4:5:355:MET:SD	2.77	0.73
1:D:802:GLU:O	1:D:806:MET:HG3	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:829:TRP:CD1	2:E:67:MET:HG2	2.24	0.73
3:F:24:LYS:CA	3:F:63:ILE:O	2.36	0.73
1:G:410:ASN:OD1	4:6:335:ARG:N	2.21	0.73
1:J:530:MET:CE	4:7:355:MET:SD	2.77	0.73
1:J:640:LYS:O	1:J:645:SER:OG	2.06	0.73
1:J:790:THR:N	3:L:87:PHE:CE2	2.57	0.73
4:0:253:GLU:HA	4:0:256:ARG:HG3	1.69	0.73
4:7:288:ASP:H	4:V:203:THR:HG22	1.52	0.73
1:A:97:LEU:CD2	1:A:712:PRO:HB3	2.19	0.73
1:A:536:LEU:HD13	1:A:550:PHE:CZ	2.24	0.73
1:D:557:GLU:N	4:7:48:GLY:HA3	1.90	0.73
1:G:93:MET:HE2	1:G:764:MLY:CG	2.13	0.73
1:G:190:MLY:HE3	1:G:230:GLU:OE2	1.89	0.73
1:G:635:GLY:HA3	4:6:341:ILE:CD1	2.14	0.73
1:J:436:MLY:HE3	1:J:626:TYR:CE1	2.23	0.73
1:A:410:ASN:OD1	4:4:335:ARG:N	2.22	0.73
1:D:441:MET:O	1:D:445:ILE:HG13	1.88	0.73
1:D:486:MLY:HH13	1:D:527:GLU:OE1	1.88	0.73
1:G:733:PRO:C	1:G:737:PHE:CD1	2.62	0.73
2:H:144:VAL:CB	2:H:153:ILE:HD11	2.19	0.73
4:5:290:ARG:HH22	4:7:202:THR:HG23	1.50	0.73
1:A:735:GLY:CA	1:A:743:ALA:HA	2.18	0.73
1:D:190:MLY:HE3	1:D:230:GLU:OE2	1.89	0.73
1:D:410:ASN:OD1	4:5:335:ARG:N	2.22	0.73
1:D:618:THR:O	1:D:622:LEU:HD13	1.89	0.73
1:D:769:ALA:HB1	1:D:770:GLY:HA3	1.71	0.73
1:G:272:MLY:HH13	1:G:435:GLU:OE1	1.88	0.73
1:G:410:ASN:CG	4:6:334:GLU:CA	2.47	0.73
1:G:640:LYS:O	4:6:23:GLY:O	2.06	0.73
1:G:802:GLU:O	1:G:806:MET:HG3	1.88	0.73
1:J:190:MLY:HE3	1:J:230:GLU:OE2	1.89	0.73
1:J:237:THR:HG22	1:J:239:ARG:H	1.54	0.73
1:J:732:ILE:N	1:J:733:PRO:CD	2.51	0.73
4:Z:253:GLU:HA	4:Z:256:ARG:HG3	1.69	0.73
1:D:36:SER:O	1:D:52:ILE:HG12	1.89	0.72
1:D:214:MET:HA	1:D:340:ILE:HD11	1.71	0.72
1:D:640:LYS:O	1:D:645:SER:OG	2.06	0.72
1:G:436:MLY:HE3	1:G:626:TYR:CE1	2.23	0.72
1:G:538:GLU:O	4:6:349:LEU:HG	1.87	0.72
1:G:817:GLN:CG	2:H:127:ARG:HB2	2.16	0.72
1:J:215:GLN:NE2	1:J:336:SER:O	2.21	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:410:ASN:OD1	4:7:335:ARG:N	2.21	0.72
1:J:553:MLY:NZ	4:V:45:VAL:HA	1.84	0.72
1:A:441:MET:O	1:A:445:ILE:HG13	1.88	0.72
1:A:721:LYS:CB	1:A:736:GLN:CD	2.56	0.72
1:A:802:GLU:O	1:A:806:MET:HG3	1.89	0.72
1:A:834:LEU:HD21	2:B:54:MET:SD	2.29	0.72
1:D:237:THR:HG22	1:D:239:ARG:H	1.54	0.72
1:G:21:GLU:O	1:G:25:ILE:HG13	1.89	0.72
1:J:21:GLU:O	1:J:25:ILE:HG13	1.89	0.72
1:J:36:SER:O	1:J:52:ILE:HG12	1.89	0.72
1:J:557:GLU:N	4:V:48:GLY:HA2	1.90	0.72
1:J:618:THR:O	1:J:622:LEU:HD13	1.89	0.72
1:J:802:GLU:O	1:J:806:MET:HG3	1.88	0.72
3:L:24:LYS:CA	3:L:63:ILE:O	2.37	0.72
4:2:253:GLU:HA	4:2:256:ARG:HG3	1.69	0.72
1:A:272:MLY:HH13	1:A:435:GLU:OE1	1.88	0.72
1:A:534:SER:CA	4:4:351:THR:HA	2.18	0.72
1:A:641:LYS:HD2	1:A:647:GLN:OE1	1.81	0.72
1:D:536:LEU:HD13	1:D:550:PHE:CZ	2.24	0.72
2:E:144:VAL:CB	2:E:153:ILE:HD11	2.19	0.72
1:J:409:GLY:HA3	4:7:333:PRO:N	2.03	0.72
1:J:542:PHE:CD2	4:7:143:TYR:CE1	2.77	0.72
1:J:754:ASP:HB3	1:J:757:GLN:HG2	1.71	0.72
1:D:735:GLY:CA	1:D:743:ALA:HA	2.18	0.72
2:E:117:LEU:CB	2:E:147:ASN:ND2	2.35	0.72
1:G:214:MET:HA	1:G:340:ILE:HD11	1.70	0.72
1:G:618:THR:O	1:G:622:LEU:HD13	1.89	0.72
1:G:640:LYS:O	1:G:645:SER:OG	2.06	0.72
1:J:95:THR:CB	1:J:713:SER:HB3	2.20	0.72
1:J:214:MET:HA	1:J:340:ILE:HD11	1.70	0.72
1:J:295:MLY:HG3	1:J:332:MET:CE	2.19	0.72
1:J:536:LEU:HD13	1:J:550:PHE:CZ	2.24	0.72
3:L:4:LYS:N	3:L:5:ALA:O	2.16	0.72
3:C:24:LYS:CA	3:C:63:ILE:O	2.37	0.72
1:D:295:MLY:HG3	1:D:332:MET:CE	2.20	0.72
1:D:789:ALA:HB2	3:F:81:GLN:HG2	1.72	0.72
1:G:176:LEU:HD12	1:G:176:LEU:N	2.05	0.72
1:G:754:ASP:HB3	1:G:757:GLN:HG2	1.72	0.72
1:G:817:GLN:CB	2:H:127:ARG:HH11	2.02	0.72
1:J:721:LYS:CB	1:J:736:GLN:CD	2.56	0.72
4:0:290:ARG:HH22	4:2:202:THR:HG23	1.50	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:3:ASP:HA	4:4:6:THR:CB	2.18	0.72
1:A:21:GLU:O	1:A:25:ILE:HG13	1.88	0.72
1:A:36:SER:O	1:A:52:ILE:HG12	1.89	0.72
1:A:486:MLY:HH22	1:A:527:GLU:OE2	1.90	0.72
1:A:519:LEU:HD12	1:A:519:LEU:N	2.04	0.72
1:G:93:MET:HE1	1:G:763:THR:HG22	1.67	0.72
1:J:769:ALA:HB3	1:J:770:GLY:N	2.04	0.72
2:K:144:VAL:CB	2:K:153:ILE:HD11	2.19	0.72
4:Y:3:ASP:HA	4:Y:6:THR:CB	2.18	0.72
1:A:290:GLN:C	1:A:331:LEU:HD12	2.09	0.72
1:A:707:CYS:CA	1:A:714:ARG:NH1	2.50	0.72
1:D:21:GLU:O	1:D:25:ILE:HG13	1.88	0.72
1:D:817:GLN:OE1	2:E:127:ARG:NE	2.22	0.72
1:G:486:MLY:HH22	1:G:527:GLU:OE2	1.90	0.72
1:G:530:MET:CE	4:6:355:MET:SD	2.78	0.72
1:G:731:ALA:HB2	3:I:109:HIS:ND1	2.04	0.72
2:H:117:LEU:HD12	2:H:147:ASN:CA	2.19	0.72
4:W:3:ASP:HA	4:W:6:THR:CB	2.18	0.72
1:G:237:THR:HG22	1:G:239:ARG:H	1.54	0.72
1:G:290:GLN:C	1:G:331:LEU:HD12	2.09	0.72
1:G:441:MET:O	1:G:445:ILE:HG13	1.88	0.72
1:J:131:TRP:C	1:J:132:LEU:HD12	2.09	0.72
1:J:510:TRP:CZ3	1:J:768:MLY:HH12	2.23	0.72
1:J:795:ARG:HD2	3:L:35:ARG:HH12	1.54	0.72
1:D:217:THR:C	1:D:221:GLN:HE21	1.92	0.72
1:D:290:GLN:C	1:D:331:LEU:HD12	2.09	0.72
1:D:292:MET:HE3	1:D:309:PRO:HA	1.71	0.72
1:D:641:LYS:HD2	1:D:647:GLN:OE1	1.81	0.72
1:D:754:ASP:HB3	1:D:757:GLN:HG2	1.72	0.72
1:G:732:ILE:HG23	1:G:747:LEU:CB	1.84	0.72
2:K:136:MET:O	2:K:140:PHE:HB2	1.90	0.72
4:3:290:ARG:NH1	4:5:202:THR:CG2	2.49	0.72
4:W:290:ARG:HH22	4:Y:202:THR:HG23	1.51	0.72
1:A:14:ALA:HB3	1:A:15:PRO:HD3	1.72	0.72
2:B:144:VAL:CB	2:B:153:ILE:HD11	2.19	0.72
1:D:486:MLY:HH22	1:D:527:GLU:OE2	1.90	0.72
1:G:14:ALA:HB3	1:G:15:PRO:HD3	1.72	0.72
1:G:721:LYS:CB	1:G:736:GLN:CD	2.56	0.72
1:A:217:THR:C	1:A:221:GLN:HE21	1.93	0.71
1:A:754:ASP:HB3	1:A:757:GLN:HG2	1.72	0.71
1:A:795:ARG:HD2	3:C:35:ARG:NH2	2.01	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:834:LEU:HD13	2:E:51:PHE:HA	1.71	0.71
1:J:176:LEU:HD12	1:J:176:LEU:N	2.05	0.71
4:1:3:ASP:HA	4:1:6:THR:CB	2.18	0.71
4:5:3:ASP:HA	4:5:6:THR:CB	2.18	0.71
1:A:217:THR:O	1:A:220:ASP:HB2	1.91	0.71
1:A:487:LEU:O	1:A:490:PHE:HB3	1.88	0.71
1:D:176:LEU:HD12	1:D:176:LEU:N	2.05	0.71
1:D:519:LEU:HD12	1:D:519:LEU:N	2.05	0.71
1:G:131:TRP:C	1:G:132:LEU:HD12	2.09	0.71
1:G:519:LEU:HD12	1:G:519:LEU:N	2.05	0.71
1:G:542:PHE:CD2	4:6:143:TYR:CE1	2.78	0.71
1:G:739:ASP:CB	1:G:742:LYS:HB3	2.12	0.71
1:J:486:MLY:HH22	1:J:527:GLU:OE2	1.90	0.71
1:J:800:ARG:CG	3:L:149:VAL:HG23	2.12	0.71
1:J:816:ILE:HD11	2:K:100:ALA:CB	2.19	0.71
1:A:190:MLY:HE3	1:A:230:GLU:OE2	1.89	0.71
1:A:836:PHE:CE1	2:B:159:HIS:CA	2.71	0.71
1:D:131:TRP:C	1:D:132:LEU:HD12	2.09	0.71
1:D:217:THR:O	1:D:220:ASP:HB2	1.90	0.71
2:E:136:MET:O	2:E:140:PHE:HB2	1.90	0.71
1:G:84:MLY:HH11	1:G:715:VAL:HG11	1.70	0.71
1:G:798:LEU:HD13	3:I:126:LEU:HD21	0.72	0.71
1:J:290:GLN:C	1:J:331:LEU:HD12	2.09	0.71
4:8:3:ASP:HA	4:8:6:THR:CB	2.18	0.71
1:A:793:ARG:HG3	3:C:146:ILE:CG2	2.21	0.71
1:G:534:SER:CA	4:6:351:THR:HA	2.20	0.71
1:G:795:ARG:CB	3:I:35:ARG:HH21	1.91	0.71
1:J:72:VAL:HG13	1:J:76:GLN:CB	2.19	0.71
1:J:510:TRP:CE3	1:J:768:MLY:CH1	2.72	0.71
1:A:214:MET:HA	1:A:340:ILE:HD11	1.71	0.71
1:D:245:ARG:HD3	1:D:271:GLU:OE1	1.90	0.71
1:D:792:ALA:CB	3:F:40:ASN:HB3	2.19	0.71
1:G:36:SER:O	1:G:52:ILE:HG12	1.90	0.71
1:J:217:THR:C	1:J:221:GLN:HE21	1.92	0.71
1:J:823:PHE:CD1	2:K:156:VAL:O	2.44	0.71
1:A:166:MET:HE3	1:A:254:PHE:CD2	2.25	0.71
1:A:618:THR:O	1:A:622:LEU:HD13	1.89	0.71
1:A:640:LYS:O	1:A:645:SER:OG	2.06	0.71
2:B:136:MET:O	2:B:140:PHE:HB2	1.90	0.71
1:D:86:ASP:OD2	1:D:87:MLY:HH13	1.91	0.71
1:D:724:TYR:CA	1:D:782:MLY:NZ	2.53	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:4:LYS:N	3:F:5:ALA:O	2.16	0.71
1:G:217:THR:C	1:G:221:GLN:HE21	1.92	0.71
1:J:295:MLY:HG3	1:J:332:MET:HE1	1.72	0.71
1:J:410:ASN:CG	4:7:334:GLU:CA	2.47	0.71
1:J:519:LEU:HD12	1:J:519:LEU:N	2.04	0.71
4:X:290:ARG:HH22	4:Z:202:THR:HG23	1.50	0.71
4:Z:3:ASP:HA	4:Z:6:THR:CB	2.18	0.71
1:A:206:LYS:HD3	1:A:217:THR:HG23	0.71	0.71
1:A:295:MLY:HG3	1:A:332:MET:CE	2.19	0.71
1:A:798:LEU:HD11	3:C:126:LEU:CG	2.20	0.71
1:A:830:PRO:HG2	2:B:67:MET:CE	2.20	0.71
1:A:831:TRP:CZ3	2:B:50:THR:CG2	2.72	0.71
1:D:56:GLU:CB	1:D:59:MLY:HB3	2.19	0.71
1:G:553:MLY:HG2	4:8:47:MET:N	2.06	0.71
1:J:831:TRP:HH2	2:K:34:ILE:HG21	1.55	0.71
1:A:819:ASN:N	2:B:90:GLY:CA	2.53	0.71
1:D:800:ARG:HB3	3:F:149:VAL:HG23	1.67	0.71
1:D:817:GLN:HG3	2:E:127:ARG:CD	2.19	0.71
1:G:274:ARG:NH2	1:G:282:GLU:OE1	2.24	0.71
1:J:56:GLU:CB	1:J:59:MLY:HB3	2.19	0.71
1:J:84:MLY:CH2	1:J:716:LEU:O	2.38	0.71
1:J:757:GLN:HG3	1:J:776:GLU:HG3	1.64	0.71
4:7:290:ARG:HH22	4:V:202:THR:HG23	1.50	0.71
1:D:14:ALA:HB3	1:D:15:PRO:HD3	1.72	0.71
1:D:831:TRP:CD1	2:E:51:PHE:HZ	2.09	0.71
1:D:834:LEU:HD12	2:E:54:MET:HB2	1.73	0.71
1:G:166:MET:HE1	1:G:254:PHE:HB2	1.72	0.71
1:G:717:TYR:HD1	1:G:744:SER:HG	1.39	0.71
1:G:834:LEU:CD1	2:H:51:PHE:CD1	2.74	0.71
1:J:274:ARG:NH2	1:J:282:GLU:OE1	2.24	0.71
1:J:762:HIS:H	1:J:762:HIS:CD2	2.07	0.71
4:3:3:ASP:HA	4:3:6:THR:CB	2.18	0.71
1:D:831:TRP:CD1	2:E:51:PHE:CZ	2.79	0.71
1:G:86:ASP:OD2	1:G:87:MLY:HH13	1.91	0.71
1:J:14:ALA:HB3	1:J:15:PRO:HD3	1.72	0.71
1:J:245:ARG:HD3	1:J:271:GLU:OE1	1.90	0.71
4:2:290:ARG:HH22	4:4:202:THR:HG23	1.50	0.71
1:A:505:MLY:HB2	1:A:761:GLY:C	2.11	0.70
1:G:245:ARG:HD3	1:G:271:GLU:OE1	1.90	0.70
1:A:72:VAL:HG13	1:A:76:GLN:CB	2.19	0.70
1:A:176:LEU:N	1:A:176:LEU:HD12	2.05	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:530:MET:HE2	4:5:354:GLN:HG3	1.73	0.70
1:D:579:PHE:HD2	1:D:592:ILE:HD11	1.56	0.70
1:G:295:MLY:HG3	1:G:332:MET:CE	2.20	0.70
1:G:550:PHE:HA	4:8:46:GLY:HA3	1.66	0.70
1:G:792:ALA:HA	3:I:35:ARG:NH1	2.04	0.70
1:G:793:ARG:NH1	3:I:40:ASN:HD21	1.90	0.70
1:G:810:ARG:HG2	1:G:810:ARG:HH11	1.56	0.70
1:J:93:MET:SD	1:J:764:MLY:CH2	2.65	0.70
1:J:206:LYS:HD3	1:J:217:THR:HG23	0.71	0.70
1:J:217:THR:O	1:J:220:ASP:HB2	1.91	0.70
4:6:3:ASP:HA	4:6:6:THR:CB	2.18	0.70
3:C:48:LYS:HB3	3:C:52:ASN:HD21	1.57	0.70
1:D:577:ALA:O	1:D:578:HIS:CG	2.45	0.70
1:D:643:GLY:N	4:5:24:ASP:CA	2.46	0.70
1:D:800:ARG:CD	3:F:149:VAL:HG22	2.21	0.70
1:J:86:ASP:OD2	1:J:87:MLY:HH13	1.91	0.70
1:J:754:ASP:CG	1:J:776:GLU:CA	2.59	0.70
1:J:787:ILE:HG22	1:J:788:THR:N	2.07	0.70
1:J:826:VAL:CG2	2:K:88:LEU:HD21	2.12	0.70
1:A:245:ARG:HD3	1:A:271:GLU:OE1	1.90	0.70
1:A:274:ARG:NH2	1:A:282:GLU:OE1	2.24	0.70
1:A:787:ILE:HG22	1:A:788:THR:N	2.07	0.70
1:D:641:LYS:HD2	4:5:348:SER:HA	1.73	0.70
1:D:769:ALA:HB1	1:D:770:GLY:N	2.05	0.70
1:G:579:PHE:HD2	1:G:592:ILE:HD11	1.56	0.70
1:G:721:LYS:HG2	1:G:736:GLN:CD	1.86	0.70
1:J:213:LYS:HA	1:J:220:ASP:OD1	1.92	0.70
1:A:86:ASP:OD2	1:A:87:MLY:HH13	1.91	0.70
1:A:123:CYS:HB2	1:A:158:ILE:HD11	1.73	0.70
1:A:818:TYR:HB2	2:B:90:GLY:CA	2.22	0.70
1:D:72:VAL:HG13	1:D:76:GLN:CB	2.19	0.70
1:D:274:ARG:NH2	1:D:282:GLU:OE1	2.24	0.70
1:D:789:ALA:CB	3:F:81:GLN:O	2.39	0.70
1:D:831:TRP:CG	2:E:51:PHE:HZ	2.10	0.70
1:G:217:THR:O	1:G:220:ASP:HB2	1.91	0.70
2:H:136:MET:O	2:H:140:PHE:HB2	1.90	0.70
1:J:630:ALA:O	4:7:25:ASP:HB2	1.91	0.70
1:D:213:LYS:HA	1:D:220:ASP:OD1	1.92	0.70
1:D:834:LEU:CD1	2:E:51:PHE:HA	2.20	0.70
3:F:25:ILE:O	3:F:63:ILE:HB	1.92	0.70
1:A:579:PHE:HD2	1:A:592:ILE:HD11	1.56	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:MLY:CD	2:B:159:HIS:CG	2.70	0.70
3:F:48:LYS:HB3	3:F:52:ASN:HD21	1.57	0.70
1:G:56:GLU:CB	1:G:59:MLY:HB3	2.19	0.70
1:J:123:CYS:HB2	1:J:158:ILE:HD11	1.73	0.70
1:J:641:LYS:HD2	4:7:348:SER:HA	1.73	0.70
1:J:810:ARG:HG2	1:J:810:ARG:HH11	1.57	0.70
1:A:814:PHE:HD1	2:B:127:ARG:NH2	1.70	0.70
1:A:839:MLY:HD2	2:B:159:HIS:CB	2.21	0.70
1:D:789:ALA:HB1	3:F:81:GLN:O	1.92	0.70
1:G:123:CYS:HB2	1:G:158:ILE:HD11	1.73	0.70
1:G:798:LEU:HD23	3:I:122:GLU:CB	2.20	0.70
1:J:577:ALA:O	1:J:578:HIS:CG	2.45	0.70
3:L:25:ILE:O	3:L:63:ILE:HB	1.92	0.70
1:A:546:THR:HG22	1:A:548:THR:N	2.05	0.70
1:A:732:ILE:HG21	1:A:747:LEU:HD11	0.73	0.70
1:G:762:HIS:H	1:G:762:HIS:CD2	2.07	0.70
1:J:800:ARG:HB2	3:L:149:VAL:CG2	2.07	0.70
1:J:818:TYR:CE1	2:K:127:ARG:CZ	2.75	0.70
1:A:813:ILE:HG22	2:B:127:ARG:NH1	2.06	0.70
2:B:111:SER:OG	2:B:148:VAL:HG12	1.92	0.70
1:D:123:CYS:HB2	1:D:158:ILE:HD11	1.73	0.70
1:D:206:LYS:HD3	1:D:217:THR:HG23	0.71	0.70
1:D:630:ALA:O	4:5:25:ASP:HB2	1.92	0.70
1:D:782:MLY:C	1:D:783:LEU:HD12	2.22	0.70
1:D:810:ARG:HG2	1:D:810:ARG:HH11	1.57	0.70
1:G:782:MLY:C	1:G:783:LEU:HD12	2.22	0.70
3:I:25:ILE:O	3:I:63:ILE:HB	1.92	0.70
1:J:215:GLN:CA	1:J:340:ILE:CG2	2.62	0.70
1:A:733:PRO:C	1:A:737:PHE:CD1	2.62	0.69
1:A:769:ALA:N	1:A:771:LEU:HB2	2.07	0.69
1:A:802:GLU:OE1	1:A:802:GLU:HA	1.92	0.69
1:D:726:VAL:H	1:D:782:MLY:HH22	1.55	0.69
1:G:546:THR:HG22	1:G:548:THR:N	2.05	0.69
1:J:838:ILE:HD11	2:K:54:MET:HE1	1.74	0.69
4:8:1:ASP:HA	4:8:4:GLU:HB3	1.74	0.69
4:W:1:ASP:HA	4:W:4:GLU:HB3	1.74	0.69
1:A:800:ARG:CG	3:C:149:VAL:CG2	2.60	0.69
1:G:643:GLY:N	4:6:24:ASP:CA	2.47	0.69
3:L:48:LYS:HB3	3:L:52:ASN:HD21	1.57	0.69
4:0:3:ASP:HA	4:0:6:THR:CB	2.18	0.69
1:A:577:ALA:O	1:A:578:HIS:CG	2.45	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:LEU:CB	2:B:147:ASN:OD1	2.39	0.69
2:E:117:LEU:HD12	2:E:147:ASN:CA	2.19	0.69
1:J:530:MET:HE2	4:7:354:GLN:HG3	1.74	0.69
1:J:579:PHE:HD2	1:J:592:ILE:HD11	1.56	0.69
1:J:630:ALA:O	4:7:25:ASP:CB	2.41	0.69
1:J:733:PRO:C	1:J:737:PHE:CD1	2.62	0.69
4:Y:1:ASP:HA	4:Y:4:GLU:HB3	1.74	0.69
1:A:834:LEU:CD2	2:B:54:MET:HG3	2.22	0.69
1:G:72:VAL:HG13	1:G:76:GLN:CB	2.19	0.69
1:G:800:ARG:HD2	3:I:149:VAL:HG23	1.72	0.69
2:H:111:SER:OG	2:H:148:VAL:HG12	1.92	0.69
2:K:111:SER:OG	2:K:148:VAL:HG12	1.92	0.69
4:1:1:ASP:HA	4:1:4:GLU:HB3	1.74	0.69
1:A:641:LYS:HD2	4:4:348:SER:HA	1.73	0.69
1:A:782:MLY:C	1:A:783:LEU:HD12	2.22	0.69
1:A:810:ARG:HG2	1:A:810:ARG:HH11	1.57	0.69
3:C:3:SER:O	3:C:4:LYS:CB	2.41	0.69
1:D:218:LEU:HB2	1:D:221:GLN:CG	2.09	0.69
1:G:93:MET:SD	1:G:716:LEU:HD11	2.32	0.69
1:J:768:MLY:HH23	1:J:772:LEU:CD1	2.21	0.69
1:J:823:PHE:CZ	2:K:156:VAL:HG12	2.27	0.69
1:A:123:CYS:HB2	1:A:158:ILE:CD1	2.23	0.69
1:A:166:MET:HE3	1:A:254:PHE:HD2	1.58	0.69
1:D:553:MLY:HG2	4:7:47:MET:N	2.07	0.69
1:G:787:ILE:HG22	1:G:788:THR:N	2.07	0.69
1:G:817:GLN:CB	2:H:127:ARG:CD	2.53	0.69
4:6:1:ASP:HA	4:6:4:GLU:HB3	1.74	0.69
1:A:553:MLY:HG2	4:6:47:MET:N	2.07	0.69
1:A:818:TYR:CB	2:B:90:GLY:N	2.56	0.69
1:D:541:MET:CG	4:5:345:ILE:O	2.41	0.69
1:G:206:LYS:HD3	1:G:217:THR:HG23	0.70	0.69
1:G:577:ALA:O	1:G:578:HIS:CG	2.45	0.69
1:G:815:CYS:O	1:G:819:ASN:HB2	1.93	0.69
1:J:752:ASP:O	1:J:780:ASP:CG	2.31	0.69
1:J:807:VAL:O	1:J:810:ARG:HB2	1.93	0.69
4:3:1:ASP:HA	4:3:4:GLU:HB3	1.74	0.69
4:7:3:ASP:HA	4:7:6:THR:CB	2.18	0.69
1:A:630:ALA:O	4:4:25:ASP:HB2	1.92	0.69
1:A:793:ARG:CG	3:C:146:ILE:HG22	2.21	0.69
1:A:798:LEU:HD21	3:C:122:GLU:HB3	1.73	0.69
1:D:510:TRP:CH2	1:D:711:PHE:HE2	2.11	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:556:ASP:HA	4:7:49:GLN:O	1.70	0.69
1:D:642:LYS:HB3	4:5:21:PHE:O	1.93	0.69
1:D:769:ALA:CA	1:D:770:GLY:C	2.61	0.69
1:D:800:ARG:HD2	3:F:149:VAL:CG2	2.22	0.69
1:D:807:VAL:O	1:D:810:ARG:HB2	1.93	0.69
1:G:123:CYS:HB2	1:G:158:ILE:CD1	2.23	0.69
1:J:218:LEU:HB2	1:J:221:GLN:CG	2.09	0.69
1:J:530:MET:HE3	4:7:354:GLN:HG2	1.71	0.69
1:J:802:GLU:OE1	1:J:802:GLU:HA	1.93	0.69
3:L:3:SER:O	3:L:4:LYS:CB	2.41	0.69
4:2:3:ASP:HA	4:2:6:THR:CB	2.18	0.69
4:5:1:ASP:HA	4:5:4:GLU:HB3	1.74	0.69
4:V:3:ASP:HA	4:V:6:THR:CB	2.18	0.69
1:A:642:LYS:HB3	4:4:21:PHE:O	1.93	0.69
1:G:641:LYS:HD2	4:6:348:SER:HA	1.73	0.69
1:G:752:ASP:C	1:G:779:ARG:HH12	1.96	0.69
1:G:820:VAL:HG11	2:H:136:MET:HE3	1.73	0.69
1:A:550:PHE:HA	4:6:46:GLY:HA3	1.66	0.69
1:G:93:MET:HE2	1:G:763:THR:HB	1.61	0.69
1:G:832:MET:SD	2:H:84:PHE:HE2	2.17	0.69
1:J:732:ILE:CG2	1:J:747:LEU:HD11	1.26	0.69
1:J:786:ILE:CG1	3:L:86:ASP:HB3	2.23	0.69
4:4:1:ASP:HA	4:4:4:GLU:HB3	1.74	0.69
4:7:1:ASP:HA	4:7:4:GLU:HB3	1.74	0.69
1:D:630:ALA:O	4:5:25:ASP:CB	2.41	0.68
1:D:733:PRO:C	1:D:737:PHE:CD1	2.62	0.68
1:D:797:PHE:CE2	3:F:126:LEU:CD2	2.75	0.68
1:D:817:GLN:CD	2:E:127:ARG:CD	2.61	0.68
2:E:117:LEU:CB	2:E:147:ASN:OD1	2.39	0.68
1:G:652:LEU:O	1:G:655:GLU:N	2.27	0.68
3:I:3:SER:O	3:I:4:LYS:CB	2.41	0.68
1:J:538:GLU:CD	4:7:355:MET:HE1	2.12	0.68
1:J:546:THR:HG22	1:J:548:THR:N	2.05	0.68
1:J:769:ALA:CB	1:J:770:GLY:N	2.57	0.68
1:A:52:ILE:HD13	1:A:52:ILE:N	2.08	0.68
1:A:502:GLU:HG2	1:A:764:MLY:O	1.93	0.68
1:A:815:CYS:O	1:A:819:ASN:HB2	1.93	0.68
2:B:117:LEU:HD12	2:B:147:ASN:CA	2.20	0.68
1:D:732:ILE:HG21	1:D:747:LEU:HD11	0.72	0.68
1:D:815:CYS:O	1:D:819:ASN:HB2	1.93	0.68
1:J:541:MET:CG	4:7:345:ILE:O	2.40	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:160:THR:HG21	4:5:274:ILE:HD11	1.76	0.68
4:V:1:ASP:HA	4:V:4:GLU:HB3	1.74	0.68
1:A:213:LYS:HA	1:A:220:ASP:OD1	1.92	0.68
1:D:62:VAL:HG12	1:D:63:MLY:O	1.93	0.68
2:E:111:SER:OG	2:E:148:VAL:HG12	1.92	0.68
3:F:48:LYS:C	3:F:52:ASN:HD21	1.96	0.68
1:G:213:LYS:HA	1:G:220:ASP:OD1	1.92	0.68
1:G:533:PHE:O	1:G:537:GLU:HG2	1.93	0.68
1:G:807:VAL:O	1:G:810:ARG:HB2	1.93	0.68
1:J:90:ASP:OD1	1:J:764:MLY:HH11	1.92	0.68
1:J:538:GLU:CD	4:7:355:MET:CE	2.62	0.68
4:1:160:THR:HG21	4:1:274:ILE:HD11	1.76	0.68
4:3:160:THR:HG21	4:3:274:ILE:HD11	1.76	0.68
1:A:166:MET:HE1	1:A:254:PHE:HB2	1.75	0.68
1:A:652:LEU:O	1:A:655:GLU:N	2.27	0.68
2:E:117:LEU:HD11	2:E:147:ASN:HB3	1.75	0.68
3:F:3:SER:O	3:F:4:LYS:CB	2.41	0.68
1:G:52:ILE:HD13	1:G:52:ILE:N	2.09	0.68
2:H:117:LEU:CB	2:H:147:ASN:OD1	2.39	0.68
1:J:90:ASP:HB2	1:J:764:MLY:HH21	1.74	0.68
1:J:553:MLY:HG2	4:V:47:MET:N	2.07	0.68
4:2:1:ASP:HA	4:2:4:GLU:HB3	1.74	0.68
4:7:160:THR:HG21	4:7:274:ILE:HD11	1.76	0.68
4:Z:1:ASP:HA	4:Z:4:GLU:HB3	1.74	0.68
1:A:732:ILE:CG2	1:A:747:LEU:HD11	1.26	0.68
1:D:533:PHE:O	1:D:537:GLU:HG2	1.93	0.68
1:D:762:HIS:H	1:D:762:HIS:CD2	2.08	0.68
1:D:787:ILE:HG22	1:D:788:THR:N	2.07	0.68
2:H:114:LYS:HA	2:H:146:GLY:C	2.02	0.68
3:I:48:LYS:C	3:I:52:ASN:HD21	1.96	0.68
1:J:533:PHE:O	1:J:537:GLU:HG2	1.93	0.68
2:K:117:LEU:HD12	2:K:147:ASN:CA	2.19	0.68
4:V:160:THR:HG21	4:V:274:ILE:HD11	1.75	0.68
4:X:1:ASP:HA	4:X:4:GLU:HB3	1.74	0.68
4:X:3:ASP:HA	4:X:6:THR:CB	2.18	0.68
4:Y:160:THR:HG21	4:Y:274:ILE:HD11	1.76	0.68
1:A:807:VAL:O	1:A:810:ARG:HB2	1.93	0.68
3:C:25:ILE:O	3:C:63:ILE:HB	1.92	0.68
1:J:166:MET:HE3	1:J:254:PHE:HD2	1.56	0.68
1:J:798:LEU:HD21	3:L:126:LEU:CD1	2.21	0.68
2:K:117:LEU:CB	2:K:147:ASN:ND2	2.35	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:0:1:ASP:HA	4:0:4:GLU:HB3	1.74	0.68
4:Z:153:LEU:HD11	4:Z:274:ILE:HG13	1.76	0.68
1:A:408:VAL:HG12	4:4:332:PRO:HB3	1.76	0.68
3:C:4:LYS:N	3:C:5:ALA:O	2.16	0.68
1:D:123:CYS:HB2	1:D:158:ILE:CD1	2.23	0.68
1:D:550:PHE:HE2	1:D:592:ILE:HG23	1.59	0.68
1:G:408:VAL:HG12	4:6:332:PRO:HB3	1.76	0.68
3:I:48:LYS:HB3	3:I:52:ASN:HD21	1.57	0.68
1:J:707:CYS:CA	1:J:714:ARG:HH22	2.07	0.68
1:J:800:ARG:NH1	3:L:149:VAL:CG2	2.35	0.68
1:J:817:GLN:HG3	2:K:128:PHE:CE1	2.29	0.68
4:2:153:LEU:HD11	4:2:274:ILE:HG13	1.76	0.68
1:A:630:ALA:O	4:4:25:ASP:CB	2.41	0.68
2:B:117:LEU:CB	2:B:147:ASN:ND2	2.35	0.68
1:D:507:GLY:O	1:D:762:HIS:N	2.27	0.68
1:D:538:GLU:CD	4:5:355:MET:CE	2.62	0.68
1:D:789:ALA:C	3:F:87:PHE:CE2	2.67	0.68
1:D:802:GLU:OE1	1:D:802:GLU:HA	1.93	0.68
3:F:102:VAL:HG23	3:F:139:TYR:HD1	1.59	0.68
1:G:166:MET:HE3	1:G:254:PHE:CD2	2.29	0.68
1:G:541:MET:CG	4:6:345:ILE:O	2.41	0.68
1:G:550:PHE:HE2	1:G:592:ILE:HG23	1.59	0.68
1:G:819:ASN:OD1	2:H:90:GLY:O	2.12	0.68
1:J:537:GLU:HG3	4:7:350:SER:O	1.78	0.68
1:J:782:MLY:C	1:J:783:LEU:HD12	2.22	0.68
1:A:793:ARG:HE	3:C:147:MET:CA	2.06	0.68
1:D:530:MET:HE3	4:5:354:GLN:HG2	1.73	0.68
1:D:817:GLN:CG	2:E:127:ARG:HD3	2.22	0.68
1:D:830:PRO:CB	2:E:51:PHE:CZ	2.68	0.68
1:D:831:TRP:CH2	2:E:47:LEU:HD23	2.26	0.68
2:E:117:LEU:CG	2:E:147:ASN:HB3	2.24	0.68
1:G:642:LYS:HB3	4:6:21:PHE:O	1.92	0.68
1:J:62:VAL:HG12	1:J:63:MLY:O	1.93	0.68
1:J:815:CYS:O	1:J:819:ASN:HB2	1.93	0.68
2:K:117:LEU:CB	2:K:147:ASN:OD1	2.39	0.68
4:0:153:LEU:HD11	4:0:274:ILE:HG13	1.76	0.68
1:A:56:GLU:CB	1:A:59:MLY:HB3	2.20	0.67
1:A:58:GLY:HA2	1:A:74:GLU:OE1	1.94	0.67
1:A:541:MET:CG	4:4:345:ILE:O	2.40	0.67
1:D:215:GLN:HA	1:D:340:ILE:CB	2.23	0.67
1:D:652:LEU:O	1:D:655:GLU:N	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:735:GLY:C	1:D:743:ALA:HB1	1.84	0.67
1:G:768:MLY:CD	1:G:772:LEU:CD2	2.68	0.67
1:G:792:ALA:HB3	3:I:40:ASN:HB3	1.76	0.67
2:H:117:LEU:CG	2:H:147:ASN:HB3	2.24	0.67
1:J:612:GLN:NE2	1:J:627:GLY:N	2.43	0.67
4:V:153:LEU:HD11	4:V:274:ILE:HG13	1.76	0.67
4:W:160:THR:HG21	4:W:274:ILE:HD11	1.76	0.67
4:X:153:LEU:HD11	4:X:274:ILE:HG13	1.76	0.67
4:X:160:THR:HG21	4:X:274:ILE:HD11	1.76	0.67
1:A:762:HIS:H	1:A:762:HIS:CD2	2.08	0.67
1:A:800:ARG:CZ	3:C:149:VAL:C	2.62	0.67
1:A:836:PHE:CE1	2:B:159:HIS:HA	2.26	0.67
1:D:52:ILE:HD13	1:D:52:ILE:N	2.09	0.67
1:D:788:THR:HG23	3:F:42:THR:CG2	2.20	0.67
1:J:123:CYS:HB2	1:J:158:ILE:CD1	2.23	0.67
1:J:546:THR:H	1:J:549:SER:HB3	1.59	0.67
1:A:797:PHE:CD2	3:C:126:LEU:HD22	2.29	0.67
2:B:141:PRO:O	2:B:145:ALA:CB	2.43	0.67
1:D:723:ARG:NH2	1:D:783:LEU:HD11	2.08	0.67
1:D:795:ARG:CZ	3:F:43:ASN:CG	2.62	0.67
1:G:538:GLU:CD	4:6:355:MET:CE	2.62	0.67
3:I:24:LYS:HA	3:I:63:ILE:O	1.95	0.67
1:J:750:GLY:HA2	3:L:114:LEU:CD2	2.25	0.67
1:J:795:ARG:HB3	3:L:35:ARG:NH2	2.09	0.67
2:K:114:LYS:HA	2:K:146:GLY:C	2.03	0.67
4:8:160:THR:HG21	4:8:274:ILE:HD11	1.76	0.67
1:A:546:THR:H	1:A:549:SER:HB3	1.60	0.67
1:D:538:GLU:CD	4:5:355:MET:HE1	2.13	0.67
2:E:162:ASP:O	2:K:21:GLU:CB	2.41	0.67
1:J:374:GLN:HG3	1:J:375:ALA:H	1.59	0.67
1:J:642:LYS:HB3	4:7:21:PHE:O	1.92	0.67
1:J:821:ARG:HH22	2:K:127:ARG:NE	1.91	0.67
1:J:838:ILE:HD11	2:K:54:MET:SD	2.34	0.67
1:D:546:THR:H	1:D:549:SER:HB3	1.59	0.67
1:G:58:GLY:HA2	1:G:74:GLU:OE1	1.95	0.67
1:J:769:ALA:HB3	1:J:770:GLY:HA3	1.68	0.67
1:J:798:LEU:HD23	3:L:122:GLU:HB3	1.75	0.67
2:K:117:LEU:CG	2:K:147:ASN:HB3	2.25	0.67
3:L:102:VAL:HG23	3:L:139:TYR:HD1	1.59	0.67
4:4:153:LEU:HD11	4:4:274:ILE:HG13	1.76	0.67
4:6:153:LEU:HD11	4:6:274:ILE:HG13	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:831:TRP:CZ3	2:E:50:THR:HB	2.29	0.67
1:G:84:MLY:HH12	1:G:715:VAL:HG12	1.67	0.67
1:G:217:THR:O	1:G:221:GLN:HG2	1.95	0.67
1:G:784:ALA:O	1:G:788:THR:HB	1.94	0.67
1:J:480:ILE:HG22	1:J:481:ASN:ND2	2.09	0.67
1:J:643:GLY:N	4:7:24:ASP:CA	2.46	0.67
1:J:795:ARG:CD	3:L:35:ARG:NH1	2.53	0.67
4:7:153:LEU:HD11	4:7:274:ILE:HG13	1.76	0.67
1:A:217:THR:O	1:A:221:GLN:HG2	1.95	0.67
3:C:102:VAL:HG23	3:C:139:TYR:HD1	1.60	0.67
1:D:480:ILE:HG22	1:D:481:ASN:ND2	2.09	0.67
1:D:732:ILE:HG22	1:D:747:LEU:CD1	1.55	0.67
1:D:769:ALA:CA	1:D:771:LEU:N	2.57	0.67
1:J:652:LEU:O	1:J:655:GLU:N	2.27	0.67
3:L:24:LYS:HA	3:L:63:ILE:O	1.95	0.67
4:Z:160:THR:HG21	4:Z:274:ILE:HD11	1.76	0.67
3:C:24:LYS:HA	3:C:63:ILE:O	1.95	0.67
1:D:131:TRP:O	1:D:132:LEU:HD12	1.95	0.67
1:D:546:THR:HG22	1:D:548:THR:N	2.05	0.67
1:G:62:VAL:HG12	1:G:63:MLY:O	1.94	0.67
1:G:202:SER:HA	1:G:207:LYS:HE3	1.72	0.67
1:G:292:MET:HE3	1:G:309:PRO:HA	1.77	0.67
1:J:58:GLY:HA2	1:J:74:GLU:OE1	1.95	0.67
1:J:290:GLN:O	1:J:331:LEU:HD12	1.95	0.67
1:A:61:THR:HG23	1:A:71:THR:OG1	1.94	0.67
1:A:62:VAL:HG12	1:A:63:MLY:O	1.93	0.67
1:A:533:PHE:O	1:A:537:GLU:HG2	1.93	0.67
2:B:144:VAL:CG1	2:B:153:ILE:HD13	2.20	0.67
1:D:612:GLN:NE2	1:D:627:GLY:N	2.43	0.67
1:D:642:LYS:CD	4:5:24:ASP:O	2.42	0.67
1:D:739:ASP:CB	1:D:742:LYS:HB3	2.12	0.67
1:G:290:GLN:O	1:G:331:LEU:HD12	1.95	0.67
1:G:802:GLU:OE1	1:G:802:GLU:HA	1.93	0.67
2:K:141:PRO:O	2:K:145:ALA:CB	2.43	0.67
4:6:160:THR:HG21	4:6:274:ILE:HD11	1.76	0.67
1:A:504:MLY:C	1:A:762:HIS:NE2	2.57	0.67
1:A:550:PHE:HE2	1:A:592:ILE:HG23	1.59	0.67
1:A:818:TYR:CB	2:B:89:LYS:C	2.63	0.67
1:D:58:GLY:HA2	1:D:74:GLU:OE1	1.95	0.67
1:G:78:PHE:HB3	1:G:98:HIS:CD2	2.30	0.67
1:G:537:GLU:C	4:6:351:THR:H	1.99	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:546:THR:H	1:G:549:SER:HB3	1.59	0.67
1:J:131:TRP:O	1:J:132:LEU:HD12	1.95	0.67
1:J:749:GLY:C	3:L:114:LEU:HD21	2.15	0.67
4:O:160:THR:HG21	4:O:274:ILE:HD11	1.76	0.67
4:2:160:THR:HG21	4:2:274:ILE:HD11	1.76	0.67
4:4:160:THR:HG21	4:4:274:ILE:HD11	1.76	0.67
1:A:78:PHE:HB3	1:A:98:HIS:CD2	2.30	0.66
1:D:374:GLN:HG3	1:D:375:ALA:H	1.60	0.66
1:D:648:THR:CB	4:5:350:SER:OG	2.43	0.66
2:E:141:PRO:O	2:E:145:ALA:CB	2.43	0.66
2:H:141:PRO:O	2:H:145:ALA:CB	2.43	0.66
1:J:408:VAL:HG12	4:7:332:PRO:HB3	1.76	0.66
1:J:541:MET:O	4:7:143:TYR:OH	2.14	0.66
1:J:635:GLY:O	4:7:341:ILE:HG21	1.95	0.66
1:J:831:TRP:CE3	2:K:34:ILE:CD1	2.77	0.66
1:A:290:GLN:O	1:A:331:LEU:HD12	1.95	0.66
1:A:795:ARG:CD	3:C:35:ARG:NH1	2.43	0.66
1:D:418:THR:HG22	1:D:419:VAL:N	2.11	0.66
1:D:724:TYR:HE1	1:D:778:MET:CG	2.08	0.66
1:G:174:SER:O	1:G:670:HIS:HB2	1.96	0.66
1:G:599:ASN:OD1	1:G:649:VAL:N	2.29	0.66
2:K:117:LEU:HD11	2:K:147:ASN:HB3	1.76	0.66
4:5:153:LEU:HD11	4:5:274:ILE:HG13	1.76	0.66
1:A:174:SER:O	1:A:670:HIS:HB2	1.96	0.66
1:A:648:THR:CB	4:4:350:SER:OG	2.43	0.66
1:G:93:MET:HE1	1:G:763:THR:O	1.94	0.66
1:G:131:TRP:O	1:G:132:LEU:HD12	1.95	0.66
1:G:783:LEU:O	1:G:787:ILE:CA	2.43	0.66
1:J:52:ILE:HD13	1:J:52:ILE:N	2.09	0.66
1:J:322:VAL:HB	1:J:325:ILE:CD1	2.26	0.66
1:J:550:PHE:HE2	1:J:592:ILE:HG23	1.59	0.66
4:8:153:LEU:HD11	4:8:274:ILE:HG13	1.76	0.66
1:A:418:THR:HG22	1:A:419:VAL:N	2.11	0.66
1:A:817:GLN:HE21	2:B:127:ARG:HG2	1.59	0.66
2:B:117:LEU:CG	2:B:147:ASN:HB3	2.24	0.66
2:E:141:PRO:O	2:E:145:ALA:HB2	1.96	0.66
1:G:61:THR:HG23	1:G:71:THR:OG1	1.94	0.66
1:J:339:ASP:OD1	1:J:348:MLY:HH13	1.95	0.66
4:1:153:LEU:HD11	4:1:274:ILE:HG13	1.76	0.66
1:A:502:GLU:HA	1:A:761:GLY:C	2.15	0.66
1:A:537:GLU:C	4:4:351:THR:H	1.99	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:LEU:HD21	2:B:54:MET:HG3	1.76	0.66
1:D:226:ASN:HB2	1:D:227:PRO:HD3	1.78	0.66
1:D:290:GLN:O	1:D:331:LEU:HD12	1.95	0.66
1:D:339:ASP:OD1	1:D:348:MLY:HH13	1.95	0.66
1:D:408:VAL:HG12	4:5:332:PRO:HB3	1.76	0.66
1:D:599:ASN:OD1	1:D:649:VAL:N	2.28	0.66
1:G:648:THR:CB	4:6:350:SER:OG	2.44	0.66
1:J:707:CYS:CB	1:J:714:ARG:HH22	2.08	0.66
1:J:754:ASP:CB	1:J:776:GLU:CB	2.56	0.66
1:A:480:ILE:HG22	1:A:481:ASN:ND2	2.10	0.66
1:A:541:MET:HG2	4:4:345:ILE:C	2.16	0.66
1:A:642:LYS:CD	4:4:24:ASP:O	2.42	0.66
1:D:174:SER:O	1:D:670:HIS:HB2	1.96	0.66
1:D:507:GLY:HA3	1:D:762:HIS:CB	2.24	0.66
1:D:537:GLU:C	4:5:351:THR:H	1.98	0.66
1:G:612:GLN:NE2	1:G:627:GLY:N	2.42	0.66
1:G:800:ARG:NH1	3:I:149:VAL:C	2.49	0.66
3:I:102:VAL:HG23	3:I:139:TYR:HD1	1.59	0.66
1:J:166:MET:HE1	1:J:254:PHE:HB2	1.78	0.66
1:J:174:SER:O	1:J:670:HIS:HB2	1.96	0.66
1:J:648:THR:CB	4:7:350:SER:OG	2.43	0.66
1:J:754:ASP:HB2	1:J:776:GLU:CB	2.14	0.66
1:J:831:TRP:CH2	2:K:47:LEU:HD23	2.31	0.66
2:K:146:GLY:O	2:K:147:ASN:HB2	1.96	0.66
4:3:153:LEU:HD11	4:3:274:ILE:HG13	1.76	0.66
1:A:91:MET:HE3	1:A:119:SER:HB2	1.78	0.66
1:A:131:TRP:O	1:A:132:LEU:HD12	1.95	0.66
2:B:141:PRO:O	2:B:145:ALA:HB2	1.96	0.66
1:D:322:VAL:HB	1:D:325:ILE:CD1	2.26	0.66
3:F:48:LYS:O	3:F:52:ASN:CG	2.34	0.66
1:G:374:GLN:HG3	1:G:375:ALA:H	1.60	0.66
1:G:553:MLY:CE	4:8:45:VAL:CA	2.49	0.66
1:G:797:PHE:CD1	3:I:149:VAL:HG12	2.25	0.66
1:J:78:PHE:HB3	1:J:98:HIS:CD2	2.30	0.66
1:J:790:THR:CA	3:L:87:PHE:CE2	2.79	0.66
1:J:795:ARG:NE	3:L:118:MET:HE1	2.01	0.66
2:K:141:PRO:O	2:K:145:ALA:HB2	1.96	0.66
1:A:538:GLU:HA	4:4:349:LEU:HB3	1.78	0.66
1:A:612:GLN:NE2	1:A:627:GLY:N	2.43	0.66
1:A:717:TYR:HD1	1:A:744:SER:HG	1.44	0.66
1:A:818:TYR:HB3	2:B:89:LYS:C	2.16	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:541:MET:O	4:5:143:TYR:OH	2.14	0.66
2:E:146:GLY:O	2:E:147:ASN:HB2	1.96	0.66
1:G:757:GLN:CD	1:G:772:LEU:HG	2.15	0.66
1:G:831:TRP:NE1	2:H:67:MET:CB	2.55	0.66
2:H:117:LEU:CB	2:H:147:ASN:ND2	2.35	0.66
2:H:146:GLY:O	2:H:147:ASN:HB2	1.96	0.66
1:J:226:ASN:HB2	1:J:227:PRO:HD3	1.78	0.66
1:J:541:MET:HG2	4:7:345:ILE:C	2.16	0.66
4:W:153:LEU:HD11	4:W:274:ILE:HG13	1.76	0.66
1:A:530:MET:CG	4:4:354:GLN:CG	2.71	0.66
1:G:226:ASN:HB2	1:G:227:PRO:HD3	1.78	0.66
1:G:635:GLY:O	4:6:341:ILE:HG21	1.95	0.66
1:J:537:GLU:C	4:7:351:THR:H	1.98	0.66
1:J:599:ASN:OD1	1:J:649:VAL:N	2.28	0.66
2:K:150:TYR:C	2:K:151:LYS:CG	2.49	0.66
1:A:144:ARG:NH1	1:A:160:ASP:OD1	2.29	0.66
1:A:161:ASN:O	1:A:165:PHE:HB2	1.96	0.66
1:A:339:ASP:OD1	1:A:348:MLY:HH13	1.95	0.66
1:A:530:MET:CA	4:4:354:GLN:CB	2.74	0.66
3:C:45:GLU:O	3:C:49:ILE:HG13	1.96	0.66
1:G:541:MET:HG2	4:6:345:ILE:C	2.17	0.66
2:H:117:LEU:HD11	2:H:147:ASN:HB3	1.75	0.66
1:J:144:ARG:NH1	1:J:160:ASP:OD1	2.29	0.66
1:A:296:MLY:HH11	1:A:348:MLY:HH21	1.78	0.65
1:A:643:GLY:N	4:4:24:ASP:CA	2.46	0.65
1:D:466:GLY:HA2	1:D:484:ASN:HD21	1.61	0.65
1:D:635:GLY:O	4:5:341:ILE:HG21	1.95	0.65
1:D:769:ALA:CA	1:D:771:LEU:CA	2.63	0.65
1:G:144:ARG:NH1	1:G:160:ASP:OD1	2.29	0.65
1:G:480:ILE:HG22	1:G:481:ASN:ND2	2.10	0.65
1:G:480:ILE:HG22	1:G:481:ASN:N	2.11	0.65
1:G:530:MET:HE2	4:6:354:GLN:HG3	1.76	0.65
1:G:557:GLU:N	4:8:48:GLY:HA3	1.90	0.65
3:I:48:LYS:O	3:I:52:ASN:CG	2.34	0.65
1:J:90:ASP:OD2	1:J:764:MLY:HH13	1.96	0.65
1:J:418:THR:HG22	1:J:419:VAL:N	2.11	0.65
3:L:45:GLU:O	3:L:49:ILE:HG13	1.96	0.65
3:L:48:LYS:C	3:L:52:ASN:HD21	1.96	0.65
1:A:538:GLU:CD	4:4:355:MET:CE	2.62	0.65
1:D:217:THR:O	1:D:221:GLN:HG2	1.94	0.65
1:D:691:VAL:O	1:D:695:LEU:HD13	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:818:TYR:CB	2:E:89:LYS:C	2.65	0.65
1:G:161:ASN:O	1:G:165:PHE:HB2	1.96	0.65
1:G:541:MET:O	4:6:143:TYR:OH	2.13	0.65
1:G:769:ALA:O	1:G:773:GLY:HA3	1.95	0.65
1:J:61:THR:HG23	1:J:71:THR:OG1	1.95	0.65
1:J:217:THR:O	1:J:221:GLN:HG2	1.95	0.65
1:J:642:LYS:HA	4:7:21:PHE:O	1.96	0.65
1:J:691:VAL:O	1:J:695:LEU:HD13	1.96	0.65
1:A:502:GLU:HA	1:A:761:GLY:CA	2.26	0.65
1:A:822:SER:HG	2:B:88:LEU:HA	1.60	0.65
1:A:831:TRP:CH2	2:B:34:ILE:HG23	2.31	0.65
1:D:61:THR:HG23	1:D:71:THR:OG1	1.95	0.65
1:D:78:PHE:HB3	1:D:98:HIS:CD2	2.30	0.65
1:D:709:LYS:O	1:D:710:GLY:HA2	1.96	0.65
1:G:296:MLY:HH11	1:G:348:MLY:HH21	1.78	0.65
1:G:339:ASP:OD1	1:G:348:MLY:HH13	1.95	0.65
1:G:466:GLY:HA2	1:G:484:ASN:HD21	1.61	0.65
1:G:538:GLU:CD	4:6:355:MET:HE3	2.17	0.65
2:H:141:PRO:O	2:H:145:ALA:HB2	1.96	0.65
4:Y:153:LEU:HD11	4:Y:274:ILE:HG13	1.76	0.65
1:D:530:MET:CA	4:5:354:GLN:CB	2.74	0.65
2:E:114:LYS:HA	2:E:146:GLY:C	2.03	0.65
3:F:24:LYS:HA	3:F:63:ILE:O	1.95	0.65
3:I:45:GLU:O	3:I:49:ILE:HG13	1.97	0.65
1:A:635:GLY:O	4:4:341:ILE:HG21	1.95	0.65
1:A:691:VAL:O	1:A:695:LEU:HD13	1.97	0.65
1:A:739:ASP:CB	1:A:742:LYS:HB3	2.12	0.65
1:D:530:MET:CG	4:5:354:GLN:CG	2.71	0.65
1:D:541:MET:HG2	4:5:345:ILE:C	2.16	0.65
1:G:691:VAL:O	1:G:695:LEU:HD13	1.97	0.65
1:G:769:ALA:CB	1:G:770:GLY:N	2.59	0.65
1:G:820:VAL:HG11	2:H:136:MET:CE	2.26	0.65
1:G:822:SER:O	1:G:825:ASN:HB2	1.97	0.65
1:J:84:MLY:NZ	1:J:719:ASP:O	2.13	0.65
1:J:161:ASN:O	1:J:165:PHE:HB2	1.96	0.65
1:J:818:TYR:HB3	2:K:90:GLY:HA2	1.75	0.65
3:L:3:SER:HG	3:L:5:ALA:N	1.95	0.65
1:A:107:MLY:HB3	1:A:686:MET:CE	2.27	0.65
1:A:480:ILE:HG22	1:A:481:ASN:N	2.11	0.65
1:A:501:GLU:O	1:A:762:HIS:CG	2.48	0.65
1:A:599:ASN:OD1	1:A:649:VAL:N	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:ARG:CZ	3:C:147:MET:HG2	2.27	0.65
1:D:612:GLN:HE22	1:D:627:GLY:N	1.94	0.65
1:D:822:SER:O	1:D:825:ASN:HB2	1.97	0.65
1:G:769:ALA:HB2	1:G:770:GLY:N	2.09	0.65
1:A:226:ASN:HB2	1:A:227:PRO:HD3	1.77	0.65
1:A:322:VAL:HB	1:A:325:ILE:CD1	2.26	0.65
3:F:45:GLU:O	3:F:49:ILE:HG13	1.97	0.65
1:G:466:GLY:HA2	1:G:484:ASN:ND2	2.12	0.65
1:G:530:MET:CG	4:6:354:GLN:CG	2.72	0.65
1:G:725:ARG:NE	1:G:737:PHE:HE1	1.95	0.65
3:I:48:LYS:C	3:I:52:ASN:HD22	1.97	0.65
1:J:95:THR:CA	1:J:713:SER:HB3	2.27	0.65
1:J:530:MET:CA	4:7:354:GLN:CB	2.74	0.65
1:J:725:ARG:NE	1:J:737:PHE:HE1	1.95	0.65
1:A:217:THR:HB	1:A:220:ASP:OD2	1.97	0.65
1:A:818:TYR:HB3	2:B:90:GLY:N	2.12	0.65
1:D:94:MET:HE1	1:D:101:ALA:HB1	1.79	0.65
1:D:725:ARG:NE	1:D:737:PHE:HE1	1.95	0.65
1:G:418:THR:HG22	1:G:419:VAL:N	2.11	0.65
1:G:798:LEU:HD11	3:I:126:LEU:HG	1.78	0.65
1:J:792:ALA:HB1	3:L:40:ASN:HB3	0.73	0.65
1:A:374:GLN:HG3	1:A:375:ALA:H	1.60	0.65
1:A:636:LYS:HG3	4:4:334:GLU:CD	2.17	0.65
1:A:822:SER:O	1:A:825:ASN:HB2	1.97	0.65
3:C:49:ILE:HA	3:C:52:ASN:ND2	2.05	0.65
1:D:642:LYS:CD	4:5:340:TRP:CZ3	2.79	0.65
1:J:822:SER:O	1:J:825:ASN:HB2	1.97	0.65
1:A:94:MET:HE1	1:A:101:ALA:HB1	1.79	0.65
1:A:642:LYS:HA	4:4:21:PHE:O	1.96	0.65
1:D:144:ARG:NH1	1:D:160:ASP:OD1	2.29	0.65
1:D:202:SER:CA	1:D:207:LYS:HE3	2.27	0.65
1:G:90:ASP:O	1:G:764:MLY:CH2	2.44	0.65
1:G:93:MET:HE3	1:G:763:THR:CG2	2.08	0.65
1:G:818:TYR:CD1	2:H:127:ARG:NH1	2.65	0.65
1:J:636:LYS:HG3	4:7:334:GLU:CD	2.17	0.65
2:K:144:VAL:CG1	2:K:153:ILE:HD13	2.20	0.65
1:A:292:MET:HE3	1:A:309:PRO:HA	1.78	0.64
1:A:466:GLY:HA2	1:A:484:ASN:ND2	2.12	0.64
1:A:642:LYS:CD	4:4:340:TRP:CZ3	2.79	0.64
1:D:479:CYS:HB3	1:D:653:PHE:CE2	2.32	0.64
1:D:636:LYS:O	1:D:637:LYS:CB	2.45	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:642:LYS:HA	4:5:21:PHE:O	1.96	0.64
1:D:831:TRP:NE1	2:E:47:LEU:CD2	2.36	0.64
1:G:107:MLY:HB3	1:G:686:MET:CE	2.26	0.64
1:J:823:PHE:CE2	2:K:140:PHE:CZ	2.86	0.64
3:L:48:LYS:O	3:L:52:ASN:CG	2.34	0.64
1:A:93:MET:O	1:A:713:SER:HB3	1.97	0.64
1:A:505:MLY:HG3	1:A:741:LYS:HZ2	1.63	0.64
1:A:814:PHE:HA	2:B:127:ARG:HH22	1.54	0.64
1:D:161:ASN:O	1:D:165:PHE:HB2	1.96	0.64
1:D:480:ILE:HG22	1:D:481:ASN:N	2.11	0.64
1:D:636:LYS:HG3	4:5:334:GLU:CD	2.17	0.64
1:D:834:LEU:HD21	2:E:54:MET:CE	2.27	0.64
1:G:322:VAL:HB	1:G:325:ILE:CD1	2.26	0.64
1:G:538:GLU:HA	4:6:349:LEU:HB3	1.79	0.64
1:A:466:GLY:HA2	1:A:484:ASN:HD21	1.61	0.64
1:D:806:MET:O	1:D:809:ARG:HB2	1.98	0.64
3:F:3:SER:HG	3:F:5:ALA:N	1.95	0.64
1:G:642:LYS:CD	4:6:24:ASP:O	2.43	0.64
1:G:642:LYS:HA	4:6:21:PHE:O	1.97	0.64
1:J:107:MLY:HB3	1:J:686:MET:CE	2.27	0.64
1:J:133:PRO:O	1:J:136:ASN:HB2	1.98	0.64
1:J:466:GLY:HA2	1:J:484:ASN:ND2	2.12	0.64
1:J:612:GLN:HE22	1:J:627:GLY:N	1.94	0.64
1:J:783:LEU:HD12	1:J:783:LEU:N	2.13	0.64
1:J:793:ARG:HG3	3:L:146:ILE:HG22	1.79	0.64
1:J:795:ARG:HH11	3:L:35:ARG:CZ	2.09	0.64
1:A:133:PRO:O	1:A:136:ASN:HB2	1.97	0.64
1:A:218:LEU:CD2	1:A:222:ILE:HG12	2.28	0.64
1:A:557:GLU:N	4:6:48:GLY:HA3	1.90	0.64
1:A:612:GLN:HE22	1:A:627:GLY:N	1.94	0.64
2:B:140:PHE:HB3	2:B:144:VAL:CG1	2.28	0.64
1:D:466:GLY:HA2	1:D:484:ASN:ND2	2.12	0.64
1:G:84:MLY:HH11	1:G:720:PHE:N	2.13	0.64
1:G:210:GLN:O	1:G:211:SER:OG	2.15	0.64
1:J:217:THR:HB	1:J:220:ASP:OD2	1.97	0.64
1:J:479:CYS:HB3	1:J:653:PHE:CE2	2.33	0.64
2:K:117:LEU:CG	2:K:147:ASN:CB	2.76	0.64
1:A:202:SER:CA	1:A:207:LYS:HE3	2.27	0.64
1:D:107:MLY:HB3	1:D:686:MET:CE	2.26	0.64
1:D:217:THR:HB	1:D:220:ASP:OD2	1.97	0.64
1:D:296:MLY:HH11	1:D:348:MLY:HH21	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:133:PRO:O	1:G:136:ASN:HB2	1.98	0.64
1:G:217:THR:HB	1:G:220:ASP:OD2	1.97	0.64
1:J:90:ASP:CG	1:J:764:MLY:HH21	2.18	0.64
1:J:466:GLY:HA2	1:J:484:ASN:HD21	1.61	0.64
1:J:806:MET:O	1:J:809:ARG:HB2	1.98	0.64
1:J:819:ASN:N	2:K:90:GLY:O	2.29	0.64
1:J:831:TRP:HH2	2:K:47:LEU:HD23	1.61	0.64
1:A:553:MLY:CE	4:6:45:VAL:CA	2.49	0.64
1:A:642:LYS:CA	4:4:21:PHE:O	2.46	0.64
3:C:48:LYS:O	3:C:52:ASN:CG	2.34	0.64
2:E:140:PHE:O	2:E:141:PRO:C	2.33	0.64
1:G:218:LEU:CD2	1:G:222:ILE:HG12	2.28	0.64
1:G:406:VAL:HG12	1:G:407:GLY:N	2.13	0.64
1:G:530:MET:CA	4:6:354:GLN:CB	2.75	0.64
1:G:612:GLN:HE22	1:G:627:GLY:N	1.94	0.64
1:G:636:LYS:HG3	4:6:334:GLU:CD	2.18	0.64
1:G:730:SER:CB	3:I:109:HIS:CD2	2.80	0.64
2:H:140:PHE:HB3	2:H:144:VAL:CG1	2.28	0.64
1:J:296:MLY:HH11	1:J:348:MLY:HH21	1.78	0.64
1:J:538:GLU:HA	4:7:349:LEU:HB3	1.78	0.64
1:J:642:LYS:CA	4:7:21:PHE:O	2.45	0.64
2:K:140:PHE:HB3	2:K:144:VAL:CG1	2.28	0.64
1:A:534:SER:C	4:4:351:THR:CA	2.47	0.64
1:A:725:ARG:NE	1:A:737:PHE:HE1	1.95	0.64
2:E:140:PHE:HB3	2:E:144:VAL:CG1	2.27	0.64
2:E:149:ASP:OD2	2:E:150:TYR:C	2.36	0.64
1:G:541:MET:HG2	4:6:345:ILE:O	1.98	0.64
1:J:510:TRP:CZ3	1:J:772:LEU:CD2	2.80	0.64
1:J:537:GLU:C	4:7:351:THR:N	2.51	0.64
1:J:636:LYS:O	1:J:637:LYS:CB	2.45	0.64
1:J:795:ARG:CD	3:L:35:ARG:HH12	2.11	0.64
2:K:144:VAL:HA	2:K:153:ILE:HD11	1.80	0.64
1:A:479:CYS:HB3	1:A:653:PHE:CE2	2.32	0.64
1:A:636:LYS:O	1:A:637:LYS:CB	2.45	0.64
1:D:795:ARG:NH2	3:F:116:GLU:OE1	2.29	0.64
1:D:830:PRO:CB	2:E:67:MET:HE3	2.23	0.64
2:E:117:LEU:CG	2:E:147:ASN:CB	2.76	0.64
1:G:166:MET:HE3	1:G:254:PHE:HD2	1.61	0.64
1:G:642:LYS:CA	4:6:21:PHE:O	2.46	0.64
1:J:127:ASN:HD22	1:J:128:PRO:CD	2.11	0.64
4:4:190:MET:SD	4:4:209:VAL:HG11	2.38	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:MET:O	4:4:143:TYR:OH	2.14	0.64
1:D:127:ASN:HD22	1:D:128:PRO:CD	2.11	0.64
1:D:537:GLU:HB3	1:D:648:THR:HB	1.80	0.64
1:D:818:TYR:HB2	2:E:89:LYS:C	2.18	0.64
1:G:479:CYS:HB3	1:G:653:PHE:CE2	2.32	0.64
1:G:751:GLY:N	3:I:114:LEU:CD1	2.61	0.64
1:J:292:MET:HE3	1:J:309:PRO:HA	1.78	0.64
1:J:636:LYS:N	4:7:334:GLU:OE1	2.31	0.64
1:J:642:LYS:CD	4:7:340:TRP:CZ3	2.79	0.64
1:J:838:ILE:CD1	2:K:54:MET:HE3	2.27	0.64
4:V:190:MET:SD	4:V:209:VAL:HG11	2.38	0.64
4:X:190:MET:SD	4:X:209:VAL:HG11	2.38	0.64
1:A:530:MET:HE3	4:4:354:GLN:CG	2.23	0.64
1:A:806:MET:O	1:A:809:ARG:HB2	1.98	0.64
1:A:831:TRP:NE1	2:B:51:PHE:CE2	2.63	0.64
1:G:529:PRO:C	4:6:354:GLN:CB	2.50	0.64
1:G:724:TYR:HB3	1:G:727:LEU:HD12	1.80	0.64
1:G:784:ALA:O	1:G:788:THR:CB	2.45	0.64
3:I:49:ILE:HA	3:I:52:ASN:ND2	2.05	0.64
1:J:406:VAL:HG12	1:J:407:GLY:N	2.13	0.64
4:2:190:MET:SD	4:2:209:VAL:HG11	2.38	0.64
1:A:538:GLU:HA	4:4:349:LEU:CG	2.27	0.63
1:D:830:PRO:CB	2:E:67:MET:CE	2.74	0.63
1:J:480:ILE:HG22	1:J:481:ASN:N	2.11	0.63
1:J:577:ALA:O	1:J:578:HIS:CD2	2.51	0.63
4:5:190:MET:SD	4:5:209:VAL:HG11	2.38	0.63
1:A:636:LYS:N	4:4:334:GLU:OE1	2.31	0.63
1:A:724:TYR:HB3	1:A:727:LEU:HD12	1.80	0.63
2:B:132:GLU:O	2:B:136:MET:HG2	1.99	0.63
2:B:146:GLY:O	2:B:147:ASN:HB2	1.96	0.63
1:G:91:MET:HE3	1:G:119:SER:HB2	1.80	0.63
1:G:215:GLN:CA	1:G:340:ILE:CG2	2.63	0.63
1:G:577:ALA:O	1:G:578:HIS:CD2	2.52	0.63
1:G:724:TYR:HD1	1:G:727:LEU:HD11	1.64	0.63
1:G:829:TRP:CZ2	2:H:87:LYS:HE2	2.34	0.63
1:J:725:ARG:NE	1:J:737:PHE:CE1	2.66	0.63
1:A:502:GLU:OE2	1:A:764:MLY:N	2.31	0.63
1:A:795:ARG:CB	3:C:35:ARG:CZ	2.75	0.63
1:A:822:SER:CB	2:B:88:LEU:CD2	2.67	0.63
1:D:218:LEU:CD2	1:D:222:ILE:HG12	2.28	0.63
1:D:577:ALA:O	1:D:578:HIS:CD2	2.51	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:537:GLU:HB3	1:G:648:THR:HB	1.80	0.63
1:G:754:ASP:CG	1:G:776:GLU:OE2	2.36	0.63
1:G:783:LEU:HD12	1:G:783:LEU:N	2.13	0.63
1:J:642:LYS:CG	4:7:22:ALA:C	2.67	0.63
1:A:406:VAL:HG12	1:A:407:GLY:N	2.13	0.63
1:A:530:MET:HA	4:4:354:GLN:CB	2.29	0.63
1:A:725:ARG:NE	1:A:737:PHE:CE1	2.67	0.63
1:D:133:PRO:O	1:D:136:ASN:HB2	1.98	0.63
1:D:783:LEU:HD12	1:D:783:LEU:N	2.13	0.63
1:D:817:GLN:CD	2:E:127:ARG:HE	1.90	0.63
1:G:642:LYS:CG	4:6:22:ALA:C	2.67	0.63
1:G:643:GLY:H	4:6:23:GLY:C	2.02	0.63
1:J:534:SER:C	4:7:351:THR:CA	2.47	0.63
4:0:190:MET:SD	4:0:209:VAL:HG11	2.38	0.63
4:7:190:MET:SD	4:7:209:VAL:HG11	2.38	0.63
1:A:577:ALA:O	1:A:578:HIS:CD2	2.52	0.63
2:B:117:LEU:CG	2:B:147:ASN:CB	2.76	0.63
1:D:538:GLU:HA	4:5:349:LEU:HB3	1.78	0.63
1:G:827:MLY:HH21	2:H:139:ALA:HB3	1.81	0.63
1:G:829:TRP:CH2	2:H:87:LYS:NZ	2.66	0.63
1:J:541:MET:CA	4:7:143:TYR:OH	2.46	0.63
1:J:724:TYR:HB3	1:J:727:LEU:HD12	1.80	0.63
2:K:146:GLY:O	2:K:147:ASN:CB	2.46	0.63
4:0:257:CYS:HB3	4:0:258:PRO:HD3	1.81	0.63
4:7:257:CYS:HB3	4:7:258:PRO:HD3	1.81	0.63
4:V:257:CYS:HB3	4:V:258:PRO:HD3	1.81	0.63
1:A:537:GLU:C	4:4:351:THR:N	2.52	0.63
1:A:542:PHE:CZ	1:A:553:MLY:HH11	2.34	0.63
1:A:724:TYR:HD1	1:A:727:LEU:HD11	1.64	0.63
1:A:800:ARG:HD2	3:C:149:VAL:CB	2.27	0.63
2:B:144:VAL:HA	2:B:153:ILE:HD11	1.80	0.63
1:D:793:ARG:HE	3:F:147:MET:CA	2.11	0.63
1:D:829:TRP:NE1	2:E:67:MET:CG	2.39	0.63
2:E:132:GLU:O	2:E:136:MET:HG2	1.99	0.63
1:G:636:LYS:O	1:G:637:LYS:CB	2.45	0.63
1:G:771:LEU:O	1:G:774:LEU:N	2.32	0.63
2:H:117:LEU:CG	2:H:147:ASN:CB	2.76	0.63
1:J:141:LEU:H	1:J:141:LEU:HD12	1.64	0.63
1:J:278:GLN:CG	1:J:317:GLU:HB2	2.27	0.63
3:L:49:ILE:HA	3:L:52:ASN:ND2	2.06	0.63
4:3:257:CYS:HB3	4:3:258:PRO:HD3	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:257:CYS:HB3	4:X:258:PRO:HD3	1.81	0.63
4:Z:257:CYS:HB3	4:Z:258:PRO:HD3	1.81	0.63
1:A:541:MET:HG2	4:4:345:ILE:O	1.98	0.63
1:D:818:TYR:HD2	2:E:89:LYS:O	1.81	0.63
2:E:146:GLY:O	2:E:147:ASN:CB	2.46	0.63
3:F:24:LYS:HB3	3:F:63:ILE:H	1.64	0.63
1:G:806:MET:O	1:G:809:ARG:HB2	1.98	0.63
1:J:218:LEU:CD2	1:J:222:ILE:HG12	2.28	0.63
1:J:537:GLU:HB3	1:J:648:THR:HB	1.80	0.63
1:J:541:MET:HG2	4:7:345:ILE:O	1.98	0.63
1:J:768:MLY:HH21	1:J:772:LEU:HD22	1.66	0.63
1:A:127:ASN:HD22	1:A:128:PRO:CD	2.11	0.63
1:A:831:TRP:HZ3	2:B:50:THR:CG2	2.11	0.63
2:B:121:LEU:HA	2:B:128:PHE:CG	2.34	0.63
2:B:146:GLY:O	2:B:147:ASN:CB	2.46	0.63
1:D:538:GLU:HA	4:5:349:LEU:CG	2.28	0.63
1:D:725:ARG:NE	1:D:737:PHE:CE1	2.66	0.63
1:G:141:LEU:H	1:G:141:LEU:HD12	1.64	0.63
1:G:541:MET:CA	4:6:143:TYR:OH	2.47	0.63
1:J:84:MLY:HH11	1:J:715:VAL:HG12	1.76	0.63
1:J:641:LYS:CE	1:J:647:GLN:CB	2.75	0.63
2:K:132:GLU:O	2:K:136:MET:HG2	1.99	0.63
1:A:93:MET:HE1	1:A:716:LEU:H	1.64	0.63
1:A:707:CYS:CA	1:A:714:ARG:CZ	2.77	0.63
3:C:24:LYS:HB3	3:C:63:ILE:H	1.64	0.63
1:D:166:MET:HE3	1:D:254:PHE:CD2	2.34	0.63
1:D:278:GLN:CG	1:D:317:GLU:HB2	2.27	0.63
1:D:411:GLU:N	4:5:333:PRO:HB2	2.11	0.63
1:D:541:MET:HG2	4:5:345:ILE:O	1.98	0.63
1:D:642:LYS:CG	4:5:22:ALA:C	2.67	0.63
1:D:726:VAL:HB	1:D:782:MLY:HH13	0.82	0.63
1:D:771:LEU:O	1:D:774:LEU:N	2.32	0.63
1:G:251:ARG:HB2	1:G:264:ASP:CB	2.29	0.63
1:G:537:GLU:C	4:6:351:THR:N	2.51	0.63
1:G:831:TRP:NE1	2:H:67:MET:HB3	2.14	0.63
1:J:553:MLY:O	4:V:48:GLY:HA2	1.99	0.63
4:1:190:MET:SD	4:1:209:VAL:HG11	2.38	0.63
4:2:257:CYS:HB3	4:2:258:PRO:HD3	1.81	0.63
4:5:257:CYS:HB3	4:5:258:PRO:HD3	1.81	0.63
4:W:190:MET:SD	4:W:209:VAL:HG11	2.38	0.63
1:A:541:MET:CA	4:4:143:TYR:OH	2.47	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:HIS:CB	1:A:592:ILE:HD12	2.29	0.62
1:A:817:GLN:HE21	2:B:127:ARG:CG	2.12	0.62
1:D:210:GLN:O	1:D:211:SER:OG	2.15	0.62
1:D:551:MLY:C	4:7:46:GLY:O	2.47	0.62
1:D:793:ARG:NE	3:F:147:MET:HA	2.14	0.62
1:G:636:LYS:N	4:6:334:GLU:OE1	2.31	0.62
1:G:725:ARG:NE	1:G:737:PHE:CE1	2.67	0.62
1:G:728:ASN:HD22	3:I:113:THR:HG1	1.46	0.62
1:G:791:GLN:CD	3:I:116:GLU:HB2	2.20	0.62
2:H:149:ASP:OD2	2:H:150:TYR:C	2.36	0.62
3:I:3:SER:HG	3:I:5:ALA:N	1.96	0.62
1:J:541:MET:HE1	4:7:346:LEU:HD12	1.81	0.62
4:3:190:MET:SD	4:3:209:VAL:HG11	2.38	0.62
4:8:190:MET:SD	4:8:209:VAL:HG11	2.38	0.62
4:Z:190:MET:SD	4:Z:209:VAL:HG11	2.38	0.62
1:A:274:ARG:HB2	1:A:285:TYR:CE2	2.34	0.62
1:A:502:GLU:CD	1:A:764:MLY:O	2.37	0.62
1:A:542:PHE:N	4:4:143:TYR:OH	2.33	0.62
1:A:643:GLY:H	4:4:23:GLY:C	2.02	0.62
1:A:783:LEU:HD12	1:A:783:LEU:N	2.13	0.62
1:D:724:TYR:HB3	1:D:727:LEU:HD12	1.80	0.62
1:D:724:TYR:HD1	1:D:727:LEU:HD11	1.64	0.62
1:D:767:PHE:HB3	1:D:771:LEU:HD11	1.80	0.62
1:D:800:ARG:HB2	3:F:149:VAL:HG22	1.80	0.62
2:E:121:LEU:HA	2:E:128:PHE:CG	2.34	0.62
1:G:544:LYS:HB2	4:6:147:ARG:HA	1.80	0.62
2:H:111:SER:OG	2:H:148:VAL:CG1	2.47	0.62
2:H:121:LEU:HA	2:H:128:PHE:CG	2.34	0.62
1:J:94:MET:HE1	1:J:101:ALA:HB1	1.80	0.62
1:J:817:GLN:HG2	2:K:127:ARG:HB2	1.81	0.62
1:A:251:ARG:HB2	1:A:264:ASP:CB	2.29	0.62
1:A:501:GLU:CG	1:A:762:HIS:ND1	2.45	0.62
1:A:537:GLU:HB3	1:A:648:THR:HB	1.80	0.62
1:A:551:MLY:C	4:6:46:GLY:O	2.47	0.62
1:D:251:ARG:HB2	1:D:264:ASP:CB	2.29	0.62
1:D:507:GLY:HA2	1:D:762:HIS:ND1	2.15	0.62
1:D:642:LYS:CA	4:5:21:PHE:O	2.46	0.62
1:D:795:ARG:C	3:F:35:ARG:HD3	2.20	0.62
1:G:202:SER:CA	1:G:207:LYS:HE3	2.28	0.62
1:G:508:ILE:HG21	1:G:711:PHE:HZ	1.64	0.62
1:J:278:GLN:HG3	1:J:318:GLY:N	2.15	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:771:LEU:O	1:J:774:LEU:N	2.32	0.62
4:1:257:CYS:HB3	4:1:258:PRO:HD3	1.81	0.62
4:4:257:CYS:HB3	4:4:258:PRO:HD3	1.81	0.62
4:6:190:MET:SD	4:6:209:VAL:HG11	2.38	0.62
1:A:302:MET:HG2	1:A:303:LEU:CD1	2.30	0.62
1:A:797:PHE:CE2	3:C:126:LEU:HD22	2.33	0.62
2:B:149:ASP:OD2	2:B:150:TYR:C	2.37	0.62
1:D:541:MET:HE2	4:5:346:LEU:HD12	1.82	0.62
1:D:542:PHE:CZ	1:D:553:MLY:HH11	2.34	0.62
1:D:580:SER:HA	1:D:588:VAL:O	2.00	0.62
1:D:636:LYS:N	4:5:334:GLU:OE1	2.31	0.62
2:H:146:GLY:O	2:H:147:ASN:CB	2.46	0.62
3:I:24:LYS:HB3	3:I:63:ILE:H	1.64	0.62
1:J:544:LYS:HB2	4:7:147:ARG:HA	1.80	0.62
1:J:551:MLY:C	4:V:46:GLY:O	2.47	0.62
1:J:724:TYR:HD1	1:J:727:LEU:HD11	1.64	0.62
3:L:24:LYS:HB3	3:L:63:ILE:H	1.64	0.62
4:6:361:GLU:HB3	4:6:369:ILE:HG12	1.82	0.62
1:A:506:GLU:N	1:A:761:GLY:HA2	2.13	0.62
1:A:543:PRO:HG2	4:4:143:TYR:O	1.98	0.62
1:A:544:LYS:HB2	4:4:147:ARG:HA	1.80	0.62
1:G:542:PHE:N	4:6:143:TYR:OH	2.33	0.62
1:J:251:ARG:HB2	1:J:264:ASP:CB	2.29	0.62
1:J:580:SER:HA	1:J:588:VAL:O	2.00	0.62
2:K:149:ASP:OD2	2:K:150:TYR:C	2.36	0.62
4:0:361:GLU:HB3	4:0:369:ILE:HG12	1.82	0.62
4:4:361:GLU:HB3	4:4:369:ILE:HG12	1.82	0.62
2:B:114:LYS:HA	2:B:146:GLY:C	2.03	0.62
1:D:730:SER:C	1:D:733:PRO:HD2	2.20	0.62
1:J:161:ASN:HA	1:J:164:GLN:HE21	1.63	0.62
2:K:111:SER:OG	2:K:148:VAL:CG1	2.47	0.62
4:2:361:GLU:HB3	4:2:369:ILE:HG12	1.82	0.62
4:5:361:GLU:HB3	4:5:369:ILE:HG12	1.82	0.62
4:6:257:CYS:HB3	4:6:258:PRO:HD3	1.81	0.62
4:7:361:GLU:HB3	4:7:369:ILE:HG12	1.82	0.62
4:8:361:GLU:HB3	4:8:369:ILE:HG12	1.82	0.62
1:A:161:ASN:HA	1:A:164:GLN:HE21	1.63	0.62
1:A:520:ALA:O	1:A:524:GLU:HG2	2.00	0.62
1:A:541:MET:HE2	4:4:346:LEU:HD12	1.82	0.62
1:D:91:MET:HE3	1:D:119:SER:HB2	1.82	0.62
1:D:537:GLU:C	4:5:351:THR:N	2.51	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:578:HIS:CB	1:D:592:ILE:HD12	2.30	0.62
2:E:111:SER:OG	2:E:148:VAL:CG1	2.48	0.62
1:G:127:ASN:HD22	1:G:128:PRO:CD	2.11	0.62
1:G:154:HIS:CE1	1:G:156:PHE:CD2	2.88	0.62
1:G:543:PRO:HG2	4:6:143:TYR:O	1.98	0.62
1:G:553:MLY:O	4:8:48:GLY:HA2	1.99	0.62
1:G:580:SER:HA	1:G:588:VAL:O	2.00	0.62
1:G:798:LEU:HD21	3:I:122:GLU:O	2.00	0.62
1:J:530:MET:CG	4:7:354:GLN:CG	2.72	0.62
1:J:538:GLU:HA	4:7:349:LEU:CG	2.28	0.62
1:J:542:PHE:CZ	1:J:553:MLY:HH11	2.34	0.62
1:J:732:ILE:HG21	1:J:747:LEU:HD11	0.73	0.62
1:J:754:ASP:CG	1:J:776:GLU:HA	2.20	0.62
2:K:121:LEU:HA	2:K:128:PHE:CG	2.34	0.62
4:W:361:GLU:HB3	4:W:369:ILE:HG12	1.82	0.62
4:Y:190:MET:SD	4:Y:209:VAL:HG11	2.38	0.62
1:D:295:MLY:HG3	1:D:332:MET:HE1	1.80	0.62
1:D:542:PHE:CB	4:5:143:TYR:HE1	2.13	0.62
1:D:831:TRP:N	2:E:51:PHE:CE1	2.68	0.62
1:G:98:HIS:HB3	1:G:100:PRO:CD	2.25	0.62
1:G:278:GLN:HG3	1:G:318:GLY:N	2.14	0.62
1:G:510:TRP:CE3	1:G:768:MLY:CH1	2.83	0.62
1:G:541:MET:C	4:6:143:TYR:CZ	2.73	0.62
1:G:578:HIS:CB	1:G:592:ILE:HD12	2.30	0.62
1:J:541:MET:C	4:7:143:TYR:CZ	2.72	0.62
1:J:707:CYS:HB3	1:J:714:ARG:NH2	2.14	0.62
4:1:361:GLU:HB3	4:1:369:ILE:HG12	1.82	0.62
4:V:361:GLU:HB3	4:V:369:ILE:HG12	1.82	0.62
4:X:361:GLU:HB3	4:X:369:ILE:HG12	1.82	0.62
4:Y:257:CYS:HB3	4:Y:258:PRO:HD3	1.81	0.62
4:Y:361:GLU:HB3	4:Y:369:ILE:HG12	1.82	0.62
4:Z:361:GLU:HB3	4:Z:369:ILE:HG12	1.82	0.62
1:A:98:HIS:HB3	1:A:100:PRO:CD	2.25	0.62
1:A:643:GLY:O	1:A:644:SER:CB	2.48	0.62
1:D:161:ASN:HA	1:D:164:GLN:HE21	1.64	0.62
1:D:302:MET:HG2	1:D:303:LEU:CD1	2.30	0.62
1:D:406:VAL:HG12	1:D:407:GLY:N	2.13	0.62
1:D:520:ALA:O	1:D:524:GLU:HG2	2.00	0.62
1:D:541:MET:CA	4:5:143:TYR:OH	2.47	0.62
1:D:830:PRO:CG	2:E:67:MET:HE2	2.15	0.62
1:G:302:MET:HG2	1:G:303:LEU:CD1	2.30	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:542:PHE:CZ	1:G:553:MLY:HH11	2.34	0.62
1:G:730:SER:C	1:G:733:PRO:HD2	2.20	0.62
1:G:768:MLY:CH2	1:G:772:LEU:HD22	2.27	0.62
1:G:791:GLN:OE1	3:I:116:GLU:CG	2.48	0.62
1:A:553:MLY:O	4:6:48:GLY:HA2	1.99	0.62
1:A:580:SER:HA	1:A:588:VAL:O	2.00	0.62
1:A:730:SER:C	1:A:733:PRO:HD2	2.20	0.62
1:A:771:LEU:O	1:A:774:LEU:N	2.32	0.62
3:C:50:LEU:O	3:C:53:PRO:HD2	2.00	0.62
1:D:202:SER:HA	1:D:207:LYS:HE3	1.72	0.62
1:J:557:GLU:HG3	1:J:557:GLU:O	2.00	0.62
1:J:730:SER:C	1:J:733:PRO:HD2	2.20	0.62
1:J:817:GLN:CG	2:K:127:ARG:CD	2.75	0.62
4:3:361:GLU:HB3	4:3:369:ILE:HG12	1.82	0.62
1:A:81:ASN:OD1	1:A:96:HIS:HB2	2.00	0.61
1:A:141:LEU:H	1:A:141:LEU:HD12	1.64	0.61
1:A:278:GLN:HG3	1:A:318:GLY:N	2.15	0.61
1:A:579:PHE:CE1	1:A:581:LEU:HD13	2.35	0.61
1:A:732:ILE:HG22	1:A:747:LEU:CD1	1.55	0.61
1:A:818:TYR:HB2	2:B:90:GLY:N	2.15	0.61
1:D:278:GLN:HG3	1:D:318:GLY:N	2.15	0.61
1:D:507:GLY:HA2	1:D:762:HIS:CG	2.34	0.61
1:D:543:PRO:HG2	4:5:143:TYR:O	1.98	0.61
1:G:551:MLY:C	4:8:46:GLY:O	2.48	0.61
4:8:257:CYS:HB3	4:8:258:PRO:HD3	1.81	0.61
4:W:257:CYS:HB3	4:W:258:PRO:HD3	1.81	0.61
1:A:154:HIS:CE1	1:A:156:PHE:CD2	2.88	0.61
1:A:278:GLN:CG	1:A:317:GLU:HB2	2.27	0.61
1:D:544:LYS:HB2	4:5:147:ARG:HA	1.80	0.61
3:F:50:LEU:O	3:F:53:PRO:HD2	2.00	0.61
1:G:278:GLN:CG	1:G:317:GLU:HB2	2.26	0.61
2:H:132:GLU:O	2:H:136:MET:HG2	1.99	0.61
3:I:50:LEU:O	3:I:53:PRO:HD2	2.00	0.61
1:J:542:PHE:CB	4:7:143:TYR:HE1	2.13	0.61
1:J:732:ILE:HG22	1:J:747:LEU:CD1	1.55	0.61
1:A:642:LYS:CG	4:4:22:ALA:C	2.67	0.61
1:A:686:MET:HG3	1:A:691:VAL:HG21	1.83	0.61
1:A:797:PHE:CD2	3:C:126:LEU:HD21	2.35	0.61
3:C:3:SER:HG	3:C:5:ALA:N	1.97	0.61
3:C:48:LYS:C	3:C:52:ASN:HD21	1.97	0.61
1:D:141:LEU:H	1:D:141:LEU:HD12	1.64	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:553:MLY:O	4:7:48:GLY:HA2	1.99	0.61
1:D:831:TRP:CZ2	2:E:47:LEU:C	2.70	0.61
1:G:728:ASN:HD21	3:I:110:VAL:CA	2.13	0.61
1:G:797:PHE:CB	3:I:149:VAL:HG11	2.29	0.61
1:J:411:GLU:N	4:7:333:PRO:HB2	2.11	0.61
1:A:99:GLU:OE2	1:A:696:ARG:NH2	2.30	0.61
1:D:274:ARG:HB2	1:D:285:TYR:CE2	2.34	0.61
1:D:634:GLY:N	4:5:25:ASP:O	2.31	0.61
2:E:114:LYS:HG3	2:E:146:GLY:HA2	1.82	0.61
1:G:81:ASN:OD1	1:G:96:HIS:HB2	2.00	0.61
1:G:161:ASN:HA	1:G:164:GLN:HE21	1.63	0.61
1:G:579:PHE:CE1	1:G:581:LEU:HD13	2.35	0.61
1:G:639:GLY:N	4:6:344:SER:C	2.54	0.61
1:G:732:ILE:HG22	1:G:747:LEU:CD1	1.55	0.61
2:H:144:VAL:HA	2:H:153:ILE:HD11	1.80	0.61
1:J:578:HIS:CB	1:J:592:ILE:HD12	2.30	0.61
1:J:642:LYS:CD	4:7:24:ASP:O	2.43	0.61
2:K:114:LYS:HG3	2:K:146:GLY:HA2	1.82	0.61
3:L:52:ASN:N	3:L:53:PRO:HD2	2.16	0.61
1:A:800:ARG:CD	3:C:149:VAL:CG2	2.41	0.61
2:B:117:LEU:HD11	2:B:147:ASN:HB3	1.76	0.61
1:D:831:TRP:CA	2:E:51:PHE:CE1	2.83	0.61
2:E:144:VAL:HA	2:E:153:ILE:HD11	1.80	0.61
1:G:541:MET:HE2	4:6:346:LEU:HD12	1.82	0.61
1:J:274:ARG:HB2	1:J:285:TYR:CE2	2.34	0.61
1:J:579:PHE:CE1	1:J:581:LEU:HD13	2.35	0.61
1:J:643:GLY:H	4:7:23:GLY:C	2.01	0.61
1:A:798:LEU:HD23	3:C:122:GLU:HB3	1.83	0.61
1:D:507:GLY:CA	1:D:762:HIS:CD2	2.84	0.61
1:D:541:MET:C	4:5:143:TYR:CZ	2.73	0.61
1:D:557:GLU:HG3	1:D:557:GLU:O	2.00	0.61
1:D:724:TYR:C	1:D:782:MLY:CH2	2.66	0.61
1:G:274:ARG:HB2	1:G:285:TYR:CE2	2.34	0.61
1:G:643:GLY:O	1:G:644:SER:CB	2.48	0.61
1:J:95:THR:HA	1:J:713:SER:HB3	1.82	0.61
1:J:99:GLU:OE2	1:J:696:ARG:NH2	2.30	0.61
1:J:623:PHE:CG	1:J:623:PHE:HA	2.35	0.61
1:J:813:ILE:O	1:J:817:GLN:N	2.30	0.61
1:A:530:MET:HE2	4:4:354:GLN:HG3	1.80	0.61
1:A:542:PHE:CB	4:4:143:TYR:HE1	2.12	0.61
2:B:111:SER:OG	2:B:148:VAL:CG1	2.47	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:541:MET:SD	4:5:346:LEU:O	2.48	0.61
1:D:686:MET:HG3	1:D:691:VAL:HG21	1.83	0.61
3:F:52:ASN:HB2	3:F:53:PRO:CD	2.28	0.61
1:G:524:GLU:O	1:G:528:MLY:HB3	2.01	0.61
1:G:821:ARG:HH22	2:H:127:ARG:HG2	0.78	0.61
1:J:302:MET:HG2	1:J:303:LEU:CD1	2.30	0.61
1:J:639:GLY:N	4:7:344:SER:C	2.54	0.61
1:J:643:GLY:O	1:J:644:SER:CB	2.49	0.61
2:B:34:ILE:O	2:B:46:ASP:HB3	2.01	0.61
1:D:217:THR:C	1:D:221:GLN:HG2	2.21	0.61
1:G:792:ALA:HA	3:I:35:ARG:CZ	2.31	0.61
2:H:144:VAL:CG1	2:H:153:ILE:HD13	2.19	0.61
1:J:93:MET:SD	1:J:764:MLY:HH23	2.33	0.61
2:B:114:LYS:HG3	2:B:146:GLY:HA2	1.82	0.61
3:C:63:ILE:HG22	3:C:64:THR:O	2.01	0.61
1:D:154:HIS:CE1	1:D:156:PHE:CD2	2.88	0.61
1:D:576:GLU:CG	1:D:577:ALA:N	2.44	0.61
1:D:579:PHE:CE1	1:D:581:LEU:HD13	2.35	0.61
3:F:49:ILE:HA	3:F:52:ASN:ND2	2.05	0.61
1:G:557:GLU:HG3	1:G:557:GLU:O	2.01	0.61
1:G:730:SER:OG	3:I:109:HIS:CE1	2.53	0.61
1:J:154:HIS:CE1	1:J:156:PHE:CD2	2.88	0.61
1:J:202:SER:HA	1:J:207:LYS:HE3	1.72	0.61
1:J:769:ALA:CB	1:J:770:GLY:HA3	2.28	0.61
4:5:223:PHE:HD2	4:5:312:ARG:NH2	1.99	0.61
1:A:411:GLU:N	4:4:333:PRO:HB2	2.11	0.61
1:D:643:GLY:O	1:D:644:SER:CB	2.48	0.61
1:D:643:GLY:H	4:5:23:GLY:C	2.02	0.61
3:F:52:ASN:N	3:F:53:PRO:HD2	2.15	0.61
1:G:94:MET:HE1	1:G:101:ALA:HB1	1.80	0.61
1:G:530:MET:HE3	4:6:354:GLN:CG	2.25	0.61
1:G:686:MET:HG3	1:G:691:VAL:HG21	1.83	0.61
1:G:732:ILE:HG21	1:G:747:LEU:HD11	0.72	0.61
1:G:769:ALA:O	1:G:773:GLY:HA2	2.01	0.61
1:G:838:ILE:CG1	2:H:54:MET:HE1	2.30	0.61
1:J:798:LEU:CD2	3:L:126:LEU:HG	2.18	0.61
3:L:50:LEU:O	3:L:53:PRO:HD2	2.00	0.61
4:4:223:PHE:HD2	4:4:312:ARG:NH2	1.99	0.61
1:A:40:VAL:HG22	1:A:41:VAL:N	2.16	0.60
1:A:156:PHE:CD1	1:A:195:TYR:CD1	2.89	0.60
1:D:530:MET:CG	4:5:354:GLN:HG3	2.30	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:578:HIS:CD2	1:D:591:ASN:HA	2.32	0.60
1:D:623:PHE:CG	1:D:623:PHE:HA	2.36	0.60
1:G:520:ALA:O	1:G:524:GLU:HG2	2.00	0.60
1:G:755:HIS:HA	1:G:758:TYR:HE1	1.64	0.60
2:H:114:LYS:HG3	2:H:146:GLY:HA2	1.82	0.60
1:J:524:GLU:O	1:J:528:MLY:HB3	2.01	0.60
1:J:795:ARG:CD	3:L:35:ARG:CZ	2.53	0.60
4:Z:223:PHE:HD2	4:Z:312:ARG:NH2	1.99	0.60
1:A:217:THR:C	1:A:221:GLN:HG2	2.21	0.60
1:A:524:GLU:O	1:A:528:MLY:HB3	2.01	0.60
1:A:813:ILE:CG2	2:B:127:ARG:CZ	2.68	0.60
3:C:52:ASN:N	3:C:53:PRO:HD2	2.16	0.60
1:D:38:VAL:HB	1:D:52:ILE:HD11	1.84	0.60
1:D:81:ASN:OD1	1:D:96:HIS:HB2	2.00	0.60
1:G:40:VAL:HG22	1:G:41:VAL:N	2.16	0.60
1:G:124:VAL:CG1	1:G:675:ILE:HD13	2.31	0.60
1:G:553:MLY:NZ	4:8:45:VAL:HG13	2.16	0.60
1:J:81:ASN:OD1	1:J:96:HIS:HB2	2.00	0.60
1:J:95:THR:HG23	1:J:96:HIS:ND1	2.17	0.60
1:J:520:ALA:O	1:J:524:GLU:HG2	2.00	0.60
1:J:543:PRO:HG2	4:7:143:TYR:O	1.98	0.60
1:J:665:ARG:C	1:J:667:THR:H	2.05	0.60
1:J:686:MET:HG3	1:J:691:VAL:HG21	1.83	0.60
2:K:34:ILE:O	2:K:46:ASP:HB3	2.01	0.60
4:2:223:PHE:HD2	4:2:312:ARG:NH2	1.99	0.60
1:A:557:GLU:HG3	1:A:557:GLU:O	2.00	0.60
1:A:665:ARG:C	1:A:667:THR:H	2.05	0.60
1:D:166:MET:HE3	1:D:254:PHE:HD2	1.66	0.60
1:D:410:ASN:CG	4:5:334:GLU:CA	2.47	0.60
1:D:721:LYS:HG2	1:D:736:GLN:CD	1.86	0.60
1:D:837:MLY:O	1:D:840:PRO:HD2	2.02	0.60
1:J:217:THR:C	1:J:221:GLN:HG2	2.21	0.60
1:A:553:MLY:NZ	4:6:45:VAL:HG13	2.16	0.60
1:J:530:MET:CG	4:7:354:GLN:HG3	2.30	0.60
1:A:40:VAL:HG22	1:A:41:VAL:H	1.67	0.60
1:A:124:VAL:CG1	1:A:675:ILE:HD13	2.31	0.60
1:A:546:THR:HG22	1:A:547:ASP:N	2.17	0.60
1:D:40:VAL:HG22	1:D:41:VAL:N	2.16	0.60
1:D:124:VAL:CG1	1:D:675:ILE:HD13	2.31	0.60
1:D:612:GLN:HE22	1:D:627:GLY:HA2	1.66	0.60
1:D:817:GLN:CG	2:E:127:ARG:CD	2.78	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:38:VAL:HB	1:G:52:ILE:HD11	1.83	0.60
1:G:623:PHE:CG	1:G:623:PHE:HA	2.36	0.60
1:G:730:SER:HB2	3:I:109:HIS:NE2	2.17	0.60
1:J:38:VAL:HB	1:J:52:ILE:HD11	1.83	0.60
1:J:546:THR:HG22	1:J:547:ASP:N	2.17	0.60
1:J:823:PHE:CD1	2:K:157:ILE:HA	2.36	0.60
1:J:837:MLY:O	1:J:840:PRO:HD2	2.02	0.60
2:K:130:PRO:HA	2:K:133:ILE:HD12	1.83	0.60
3:L:63:ILE:HG22	3:L:64:THR:O	2.01	0.60
4:6:223:PHE:HD2	4:6:312:ARG:NH2	1.99	0.60
4:Y:287:ILE:H	4:Y:287:ILE:HD12	1.67	0.60
1:A:38:VAL:HB	1:A:52:ILE:HD11	1.84	0.60
1:A:787:ILE:O	1:A:790:THR:N	2.35	0.60
1:D:530:MET:HA	4:5:354:GLN:CB	2.29	0.60
1:D:542:PHE:N	4:5:143:TYR:OH	2.32	0.60
2:E:34:ILE:O	2:E:46:ASP:HB3	2.01	0.60
1:G:542:PHE:CB	4:6:143:TYR:HE1	2.13	0.60
1:G:837:MLY:O	1:G:840:PRO:HD2	2.02	0.60
1:J:60:VAL:O	1:J:71:THR:HA	2.02	0.60
1:J:124:VAL:HG13	1:J:675:ILE:HD13	1.84	0.60
1:J:202:SER:CA	1:J:207:LYS:HE3	2.27	0.60
1:J:542:PHE:N	4:7:143:TYR:OH	2.33	0.60
4:2:287:ILE:H	4:2:287:ILE:HD12	1.67	0.60
4:3:223:PHE:HD2	4:3:312:ARG:NH2	1.99	0.60
4:5:287:ILE:H	4:5:287:ILE:HD12	1.67	0.60
4:V:287:ILE:H	4:V:287:ILE:HD12	1.67	0.60
4:X:223:PHE:HD2	4:X:312:ARG:NH2	1.99	0.60
1:A:504:MLY:HB2	1:A:762:HIS:CE1	2.37	0.60
1:A:550:PHE:CE2	1:A:592:ILE:HG23	2.37	0.60
1:A:837:MLY:O	1:A:840:PRO:HD2	2.02	0.60
1:D:524:GLU:O	1:D:528:MLY:HB3	2.01	0.60
1:D:639:GLY:N	4:5:344:SER:C	2.54	0.60
1:D:796:GLY:HA2	3:F:35:ARG:HB3	1.83	0.60
2:E:130:PRO:HA	2:E:133:ILE:HD12	1.84	0.60
2:E:144:VAL:CG1	2:E:153:ILE:HD13	2.19	0.60
1:G:60:VAL:O	1:G:71:THR:HA	2.02	0.60
1:G:84:MLY:CH1	1:G:716:LEU:O	2.50	0.60
1:G:156:PHE:CD1	1:G:195:TYR:CD1	2.90	0.60
1:J:40:VAL:HG22	1:J:41:VAL:N	2.16	0.60
1:J:124:VAL:CG1	1:J:675:ILE:HD13	2.31	0.60
1:J:578:HIS:CD2	1:J:591:ASN:HA	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:787:ILE:O	1:J:790:THR:N	2.35	0.60
4:3:287:ILE:H	4:3:287:ILE:HD12	1.67	0.60
4:X:287:ILE:H	4:X:287:ILE:HD12	1.67	0.60
4:Y:223:PHE:HD2	4:Y:312:ARG:NH2	1.99	0.60
1:A:60:VAL:O	1:A:71:THR:HA	2.02	0.60
1:A:634:GLY:N	4:4:25:ASP:O	2.31	0.60
1:J:827:MLY:HH21	2:K:139:ALA:HB3	1.83	0.60
4:7:287:ILE:HD12	4:7:287:ILE:H	1.67	0.60
1:A:506:GLU:OE2	1:A:760:PHE:CD2	2.49	0.60
1:A:542:PHE:CD1	4:4:143:TYR:CE1	2.90	0.60
3:C:46:ILE:O	3:C:50:LEU:CG	2.47	0.60
3:C:52:ASN:N	3:C:53:PRO:CD	2.65	0.60
1:D:49:MLY:HH13	1:D:108:GLU:OE2	2.02	0.60
1:D:124:VAL:HG13	1:D:675:ILE:HD13	1.84	0.60
1:D:553:MLY:NZ	4:7:45:VAL:HG13	2.16	0.60
1:D:665:ARG:C	1:D:667:THR:H	2.05	0.60
1:D:769:ALA:HA	1:D:771:LEU:HB2	1.81	0.60
1:D:789:ALA:O	3:F:87:PHE:CZ	2.55	0.60
1:J:786:ILE:HG12	3:L:86:ASP:CB	2.30	0.60
3:L:52:ASN:N	3:L:53:PRO:CD	2.65	0.60
4:0:223:PHE:HD2	4:0:312:ARG:NH2	1.99	0.60
4:0:287:ILE:H	4:0:287:ILE:HD12	1.67	0.60
4:Z:287:ILE:HD12	4:Z:287:ILE:H	1.67	0.60
1:A:95:THR:HG23	1:A:96:HIS:ND1	2.16	0.60
1:G:217:THR:C	1:G:221:GLN:HG2	2.21	0.60
1:G:578:HIS:CD2	1:G:591:ASN:HA	2.31	0.60
1:A:505:MLY:HH23	1:A:762:HIS:O	2.02	0.59
1:A:541:MET:SD	4:4:346:LEU:O	2.48	0.59
3:C:49:ILE:CA	3:C:52:ASN:ND2	2.53	0.59
1:D:536:LEU:HD13	1:D:550:PHE:CE1	2.37	0.59
1:D:755:HIS:HA	1:D:758:TYR:HE1	1.64	0.59
3:F:63:ILE:HG22	3:F:64:THR:O	2.01	0.59
1:G:665:ARG:C	1:G:667:THR:H	2.05	0.59
2:H:34:ILE:O	2:H:46:ASP:HB3	2.01	0.59
3:I:63:ILE:HG22	3:I:64:THR:O	2.01	0.59
1:J:768:MLY:CH2	1:J:772:LEU:HD13	2.32	0.59
1:J:820:VAL:CG1	2:K:136:MET:CE	2.80	0.59
4:4:287:ILE:H	4:4:287:ILE:HD12	1.67	0.59
1:D:60:VAL:O	1:D:71:THR:HA	2.02	0.59
1:D:95:THR:HG23	1:D:96:HIS:ND1	2.17	0.59
1:G:536:LEU:HD13	1:G:550:PHE:CE1	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:52:ASN:HB2	3:I:53:PRO:CD	2.28	0.59
3:I:52:ASN:N	3:I:53:PRO:CD	2.65	0.59
3:L:49:ILE:CA	3:L:52:ASN:ND2	2.54	0.59
4:1:287:ILE:H	4:1:287:ILE:HD12	1.67	0.59
4:W:287:ILE:H	4:W:287:ILE:HD12	1.67	0.59
1:A:530:MET:CG	4:4:354:GLN:HG3	2.30	0.59
1:A:536:LEU:HD13	1:A:550:PHE:CE1	2.37	0.59
1:D:549:SER:OG	1:D:550:PHE:N	2.36	0.59
1:G:541:MET:SD	4:6:346:LEU:O	2.48	0.59
1:G:546:THR:HG22	1:G:547:ASP:N	2.17	0.59
1:J:549:SER:OG	1:J:550:PHE:N	2.35	0.59
1:A:116:TYR:HB2	1:A:153:PRO:O	2.03	0.59
1:A:135:TYR:N	1:A:135:TYR:CD1	2.70	0.59
1:A:195:TYR:O	1:A:199:ILE:HG23	2.03	0.59
1:D:7:MET:HE3	1:D:14:ALA:HB1	1.84	0.59
1:D:599:ASN:CB	1:D:649:VAL:HB	2.32	0.59
1:D:776:GLU:O	1:D:779:ARG:HB3	2.03	0.59
1:D:783:LEU:O	1:D:787:ILE:N	2.28	0.59
1:D:787:ILE:O	1:D:790:THR:N	2.35	0.59
1:G:7:MET:HE3	1:G:14:ALA:HB1	1.83	0.59
1:G:550:PHE:CE2	1:G:592:ILE:HG23	2.37	0.59
1:G:787:ILE:O	1:G:790:THR:N	2.35	0.59
1:G:792:ALA:CB	3:I:40:ASN:HB3	2.32	0.59
1:J:156:PHE:CD1	1:J:195:TYR:CD1	2.90	0.59
1:J:530:MET:HA	4:7:354:GLN:CB	2.28	0.59
4:8:223:PHE:HD2	4:8:312:ARG:NH2	1.99	0.59
1:A:578:HIS:CD2	1:A:591:ASN:HA	2.31	0.59
1:A:623:PHE:CG	1:A:623:PHE:HA	2.36	0.59
1:A:776:GLU:O	1:A:779:ARG:HB3	2.03	0.59
1:G:530:MET:CG	4:6:354:GLN:HG3	2.30	0.59
1:G:538:GLU:HA	4:6:349:LEU:CG	2.28	0.59
1:G:728:ASN:HA	3:I:113:THR:OG1	2.03	0.59
1:G:817:GLN:OE1	2:H:127:ARG:CD	2.47	0.59
1:G:818:TYR:CG	2:H:127:ARG:NH1	2.70	0.59
3:I:52:ASN:N	3:I:53:PRO:HD2	2.16	0.59
1:J:542:PHE:CD1	4:7:143:TYR:CE1	2.91	0.59
4:W:223:PHE:HD2	4:W:312:ARG:NH2	1.99	0.59
1:A:295:MLY:HG3	1:A:332:MET:HE1	1.85	0.59
1:A:529:PRO:HG3	4:4:353:GLN:OE1	2.03	0.59
1:D:156:PHE:CD1	1:D:195:TYR:CD1	2.90	0.59
1:D:464:ILE:HG22	1:D:465:ALA:N	2.18	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:534:SER:C	4:5:351:THR:CA	2.47	0.59
1:G:599:ASN:CB	1:G:649:VAL:HB	2.32	0.59
1:J:49:MLY:HH13	1:J:108:GLU:OE2	2.02	0.59
1:J:230:GLU:O	1:J:234:ASN:HB2	2.03	0.59
1:A:735:GLY:O	1:A:743:ALA:HA	1.94	0.59
1:D:40:VAL:HG22	1:D:41:VAL:H	1.67	0.59
1:D:542:PHE:CD1	4:5:143:TYR:CE1	2.90	0.59
1:D:831:TRP:CH2	2:E:50:THR:HB	2.37	0.59
3:F:52:ASN:N	3:F:53:PRO:CD	2.65	0.59
1:G:40:VAL:HG22	1:G:41:VAL:H	1.67	0.59
1:G:93:MET:CB	1:G:716:LEU:HD12	2.33	0.59
1:G:195:TYR:O	1:G:199:ILE:HG23	2.03	0.59
1:G:549:SER:OG	1:G:550:PHE:N	2.36	0.59
1:G:646:PHE:CD2	1:G:652:LEU:CD1	2.85	0.59
1:G:715:VAL:HG11	1:G:720:PHE:HD1	1.68	0.59
1:G:836:PHE:CE1	2:H:159:HIS:CA	2.63	0.59
1:J:265:ILE:HG22	1:J:266:GLU:N	2.18	0.59
1:J:550:PHE:CE2	1:J:592:ILE:HG23	2.37	0.59
1:J:817:GLN:HG2	2:K:127:ARG:CB	2.32	0.59
4:1:223:PHE:HD2	4:1:312:ARG:NH2	1.99	0.59
1:A:48:VAL:HG22	1:A:49:MLY:N	2.18	0.59
1:A:265:ILE:HG22	1:A:266:GLU:N	2.18	0.59
1:D:601:ASP:N	1:D:602:PRO:HD3	2.18	0.59
1:D:724:TYR:CE1	1:D:778:MET:CG	2.86	0.59
1:G:542:PHE:CD1	4:6:143:TYR:CE1	2.91	0.59
1:J:599:ASN:CB	1:J:649:VAL:HB	2.32	0.59
1:A:230:GLU:O	1:A:234:ASN:HB2	2.03	0.59
1:D:792:ALA:CB	3:F:40:ASN:CB	2.75	0.59
1:G:116:TYR:HB2	1:G:153:PRO:O	2.03	0.59
1:J:776:GLU:O	1:J:779:ARG:HB3	2.02	0.59
1:J:784:ALA:O	1:J:788:THR:HB	2.02	0.59
4:V:223:PHE:HD2	4:V:312:ARG:NH2	1.99	0.59
1:A:599:ASN:CB	1:A:649:VAL:HB	2.32	0.59
1:A:601:ASP:N	1:A:602:PRO:HD3	2.18	0.59
1:A:755:HIS:HA	1:A:758:TYR:HE1	1.64	0.59
1:D:135:TYR:N	1:D:135:TYR:CD1	2.69	0.59
1:D:141:LEU:O	1:D:144:ARG:HB3	2.03	0.59
1:D:649:VAL:HA	1:D:649:VAL:HG22	1.80	0.59
1:D:817:GLN:NE2	2:E:127:ARG:CD	2.66	0.59
1:D:831:TRP:N	2:E:51:PHE:HZ	1.98	0.59
1:J:195:TYR:O	1:J:199:ILE:HG23	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:536:LEU:HD13	1:J:550:PHE:CE1	2.37	0.59
1:J:715:VAL:HG11	1:J:720:PHE:HD1	1.68	0.59
1:D:722:GLN:O	1:D:782:MLY:HH23	2.02	0.58
1:D:769:ALA:CB	1:D:771:LEU:N	2.66	0.58
1:G:95:THR:HG23	1:G:96:HIS:ND1	2.17	0.58
1:G:124:VAL:HG13	1:G:675:ILE:HD13	1.84	0.58
1:G:135:TYR:N	1:G:135:TYR:CD1	2.69	0.58
1:G:230:GLU:O	1:G:234:ASN:HB2	2.03	0.58
1:J:7:MET:HE3	1:J:14:ALA:HB1	1.85	0.58
1:J:210:GLN:O	1:J:211:SER:OG	2.15	0.58
1:J:601:ASP:N	1:J:602:PRO:HD3	2.18	0.58
1:J:643:GLY:HA2	4:7:24:ASP:OD1	2.04	0.58
4:6:287:ILE:H	4:6:287:ILE:HD12	1.67	0.58
1:A:538:GLU:O	1:A:541:MET:HB2	2.04	0.58
1:A:794:CYS:O	1:A:798:LEU:N	2.37	0.58
1:A:831:TRP:CH2	2:B:50:THR:CB	2.81	0.58
1:D:124:VAL:HG13	1:D:675:ILE:CD1	2.33	0.58
1:D:550:PHE:CE2	1:D:592:ILE:HG23	2.37	0.58
1:D:629:GLU:HB3	1:D:645:SER:N	2.18	0.58
1:J:553:MLY:NZ	4:V:45:VAL:HG13	2.17	0.58
1:J:754:ASP:OD2	1:J:776:GLU:HB3	2.01	0.58
1:A:410:ASN:CG	4:4:334:GLU:CA	2.48	0.58
1:A:549:SER:OG	1:A:550:PHE:N	2.36	0.58
1:D:529:PRO:HG3	4:5:353:GLN:OE1	2.03	0.58
1:D:794:CYS:O	1:D:798:LEU:N	2.36	0.58
1:G:265:ILE:HG22	1:G:266:GLU:N	2.18	0.58
1:G:464:ILE:HG22	1:G:465:ALA:N	2.18	0.58
2:H:130:PRO:HA	2:H:133:ILE:HD12	1.84	0.58
1:J:116:TYR:HB2	1:J:153:PRO:O	2.03	0.58
1:J:646:PHE:CD2	1:J:652:LEU:CD1	2.85	0.58
1:J:820:VAL:CG1	2:K:136:MET:HE1	2.33	0.58
1:A:7:MET:HE3	1:A:14:ALA:HB1	1.84	0.58
1:A:715:VAL:HG11	1:A:720:PHE:HD1	1.68	0.58
1:A:831:TRP:CZ3	2:B:34:ILE:HG12	2.39	0.58
2:B:140:PHE:O	2:B:141:PRO:C	2.33	0.58
1:D:218:LEU:N	1:D:221:GLN:HE21	2.01	0.58
1:D:643:GLY:HA2	4:5:24:ASP:OD1	2.04	0.58
1:D:813:ILE:O	1:D:817:GLN:N	2.30	0.58
1:G:601:ASP:N	1:G:602:PRO:HD3	2.18	0.58
1:G:642:LYS:CG	4:6:22:ALA:CA	2.80	0.58
1:J:40:VAL:HG22	1:J:41:VAL:H	1.67	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:629:GLU:HB3	1:J:645:SER:N	2.18	0.58
1:J:649:VAL:HA	1:J:649:VAL:HG22	1.80	0.58
3:L:52:ASN:HB2	3:L:53:PRO:CD	2.28	0.58
1:A:124:VAL:HG13	1:A:675:ILE:HD13	1.84	0.58
1:D:48:VAL:HG22	1:D:49:MLY:N	2.18	0.58
1:D:220:ASP:O	1:D:224:SER:N	2.27	0.58
1:D:546:THR:HG22	1:D:547:ASP:N	2.17	0.58
1:D:715:VAL:HG11	1:D:720:PHE:HD1	1.68	0.58
1:G:629:GLU:HB3	1:G:645:SER:N	2.18	0.58
1:G:751:GLY:HA2	3:I:114:LEU:CD1	2.24	0.58
1:G:836:PHE:CE2	2:H:160:GLY:CA	2.86	0.58
1:J:48:VAL:HG22	1:J:49:MLY:N	2.18	0.58
1:J:135:TYR:N	1:J:135:TYR:CD1	2.69	0.58
1:J:529:PRO:HG3	4:7:353:GLN:OE1	2.04	0.58
4:8:287:ILE:H	4:8:287:ILE:HD12	1.67	0.58
1:A:839:MLY:CD	2:B:159:HIS:HB3	2.33	0.58
1:D:127:ASN:ND2	1:D:128:PRO:HD2	2.16	0.58
1:D:230:GLU:O	1:D:234:ASN:HB2	2.03	0.58
1:D:538:GLU:O	1:D:541:MET:HB2	2.04	0.58
1:G:124:VAL:HG13	1:G:675:ILE:CD1	2.33	0.58
1:G:508:ILE:CD1	1:G:759:ALA:CB	2.49	0.58
1:G:538:GLU:O	1:G:541:MET:HB2	2.04	0.58
1:G:776:GLU:O	1:G:779:ARG:HB3	2.03	0.58
1:J:218:LEU:N	1:J:221:GLN:HE21	2.01	0.58
1:J:510:TRP:CE2	1:J:768:MLY:CH1	2.86	0.58
1:A:64:THR:HG22	1:A:65:GLU:N	2.19	0.58
1:A:124:VAL:HG13	1:A:675:ILE:CD1	2.33	0.58
1:D:175:ILE:HA	1:D:670:HIS:O	2.03	0.58
1:G:64:THR:HG22	1:G:65:GLU:N	2.19	0.58
1:G:254:PHE:CE2	1:G:459:ILE:HD12	2.39	0.58
1:G:831:TRP:CE2	2:H:67:MET:CG	2.86	0.58
1:G:831:TRP:CE2	2:H:67:MET:HB3	2.38	0.58
1:J:127:ASN:ND2	1:J:128:PRO:HD2	2.16	0.58
1:J:175:ILE:HA	1:J:670:HIS:O	2.03	0.58
1:J:755:HIS:HA	1:J:758:TYR:HE1	1.64	0.58
3:L:102:VAL:HG11	3:L:107:LEU:HB2	1.84	0.58
2:B:130:PRO:HA	2:B:133:ILE:HD12	1.84	0.58
1:D:818:TYR:HB2	2:E:90:GLY:HA3	1.86	0.58
1:J:279:LEU:HB3	1:J:280:PRO:HD2	1.86	0.58
1:J:464:ILE:HG22	1:J:465:ALA:N	2.18	0.58
1:J:481:ASN:N	1:J:481:ASN:ND2	2.51	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:MLY:HH13	1:A:108:GLU:OE2	2.03	0.58
1:A:141:LEU:O	1:A:144:ARG:HB3	2.03	0.58
1:A:175:ILE:HA	1:A:670:HIS:O	2.04	0.58
1:A:409:GLY:HA3	4:4:333:PRO:CD	2.34	0.58
1:A:541:MET:C	4:4:143:TYR:CZ	2.73	0.58
1:A:642:LYS:CG	4:4:22:ALA:CA	2.81	0.58
1:D:279:LEU:HB3	1:D:280:PRO:HD2	1.86	0.58
1:D:724:TYR:CA	1:D:782:MLY:CH2	2.81	0.58
1:D:735:GLY:O	1:D:743:ALA:HA	1.94	0.58
1:G:529:PRO:HG3	4:6:353:GLN:OE1	2.04	0.58
1:G:568:PRO:HG3	1:G:578:HIS:H	1.69	0.58
1:D:254:PHE:CE2	1:D:459:ILE:HD12	2.39	0.58
1:D:506:GLU:OE2	1:D:764:MLY:HH22	2.04	0.58
1:G:48:VAL:HG22	1:G:49:MLY:N	2.18	0.58
1:J:538:GLU:O	1:J:541:MET:HB2	2.03	0.58
1:A:813:ILE:O	1:A:817:GLN:N	2.30	0.57
1:A:814:PHE:CA	2:B:127:ARG:HH22	2.17	0.57
3:C:102:VAL:HG11	3:C:107:LEU:HB2	1.85	0.57
1:D:817:GLN:OE1	2:E:127:ARG:NH2	2.37	0.57
2:E:112:ILE:C	2:E:147:ASN:O	2.42	0.57
1:G:49:MLY:HH13	1:G:108:GLU:OE2	2.03	0.57
1:G:84:MLY:CH1	1:G:719:ASP:C	2.50	0.57
1:G:141:LEU:O	1:G:144:ARG:HB3	2.03	0.57
1:J:95:THR:HA	1:J:713:SER:CA	2.32	0.57
1:J:124:VAL:HG13	1:J:675:ILE:CD1	2.33	0.57
1:J:541:MET:SD	4:7:346:LEU:O	2.48	0.57
1:A:464:ILE:HG22	1:A:465:ALA:N	2.18	0.57
1:A:629:GLU:HB3	1:A:645:SER:N	2.18	0.57
1:A:676:ILE:HG23	1:A:676:ILE:O	2.03	0.57
1:A:831:TRP:CZ2	2:B:51:PHE:CZ	2.88	0.57
1:D:265:ILE:HG22	1:D:266:GLU:N	2.18	0.57
1:D:322:VAL:HG11	1:D:325:ILE:HD11	1.86	0.57
1:D:676:ILE:HG23	1:D:676:ILE:O	2.03	0.57
1:D:717:TYR:HD1	1:D:744:SER:HG	1.52	0.57
1:G:99:GLU:OE2	1:G:696:ARG:NH2	2.30	0.57
1:G:279:LEU:HB3	1:G:280:PRO:HD2	1.86	0.57
1:G:411:GLU:N	4:6:333:PRO:HB2	2.10	0.57
1:A:254:PHE:CE2	1:A:459:ILE:HD12	2.39	0.57
1:A:783:LEU:O	1:A:787:ILE:N	2.28	0.57
1:D:541:MET:HG2	4:5:345:ILE:CG2	2.35	0.57
1:D:831:TRP:CD2	2:E:51:PHE:CZ	2.92	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:102:VAL:HG11	3:F:107:LEU:HB2	1.84	0.57
1:G:295:MLY:HG3	1:G:332:MET:HE1	1.87	0.57
1:J:322:VAL:HG11	1:J:325:ILE:HD11	1.86	0.57
1:J:717:TYR:HD1	1:J:744:SER:HG	1.52	0.57
1:A:279:LEU:HB3	1:A:280:PRO:HD2	1.86	0.57
1:A:418:THR:HG22	1:A:419:VAL:H	1.69	0.57
1:A:831:TRP:CD2	2:B:51:PHE:CZ	2.88	0.57
1:D:418:THR:HG22	1:D:419:VAL:H	1.69	0.57
1:G:409:GLY:HA3	4:6:333:PRO:CD	2.35	0.57
1:G:813:ILE:O	1:G:816:ILE:N	2.37	0.57
3:I:102:VAL:HG11	3:I:107:LEU:HB2	1.85	0.57
1:J:64:THR:HG22	1:J:65:GLU:N	2.19	0.57
1:J:254:PHE:CE2	1:J:459:ILE:HD12	2.39	0.57
1:J:676:ILE:HG23	1:J:676:ILE:O	2.03	0.57
1:J:784:ALA:O	1:J:788:THR:CB	2.52	0.57
1:A:220:ASP:O	1:A:224:SER:N	2.27	0.57
1:A:635:GLY:HA3	4:4:334:GLU:CG	2.30	0.57
1:A:768:MLY:C	1:A:771:LEU:HB3	2.35	0.57
2:B:112:ILE:C	2:B:147:ASN:O	2.42	0.57
1:D:64:THR:HG22	1:D:65:GLU:N	2.19	0.57
1:D:195:TYR:O	1:D:199:ILE:HG23	2.03	0.57
1:D:831:TRP:CA	2:E:51:PHE:HE1	2.17	0.57
1:G:218:LEU:N	1:G:221:GLN:HE21	2.01	0.57
1:G:508:ILE:HD11	1:G:759:ALA:HB2	0.75	0.57
1:J:91:MET:HE3	1:J:119:SER:HB2	1.85	0.57
1:J:409:GLY:HA3	4:7:333:PRO:CD	2.35	0.57
1:J:794:CYS:O	1:J:798:LEU:N	2.36	0.57
1:A:173:GLN:C	1:A:667:THR:HG23	2.25	0.57
1:A:541:MET:HG2	4:4:345:ILE:CG2	2.35	0.57
1:A:818:TYR:HB2	2:B:90:GLY:HA3	1.86	0.57
3:C:102:VAL:HG23	3:C:139:TYR:CD1	2.39	0.57
1:D:22:LYS:O	1:D:26:GLU:N	2.29	0.57
1:D:173:GLN:C	1:D:667:THR:HG23	2.25	0.57
1:D:579:PHE:CD2	1:D:592:ILE:HD11	2.39	0.57
1:D:822:SER:HG	2:E:87:LYS:C	2.07	0.57
3:F:102:VAL:HG23	3:F:139:TYR:CD1	2.39	0.57
1:G:599:ASN:CG	1:G:649:VAL:HB	2.25	0.57
1:G:813:ILE:O	1:G:817:GLN:N	2.30	0.57
1:J:82:PRO:HD2	1:J:85:TYR:CD2	2.40	0.57
1:J:141:LEU:O	1:J:144:ARG:HB3	2.04	0.57
1:J:541:MET:HG2	4:7:345:ILE:CG2	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:789:ALA:HB2	3:L:81:GLN:HG2	1.86	0.57
1:A:218:LEU:N	1:A:221:GLN:HE21	2.02	0.57
1:D:409:GLY:HA3	4:5:333:PRO:CD	2.35	0.57
1:D:834:LEU:HD21	2:E:54:MET:HE2	1.86	0.57
1:G:175:ILE:HA	1:G:670:HIS:O	2.04	0.57
1:J:173:GLN:C	1:J:667:THR:HG23	2.25	0.57
1:J:752:ASP:O	1:J:780:ASP:OD2	2.23	0.57
1:A:322:VAL:HG11	1:A:325:ILE:HD11	1.86	0.57
1:A:502:GLU:CG	1:A:761:GLY:C	2.69	0.57
1:A:639:GLY:N	4:4:344:SER:C	2.54	0.57
1:D:82:PRO:HD2	1:D:85:TYR:CD2	2.40	0.57
1:D:116:TYR:HB2	1:D:153:PRO:O	2.03	0.57
1:D:813:ILE:O	1:D:816:ILE:N	2.38	0.57
1:D:830:PRO:C	2:E:51:PHE:CE1	2.78	0.57
1:G:173:GLN:C	1:G:667:THR:HG23	2.25	0.57
1:G:642:LYS:CD	4:6:340:TRP:CZ3	2.80	0.57
1:A:109:ARG:O	1:A:114:MET:N	2.37	0.57
1:A:643:GLY:HA2	4:4:24:ASP:OD1	2.04	0.57
1:A:813:ILE:O	1:A:816:ILE:N	2.37	0.57
1:D:481:ASN:N	1:D:481:ASN:ND2	2.51	0.57
1:D:530:MET:CA	4:5:354:GLN:HB3	2.35	0.57
1:J:530:MET:CA	4:7:354:GLN:HB3	2.35	0.57
1:J:579:PHE:CD2	1:J:592:ILE:HD11	2.40	0.57
1:J:783:LEU:O	1:J:787:ILE:CB	2.52	0.57
1:A:529:PRO:CG	4:4:353:GLN:OE1	2.53	0.57
1:A:768:MLY:HB3	1:A:771:LEU:CG	2.35	0.57
1:A:795:ARG:NH2	3:C:116:GLU:CG	2.68	0.57
1:D:646:PHE:CD2	1:D:652:LEU:CD1	2.85	0.57
1:D:724:TYR:OH	1:D:778:MET:SD	2.63	0.57
1:G:82:PRO:HD2	1:G:85:TYR:CD2	2.40	0.57
1:G:612:GLN:HE22	1:G:627:GLY:HA2	1.66	0.57
1:G:820:VAL:CG1	2:H:136:MET:HE1	2.34	0.57
1:J:747:LEU:O	1:J:747:LEU:HD23	2.05	0.57
1:A:82:PRO:HD2	1:A:85:TYR:CD2	2.40	0.56
1:A:599:ASN:CG	1:A:649:VAL:HB	2.25	0.56
1:A:795:ARG:CG	3:C:118:MET:CE	2.82	0.56
1:A:830:PRO:HG2	2:B:67:MET:HE1	1.87	0.56
1:D:599:ASN:CG	1:D:649:VAL:HB	2.25	0.56
1:D:831:TRP:HE1	2:E:47:LEU:HD22	1.58	0.56
1:G:541:MET:HG2	4:6:345:ILE:CG2	2.35	0.56
1:G:747:LEU:HD23	1:G:747:LEU:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:797:PHE:HE2	3:I:126:LEU:HD23	1.69	0.56
1:G:831:TRP:CZ2	2:H:67:MET:HB3	2.40	0.56
1:J:677:PRO:HB2	1:J:678:ASN:ND2	2.20	0.56
1:J:768:MLY:NZ	1:J:772:LEU:CD2	2.40	0.56
1:A:481:ASN:N	1:A:481:ASN:ND2	2.51	0.56
1:A:753:VAL:HG12	1:A:775:LEU:HG	1.86	0.56
1:A:834:LEU:HD21	2:B:54:MET:CG	2.35	0.56
1:D:411:GLU:H	4:5:333:PRO:HG2	1.70	0.56
1:D:568:PRO:HG3	1:D:578:HIS:H	1.69	0.56
1:D:724:TYR:CZ	1:D:778:MET:HB3	2.37	0.56
1:D:733:PRO:CB	1:D:737:PHE:HE1	2.19	0.56
1:J:821:ARG:NH2	2:K:127:ARG:HD3	2.18	0.56
3:L:46:ILE:O	3:L:50:LEU:CG	2.47	0.56
3:L:102:VAL:HG23	3:L:139:TYR:CD1	2.39	0.56
1:A:135:TYR:N	1:A:135:TYR:HD1	2.04	0.56
1:A:302:MET:HG2	1:A:303:LEU:HD13	1.87	0.56
1:A:411:GLU:H	4:4:333:PRO:HG2	1.71	0.56
1:A:568:PRO:HG3	1:A:578:HIS:H	1.69	0.56
1:A:640:LYS:C	4:4:23:GLY:CA	2.64	0.56
1:A:733:PRO:CA	1:A:737:PHE:HE1	2.19	0.56
1:A:831:TRP:CH2	2:B:50:THR:CG2	2.88	0.56
1:D:22:LYS:HA	1:D:25:ILE:HB	1.87	0.56
1:D:733:PRO:CA	1:D:737:PHE:HE1	2.18	0.56
1:D:831:TRP:NE1	2:E:67:MET:SD	2.77	0.56
2:E:163:ALA:C	2:K:22:THR:CB	2.74	0.56
1:G:302:MET:HG2	1:G:303:LEU:HD13	1.88	0.56
1:G:322:VAL:HG11	1:G:325:ILE:HD11	1.86	0.56
1:G:338:ILE:HG21	1:G:348:MLY:HB3	1.87	0.56
1:G:642:LYS:CA	4:6:22:ALA:C	2.70	0.56
1:G:643:GLY:N	4:6:23:GLY:C	2.55	0.56
1:G:676:ILE:HG23	1:G:676:ILE:O	2.03	0.56
1:G:677:PRO:HB2	1:G:678:ASN:ND2	2.20	0.56
1:G:757:GLN:NE2	1:G:772:LEU:HG	2.20	0.56
2:H:112:ILE:C	2:H:147:ASN:O	2.42	0.56
3:I:102:VAL:HG23	3:I:139:TYR:CD1	2.39	0.56
1:J:568:PRO:HG3	1:J:578:HIS:H	1.69	0.56
1:J:735:GLY:O	1:J:743:ALA:HA	1.94	0.56
1:J:813:ILE:O	1:J:816:ILE:N	2.37	0.56
4:7:223:PHE:HD2	4:7:312:ARG:NH2	1.99	0.56
1:A:210:GLN:O	1:A:211:SER:OG	2.15	0.56
1:A:630:ALA:CA	4:4:25:ASP:OD2	2.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:MLY:HG2	1:A:771:LEU:HD13	1.87	0.56
1:A:800:ARG:HD2	3:C:149:VAL:CA	2.35	0.56
1:A:830:PRO:HG2	2:B:67:MET:HE2	1.87	0.56
1:A:839:MLY:HD2	2:B:159:HIS:CD2	2.38	0.56
1:D:135:TYR:N	1:D:135:TYR:HD1	2.04	0.56
1:D:677:PRO:HB2	1:D:678:ASN:ND2	2.20	0.56
1:D:786:ILE:HG12	3:F:86:ASP:HB3	1.87	0.56
1:D:815:CYS:HA	2:E:90:GLY:HA2	1.87	0.56
1:J:418:THR:HG22	1:J:419:VAL:H	1.69	0.56
1:J:638:GLY:CA	4:7:345:ILE:H	2.18	0.56
1:A:649:VAL:HA	1:A:649:VAL:HG23	1.83	0.56
1:A:677:PRO:HB2	1:A:678:ASN:ND2	2.20	0.56
1:A:753:VAL:CG1	1:A:775:LEU:HG	2.36	0.56
1:A:834:LEU:HD21	2:B:54:MET:CE	2.36	0.56
3:C:48:LYS:C	3:C:52:ASN:HD22	1.97	0.56
1:D:116:TYR:CE2	1:D:154:HIS:CD2	2.94	0.56
1:D:406:VAL:HG12	1:D:407:GLY:H	1.71	0.56
1:G:733:PRO:CA	1:G:737:PHE:HE1	2.19	0.56
1:G:817:GLN:HG2	2:H:127:ARG:CD	2.34	0.56
1:J:116:TYR:CE2	1:J:154:HIS:CD2	2.94	0.56
1:J:338:ILE:HG21	1:J:348:MLY:HB3	1.87	0.56
1:A:338:ILE:HG21	1:A:348:MLY:HB3	1.87	0.56
1:A:546:THR:HG21	1:A:548:THR:HB	1.88	0.56
1:A:646:PHE:CD2	1:A:652:LEU:CD1	2.85	0.56
1:A:649:VAL:HG22	1:A:649:VAL:HA	1.80	0.56
1:A:733:PRO:CB	1:A:737:PHE:HE1	2.19	0.56
2:B:150:TYR:C	2:B:151:LYS:CG	2.49	0.56
1:G:135:TYR:N	1:G:135:TYR:HD1	2.04	0.56
1:J:599:ASN:CG	1:J:649:VAL:HB	2.25	0.56
1:A:116:TYR:CE2	1:A:154:HIS:CD2	2.94	0.56
1:A:747:LEU:HD23	1:A:747:LEU:O	2.05	0.56
1:A:768:MLY:CG	1:A:771:LEU:HD13	2.35	0.56
1:A:797:PHE:HD2	3:C:126:LEU:CD2	2.18	0.56
1:D:215:GLN:CA	1:D:340:ILE:CG2	2.63	0.56
1:D:834:LEU:HD22	2:E:50:THR:HG22	1.87	0.56
1:G:84:MLY:HH11	1:G:720:PHE:CA	2.35	0.56
1:G:638:GLY:CA	4:6:345:ILE:H	2.18	0.56
1:G:643:GLY:HA2	4:6:24:ASP:OD1	2.04	0.56
1:J:95:THR:HA	1:J:713:SER:CB	2.36	0.56
1:J:135:TYR:N	1:J:135:TYR:HD1	2.04	0.56
1:J:503:TYR:OH	1:J:711:PHE:CD2	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:630:ALA:CA	4:7:25:ASP:OD2	2.53	0.56
1:J:754:ASP:OD1	1:J:779:ARG:HD2	2.06	0.56
1:A:206:LYS:HB3	1:A:217:THR:OG1	2.06	0.56
1:A:502:GLU:HA	1:A:762:HIS:H	1.71	0.56
1:A:530:MET:CA	4:4:354:GLN:HB3	2.34	0.56
1:A:795:ARG:HG2	3:C:118:MET:CE	2.35	0.56
1:D:435:GLU:O	1:D:438:PHE:HB3	2.06	0.56
1:D:747:LEU:HD23	1:D:747:LEU:O	2.05	0.56
1:D:834:LEU:CD2	2:E:54:MET:CG	2.61	0.56
1:G:109:ARG:O	1:G:114:MET:N	2.37	0.56
1:G:538:GLU:CG	4:6:351:THR:C	2.73	0.56
1:A:217:THR:HG22	1:A:218:LEU:O	2.05	0.56
1:D:99:GLU:OE2	1:D:696:ARG:NH2	2.31	0.56
1:D:529:PRO:CB	4:5:354:GLN:HA	2.36	0.56
1:D:529:PRO:CG	4:5:353:GLN:OE1	2.53	0.56
1:G:410:ASN:CG	4:6:334:GLU:C	2.64	0.56
1:G:529:PRO:CG	4:6:353:GLN:OE1	2.54	0.56
1:G:649:VAL:CG1	1:G:649:VAL:HA	2.35	0.56
1:G:733:PRO:CB	1:G:737:PHE:HE1	2.19	0.56
1:J:503:TYR:HH	1:J:711:PHE:HD2	0.72	0.56
1:J:530:MET:CB	4:7:354:GLN:HG3	2.36	0.56
1:A:22:LYS:O	1:A:26:GLU:HG3	2.06	0.56
1:A:546:THR:HB	1:A:549:SER:H	1.71	0.56
1:D:290:GLN:HG2	1:D:331:LEU:HA	1.87	0.56
1:D:630:ALA:CA	4:5:25:ASP:OD2	2.53	0.56
1:D:640:LYS:C	1:D:645:SER:OG	2.44	0.56
1:G:22:LYS:O	1:G:26:GLU:HG3	2.06	0.56
1:G:217:THR:HG22	1:G:218:LEU:O	2.06	0.56
1:G:418:THR:HG22	1:G:419:VAL:H	1.69	0.56
1:G:435:GLU:O	1:G:438:PHE:HB3	2.06	0.56
1:G:537:GLU:HB3	1:G:648:THR:CB	2.36	0.56
1:G:794:CYS:O	1:G:798:LEU:N	2.37	0.56
3:I:46:ILE:O	3:I:50:LEU:CG	2.47	0.56
1:J:530:MET:HE3	4:7:354:GLN:CG	2.30	0.56
1:J:629:GLU:O	1:J:643:GLY:HA3	2.06	0.56
1:J:733:PRO:CA	1:J:737:PHE:HE1	2.19	0.56
1:A:97:LEU:HD22	1:A:712:PRO:CB	2.32	0.55
1:A:290:GLN:HG2	1:A:331:LEU:HA	1.87	0.55
1:A:530:MET:HE3	4:4:354:GLN:CB	2.37	0.55
1:A:797:PHE:HD2	3:C:126:LEU:HD21	1.71	0.55
1:A:798:LEU:CD1	3:C:126:LEU:CG	2.79	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:PHE:CG	1:D:83:PRO:HD3	2.41	0.55
1:D:789:ALA:C	3:F:87:PHE:CZ	2.79	0.55
1:G:206:LYS:HB3	1:G:217:THR:OG1	2.06	0.55
1:G:411:GLU:H	4:6:333:PRO:HG2	1.70	0.55
1:G:530:MET:CA	4:6:354:GLN:HB3	2.35	0.55
1:G:649:VAL:HA	1:G:649:VAL:HG22	1.80	0.55
1:G:820:VAL:CG1	2:H:136:MET:CE	2.84	0.55
1:J:90:ASP:OD2	1:J:764:MLY:HH22	2.05	0.55
4:7:365:ALA:HB3	4:7:369:ILE:HB	1.88	0.55
1:A:529:PRO:CB	4:4:354:GLN:HA	2.36	0.55
1:A:538:GLU:CG	4:4:351:THR:C	2.74	0.55
1:A:640:LYS:C	1:A:645:SER:OG	2.44	0.55
1:D:638:GLY:CA	4:5:345:ILE:H	2.19	0.55
1:D:725:ARG:H	1:D:782:MLY:HH21	1.65	0.55
1:G:84:MLY:HH12	1:G:716:LEU:O	2.05	0.55
1:G:116:TYR:CE2	1:G:154:HIS:CD2	2.94	0.55
1:J:217:THR:HG22	1:J:218:LEU:O	2.05	0.55
1:J:750:GLY:HA2	3:L:114:LEU:HD23	1.87	0.55
4:V:365:ALA:HB3	4:V:369:ILE:HB	1.88	0.55
1:A:32:PHE:CG	1:A:83:PRO:HD3	2.42	0.55
1:D:530:MET:HE3	4:5:355:MET:SD	2.46	0.55
1:D:537:GLU:HB3	1:D:648:THR:CB	2.36	0.55
1:D:546:THR:HG21	1:D:548:THR:HB	1.88	0.55
2:E:162:ASP:O	2:K:21:GLU:HB2	2.07	0.55
1:J:206:LYS:HB3	1:J:217:THR:OG1	2.06	0.55
1:J:579:PHE:HE1	1:J:581:LEU:HD13	1.72	0.55
1:J:634:GLY:N	4:7:25:ASP:O	2.31	0.55
1:J:733:PRO:CB	1:J:737:PHE:HE1	2.19	0.55
3:L:123:VAL:O	3:L:127:MET:HG2	2.06	0.55
1:A:290:GLN:NE2	1:A:334:THR:OG1	2.40	0.55
1:A:345:ALA:O	1:A:349:THR:N	2.40	0.55
1:A:537:GLU:HB3	1:A:648:THR:CB	2.36	0.55
1:A:629:GLU:O	1:A:643:GLY:HA3	2.06	0.55
1:A:765:VAL:HG12	1:A:766:PHE:N	2.22	0.55
1:A:793:ARG:NH2	3:C:147:MET:HE2	2.22	0.55
1:D:217:THR:HG22	1:D:218:LEU:O	2.06	0.55
1:D:629:GLU:O	1:D:643:GLY:HA3	2.06	0.55
1:D:789:ALA:HB2	3:F:81:GLN:O	2.06	0.55
1:G:127:ASN:ND2	1:G:128:PRO:HD2	2.17	0.55
1:G:732:ILE:CG2	1:G:747:LEU:HD11	1.26	0.55
1:J:643:GLY:N	4:7:23:GLY:C	2.55	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:646:PHE:CE2	1:J:652:LEU:CG	2.90	0.55
4:5:365:ALA:HB3	4:5:369:ILE:HB	1.88	0.55
1:A:7:MET:HE3	1:A:14:ALA:CB	2.36	0.55
1:A:406:VAL:HG12	1:A:407:GLY:H	1.71	0.55
1:A:604:ASN:OD1	1:A:607:VAL:HG23	2.06	0.55
1:D:604:ASN:OD1	1:D:607:VAL:HG23	2.06	0.55
1:D:646:PHE:CE2	1:D:652:LEU:CG	2.90	0.55
1:G:22:LYS:HA	1:G:25:ILE:HB	1.87	0.55
1:G:93:MET:HB2	1:G:764:MLY:NZ	2.18	0.55
1:G:629:GLU:O	1:G:643:GLY:HA3	2.06	0.55
1:G:646:PHE:CE2	1:G:652:LEU:CG	2.90	0.55
1:J:7:MET:HE3	1:J:14:ALA:CB	2.36	0.55
1:J:302:MET:HG2	1:J:303:LEU:HD13	1.87	0.55
1:J:406:VAL:HG12	1:J:407:GLY:H	1.71	0.55
1:J:640:LYS:C	1:J:645:SER:OG	2.44	0.55
1:J:768:MLY:CH2	1:J:772:LEU:CD1	2.83	0.55
3:L:35:ARG:HA	3:L:39:GLN:O	2.07	0.55
4:1:365:ALA:HB3	4:1:369:ILE:HB	1.88	0.55
1:A:612:GLN:HE22	1:A:627:GLY:HA2	1.66	0.55
2:E:156:VAL:HA	2:E:159:HIS:O	2.07	0.55
1:G:579:PHE:HE1	1:G:581:LEU:HD13	1.72	0.55
1:G:604:ASN:OD1	1:G:607:VAL:HG23	2.06	0.55
1:G:795:ARG:HE	3:I:118:MET:HE1	1.72	0.55
1:J:32:PHE:CG	1:J:83:PRO:HD3	2.41	0.55
1:J:410:ASN:CG	4:7:334:GLU:C	2.65	0.55
1:J:435:GLU:O	1:J:438:PHE:HB3	2.06	0.55
4:X:365:ALA:HB3	4:X:369:ILE:HB	1.88	0.55
1:A:530:MET:CB	4:4:354:GLN:HG3	2.36	0.55
1:A:642:LYS:CA	4:4:22:ALA:C	2.71	0.55
1:A:725:ARG:HG3	1:A:733:PRO:CA	2.36	0.55
1:A:757:GLN:OE1	1:A:771:LEU:HD12	2.06	0.55
1:D:338:ILE:HG21	1:D:348:MLY:HB3	1.87	0.55
1:D:530:MET:CB	4:5:354:GLN:HG3	2.36	0.55
1:G:7:MET:HE3	1:G:14:ALA:CB	2.37	0.55
1:G:290:GLN:NE2	1:G:334:THR:OG1	2.40	0.55
1:G:546:THR:HB	1:G:549:SER:H	1.71	0.55
3:I:35:ARG:HA	3:I:39:GLN:O	2.07	0.55
1:J:22:LYS:HA	1:J:25:ILE:HB	1.87	0.55
1:J:82:PRO:HD2	1:J:85:TYR:HD2	1.72	0.55
1:J:345:ALA:O	1:J:349:THR:N	2.40	0.55
1:J:529:PRO:CB	4:7:354:GLN:HA	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:725:ARG:HG3	1:J:733:PRO:CA	2.36	0.55
4:3:365:ALA:HB3	4:3:369:ILE:HB	1.88	0.55
1:D:302:MET:HG2	1:D:303:LEU:HD13	1.87	0.55
1:D:723:ARG:HH21	1:D:783:LEU:HD11	1.71	0.55
1:G:640:LYS:C	1:G:645:SER:OG	2.44	0.55
2:H:156:VAL:HA	2:H:159:HIS:O	2.07	0.55
1:J:411:GLU:H	4:7:333:PRO:HG2	1.71	0.55
1:J:635:GLY:HA3	4:7:334:GLU:CG	2.30	0.55
2:K:156:VAL:HA	2:K:159:HIS:O	2.07	0.55
1:A:292:MET:HE1	1:A:309:PRO:CD	2.37	0.55
1:A:646:PHE:CE2	1:A:652:LEU:CG	2.90	0.55
1:A:817:GLN:NE2	2:B:127:ARG:CG	2.70	0.55
3:C:35:ARG:HA	3:C:39:GLN:O	2.07	0.55
1:D:7:MET:HE3	1:D:14:ALA:CB	2.36	0.55
1:D:135:TYR:HD2	1:D:191:ARG:HG2	1.72	0.55
1:D:206:LYS:HB3	1:D:217:THR:OG1	2.07	0.55
2:E:121:LEU:CA	2:E:128:PHE:CG	2.89	0.55
3:F:46:ILE:O	3:F:50:LEU:CG	2.47	0.55
1:G:290:GLN:HG2	1:G:331:LEU:HA	1.87	0.55
1:G:730:SER:HG	3:I:109:HIS:CG	2.20	0.55
1:G:751:GLY:N	3:I:114:LEU:HD11	2.21	0.55
2:H:121:LEU:CA	2:H:128:PHE:CG	2.89	0.55
2:H:140:PHE:O	2:H:141:PRO:C	2.33	0.55
1:J:290:GLN:HG2	1:J:331:LEU:HA	1.88	0.55
1:J:529:PRO:CG	4:7:353:GLN:OE1	2.54	0.55
1:J:723:ARG:HH11	1:J:723:ARG:CG	2.20	0.55
4:Y:365:ALA:HB3	4:Y:369:ILE:HB	1.88	0.55
1:A:127:ASN:ND2	1:A:128:PRO:HD2	2.16	0.55
1:A:643:GLY:N	4:4:23:GLY:C	2.55	0.55
1:A:723:ARG:CG	1:A:723:ARG:HH11	2.20	0.55
1:G:553:MLY:HG3	4:8:44:MET:O	2.07	0.55
1:G:638:GLY:HA2	4:6:345:ILE:H	1.71	0.55
1:G:723:ARG:HH11	1:G:723:ARG:CG	2.20	0.55
1:J:84:MLY:CH1	1:J:719:ASP:C	2.63	0.55
4:W:365:ALA:HB3	4:W:369:ILE:HB	1.88	0.55
1:A:10:PHE:O	1:A:12:GLU:N	2.41	0.54
1:A:22:LYS:HA	1:A:25:ILE:HB	1.88	0.54
1:A:435:GLU:O	1:A:438:PHE:HB3	2.06	0.54
1:A:630:ALA:HA	4:4:25:ASP:OD2	2.07	0.54
1:A:638:GLY:CA	4:4:345:ILE:H	2.19	0.54
1:A:638:GLY:HA2	4:4:345:ILE:H	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:ARG:CG	3:C:118:MET:HE3	2.37	0.54
1:D:305:ILE:HG22	1:D:312:TYR:CE2	2.42	0.54
1:D:635:GLY:HA3	4:5:334:GLU:CG	2.30	0.54
1:D:638:GLY:HA2	4:5:345:ILE:H	1.72	0.54
1:D:788:THR:HG22	3:F:81:GLN:NE2	2.22	0.54
1:D:819:ASN:H	2:E:90:GLY:HA3	1.72	0.54
1:G:508:ILE:HG21	1:G:711:PHE:CZ	2.42	0.54
1:G:649:VAL:HA	1:G:649:VAL:HG23	1.83	0.54
1:J:290:GLN:NE2	1:J:334:THR:OG1	2.40	0.54
1:J:292:MET:HE1	1:J:309:PRO:CD	2.37	0.54
1:J:604:ASN:OD1	1:J:607:VAL:HG23	2.06	0.54
1:J:649:VAL:CG1	1:J:649:VAL:HA	2.35	0.54
4:Z:365:ALA:HB3	4:Z:369:ILE:HB	1.88	0.54
1:A:82:PRO:HD2	1:A:85:TYR:HD2	1.72	0.54
1:A:305:ILE:HG22	1:A:312:TYR:CE2	2.43	0.54
1:A:797:PHE:CG	3:C:149:VAL:HG11	2.35	0.54
3:C:123:VAL:O	3:C:127:MET:HG2	2.06	0.54
1:D:470:PHE:O	1:D:473:ASN:ND2	2.40	0.54
1:D:553:MLY:HG3	4:7:44:MET:O	2.07	0.54
1:D:649:VAL:CG1	1:D:649:VAL:HA	2.35	0.54
1:D:793:ARG:HE	3:F:147:MET:HG2	1.71	0.54
1:D:839:MLY:HH11	2:E:159:HIS:CG	2.30	0.54
3:F:123:VAL:O	3:F:127:MET:HG2	2.07	0.54
1:G:32:PHE:CG	1:G:83:PRO:HD3	2.41	0.54
1:G:78:PHE:HB3	1:G:98:HIS:NE2	2.23	0.54
1:G:126:VAL:HG13	1:G:675:ILE:HG22	1.89	0.54
1:G:735:GLY:O	1:G:743:ALA:HA	1.94	0.54
1:G:751:GLY:CA	3:I:114:LEU:CD1	2.84	0.54
1:G:765:VAL:HG12	1:G:766:PHE:N	2.22	0.54
1:J:470:PHE:O	1:J:473:ASN:ND2	2.40	0.54
1:J:546:THR:HG21	1:J:548:THR:HB	1.88	0.54
1:J:556:ASP:CA	4:V:49:GLN:O	2.51	0.54
1:J:797:PHE:CD2	3:L:126:LEU:CD2	2.91	0.54
4:8:365:ALA:HB3	4:8:369:ILE:HB	1.88	0.54
1:A:78:PHE:HB3	1:A:98:HIS:NE2	2.22	0.54
1:A:126:VAL:HG13	1:A:675:ILE:HG22	1.90	0.54
1:D:22:LYS:O	1:D:26:GLU:HG3	2.07	0.54
1:D:724:TYR:OH	1:D:778:MET:HB2	2.07	0.54
1:G:82:PRO:HD2	1:G:85:TYR:HD2	1.72	0.54
1:G:220:ASP:O	1:G:224:SER:N	2.27	0.54
1:G:530:MET:CB	4:6:354:GLN:HG3	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:546:THR:HG21	1:G:548:THR:HB	1.88	0.54
3:I:123:VAL:O	3:I:127:MET:HG2	2.07	0.54
1:J:756:THR:HB	1:J:776:GLU:CD	2.28	0.54
4:0:365:ALA:HB3	4:0:369:ILE:HB	1.88	0.54
4:2:365:ALA:HB3	4:2:369:ILE:HB	1.88	0.54
1:A:579:PHE:HE1	1:A:581:LEU:HD13	1.71	0.54
1:D:10:PHE:O	1:D:12:GLU:N	2.41	0.54
1:D:82:PRO:HD2	1:D:85:TYR:HD2	1.72	0.54
1:D:126:VAL:HG13	1:D:675:ILE:HG22	1.90	0.54
1:D:290:GLN:NE2	1:D:334:THR:OG1	2.40	0.54
1:G:38:VAL:CB	1:G:52:ILE:HD11	2.38	0.54
1:G:305:ILE:HG22	1:G:312:TYR:CZ	2.42	0.54
1:G:345:ALA:O	1:G:349:THR:N	2.40	0.54
1:G:783:LEU:HA	1:G:786:ILE:HB	1.87	0.54
1:J:305:ILE:HG22	1:J:312:TYR:CE2	2.43	0.54
2:K:146:GLY:O	2:K:147:ASN:ND2	2.41	0.54
4:4:288:ASP:CA	4:6:204:ALA:HB2	2.31	0.54
2:B:156:VAL:HA	2:B:159:HIS:O	2.07	0.54
1:D:571:ALA:O	1:D:572:LYS:CB	2.56	0.54
1:D:739:ASP:CB	1:D:742:LYS:CB	2.81	0.54
1:G:305:ILE:HG22	1:G:312:TYR:CE2	2.42	0.54
1:G:406:VAL:HG12	1:G:407:GLY:H	1.71	0.54
1:G:529:PRO:CB	4:6:354:GLN:HA	2.37	0.54
1:J:126:VAL:HG13	1:J:675:ILE:HG22	1.90	0.54
1:J:305:ILE:HG22	1:J:312:TYR:CZ	2.42	0.54
1:J:537:GLU:HB3	1:J:648:THR:CB	2.36	0.54
1:J:757:GLN:OE1	1:J:773:GLY:N	2.40	0.54
4:4:365:ALA:HB3	4:4:369:ILE:HB	1.88	0.54
4:6:365:ALA:HB3	4:6:369:ILE:HB	1.88	0.54
1:A:95:THR:OG1	1:A:769:ALA:CA	2.53	0.54
1:A:571:ALA:O	1:A:572:LYS:CB	2.56	0.54
1:A:629:GLU:CB	1:A:643:GLY:C	2.75	0.54
1:A:800:ARG:HH11	3:C:149:VAL:CB	2.20	0.54
1:D:78:PHE:HB3	1:D:98:HIS:NE2	2.22	0.54
1:D:292:MET:HE1	1:D:309:PRO:CD	2.37	0.54
1:D:345:ALA:O	1:D:349:THR:N	2.40	0.54
1:D:630:ALA:HA	4:5:25:ASP:OD2	2.07	0.54
1:D:649:VAL:HA	1:D:649:VAL:HG23	1.82	0.54
1:G:836:PHE:CD2	2:H:160:GLY:N	2.75	0.54
2:H:117:LEU:CG	2:H:147:ASN:OD1	2.52	0.54
1:J:10:PHE:O	1:J:12:GLU:N	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:78:PHE:HB3	1:J:98:HIS:NE2	2.22	0.54
1:J:538:GLU:CG	4:7:351:THR:C	2.73	0.54
1:J:546:THR:HB	1:J:549:SER:H	1.71	0.54
1:J:831:TRP:CZ3	2:K:34:ILE:HG21	2.42	0.54
1:A:642:LYS:HG2	4:4:22:ALA:C	2.28	0.54
1:A:721:LYS:C	1:A:736:GLN:OE1	2.46	0.54
1:D:38:VAL:CB	1:D:52:ILE:HD11	2.38	0.54
1:D:640:LYS:C	4:5:23:GLY:CA	2.64	0.54
1:D:792:ALA:O	3:F:40:ASN:HB3	2.06	0.54
1:G:530:MET:HE3	4:6:354:GLN:CB	2.38	0.54
1:G:725:ARG:HG3	1:G:733:PRO:CA	2.36	0.54
1:G:791:GLN:O	1:G:794:CYS:HB2	2.08	0.54
1:J:22:LYS:O	1:J:26:GLU:HG3	2.07	0.54
1:J:135:TYR:HD2	1:J:191:ARG:HG2	1.72	0.54
1:J:503:TYR:CE1	1:J:711:PHE:CE2	2.94	0.54
1:J:791:GLN:O	1:J:794:CYS:HB2	2.08	0.54
1:A:135:TYR:HD2	1:A:191:ARG:HG2	1.72	0.54
1:A:410:ASN:CG	4:4:334:GLU:C	2.65	0.54
1:A:649:VAL:CG1	1:A:649:VAL:HA	2.35	0.54
1:D:218:LEU:HA	1:D:221:GLN:HG3	1.71	0.54
1:D:218:LEU:CD2	1:D:222:ILE:CG1	2.86	0.54
1:D:721:LYS:C	1:D:736:GLN:OE1	2.46	0.54
1:D:732:ILE:CG2	1:D:747:LEU:HD11	1.26	0.54
1:G:10:PHE:O	1:G:12:GLU:N	2.41	0.54
1:G:292:MET:HE1	1:G:309:PRO:CD	2.37	0.54
1:J:493:HIS:ND1	1:J:514:ASP:OD2	2.41	0.54
1:J:629:GLU:CB	1:J:643:GLY:C	2.76	0.54
1:J:638:GLY:HA2	4:7:345:ILE:H	1.72	0.54
3:L:92:ARG:HA	3:L:139:TYR:OH	2.08	0.54
1:A:305:ILE:HG22	1:A:312:TYR:CZ	2.43	0.54
1:A:470:PHE:O	1:A:473:ASN:ND2	2.40	0.54
1:D:305:ILE:HG22	1:D:312:TYR:CZ	2.43	0.54
1:D:724:TYR:OH	1:D:778:MET:CB	2.56	0.54
2:E:146:GLY:O	2:E:147:ASN:ND2	2.41	0.54
1:G:404:PRO:CG	1:G:417:GLU:HG3	2.38	0.54
1:G:470:PHE:O	1:G:473:ASN:ND2	2.40	0.54
1:G:493:HIS:ND1	1:G:514:ASP:OD2	2.41	0.54
1:G:629:GLU:CB	1:G:643:GLY:C	2.76	0.54
1:A:38:VAL:CB	1:A:52:ILE:HD11	2.38	0.54
1:A:538:GLU:HG3	4:4:352:PHE:CA	2.38	0.54
2:B:146:GLY:O	2:B:147:ASN:ND2	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:507:GLY:CA	1:D:762:HIS:ND1	2.71	0.54
1:D:546:THR:HB	1:D:549:SER:H	1.71	0.54
1:D:765:VAL:HG12	1:D:766:PHE:N	2.22	0.54
1:D:792:ALA:C	3:F:40:ASN:CB	2.69	0.54
1:G:571:ALA:O	1:G:572:LYS:CB	2.56	0.54
1:G:576:GLU:CG	1:G:577:ALA:N	2.43	0.54
1:D:98:HIS:HB3	1:D:100:PRO:CD	2.25	0.53
1:D:793:ARG:HE	3:F:147:MET:CB	2.21	0.53
1:G:539:GLU:OE2	4:8:45:VAL:C	2.47	0.53
1:G:769:ALA:C	1:G:773:GLY:HA3	2.29	0.53
3:I:92:ARG:HA	3:I:139:TYR:OH	2.08	0.53
1:J:38:VAL:CB	1:J:52:ILE:HD11	2.38	0.53
1:J:553:MLY:O	4:V:48:GLY:CA	2.56	0.53
1:J:630:ALA:HA	4:7:25:ASP:OD2	2.07	0.53
1:J:640:LYS:C	4:7:23:GLY:CA	2.64	0.53
1:J:642:LYS:HG2	4:7:22:ALA:C	2.27	0.53
1:J:800:ARG:HB3	3:L:149:VAL:HG23	1.85	0.53
1:A:218:LEU:N	1:A:221:GLN:HG2	2.24	0.53
1:A:404:PRO:CG	1:A:417:GLU:HG3	2.38	0.53
1:A:553:MLY:O	4:6:48:GLY:CA	2.56	0.53
1:A:584:TYR:CD1	1:A:585:ALA:N	2.77	0.53
1:A:836:PHE:CE2	2:B:160:GLY:C	2.82	0.53
1:D:529:PRO:HB2	4:5:354:GLN:HA	1.91	0.53
1:D:629:GLU:CB	1:D:643:GLY:C	2.76	0.53
1:D:815:CYS:O	2:E:90:GLY:HA3	2.08	0.53
1:G:135:TYR:HD2	1:G:191:ARG:HD3	1.73	0.53
1:G:135:TYR:HD2	1:G:191:ARG:HG2	1.73	0.53
1:G:538:GLU:HG3	4:6:352:PHE:CA	2.38	0.53
1:G:640:LYS:C	4:6:23:GLY:CA	2.64	0.53
1:G:795:ARG:HH22	3:I:43:ASN:HB2	1.73	0.53
2:H:146:GLY:O	2:H:147:ASN:ND2	2.41	0.53
1:J:135:TYR:HD2	1:J:191:ARG:HD3	1.73	0.53
1:J:530:MET:HE3	4:7:355:MET:SD	2.48	0.53
1:J:538:GLU:HG3	4:7:352:PHE:CA	2.38	0.53
1:J:707:CYS:C	1:J:714:ARG:HH22	2.11	0.53
4:X:185:LEU:HD23	4:X:306:TYR:OH	2.09	0.53
1:D:508:ILE:HG23	1:D:766:PHE:CD1	2.44	0.53
1:D:723:ARG:CG	1:D:723:ARG:HH11	2.20	0.53
1:G:661:MET:O	1:G:665:ARG:HG3	2.08	0.53
1:J:553:MLY:HG3	4:V:44:MET:O	2.07	0.53
1:J:793:ARG:HG2	3:L:147:MET:HG2	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:TYR:HD2	1:A:191:ARG:HD3	1.73	0.53
1:A:800:ARG:HH11	3:C:149:VAL:CA	2.21	0.53
2:B:121:LEU:CA	2:B:128:PHE:CG	2.89	0.53
1:D:553:MLY:O	4:7:48:GLY:CA	2.56	0.53
1:D:579:PHE:HE1	1:D:581:LEU:HD13	1.72	0.53
3:F:35:ARG:HA	3:F:39:GLN:O	2.07	0.53
1:G:732:ILE:H	1:G:733:PRO:HD2	1.74	0.53
1:J:109:ARG:O	1:J:114:MET:N	2.37	0.53
1:J:721:LYS:C	1:J:736:GLN:OE1	2.46	0.53
1:A:295:MLY:HE2	1:A:332:MET:HE1	1.91	0.53
1:A:529:PRO:HB2	4:4:354:GLN:HA	1.91	0.53
1:D:42:HIS:HB3	1:D:45:GLN:O	2.09	0.53
1:D:404:PRO:CG	1:D:417:GLU:HG3	2.38	0.53
1:D:584:TYR:CD1	1:D:585:ALA:N	2.77	0.53
1:D:724:TYR:CA	1:D:782:MLY:HH21	2.38	0.53
2:E:114:LYS:O	2:E:147:ASN:ND2	2.41	0.53
2:E:162:ASP:O	2:K:21:GLU:HB3	2.08	0.53
1:G:730:SER:HB2	3:I:109:HIS:CE1	2.43	0.53
1:G:818:TYR:CD1	2:H:127:ARG:CZ	2.79	0.53
1:J:32:PHE:CD1	1:J:83:PRO:HD3	2.43	0.53
1:J:295:MLY:CG	1:J:332:MET:HE1	2.39	0.53
1:J:404:PRO:CG	1:J:417:GLU:HG3	2.38	0.53
1:J:765:VAL:HG12	1:J:766:PHE:N	2.22	0.53
1:J:834:LEU:HD11	2:K:54:MET:HG3	1.90	0.53
4:V:185:LEU:HD23	4:V:306:TYR:OH	2.09	0.53
1:A:791:GLN:O	1:A:794:CYS:HB2	2.08	0.53
1:D:135:TYR:CD2	1:D:191:ARG:HG2	2.44	0.53
1:D:277:PHE:CG	1:D:278:GLN:N	2.76	0.53
1:D:510:TRP:CZ3	1:D:711:PHE:HE2	2.26	0.53
1:D:830:PRO:HD2	2:E:67:MET:HE2	1.90	0.53
1:G:32:PHE:CD1	1:G:83:PRO:HD3	2.44	0.53
1:G:251:ARG:HB2	1:G:264:ASP:HB2	1.91	0.53
1:G:553:MLY:O	4:8:48:GLY:CA	2.56	0.53
1:G:728:ASN:ND2	3:I:109:HIS:O	2.41	0.53
1:J:571:ALA:O	1:J:572:LYS:CB	2.56	0.53
1:J:584:TYR:CD1	1:J:585:ALA:N	2.77	0.53
1:J:599:ASN:CG	1:J:649:VAL:H	2.12	0.53
1:J:642:LYS:CG	4:7:22:ALA:CA	2.80	0.53
1:J:661:MET:O	1:J:665:ARG:HG3	2.09	0.53
4:3:185:LEU:HD23	4:3:306:TYR:OH	2.09	0.53
4:4:185:LEU:HD23	4:4:306:TYR:OH	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LYS:O	1:A:26:GLU:N	2.30	0.53
1:A:42:HIS:HB3	1:A:45:GLN:O	2.09	0.53
1:D:135:TYR:HD2	1:D:191:ARG:HD3	1.73	0.53
1:G:149:GLN:OE1	1:G:762:HIS:HB3	2.09	0.53
1:G:277:PHE:CG	1:G:278:GLN:N	2.76	0.53
1:G:817:GLN:HB3	2:H:127:ARG:NH1	2.17	0.53
1:J:22:LYS:O	1:J:26:GLU:N	2.29	0.53
1:J:218:LEU:N	1:J:221:GLN:HG2	2.24	0.53
2:K:121:LEU:CA	2:K:128:PHE:CG	2.89	0.53
1:A:156:PHE:HD1	1:A:195:TYR:CD1	2.27	0.53
1:A:217:THR:C	1:A:221:GLN:NE2	2.62	0.53
1:A:493:HIS:ND1	1:A:514:ASP:OD2	2.41	0.53
1:A:539:GLU:OE2	4:6:45:VAL:C	2.48	0.53
1:A:579:PHE:CD2	1:A:592:ILE:HD11	2.40	0.53
1:A:739:ASP:CB	1:A:742:LYS:CB	2.81	0.53
1:D:32:PHE:CD1	1:D:83:PRO:HD3	2.43	0.53
1:D:642:LYS:HG2	4:5:22:ALA:C	2.27	0.53
1:D:661:MET:O	1:D:665:ARG:HG3	2.09	0.53
1:D:793:ARG:NE	3:F:147:MET:HG2	2.23	0.53
1:G:292:MET:CE	1:G:309:PRO:HA	2.39	0.53
1:G:636:LYS:HB2	4:6:334:GLU:OE1	2.09	0.53
1:G:797:PHE:CE2	3:I:126:LEU:CD2	2.92	0.53
1:G:798:LEU:HD21	3:I:126:LEU:HG	1.90	0.53
2:H:114:LYS:O	2:H:147:ASN:ND2	2.41	0.53
1:J:295:MLY:HE2	1:J:332:MET:HE1	1.91	0.53
1:J:404:PRO:HG3	1:J:417:GLU:HG3	1.91	0.53
2:K:114:LYS:O	2:K:147:ASN:ND2	2.41	0.53
3:L:53:PRO:HB2	3:L:55:LYS:HG3	1.91	0.53
1:A:502:GLU:OE1	1:A:763:THR:CA	2.57	0.53
1:D:599:ASN:CG	1:D:649:VAL:H	2.12	0.53
1:D:796:GLY:CA	3:F:40:ASN:OD1	2.52	0.53
2:E:114:LYS:N	2:E:146:GLY:O	2.40	0.53
3:F:92:ARG:HA	3:F:139:TYR:OH	2.08	0.53
1:G:218:LEU:N	1:G:221:GLN:HG2	2.24	0.53
1:G:295:MLY:HE2	1:G:332:MET:HE1	1.91	0.53
3:I:53:PRO:HB2	3:I:55:LYS:HG3	1.91	0.53
1:J:251:ARG:HB2	1:J:264:ASP:HB2	1.91	0.53
1:J:529:PRO:HB2	4:7:354:GLN:HA	1.91	0.53
1:J:612:GLN:HE22	1:J:627:GLY:HA2	1.66	0.53
2:K:129:THR:O	2:K:133:ILE:HG13	2.09	0.53
4:5:185:LEU:HD23	4:5:306:TYR:OH	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:287:ILE:HG22	4:Z:204:ALA:HB3	1.91	0.53
1:A:32:PHE:CD1	1:A:83:PRO:HD3	2.44	0.53
1:A:135:TYR:CD2	1:A:191:ARG:HG2	2.44	0.53
1:A:732:ILE:H	1:A:733:PRO:HD2	1.74	0.53
1:D:493:HIS:ND1	1:D:514:ASP:OD2	2.41	0.53
1:D:834:LEU:HD13	2:E:51:PHE:CD1	2.39	0.53
2:E:129:THR:O	2:E:133:ILE:HG13	2.09	0.53
1:G:534:SER:C	4:6:351:THR:CA	2.48	0.53
1:G:642:LYS:HG2	4:6:22:ALA:C	2.27	0.53
1:G:721:LYS:C	1:G:736:GLN:OE1	2.46	0.53
1:J:418:THR:CB	1:J:421:GLU:HG3	2.37	0.53
4:1:185:LEU:HD23	4:1:306:TYR:OH	2.09	0.53
4:Z:185:LEU:HD23	4:Z:306:TYR:OH	2.09	0.53
1:A:599:ASN:CG	1:A:649:VAL:H	2.12	0.52
1:A:661:MET:O	1:A:665:ARG:HG3	2.09	0.52
1:D:154:HIS:CE1	1:D:156:PHE:HD2	2.27	0.52
1:D:218:LEU:N	1:D:221:GLN:HG2	2.24	0.52
1:D:404:PRO:HG3	1:D:417:GLU:HG3	1.91	0.52
1:D:494:HIS:O	1:D:498:LEU:HB2	2.09	0.52
1:D:556:ASP:HB3	4:7:43:VAL:HG12	1.91	0.52
1:D:642:LYS:CG	4:5:22:ALA:CA	2.80	0.52
1:D:732:ILE:H	1:D:733:PRO:HD2	1.74	0.52
1:D:800:ARG:CG	3:F:149:VAL:HG22	2.37	0.52
1:G:579:PHE:CD2	1:G:592:ILE:HD11	2.39	0.52
1:G:634:GLY:N	4:6:25:ASP:O	2.31	0.52
1:J:197:ALA:O	1:J:201:ALA:HB2	2.09	0.52
1:J:510:TRP:CD2	1:J:768:MLY:CH1	2.92	0.52
1:J:707:CYS:HG	1:J:714:ARG:HH12	1.45	0.52
4:2:185:LEU:HD23	4:2:306:TYR:OH	2.09	0.52
4:3:180:LEU:HD22	4:3:267:ILE:HD11	1.92	0.52
4:V:287:ILE:HG22	4:X:204:ALA:HB3	1.91	0.52
1:A:555:TYR:N	4:6:48:GLY:N	2.58	0.52
1:D:538:GLU:HG3	4:5:352:PHE:CA	2.38	0.52
1:D:791:GLN:O	1:D:794:CYS:HB2	2.08	0.52
1:G:63:MLY:HG3	1:G:64:THR:H	1.75	0.52
1:G:404:PRO:HG3	1:G:417:GLU:HG3	1.91	0.52
1:G:584:TYR:CD1	1:G:585:ALA:N	2.77	0.52
1:G:599:ASN:CG	1:G:649:VAL:H	2.12	0.52
1:G:642:LYS:CG	4:6:22:ALA:HA	2.37	0.52
4:0:287:ILE:HG22	4:2:204:ALA:HB3	1.91	0.52
4:1:285:CYS:O	4:1:290:ARG:NH1	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2:180:LEU:HD22	4:2:267:ILE:HD11	1.92	0.52
4:2:288:ASP:CA	4:4:204:ALA:HB2	2.31	0.52
4:6:185:LEU:HD23	4:6:306:TYR:OH	2.09	0.52
4:7:287:ILE:HG22	4:V:204:ALA:HB3	1.91	0.52
4:8:185:LEU:HD23	4:8:306:TYR:OH	2.09	0.52
4:W:185:LEU:HD23	4:W:306:TYR:OH	2.09	0.52
1:A:277:PHE:CG	1:A:278:GLN:N	2.76	0.52
1:A:732:ILE:HG23	1:A:747:LEU:CD1	1.04	0.52
1:D:418:THR:CB	1:D:421:GLU:HG3	2.37	0.52
1:D:636:LYS:HB2	4:5:334:GLU:OE1	2.09	0.52
1:D:725:ARG:HG3	1:D:733:PRO:CA	2.36	0.52
1:G:84:MLY:CH1	1:G:720:PHE:N	2.72	0.52
1:J:84:MLY:HH11	1:J:720:PHE:N	2.24	0.52
1:J:135:TYR:CD2	1:J:191:ARG:HG2	2.44	0.52
1:J:220:ASP:O	1:J:224:SER:N	2.27	0.52
1:J:277:PHE:CG	1:J:278:GLN:N	2.76	0.52
1:J:732:ILE:HG23	1:J:747:LEU:CD1	1.05	0.52
1:J:797:PHE:CG	3:L:149:VAL:CG1	2.80	0.52
2:K:114:LYS:HA	2:K:147:ASN:HD22	1.74	0.52
4:6:180:LEU:HD22	4:6:267:ILE:HD11	1.92	0.52
4:7:285:CYS:O	4:7:290:ARG:NH1	2.43	0.52
4:W:285:CYS:O	4:W:290:ARG:NH1	2.43	0.52
4:X:285:CYS:O	4:X:290:ARG:NH1	2.43	0.52
4:Y:185:LEU:HD23	4:Y:306:TYR:OH	2.09	0.52
4:Y:285:CYS:O	4:Y:290:ARG:NH1	2.43	0.52
4:Z:285:CYS:O	4:Z:290:ARG:NH1	2.43	0.52
1:A:504:MLY:HB2	1:A:762:HIS:NE2	2.24	0.52
1:A:636:LYS:HB2	4:4:334:GLU:OE1	2.08	0.52
1:A:798:LEU:HD22	3:C:126:LEU:HD11	1.90	0.52
3:C:104:GLY:HA2	3:C:137:ILE:HD11	1.91	0.52
1:D:128:PRO:O	1:D:129:TYR:HB2	2.09	0.52
1:D:538:GLU:CG	4:5:351:THR:C	2.74	0.52
1:J:98:HIS:HB3	1:J:100:PRO:CD	2.25	0.52
1:J:156:PHE:HD1	1:J:195:TYR:CD1	2.27	0.52
1:J:642:LYS:CA	4:7:22:ALA:C	2.70	0.52
4:5:180:LEU:HD22	4:5:267:ILE:HD11	1.92	0.52
4:5:287:ILE:HG22	4:7:204:ALA:HB3	1.91	0.52
4:6:285:CYS:O	4:6:290:ARG:NH1	2.43	0.52
4:7:185:LEU:HD23	4:7:306:TYR:OH	2.09	0.52
4:W:180:LEU:HD22	4:W:267:ILE:HD11	1.92	0.52
1:A:63:MLY:HG3	1:A:64:THR:H	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ARG:HD3	1:A:117:THR:HB	1.92	0.52
1:A:556:ASP:HB3	4:6:43:VAL:HG12	1.91	0.52
1:D:732:ILE:H	1:D:733:PRO:CD	2.23	0.52
1:G:217:THR:C	1:G:221:GLN:NE2	2.62	0.52
1:G:530:MET:HG2	4:6:354:GLN:HB2	0.57	0.52
1:J:759:ALA:O	1:J:766:PHE:N	2.32	0.52
1:J:795:ARG:HD3	3:L:35:ARG:NH2	1.91	0.52
1:J:795:ARG:CB	3:L:35:ARG:NH2	2.73	0.52
2:K:112:ILE:C	2:K:147:ASN:O	2.42	0.52
3:L:104:GLY:HA2	3:L:137:ILE:HD11	1.92	0.52
3:L:110:VAL:HG13	3:L:114:LEU:HD12	1.92	0.52
4:5:285:CYS:O	4:5:290:ARG:NH1	2.43	0.52
4:V:180:LEU:HD22	4:V:267:ILE:HD11	1.92	0.52
4:Y:180:LEU:HD22	4:Y:267:ILE:HD11	1.92	0.52
1:A:154:HIS:CE1	1:A:156:PHE:HD2	2.27	0.52
1:A:404:PRO:HG3	1:A:417:GLU:HG3	1.91	0.52
1:A:494:HIS:O	1:A:498:LEU:HB2	2.09	0.52
1:A:732:ILE:H	1:A:733:PRO:CD	2.23	0.52
1:A:788:THR:CG2	3:C:42:THR:HG21	2.40	0.52
1:A:795:ARG:HG2	3:C:118:MET:HE3	1.90	0.52
3:F:104:GLY:HA2	3:F:137:ILE:HD11	1.92	0.52
1:G:41:VAL:HG13	1:G:42:HIS:N	2.25	0.52
1:G:42:HIS:HB3	1:G:45:GLN:O	2.09	0.52
1:G:109:ARG:HD3	1:G:117:THR:HB	1.92	0.52
1:G:510:TRP:CH2	1:G:768:MLY:HH11	2.39	0.52
1:G:732:ILE:HG23	1:G:747:LEU:CD1	1.04	0.52
2:H:114:LYS:HA	2:H:147:ASN:HD22	1.75	0.52
1:J:556:ASP:HB3	4:V:43:VAL:HG12	1.91	0.52
4:0:180:LEU:HD22	4:0:267:ILE:HD11	1.92	0.52
4:1:180:LEU:HD22	4:1:267:ILE:HD11	1.92	0.52
4:2:287:ILE:HG22	4:4:204:ALA:HB3	1.91	0.52
4:4:180:LEU:HD22	4:4:267:ILE:HD11	1.92	0.52
4:8:285:CYS:O	4:8:290:ARG:NH1	2.43	0.52
4:X:180:LEU:HD22	4:X:267:ILE:HD11	1.92	0.52
1:A:212:GLY:O	1:A:213:LYS:HB2	2.10	0.52
1:A:800:ARG:HB3	3:C:149:VAL:HG23	1.73	0.52
3:C:52:ASN:HB2	3:C:53:PRO:CD	2.28	0.52
3:C:53:PRO:HB2	3:C:55:LYS:HG3	1.91	0.52
3:C:92:ARG:HA	3:C:139:TYR:OH	2.09	0.52
1:D:41:VAL:HG13	1:D:42:HIS:N	2.25	0.52
1:D:156:PHE:HD1	1:D:195:TYR:CD1	2.28	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:491:PHE:HD1	1:D:671:PHE:CE2	2.27	0.52
1:D:538:GLU:HA	4:5:349:LEU:CB	2.40	0.52
1:G:40:VAL:HG13	1:G:41:VAL:O	2.10	0.52
1:G:128:PRO:O	1:G:129:TYR:HB2	2.09	0.52
1:G:135:TYR:CD2	1:G:191:ARG:HG2	2.44	0.52
1:G:154:HIS:CE1	1:G:156:PHE:HD2	2.26	0.52
1:G:529:PRO:HB2	4:6:354:GLN:HA	1.92	0.52
1:G:793:ARG:HH11	3:I:40:ASN:HD21	1.56	0.52
1:J:41:VAL:HG13	1:J:42:HIS:N	2.25	0.52
1:J:42:HIS:HB3	1:J:45:GLN:O	2.09	0.52
1:J:530:MET:HG2	4:7:354:GLN:HB2	0.57	0.52
1:J:817:GLN:HG3	2:K:128:PHE:CZ	2.45	0.52
4:0:185:LEU:HD23	4:0:306:TYR:OH	2.09	0.52
4:2:285:CYS:O	4:2:290:ARG:NH1	2.43	0.52
4:3:287:ILE:HG22	4:5:204:ALA:HB3	1.91	0.52
1:A:218:LEU:CD2	1:A:222:ILE:CG1	2.85	0.52
1:A:491:PHE:HD1	1:A:671:PHE:CE2	2.27	0.52
1:A:795:ARG:CD	3:C:43:ASN:OD1	2.58	0.52
1:A:798:LEU:HD11	3:C:126:LEU:HG	1.90	0.52
1:D:839:MLY:HH11	2:E:159:HIS:HB3	1.87	0.52
3:F:53:PRO:HB2	3:F:55:LYS:HG3	1.91	0.52
1:G:156:PHE:HD1	1:G:195:TYR:CD1	2.27	0.52
1:G:197:ALA:O	1:G:201:ALA:HB2	2.09	0.52
1:G:491:PHE:HD1	1:G:671:PHE:CE2	2.27	0.52
1:J:555:TYR:N	4:V:48:GLY:N	2.58	0.52
1:J:642:LYS:HG2	4:7:21:PHE:C	2.29	0.52
4:7:180:LEU:HD22	4:7:267:ILE:HD11	1.92	0.52
4:8:287:ILE:HG22	4:W:204:ALA:HB3	1.91	0.52
4:V:285:CYS:O	4:V:290:ARG:NH1	2.43	0.52
4:Z:180:LEU:HD22	4:Z:267:ILE:HD11	1.92	0.52
1:A:251:ARG:HB2	1:A:264:ASP:HB2	1.91	0.52
1:D:63:MLY:HG3	1:D:64:THR:H	1.75	0.52
1:D:251:ARG:HB2	1:D:264:ASP:HB2	1.91	0.52
1:D:830:PRO:CD	2:E:67:MET:HE2	2.38	0.52
3:F:110:VAL:HG13	3:F:114:LEU:HD12	1.91	0.52
1:J:128:PRO:O	1:J:129:TYR:HB2	2.09	0.52
1:J:154:HIS:CE1	1:J:156:PHE:HD2	2.26	0.52
4:0:285:CYS:O	4:0:290:ARG:NH1	2.43	0.52
4:8:180:LEU:HD22	4:8:267:ILE:HD11	1.92	0.52
4:W:287:ILE:HG22	4:Y:204:ALA:HB3	1.91	0.52
1:A:40:VAL:HG13	1:A:41:VAL:O	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:MET:CE	1:A:309:PRO:HA	2.39	0.52
1:A:797:PHE:CD1	3:C:149:VAL:HG12	2.20	0.52
2:B:129:THR:O	2:B:133:ILE:HG13	2.09	0.52
1:D:41:VAL:HG21	1:D:76:GLN:HG3	1.92	0.52
1:D:109:ARG:HD3	1:D:117:THR:HB	1.92	0.52
1:D:195:TYR:CE2	1:D:199:ILE:CD1	2.93	0.52
1:D:642:LYS:HG2	4:5:21:PHE:C	2.30	0.52
1:D:733:PRO:O	1:D:737:PHE:CE1	2.53	0.52
1:G:481:ASN:N	1:G:481:ASN:ND2	2.51	0.52
1:G:494:HIS:O	1:G:498:LEU:HB2	2.09	0.52
1:G:556:ASP:HB3	4:8:43:VAL:HG12	1.92	0.52
1:J:90:ASP:OD2	1:J:764:MLY:HH21	2.08	0.52
1:J:135:TYR:HD2	1:J:191:ARG:CD	2.23	0.52
1:J:232:PHE:CE1	1:J:287:ILE:HD13	2.44	0.52
1:J:491:PHE:HD1	1:J:671:PHE:CE2	2.27	0.52
1:J:510:TRP:CE2	1:J:768:MLY:HH13	2.45	0.52
1:J:553:MLY:CE	4:V:45:VAL:CA	2.49	0.52
1:J:636:LYS:HB2	4:7:334:GLU:OE1	2.09	0.52
1:J:642:LYS:HB2	4:7:24:ASP:O	1.89	0.52
3:L:100:GLY:O	3:L:138:ASN:HA	2.10	0.52
1:A:135:TYR:HD2	1:A:191:ARG:CD	2.23	0.51
1:A:538:GLU:HA	4:4:349:LEU:CB	2.39	0.51
1:A:578:HIS:O	1:A:579:PHE:HB3	2.11	0.51
1:A:642:LYS:CG	4:4:22:ALA:HA	2.38	0.51
1:A:725:ARG:O	1:A:729:ALA:HA	2.10	0.51
2:B:114:LYS:O	2:B:147:ASN:ND2	2.41	0.51
1:D:40:VAL:HG13	1:D:41:VAL:O	2.10	0.51
1:D:410:ASN:CG	4:5:334:GLU:C	2.65	0.51
1:D:555:TYR:N	4:7:48:GLY:N	2.58	0.51
2:E:114:LYS:HA	2:E:147:ASN:HD22	1.74	0.51
1:G:221:GLN:HB2	1:G:449:LEU:HD11	1.92	0.51
2:H:129:THR:O	2:H:133:ILE:HG13	2.09	0.51
3:I:110:VAL:HG13	3:I:114:LEU:HD12	1.91	0.51
1:J:40:VAL:HG13	1:J:41:VAL:O	2.10	0.51
1:J:221:GLN:HB2	1:J:449:LEU:HD11	1.92	0.51
1:J:292:MET:CE	1:J:309:PRO:HA	2.40	0.51
1:J:539:GLU:OE2	4:V:45:VAL:C	2.47	0.51
4:4:287:ILE:HG22	4:6:204:ALA:HB3	1.91	0.51
1:D:221:GLN:HB2	1:D:449:LEU:HD11	1.92	0.51
1:D:813:ILE:CB	2:E:127:ARG:NH1	2.73	0.51
1:G:93:MET:CG	1:G:716:LEU:HD12	2.39	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:727:LEU:O	3:I:113:THR:CB	2.58	0.51
1:J:63:MLY:HG3	1:J:64:THR:H	1.75	0.51
1:J:494:HIS:O	1:J:498:LEU:HB2	2.09	0.51
1:J:538:GLU:HA	4:7:349:LEU:CB	2.40	0.51
1:A:97:LEU:CD2	1:A:712:PRO:CB	2.88	0.51
1:A:408:VAL:CG1	4:4:332:PRO:HB3	2.40	0.51
1:A:501:GLU:C	1:A:762:HIS:CE1	2.84	0.51
1:A:530:MET:HG2	4:4:354:GLN:HB2	0.57	0.51
1:A:530:MET:CE	4:4:354:GLN:HG3	2.35	0.51
2:B:114:LYS:HA	2:B:147:ASN:HD22	1.74	0.51
1:D:295:MLY:HE2	1:D:332:MET:HE1	1.91	0.51
3:F:100:GLY:O	3:F:138:ASN:HA	2.11	0.51
1:G:232:PHE:CE1	1:G:287:ILE:HD13	2.45	0.51
1:G:559:LEU:HD23	1:G:559:LEU:C	2.31	0.51
1:G:762:HIS:CD2	1:G:762:HIS:N	2.78	0.51
1:J:195:TYR:CE2	1:J:199:ILE:CD1	2.93	0.51
1:A:221:GLN:HB2	1:A:449:LEU:HD11	1.92	0.51
1:A:232:PHE:CE1	1:A:287:ILE:HD13	2.45	0.51
1:A:546:THR:CG2	1:A:548:THR:HB	2.41	0.51
1:A:592:ILE:O	1:A:592:ILE:HG22	2.11	0.51
1:D:248:MLY:N	1:D:463:ASP:O	2.44	0.51
1:D:642:LYS:CA	4:5:22:ALA:C	2.71	0.51
1:G:538:GLU:HA	4:6:349:LEU:CB	2.40	0.51
1:G:546:THR:CG2	1:G:548:THR:HB	2.41	0.51
1:J:248:MLY:N	1:J:463:ASP:O	2.44	0.51
1:J:640:LYS:CA	1:J:645:SER:OG	2.58	0.51
1:J:818:TYR:CD1	2:K:127:ARG:NH1	2.78	0.51
4:1:287:ILE:HG22	4:3:204:ALA:HB3	1.91	0.51
4:3:285:CYS:O	4:3:290:ARG:NH1	2.43	0.51
1:A:195:TYR:CE2	1:A:199:ILE:CD1	2.93	0.51
1:D:232:PHE:CE1	1:D:287:ILE:HD13	2.45	0.51
1:D:538:GLU:CD	4:5:355:MET:HE3	2.29	0.51
1:G:195:TYR:CE2	1:G:199:ILE:CD1	2.93	0.51
1:G:411:GLU:H	4:6:333:PRO:CG	2.24	0.51
1:G:418:THR:O	1:G:422:VAL:HG23	2.11	0.51
1:G:578:HIS:O	1:G:579:PHE:HB3	2.11	0.51
3:I:100:GLY:O	3:I:138:ASN:HA	2.11	0.51
3:I:104:GLY:HA2	3:I:137:ILE:HD11	1.92	0.51
1:J:13:ALA:C	1:J:15:PRO:HD2	2.31	0.51
1:J:212:GLY:O	1:J:213:LYS:HB2	2.11	0.51
1:J:418:THR:O	1:J:422:VAL:HG23	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:578:HIS:O	1:J:579:PHE:HB3	2.11	0.51
1:J:687:GLU:O	1:J:691:VAL:HG23	2.11	0.51
4:4:285:CYS:O	4:4:290:ARG:NH1	2.43	0.51
1:A:38:VAL:CG1	1:A:39:PHE:N	2.74	0.51
1:A:41:VAL:HG13	1:A:42:HIS:N	2.25	0.51
1:A:248:MLY:N	1:A:463:ASP:O	2.44	0.51
1:A:559:LEU:HD23	1:A:559:LEU:C	2.31	0.51
1:A:814:PHE:CA	2:B:127:ARG:NH2	2.67	0.51
1:D:197:ALA:O	1:D:201:ALA:HB2	2.10	0.51
2:E:112:ILE:HG23	2:E:147:ASN:HB3	1.93	0.51
1:G:248:MLY:N	1:G:463:ASP:O	2.44	0.51
1:G:675:ILE:CG2	1:G:676:ILE:N	2.74	0.51
1:G:826:VAL:HG21	2:H:88:LEU:HD21	1.93	0.51
4:6:287:ILE:HG22	4:8:204:ALA:HB3	1.91	0.51
1:A:418:THR:O	1:A:422:VAL:HG23	2.11	0.51
1:A:757:GLN:HG3	1:A:771:LEU:CD1	2.30	0.51
1:D:237:THR:O	1:D:240:ASN:O	2.29	0.51
1:D:400:ALA:HB1	1:D:606:THR:HG22	1.92	0.51
1:D:411:GLU:H	4:5:333:PRO:CG	2.24	0.51
1:G:38:VAL:CG1	1:G:39:PHE:N	2.74	0.51
1:G:41:VAL:HG21	1:G:76:GLN:HG3	1.93	0.51
1:G:311:ASP:HB2	1:G:312:TYR:CE1	2.46	0.51
1:J:90:ASP:CG	1:J:764:MLY:CH2	2.79	0.51
1:J:202:SER:HB2	1:J:207:LYS:NZ	2.26	0.51
1:J:592:ILE:HG22	1:J:592:ILE:O	2.10	0.51
1:J:818:TYR:OH	2:K:127:ARG:NH2	2.35	0.51
2:K:114:LYS:N	2:K:146:GLY:O	2.40	0.51
1:A:400:ALA:HB1	1:A:606:THR:HG22	1.92	0.51
1:A:631:GLU:C	4:4:25:ASP:HB2	2.31	0.51
1:D:13:ALA:C	1:D:15:PRO:HD2	2.31	0.51
1:D:135:TYR:HD2	1:D:191:ARG:CD	2.23	0.51
1:D:217:THR:C	1:D:221:GLN:NE2	2.62	0.51
1:D:553:MLY:CE	4:7:45:VAL:CA	2.49	0.51
1:D:592:ILE:O	1:D:592:ILE:HG22	2.10	0.51
1:G:13:ALA:C	1:G:15:PRO:HD2	2.31	0.51
1:G:400:ALA:HB1	1:G:606:THR:HG22	1.93	0.51
1:G:631:GLU:C	4:6:25:ASP:HB2	2.31	0.51
1:G:725:ARG:O	1:G:729:ALA:HA	2.10	0.51
1:J:41:VAL:HG21	1:J:76:GLN:HG3	1.93	0.51
1:J:742:LYS:O	1:J:745:GLU:HB2	2.10	0.51
1:A:506:GLU:OE1	1:A:761:GLY:N	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:110:VAL:HG13	3:C:114:LEU:HD12	1.92	0.51
1:D:202:SER:HB2	1:D:207:LYS:NZ	2.26	0.51
1:D:530:MET:HG2	4:5:354:GLN:HB2	0.57	0.51
1:D:687:GLU:O	1:D:691:VAL:HG23	2.11	0.51
1:D:815:CYS:O	2:E:90:GLY:CA	2.59	0.51
2:E:121:LEU:HA	2:E:128:PHE:CD2	2.46	0.51
1:G:267:THR:HG21	1:G:438:PHE:HE2	1.76	0.51
1:J:649:VAL:HA	1:J:649:VAL:HG23	1.83	0.51
4:7:288:ASP:CA	4:V:204:ALA:HB2	2.31	0.51
1:A:128:PRO:O	1:A:129:TYR:HB2	2.09	0.51
1:A:197:ALA:O	1:A:201:ALA:HB2	2.10	0.51
1:A:311:ASP:HB2	1:A:312:TYR:CE1	2.46	0.51
1:D:38:VAL:CG1	1:D:39:PHE:N	2.74	0.51
1:D:632:GLY:HA3	1:D:643:GLY:N	2.17	0.51
1:D:725:ARG:O	1:D:729:ALA:HA	2.10	0.51
1:G:212:GLY:O	1:G:213:LYS:HB2	2.10	0.51
2:H:114:LYS:N	2:H:146:GLY:O	2.40	0.51
1:J:169:ASP:N	1:J:169:ASP:OD1	2.44	0.51
1:J:768:MLY:HH21	1:J:772:LEU:HD13	1.93	0.51
1:A:556:ASP:CA	4:6:49:GLN:O	2.52	0.50
1:A:640:LYS:CA	1:A:645:SER:OG	2.58	0.50
1:A:646:PHE:CE2	1:A:652:LEU:CD2	2.87	0.50
1:A:675:ILE:CG2	1:A:676:ILE:N	2.74	0.50
1:A:822:SER:HB3	2:B:88:LEU:CD2	2.41	0.50
1:D:212:GLY:O	1:D:213:LYS:HB2	2.11	0.50
1:D:218:LEU:N	1:D:221:GLN:CG	2.74	0.50
1:D:578:HIS:O	1:D:579:PHE:HB3	2.10	0.50
1:G:429:LEU:O	1:G:433:VAL:HG23	2.11	0.50
1:G:797:PHE:CD2	3:I:126:LEU:CD2	2.93	0.50
1:J:109:ARG:HD3	1:J:117:THR:HB	1.92	0.50
1:J:408:VAL:CG1	4:7:332:PRO:HB3	2.40	0.50
1:J:632:GLY:HA3	1:J:643:GLY:N	2.17	0.50
1:J:733:PRO:O	1:J:737:PHE:CE1	2.53	0.50
1:A:41:VAL:HG21	1:A:76:GLN:HG3	1.92	0.50
1:A:687:GLU:O	1:A:691:VAL:HG23	2.11	0.50
1:D:546:THR:CG2	1:D:548:THR:HB	2.41	0.50
1:D:559:LEU:HD23	1:D:559:LEU:C	2.31	0.50
1:D:631:GLU:C	4:5:25:ASP:HB2	2.31	0.50
1:D:818:TYR:CG	2:E:89:LYS:CB	2.93	0.50
1:D:818:TYR:HB3	2:E:90:GLY:N	2.26	0.50
1:G:135:TYR:HD2	1:G:191:ARG:CD	2.23	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:218:LEU:N	1:G:221:GLN:CG	2.74	0.50
1:G:730:SER:CB	3:I:109:HIS:CE1	2.94	0.50
1:J:218:LEU:N	1:J:221:GLN:CG	2.74	0.50
1:J:237:THR:O	1:J:240:ASN:O	2.29	0.50
1:A:629:GLU:CB	1:A:645:SER:N	2.74	0.50
1:A:759:ALA:O	1:A:766:PHE:N	2.32	0.50
1:D:169:ASP:OD1	1:D:169:ASP:N	2.44	0.50
1:D:418:THR:O	1:D:422:VAL:HG23	2.11	0.50
1:D:723:ARG:C	1:D:782:MLY:NZ	2.65	0.50
1:D:742:LYS:O	1:D:745:GLU:HB2	2.10	0.50
1:G:202:SER:HB2	1:G:207:LYS:NZ	2.26	0.50
1:G:237:THR:O	1:G:240:ASN:O	2.29	0.50
1:G:555:TYR:N	4:8:48:GLY:N	2.59	0.50
1:J:411:GLU:H	4:7:333:PRO:CG	2.25	0.50
1:J:646:PHE:HE2	1:J:652:LEU:CG	2.25	0.50
1:J:725:ARG:O	1:J:729:ALA:HA	2.10	0.50
1:J:732:ILE:H	1:J:733:PRO:CD	2.23	0.50
1:J:823:PHE:HE1	2:K:156:VAL:O	1.88	0.50
1:A:13:ALA:C	1:A:15:PRO:HD2	2.31	0.50
1:A:169:ASP:OD1	1:A:169:ASP:N	2.44	0.50
1:A:267:THR:HG21	1:A:438:PHE:HE2	1.76	0.50
1:A:817:GLN:CG	2:B:127:ARG:HG2	2.41	0.50
1:A:839:MLY:HD3	2:B:159:HIS:CB	2.40	0.50
1:D:154:HIS:CD2	1:D:155:ILE:H	2.30	0.50
1:G:538:GLU:OE1	4:6:351:THR:HB	2.12	0.50
1:G:732:ILE:H	1:G:733:PRO:CD	2.23	0.50
1:G:797:PHE:CE2	3:I:126:LEU:HD23	2.45	0.50
1:G:800:ARG:CZ	3:I:149:VAL:HG22	2.30	0.50
1:J:154:HIS:CD2	1:J:155:ILE:H	2.30	0.50
1:J:278:GLN:HG3	1:J:318:GLY:H	1.75	0.50
1:J:311:ASP:HB2	1:J:312:TYR:CE1	2.46	0.50
1:J:346:ASP:O	1:J:349:THR:HB	2.12	0.50
1:J:629:GLU:CB	1:J:645:SER:N	2.73	0.50
1:J:631:GLU:C	4:7:25:ASP:HB2	2.31	0.50
1:J:733:PRO:CA	1:J:737:PHE:CE1	2.95	0.50
3:C:100:GLY:O	3:C:138:ASN:HA	2.11	0.50
1:D:311:ASP:HB2	1:D:312:TYR:CE1	2.46	0.50
1:D:346:ASP:O	1:D:349:THR:HB	2.11	0.50
1:D:429:LEU:O	1:D:433:VAL:HG23	2.11	0.50
1:D:646:PHE:HE2	1:D:652:LEU:CG	2.25	0.50
1:G:687:GLU:O	1:G:691:VAL:HG23	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:733:PRO:O	1:G:737:PHE:CE1	2.53	0.50
1:G:742:LYS:O	1:G:745:GLU:HB2	2.10	0.50
1:A:715:VAL:O	1:A:764:MLY:HB3	2.12	0.50
1:A:732:ILE:O	1:A:736:GLN:HG3	2.12	0.50
1:D:507:GLY:O	1:D:761:GLY:C	2.49	0.50
1:D:640:LYS:CA	1:D:645:SER:OG	2.58	0.50
1:D:715:VAL:O	1:D:764:MLY:HB3	2.12	0.50
1:D:732:ILE:HG23	1:D:747:LEU:HD12	0.94	0.50
1:G:149:GLN:OE1	1:G:762:HIS:CB	2.59	0.50
1:G:592:ILE:HG22	1:G:592:ILE:O	2.10	0.50
1:G:640:LYS:CA	1:G:645:SER:OG	2.58	0.50
1:G:715:VAL:O	1:G:764:MLY:HB3	2.12	0.50
1:J:400:ALA:HB1	1:J:606:THR:HG22	1.93	0.50
1:J:538:GLU:CD	4:7:355:MET:HE3	2.30	0.50
1:J:792:ALA:CB	3:L:40:ASN:CB	2.52	0.50
2:K:112:ILE:HG23	2:K:147:ASN:HB3	1.93	0.50
1:A:218:LEU:N	1:A:221:GLN:CG	2.74	0.50
1:A:237:THR:O	1:A:240:ASN:O	2.29	0.50
1:A:601:ASP:N	1:A:602:PRO:CD	2.75	0.50
1:A:742:LYS:O	1:A:745:GLU:HB2	2.10	0.50
1:D:278:GLN:HG3	1:D:318:GLY:H	1.75	0.50
1:D:629:GLU:CA	1:D:643:GLY:C	2.73	0.50
1:D:795:ARG:HB3	3:F:35:ARG:HD3	1.91	0.50
1:D:798:LEU:HD11	3:F:126:LEU:CD2	2.19	0.50
1:G:218:LEU:CD2	1:G:222:ILE:CG1	2.85	0.50
1:G:291:ILE:HA	1:G:331:LEU:CD1	2.39	0.50
1:G:646:PHE:CE2	1:G:652:LEU:CD2	2.87	0.50
1:J:429:LEU:O	1:J:433:VAL:HG23	2.12	0.50
1:J:546:THR:CG2	1:J:548:THR:HB	2.41	0.50
1:J:559:LEU:HD23	1:J:559:LEU:C	2.31	0.50
1:J:839:MLY:HB2	1:J:840:PRO:HD3	1.94	0.50
4:0:288:ASP:CA	4:2:204:ALA:HB2	2.31	0.50
4:7:318:THR:HA	4:7:327:ILE:HG12	1.94	0.50
1:A:202:SER:HB2	1:A:207:LYS:NZ	2.26	0.50
1:A:471:ASP:HB3	1:A:573:GLY:O	2.12	0.50
1:A:576:GLU:CG	1:A:577:ALA:N	2.43	0.50
1:A:733:PRO:CA	1:A:737:PHE:CE1	2.95	0.50
1:A:769:ALA:N	1:A:771:LEU:CB	2.74	0.50
1:D:109:ARG:O	1:D:114:MET:N	2.37	0.50
1:D:408:VAL:CG1	4:5:332:PRO:HB3	2.41	0.50
1:D:471:ASP:HB3	1:D:573:GLY:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:346:ASP:O	1:G:349:THR:HB	2.11	0.50
1:G:707:CYS:C	1:G:714:ARG:NH2	2.52	0.50
1:G:733:PRO:CA	1:G:737:PHE:CE1	2.95	0.50
1:G:795:ARG:HH21	3:I:116:GLU:HB3	1.77	0.50
1:J:732:ILE:O	1:J:736:GLN:HG3	2.12	0.50
2:K:117:LEU:HG	2:K:147:ASN:HB3	1.93	0.50
4:4:70:PRO:HG3	4:4:81:ASP:HB3	1.94	0.50
1:A:95:THR:HG1	1:A:769:ALA:HA	1.76	0.50
1:A:409:GLY:N	1:A:636:LYS:CD	2.70	0.50
1:A:530:MET:HA	4:4:354:GLN:CD	2.11	0.50
1:A:547:ASP:O	1:A:550:PHE:HB3	2.12	0.50
1:A:553:MLY:HG3	4:6:44:MET:O	2.07	0.50
1:D:539:GLU:OE2	4:7:45:VAL:C	2.47	0.50
1:D:733:PRO:CA	1:D:737:PHE:CE1	2.94	0.50
1:G:471:ASP:HB3	1:G:573:GLY:O	2.12	0.50
1:G:839:MLY:N	1:G:840:PRO:CD	2.75	0.50
1:J:38:VAL:CG1	1:J:39:PHE:N	2.74	0.50
1:J:217:THR:C	1:J:221:GLN:NE2	2.62	0.50
4:8:318:THR:HA	4:8:327:ILE:HG12	1.94	0.50
1:A:411:GLU:H	4:4:333:PRO:CG	2.24	0.49
1:A:505:MLY:HB2	1:A:761:GLY:CA	2.42	0.49
1:D:291:ILE:HA	1:D:331:LEU:CD1	2.39	0.49
1:D:538:GLU:OE1	4:5:351:THR:HB	2.12	0.49
2:E:140:PHE:HB3	2:E:144:VAL:HG12	1.94	0.49
2:H:137:TRP:CA	2:H:145:ALA:CB	2.82	0.49
1:J:251:ARG:O	1:J:263:ALA:HA	2.12	0.49
1:J:642:LYS:CG	4:7:22:ALA:HA	2.37	0.49
1:J:642:LYS:HA	4:7:22:ALA:C	2.33	0.49
1:J:675:ILE:CG2	1:J:676:ILE:N	2.74	0.49
4:3:318:THR:HA	4:3:327:ILE:HG12	1.94	0.49
4:5:318:THR:HA	4:5:327:ILE:HG12	1.95	0.49
4:6:318:THR:HA	4:6:327:ILE:HG12	1.94	0.49
1:A:51:THR:C	1:A:62:VAL:HG13	2.32	0.49
1:A:756:THR:O	1:A:758:TYR:N	2.46	0.49
1:A:818:TYR:HB2	2:B:89:LYS:C	2.31	0.49
2:B:117:LEU:CG	2:B:147:ASN:OD1	2.52	0.49
2:B:140:PHE:HB3	2:B:144:VAL:HG12	1.94	0.49
1:D:769:ALA:C	1:D:770:GLY:C	2.69	0.49
2:E:162:ASP:HB2	2:K:20:ASP:HA	1.94	0.49
1:G:169:ASP:N	1:G:169:ASP:OD1	2.44	0.49
1:G:278:GLN:HG3	1:G:318:GLY:H	1.75	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:632:GLY:HA3	1:G:643:GLY:N	2.17	0.49
1:G:756:THR:O	1:G:758:TYR:N	2.45	0.49
1:J:192:VAL:O	1:J:195:TYR:HB3	2.12	0.49
1:J:538:GLU:OE1	4:7:351:THR:HB	2.12	0.49
4:W:318:THR:HA	4:W:327:ILE:HG12	1.94	0.49
4:Z:70:PRO:HG3	4:Z:81:ASP:HB3	1.94	0.49
1:A:154:HIS:CD2	1:A:155:ILE:H	2.30	0.49
1:A:715:VAL:HG12	1:A:716:LEU:O	2.13	0.49
2:B:112:ILE:HG23	2:B:147:ASN:HB3	1.93	0.49
1:D:192:VAL:O	1:D:195:TYR:HB3	2.13	0.49
1:D:251:ARG:O	1:D:263:ALA:HA	2.12	0.49
1:D:725:ARG:NE	1:D:733:PRO:CB	1.95	0.49
1:D:732:ILE:O	1:D:736:GLN:HG3	2.12	0.49
1:D:817:GLN:CD	2:E:127:ARG:CZ	2.70	0.49
1:G:543:PRO:CD	4:6:146:GLY:O	2.60	0.49
1:G:751:GLY:H	3:I:114:LEU:CD1	2.25	0.49
1:G:757:GLN:CD	1:G:772:LEU:CG	2.75	0.49
2:H:112:ILE:HG23	2:H:147:ASN:HB3	1.93	0.49
1:J:214:MET:HA	1:J:340:ILE:CD1	2.41	0.49
1:J:595:TRP:N	1:J:595:TRP:CD1	2.80	0.49
1:J:739:ASP:OD1	1:J:740:SER:N	2.45	0.49
1:J:756:THR:O	1:J:758:TYR:N	2.45	0.49
1:J:768:MLY:CE	1:J:772:LEU:CD2	2.90	0.49
1:J:795:ARG:NE	3:L:35:ARG:HH12	2.10	0.49
4:1:318:THR:HA	4:1:327:ILE:HG12	1.94	0.49
4:4:318:THR:HA	4:4:327:ILE:HG12	1.94	0.49
4:V:318:THR:HA	4:V:327:ILE:HG12	1.94	0.49
4:X:253:GLU:HA	4:X:256:ARG:CG	2.42	0.49
1:A:20:SER:HB3	1:A:23:GLU:OE1	2.13	0.49
1:A:278:GLN:HG3	1:A:318:GLY:H	1.75	0.49
1:A:291:ILE:HA	1:A:331:LEU:CD1	2.39	0.49
1:A:786:ILE:HD13	3:C:90:GLY:HA2	1.93	0.49
1:A:839:MLY:HB2	1:A:840:PRO:HD3	1.94	0.49
2:B:114:LYS:N	2:B:146:GLY:O	2.40	0.49
1:D:601:ASP:N	1:D:602:PRO:CD	2.75	0.49
1:D:831:TRP:HZ3	2:E:50:THR:HG21	1.77	0.49
2:E:93:PRO:O	2:E:97:ILE:HG13	2.13	0.49
1:G:84:MLY:HH11	1:G:715:VAL:HG12	1.76	0.49
1:J:128:PRO:O	1:J:683:PRO:HB3	2.12	0.49
1:J:471:ASP:HB3	1:J:573:GLY:O	2.12	0.49
1:J:543:PRO:CD	4:7:146:GLY:O	2.61	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:601:ASP:N	1:J:602:PRO:CD	2.75	0.49
1:J:715:VAL:O	1:J:764:MLY:HB3	2.12	0.49
4:0:70:PRO:HG3	4:0:81:ASP:HB3	1.94	0.49
4:2:70:PRO:HG3	4:2:81:ASP:HB3	1.94	0.49
4:6:70:PRO:HG3	4:6:81:ASP:HB3	1.94	0.49
4:Y:318:THR:HA	4:Y:327:ILE:HG12	1.94	0.49
1:A:543:PRO:CD	4:4:146:GLY:O	2.61	0.49
1:A:795:ARG:CD	3:C:35:ARG:CZ	2.76	0.49
1:D:543:PRO:CD	4:5:146:GLY:O	2.61	0.49
1:D:715:VAL:HG12	1:D:716:LEU:O	2.12	0.49
2:E:162:ASP:HB3	2:K:20:ASP:CB	2.37	0.49
1:G:290:GLN:HG2	1:G:331:LEU:CA	2.43	0.49
1:G:530:MET:HA	4:6:354:GLN:CD	2.11	0.49
1:G:601:ASP:N	1:G:602:PRO:CD	2.75	0.49
1:G:642:LYS:CB	4:6:24:ASP:O	2.60	0.49
1:G:715:VAL:HG12	1:G:716:LEU:O	2.12	0.49
2:H:93:PRO:O	2:H:97:ILE:HG13	2.12	0.49
1:J:97:LEU:HD13	1:J:97:LEU:N	2.28	0.49
1:J:237:THR:HG22	1:J:238:VAL:N	2.28	0.49
1:J:291:ILE:HA	1:J:331:LEU:CD1	2.39	0.49
1:J:310:TYR:CE2	1:J:320:ILE:CD1	2.94	0.49
4:0:124:PHE:CZ	4:0:132:MET:HG3	2.48	0.49
4:2:318:THR:HA	4:2:327:ILE:HG12	1.94	0.49
4:4:124:PHE:CZ	4:4:132:MET:HG3	2.48	0.49
4:8:124:PHE:CZ	4:8:132:MET:HG3	2.48	0.49
4:W:124:PHE:CZ	4:W:132:MET:HG3	2.48	0.49
1:A:312:TYR:N	1:A:312:TYR:CD1	2.80	0.49
1:A:642:LYS:HG2	4:4:21:PHE:C	2.30	0.49
2:B:121:LEU:HA	2:B:128:PHE:CD2	2.46	0.49
1:D:173:GLN:OE1	1:D:668:HIS:HB3	2.13	0.49
1:D:214:MET:HA	1:D:340:ILE:CD1	2.42	0.49
1:D:251:ARG:HB2	1:D:264:ASP:HB3	1.95	0.49
1:D:332:MET:O	1:D:336:SER:OG	2.27	0.49
1:D:642:LYS:CG	4:5:22:ALA:HA	2.37	0.49
1:D:739:ASP:OD1	1:D:740:SER:N	2.45	0.49
2:E:117:LEU:HG	2:E:147:ASN:HB3	1.93	0.49
1:G:732:ILE:O	1:G:736:GLN:HG3	2.12	0.49
3:I:50:LEU:O	3:I:55:LYS:HB2	2.13	0.49
1:J:218:LEU:HA	1:J:221:GLN:HG3	1.71	0.49
1:J:544:LYS:HD2	4:7:147:ARG:CB	2.36	0.49
1:J:715:VAL:HG12	1:J:716:LEU:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:114:LYS:HG3	2:K:137:TRP:CZ2	2.48	0.49
4:2:124:PHE:CZ	4:2:132:MET:HG3	2.48	0.49
4:6:124:PHE:CZ	4:6:132:MET:HG3	2.48	0.49
4:X:318:THR:HA	4:X:327:ILE:HG12	1.94	0.49
4:Z:124:PHE:CZ	4:Z:132:MET:HG3	2.48	0.49
1:A:173:GLN:OE1	1:A:668:HIS:HB3	2.13	0.49
1:A:354:LEU:HD12	1:A:354:LEU:HA	1.56	0.49
1:A:429:LEU:O	1:A:433:VAL:HG23	2.12	0.49
1:A:538:GLU:OE1	4:4:351:THR:HB	2.12	0.49
1:A:739:ASP:OD1	1:A:740:SER:N	2.45	0.49
1:A:834:LEU:HD13	2:B:54:MET:HG3	1.86	0.49
1:D:128:PRO:O	1:D:683:PRO:HB3	2.12	0.49
1:D:290:GLN:HG2	1:D:331:LEU:CA	2.43	0.49
1:D:507:GLY:HA2	1:D:762:HIS:CD2	2.47	0.49
1:D:538:GLU:HA	4:5:351:THR:H	1.77	0.49
1:D:732:ILE:HG21	1:D:747:LEU:CD1	0.64	0.49
1:D:822:SER:OG	2:E:88:LEU:HA	2.13	0.49
2:E:114:LYS:HG3	2:E:137:TRP:CZ2	2.48	0.49
1:G:154:HIS:CD2	1:G:155:ILE:H	2.30	0.49
1:G:642:LYS:HG2	4:6:21:PHE:C	2.30	0.49
1:G:642:LYS:HA	4:6:22:ALA:C	2.33	0.49
1:J:20:SER:HB3	1:J:23:GLU:OE1	2.13	0.49
2:K:121:LEU:O	2:K:128:PHE:CG	2.61	0.49
4:0:253:GLU:HA	4:0:256:ARG:CG	2.42	0.49
4:7:124:PHE:CZ	4:7:132:MET:HG3	2.48	0.49
4:8:70:PRO:HG3	4:8:81:ASP:HB3	1.94	0.49
4:8:198:TYR:CZ	4:8:248:ILE:HG13	2.48	0.49
4:W:198:TYR:CZ	4:W:248:ILE:HG13	2.48	0.49
1:A:720:PHE:CD2	1:A:744:SER:HB3	2.48	0.49
1:D:64:THR:CG2	1:D:65:GLU:N	2.75	0.49
1:D:237:THR:HG22	1:D:238:VAL:N	2.28	0.49
1:D:292:MET:HE1	1:D:309:PRO:HD3	1.95	0.49
1:D:310:TYR:CE2	1:D:320:ILE:CD1	2.94	0.49
1:D:642:LYS:HA	4:5:22:ALA:C	2.33	0.49
1:D:756:THR:O	1:D:758:TYR:N	2.45	0.49
1:D:793:ARG:HH21	3:F:147:MET:HB3	1.77	0.49
2:E:128:PHE:O	2:E:133:ILE:HD11	2.13	0.49
1:G:20:SER:HB3	1:G:23:GLU:OE1	2.12	0.49
1:G:51:THR:C	1:G:62:VAL:HG13	2.32	0.49
1:G:768:MLY:HD3	1:G:772:LEU:HB2	1.94	0.49
1:J:312:TYR:N	1:J:312:TYR:CD1	2.81	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:753:VAL:CA	1:J:780:ASP:OD2	2.54	0.49
1:J:768:MLY:HH11	1:J:772:LEU:HD22	1.78	0.49
4:1:198:TYR:CZ	4:1:248:ILE:HG13	2.48	0.49
4:X:70:PRO:HG3	4:X:81:ASP:HB3	1.94	0.49
4:Y:124:PHE:CZ	4:Y:132:MET:HG3	2.48	0.49
4:Z:318:THR:HA	4:Z:327:ILE:HG12	1.94	0.49
1:A:97:LEU:HD13	1:A:97:LEU:N	2.28	0.49
1:A:103:LEU:C	1:A:103:LEU:HD12	2.33	0.49
1:A:168:THR:HG22	1:A:169:ASP:OD1	2.12	0.49
1:A:192:VAL:O	1:A:195:TYR:HB3	2.13	0.49
1:A:251:ARG:O	1:A:263:ALA:HA	2.12	0.49
1:A:346:ASP:O	1:A:349:THR:HB	2.11	0.49
1:A:839:MLY:N	1:A:840:PRO:CD	2.75	0.49
1:D:51:THR:C	1:D:62:VAL:HG13	2.32	0.49
1:D:831:TRP:CZ3	2:E:50:THR:CB	2.96	0.49
1:G:41:VAL:CG1	1:G:42:HIS:N	2.75	0.49
1:G:192:VAL:O	1:G:195:TYR:HB3	2.13	0.49
1:G:237:THR:HG22	1:G:238:VAL:N	2.28	0.49
2:H:114:LYS:HG3	2:H:137:TRP:CZ2	2.48	0.49
1:J:51:THR:C	1:J:62:VAL:HG13	2.32	0.49
1:J:64:THR:CG2	1:J:65:GLU:N	2.75	0.49
1:J:173:GLN:OE1	1:J:668:HIS:HB3	2.13	0.49
1:J:251:ARG:HB2	1:J:264:ASP:HB3	1.95	0.49
3:L:50:LEU:O	3:L:55:LYS:HB2	2.13	0.49
4:0:318:THR:HA	4:0:327:ILE:HG12	1.94	0.49
4:1:213:LYS:O	4:1:217:CYS:HB2	2.13	0.49
4:3:70:PRO:HG3	4:3:81:ASP:HB3	1.94	0.49
4:6:198:TYR:CZ	4:6:248:ILE:HG13	2.48	0.49
4:X:124:PHE:CZ	4:X:132:MET:HG3	2.48	0.49
4:Y:198:TYR:CZ	4:Y:248:ILE:HG13	2.48	0.49
1:A:128:PRO:O	1:A:683:PRO:HB3	2.12	0.49
1:A:218:LEU:HD22	1:A:222:ILE:HG13	1.95	0.49
1:A:768:MLY:O	1:A:771:LEU:HB3	2.13	0.49
2:B:114:LYS:HG3	2:B:137:TRP:CZ2	2.48	0.49
3:C:50:LEU:O	3:C:55:LYS:HB2	2.13	0.49
1:D:20:SER:HB3	1:D:23:GLU:OE1	2.13	0.49
1:D:547:ASP:O	1:D:550:PHE:HB3	2.12	0.49
1:D:769:ALA:CB	1:D:770:GLY:N	2.75	0.49
1:D:830:PRO:CB	2:E:67:MET:HE1	2.41	0.49
1:D:831:TRP:CE2	2:E:47:LEU:CB	2.93	0.49
1:D:839:MLY:N	1:D:840:PRO:CD	2.75	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:50:LEU:O	3:F:55:LYS:HB2	2.13	0.49
1:G:95:THR:OG1	1:G:713:SER:CB	2.55	0.49
1:G:547:ASP:O	1:G:550:PHE:HB3	2.12	0.49
1:J:290:GLN:HG2	1:J:331:LEU:CA	2.43	0.49
1:J:405:ARG:HB2	1:J:414:THR:OG1	2.13	0.49
1:J:720:PHE:CD2	1:J:744:SER:HB3	2.48	0.49
1:J:798:LEU:HD21	3:L:122:GLU:O	2.12	0.49
1:J:831:TRP:HH2	2:K:34:ILE:CG2	2.24	0.49
2:K:93:PRO:O	2:K:97:ILE:HG13	2.12	0.49
4:5:70:PRO:HG3	4:5:81:ASP:HB3	1.94	0.49
4:5:124:PHE:CZ	4:5:132:MET:HG3	2.48	0.49
1:A:93:MET:HE2	1:A:715:VAL:HA	1.94	0.48
1:A:732:ILE:HG23	1:A:747:LEU:HD12	0.95	0.48
1:A:795:ARG:NE	3:C:43:ASN:OD1	2.10	0.48
1:A:813:ILE:HG22	2:B:127:ARG:HD2	1.25	0.48
1:D:168:THR:HG22	1:D:169:ASP:OD1	2.12	0.48
1:D:267:THR:HG21	1:D:438:PHE:HE2	1.76	0.48
1:D:793:ARG:O	1:D:797:PHE:N	2.39	0.48
1:D:839:MLY:HB2	1:D:840:PRO:HD3	1.94	0.48
1:G:128:PRO:O	1:G:683:PRO:HB3	2.12	0.48
1:G:134:VAL:C	1:G:136:ASN:H	2.16	0.48
1:G:168:THR:HG22	1:G:169:ASP:OD1	2.12	0.48
1:G:248:MLY:HE2	1:G:250:ILE:HD11	1.95	0.48
1:G:739:ASP:OD1	1:G:740:SER:N	2.46	0.48
1:G:839:MLY:HB2	1:G:840:PRO:HD3	1.94	0.48
1:J:84:MLY:CH1	1:J:715:VAL:HG11	2.17	0.48
1:J:530:MET:HE3	4:7:354:GLN:CB	2.43	0.48
4:1:70:PRO:HG3	4:1:81:ASP:HB3	1.94	0.48
4:1:124:PHE:CZ	4:1:132:MET:HG3	2.48	0.48
4:3:124:PHE:CZ	4:3:132:MET:HG3	2.48	0.48
4:3:198:TYR:CZ	4:3:248:ILE:HG13	2.48	0.48
4:V:124:PHE:CZ	4:V:132:MET:HG3	2.48	0.48
1:A:237:THR:HG22	1:A:238:VAL:N	2.28	0.48
1:A:290:GLN:HG2	1:A:331:LEU:CA	2.43	0.48
1:A:310:TYR:CE2	1:A:320:ILE:CD1	2.94	0.48
1:A:530:MET:HE3	4:4:355:MET:SD	2.53	0.48
1:A:542:PHE:CD2	4:4:143:TYR:CD1	3.02	0.48
2:B:130:PRO:O	2:B:131:GLU:C	2.52	0.48
1:G:405:ARG:HB2	1:G:414:THR:OG1	2.13	0.48
1:G:556:ASP:CA	4:8:49:GLN:O	2.51	0.48
1:G:836:PHE:CE2	2:H:160:GLY:HA3	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:117:LEU:HG	2:H:147:ASN:HB3	1.93	0.48
1:J:215:GLN:H	1:J:340:ILE:CD1	2.20	0.48
1:J:817:GLN:CD	2:K:127:ARG:CD	2.58	0.48
2:K:128:PHE:O	2:K:133:ILE:HD11	2.13	0.48
4:4:198:TYR:CZ	4:4:248:ILE:HG13	2.48	0.48
4:5:198:TYR:CZ	4:5:248:ILE:HG13	2.48	0.48
4:7:70:PRO:HG3	4:7:81:ASP:HB3	1.94	0.48
4:W:70:PRO:HG3	4:W:81:ASP:HB3	1.94	0.48
1:A:642:LYS:HA	4:4:22:ALA:C	2.34	0.48
2:B:93:PRO:O	2:B:97:ILE:HG13	2.13	0.48
1:D:292:MET:CE	1:D:309:PRO:HA	2.39	0.48
1:D:404:PRO:HD2	1:D:415:MLY:O	2.13	0.48
1:D:724:TYR:CZ	1:D:778:MET:CB	2.97	0.48
1:G:93:MET:CE	1:G:763:THR:O	2.60	0.48
1:G:530:MET:HE3	4:6:355:MET:SD	2.53	0.48
1:G:757:GLN:HE22	1:G:772:LEU:CD2	2.27	0.48
1:G:797:PHE:HB2	3:I:149:VAL:CG1	2.43	0.48
1:J:87:MLY:HD3	1:J:87:MLY:HH12	1.61	0.48
1:J:404:PRO:HD2	1:J:415:MLY:O	2.13	0.48
1:J:538:GLU:HA	4:7:351:THR:H	1.77	0.48
1:J:739:ASP:CB	1:J:742:LYS:CB	2.81	0.48
1:J:839:MLY:N	1:J:840:PRO:CD	2.75	0.48
1:A:499:GLU:OE1	1:A:499:GLU:HA	2.13	0.48
1:D:724:TYR:CA	1:D:782:MLY:CH1	2.90	0.48
1:G:251:ARG:O	1:G:263:ALA:HA	2.12	0.48
1:G:759:ALA:O	1:G:766:PHE:N	2.32	0.48
2:H:128:PHE:O	2:H:133:ILE:HD11	2.13	0.48
1:J:136:ASN:O	1:J:139:VAL:N	2.47	0.48
1:J:168:THR:HG22	1:J:169:ASP:OD1	2.12	0.48
1:J:410:ASN:HD22	4:7:336:LYS:HE2	1.78	0.48
1:J:547:ASP:O	1:J:550:PHE:HB3	2.12	0.48
1:J:732:ILE:HG21	1:J:747:LEU:CD1	0.63	0.48
1:J:817:GLN:HG2	2:K:127:ARG:CD	2.42	0.48
2:K:130:PRO:O	2:K:131:GLU:C	2.52	0.48
4:V:70:PRO:HG3	4:V:81:ASP:HB3	1.94	0.48
1:A:406:VAL:CG1	1:A:407:GLY:N	2.77	0.48
2:B:117:LEU:HG	2:B:147:ASN:HB3	1.93	0.48
1:D:405:ARG:HB2	1:D:414:THR:OG1	2.13	0.48
1:D:436:MLY:HE3	1:D:626:TYR:HE1	1.77	0.48
1:D:530:MET:HE3	4:5:354:GLN:CG	2.32	0.48
1:D:544:LYS:HD2	4:5:147:ARG:CB	2.36	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:173:GLN:OE1	1:G:668:HIS:HB3	2.13	0.48
1:G:310:TYR:CE2	1:G:320:ILE:CD1	2.94	0.48
1:G:409:GLY:N	1:G:636:LYS:CD	2.71	0.48
1:G:538:GLU:HA	4:6:351:THR:H	1.77	0.48
1:G:617:MLY:O	1:G:620:ALA:HB3	2.14	0.48
1:G:720:PHE:CD2	1:G:744:SER:HB3	2.48	0.48
1:G:723:ARG:HH11	1:G:723:ARG:HG3	1.78	0.48
1:G:800:ARG:NH1	3:I:149:VAL:CG2	2.26	0.48
1:J:289:TYR:OH	1:J:315:VAL:O	2.27	0.48
4:1:253:GLU:HA	4:1:256:ARG:CG	2.42	0.48
4:2:120:THR:HG21	4:2:370:VAL:HG11	1.95	0.48
4:8:213:LYS:O	4:8:217:CYS:HB2	2.13	0.48
4:8:253:GLU:HA	4:8:256:ARG:CG	2.42	0.48
1:A:10:PHE:CD2	1:A:17:LEU:HD23	2.49	0.48
1:A:544:LYS:HD2	4:4:147:ARG:CB	2.36	0.48
2:B:112:ILE:CG2	2:B:147:ASN:O	2.62	0.48
2:B:128:PHE:O	2:B:133:ILE:HD11	2.13	0.48
1:D:103:LEU:C	1:D:103:LEU:HD12	2.33	0.48
1:D:314:TYR:CZ	1:D:362:GLY:HA2	2.48	0.48
1:D:617:MLY:O	1:D:620:ALA:HB3	2.14	0.48
1:D:642:LYS:CB	4:5:24:ASP:O	2.59	0.48
1:D:838:ILE:C	1:D:840:PRO:HD2	2.34	0.48
1:G:64:THR:CG2	1:G:65:GLU:N	2.75	0.48
1:G:499:GLU:OE1	1:G:499:GLU:HA	2.13	0.48
1:J:41:VAL:CG1	1:J:42:HIS:N	2.76	0.48
1:J:103:LEU:C	1:J:103:LEU:HD12	2.33	0.48
1:J:267:THR:HG21	1:J:438:PHE:HE2	1.76	0.48
1:J:314:TYR:CZ	1:J:362:GLY:HA2	2.48	0.48
4:2:198:TYR:CZ	4:2:248:ILE:HG13	2.48	0.48
4:3:213:LYS:O	4:3:217:CYS:HB2	2.13	0.48
4:6:120:THR:HG21	4:6:370:VAL:HG11	1.95	0.48
4:7:198:TYR:CZ	4:7:248:ILE:HG13	2.48	0.48
4:7:213:LYS:O	4:7:217:CYS:HB2	2.13	0.48
4:V:250:ILE:HG23	4:V:253:GLU:HG2	1.96	0.48
1:A:64:THR:CG2	1:A:65:GLU:N	2.75	0.48
1:A:405:ARG:HB2	1:A:414:THR:OG1	2.13	0.48
1:A:506:GLU:OE2	1:A:760:PHE:HD2	1.97	0.48
1:D:106:LEU:HD12	1:D:117:THR:HG21	1.96	0.48
1:D:550:PHE:CE2	1:D:592:ILE:CG2	2.97	0.48
1:D:689:GLU:O	1:D:689:GLU:HG2	2.14	0.48
1:D:720:PHE:CD2	1:D:744:SER:HB3	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:LEU:C	1:G:103:LEU:HD12	2.33	0.48
1:G:728:ASN:ND2	3:I:110:VAL:HA	2.18	0.48
1:G:739:ASP:CB	1:G:742:LYS:CB	2.81	0.48
1:J:10:PHE:CD2	1:J:17:LEU:HD23	2.49	0.48
1:J:617:MLY:O	1:J:620:ALA:HB3	2.14	0.48
1:J:707:CYS:CB	1:J:714:ARG:NH2	2.73	0.48
4:7:250:ILE:HG23	4:7:253:GLU:HG2	1.96	0.48
4:V:213:LYS:O	4:V:217:CYS:HB2	2.13	0.48
4:Y:253:GLU:HA	4:Y:256:ARG:CG	2.42	0.48
1:D:790:THR:HA	3:F:87:PHE:CZ	2.47	0.48
1:G:10:PHE:CD2	1:G:17:LEU:HD23	2.49	0.48
1:G:312:TYR:N	1:G:312:TYR:CD1	2.81	0.48
1:J:664:LEU:HD12	1:J:664:LEU:HA	1.52	0.48
1:J:723:ARG:HH11	1:J:723:ARG:HG3	1.78	0.48
2:K:137:TRP:CA	2:K:145:ALA:CB	2.82	0.48
4:0:198:TYR:CZ	4:0:248:ILE:HG13	2.48	0.48
4:6:213:LYS:O	4:6:217:CYS:HB2	2.13	0.48
4:X:250:ILE:HG23	4:X:253:GLU:HG2	1.96	0.48
4:Y:70:PRO:HG3	4:Y:81:ASP:HB3	1.94	0.48
4:Z:198:TYR:CZ	4:Z:248:ILE:HG13	2.48	0.48
1:A:765:VAL:CG1	1:A:766:PHE:N	2.77	0.48
1:D:723:ARG:HH11	1:D:723:ARG:HG3	1.79	0.48
1:D:806:MET:SD	3:F:17:PHE:HE2	2.37	0.48
1:D:818:TYR:CD2	2:E:89:LYS:O	2.63	0.48
1:G:97:LEU:HD13	1:G:97:LEU:N	2.28	0.48
1:G:635:GLY:HA3	4:6:334:GLU:CG	2.30	0.48
1:G:823:PHE:CZ	2:H:156:VAL:HG12	2.48	0.48
1:G:838:ILE:C	1:G:840:PRO:HD2	2.34	0.48
2:H:130:PRO:O	2:H:131:GLU:C	2.52	0.48
2:H:140:PHE:HB3	2:H:144:VAL:HG12	1.95	0.48
1:J:768:MLY:HE2	1:J:772:LEU:HD23	1.95	0.48
4:0:250:ILE:HG23	4:0:253:GLU:HG2	1.96	0.48
4:1:120:THR:HG21	4:1:370:VAL:HG11	1.95	0.48
4:2:250:ILE:HG23	4:2:253:GLU:HG2	1.96	0.48
4:4:120:THR:HG21	4:4:370:VAL:HG11	1.95	0.48
4:6:250:ILE:HG23	4:6:253:GLU:HG2	1.96	0.48
4:V:198:TYR:CZ	4:V:248:ILE:HG13	2.48	0.48
4:W:288:ASP:CA	4:Y:204:ALA:HB2	2.31	0.48
4:X:198:TYR:CZ	4:X:248:ILE:HG13	2.48	0.48
4:Y:213:LYS:O	4:Y:217:CYS:HB2	2.13	0.48
4:Z:250:ILE:HG23	4:Z:253:GLU:HG2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:MLY:HE2	1:A:250:ILE:HD11	1.95	0.48
1:A:410:ASN:HD22	4:4:336:LYS:HE2	1.78	0.48
1:A:546:THR:CG2	1:A:547:ASP:N	2.77	0.48
1:A:550:PHE:CE2	1:A:592:ILE:CG2	2.97	0.48
1:A:617:MLY:O	1:A:620:ALA:HB3	2.14	0.48
1:A:664:LEU:HD12	1:A:664:LEU:HA	1.53	0.48
1:A:689:GLU:HG2	1:A:689:GLU:O	2.14	0.48
1:A:723:ARG:HH11	1:A:723:ARG:HG3	1.78	0.48
1:D:312:TYR:N	1:D:312:TYR:CD1	2.81	0.48
1:D:578:HIS:HB3	1:D:592:ILE:CD1	2.38	0.48
1:D:792:ALA:HB2	3:F:40:ASN:O	2.10	0.48
1:D:830:PRO:HG2	2:E:67:MET:HE3	0.48	0.48
1:J:134:VAL:C	1:J:136:ASN:H	2.16	0.48
1:J:757:GLN:OE1	1:J:773:GLY:HA2	2.14	0.48
2:K:121:LEU:HA	2:K:128:PHE:CD2	2.46	0.48
4:0:120:THR:HG21	4:0:370:VAL:HG11	1.95	0.48
4:1:250:ILE:HG23	4:1:253:GLU:HG2	1.96	0.48
4:4:250:ILE:HG23	4:4:253:GLU:HG2	1.96	0.48
4:5:250:ILE:HG23	4:5:253:GLU:HG2	1.96	0.48
4:8:120:THR:HG21	4:8:370:VAL:HG11	1.95	0.48
4:V:253:GLU:HA	4:V:256:ARG:CG	2.42	0.48
1:A:602:PRO:O	1:A:603:LEU:HD12	2.14	0.47
1:A:640:LYS:HD2	1:A:646:PHE:O	2.14	0.47
1:D:10:PHE:CD2	1:D:17:LEU:HD23	2.49	0.47
1:D:542:PHE:CD2	4:5:143:TYR:CD1	3.02	0.47
1:D:546:THR:CG2	1:D:547:ASP:N	2.77	0.47
1:D:568:PRO:HD3	1:D:579:PHE:HA	1.96	0.47
2:E:137:TRP:CA	2:E:145:ALA:CB	2.82	0.47
2:E:160:GLY:O	2:E:161:GLU:HG2	2.14	0.47
1:G:530:MET:CE	4:6:354:GLN:HG3	2.34	0.47
1:G:544:LYS:HD2	4:6:147:ARG:CB	2.36	0.47
1:G:707:CYS:CB	1:G:714:ARG:NH1	2.45	0.47
2:H:121:LEU:O	2:H:128:PHE:CG	2.61	0.47
1:J:84:MLY:HH12	1:J:715:VAL:HG12	1.84	0.47
1:J:542:PHE:CD2	4:7:143:TYR:CD1	3.02	0.47
1:J:550:PHE:CE2	1:J:592:ILE:CG2	2.97	0.47
1:J:636:LYS:O	4:7:144:ALA:HB1	2.14	0.47
1:J:768:MLY:CE	1:J:772:LEU:HD23	2.44	0.47
2:K:112:ILE:CG2	2:K:147:ASN:O	2.62	0.47
4:3:120:THR:HG21	4:3:370:VAL:HG11	1.95	0.47
4:3:250:ILE:HG23	4:3:253:GLU:HG2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:8:250:ILE:HG23	4:8:253:GLU:HG2	1.96	0.47
4:W:213:LYS:O	4:W:217:CYS:HB2	2.13	0.47
4:W:250:ILE:HG23	4:W:253:GLU:HG2	1.96	0.47
4:Y:250:ILE:HG23	4:Y:253:GLU:HG2	1.96	0.47
1:A:218:LEU:HA	1:A:221:GLN:H	1.79	0.47
1:A:501:GLU:CA	1:A:762:HIS:CE1	2.97	0.47
1:A:783:LEU:HA	1:A:786:ILE:HB	1.96	0.47
2:B:160:GLY:O	2:B:161:GLU:HG2	2.14	0.47
1:D:97:LEU:HD13	1:D:97:LEU:N	2.28	0.47
1:D:154:HIS:CE1	1:D:156:PHE:CE2	3.02	0.47
1:D:602:PRO:O	1:D:603:LEU:HD12	2.14	0.47
2:E:144:VAL:HG12	2:E:153:ILE:HD13	1.92	0.47
1:G:410:ASN:HD22	4:6:336:LYS:HE2	1.79	0.47
1:G:550:PHE:CE2	1:G:592:ILE:CG2	2.97	0.47
1:G:564:ASN:HD22	1:G:582:VAL:HB	1.79	0.47
1:G:629:GLU:CA	1:G:643:GLY:C	2.73	0.47
1:G:640:LYS:HD2	1:G:646:PHE:O	2.14	0.47
1:G:701:LEU:HA	1:G:701:LEU:HD12	1.55	0.47
1:G:795:ARG:HB2	3:I:35:ARG:CZ	2.44	0.47
1:G:826:VAL:HG21	2:H:88:LEU:CD2	2.43	0.47
1:J:218:LEU:CD2	1:J:222:ILE:CG1	2.86	0.47
1:J:765:VAL:CG1	1:J:766:PHE:N	2.77	0.47
4:5:120:THR:HG21	4:5:370:VAL:HG11	1.95	0.47
4:X:213:LYS:O	4:X:217:CYS:HB2	2.13	0.47
4:X:287:ILE:CB	4:Z:204:ALA:H	2.13	0.47
4:Y:120:THR:HG21	4:Y:370:VAL:HG11	1.95	0.47
4:Z:120:THR:HG21	4:Z:370:VAL:HG11	1.95	0.47
1:A:314:TYR:CZ	1:A:362:GLY:HA2	2.48	0.47
1:A:538:GLU:HA	4:4:351:THR:H	1.78	0.47
1:G:314:TYR:CZ	1:G:362:GLY:HA2	2.48	0.47
1:G:546:THR:CG2	1:G:547:ASP:N	2.77	0.47
1:G:793:ARG:O	1:G:797:PHE:N	2.39	0.47
1:J:546:THR:CG2	1:J:547:ASP:N	2.77	0.47
1:J:564:ASN:HD22	1:J:582:VAL:HB	1.79	0.47
4:0:213:LYS:O	4:0:217:CYS:HB2	2.13	0.47
4:Z:213:LYS:O	4:Z:217:CYS:HB2	2.13	0.47
1:A:122:PHE:CE2	1:A:700:VAL:HA	2.49	0.47
1:A:595:TRP:N	1:A:595:TRP:CD1	2.80	0.47
1:D:188:ASN:ND2	1:D:674:CYS:SG	2.88	0.47
1:D:410:ASN:HD22	4:5:336:LYS:HE2	1.78	0.47
1:D:564:ASN:HD22	1:D:582:VAL:HB	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:765:VAL:CG1	1:D:766:PHE:N	2.77	0.47
1:D:834:LEU:CD2	2:E:50:THR:HG22	2.44	0.47
1:G:22:LYS:O	1:G:26:GLU:N	2.29	0.47
1:G:93:MET:CE	1:G:764:MLY:CG	2.88	0.47
1:G:154:HIS:CE1	1:G:156:PHE:CE2	3.02	0.47
1:G:408:VAL:HG22	1:G:636:LYS:HG2	1.51	0.47
1:G:725:ARG:CG	1:G:733:PRO:HA	2.43	0.47
1:G:798:LEU:CD1	3:I:126:LEU:HD23	2.12	0.47
2:H:160:GLY:O	2:H:161:GLU:HG2	2.15	0.47
1:J:214:MET:C	1:J:340:ILE:CD1	2.82	0.47
1:J:436:MLY:HE3	1:J:626:TYR:HE1	1.77	0.47
1:J:786:ILE:CD1	3:L:86:ASP:HB3	2.45	0.47
2:K:140:PHE:HB3	2:K:144:VAL:HG12	1.94	0.47
3:L:53:PRO:O	3:L:55:LYS:HG3	2.15	0.47
4:5:213:LYS:O	4:5:217:CYS:HB2	2.13	0.47
4:V:162:ASN:OD1	4:V:277:THR:HG22	2.15	0.47
1:A:136:ASN:O	1:A:139:VAL:N	2.47	0.47
1:A:154:HIS:CE1	1:A:156:PHE:CE2	3.02	0.47
1:A:176:LEU:N	1:A:176:LEU:CD1	2.74	0.47
1:A:404:PRO:HD2	1:A:415:MLY:O	2.13	0.47
1:A:646:PHE:HE2	1:A:652:LEU:CG	2.24	0.47
1:A:838:ILE:C	1:A:840:PRO:HD2	2.35	0.47
2:B:139:ALA:C	2:B:141:PRO:HD3	2.33	0.47
1:D:636:LYS:O	4:5:144:ALA:HB1	2.14	0.47
1:G:106:LEU:HD12	1:G:117:THR:HG21	1.96	0.47
1:G:295:MLY:HG3	1:G:332:MET:HE2	1.94	0.47
1:G:602:PRO:O	1:G:603:LEU:HD12	2.14	0.47
1:G:664:LEU:HD12	1:G:664:LEU:HA	1.53	0.47
1:G:819:ASN:CB	2:H:92:ASP:HB2	2.41	0.47
2:H:112:ILE:CG2	2:H:147:ASN:O	2.62	0.47
1:J:629:GLU:CA	1:J:643:GLY:C	2.73	0.47
4:2:213:LYS:O	4:2:217:CYS:HB2	2.13	0.47
4:3:162:ASN:OD1	4:3:277:THR:HG22	2.15	0.47
4:5:288:ASP:CA	4:7:204:ALA:HB2	2.31	0.47
4:7:162:ASN:OD1	4:7:277:THR:HG22	2.15	0.47
4:8:162:ASN:OD1	4:8:277:THR:HG22	2.15	0.47
1:A:214:MET:C	1:A:340:ILE:CD1	2.82	0.47
1:D:499:GLU:OE1	1:D:499:GLU:HA	2.13	0.47
1:D:640:LYS:HD2	1:D:646:PHE:O	2.15	0.47
1:D:715:VAL:HG11	1:D:720:PHE:CD1	2.50	0.47
2:E:130:PRO:O	2:E:131:GLU:C	2.52	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:122:PHE:CE2	1:G:700:VAL:HA	2.50	0.47
1:G:292:MET:HE1	1:G:309:PRO:HD3	1.97	0.47
1:G:542:PHE:CD2	4:6:143:TYR:CD1	3.03	0.47
1:J:188:ASN:ND2	1:J:674:CYS:SG	2.88	0.47
1:J:406:VAL:CG1	1:J:407:GLY:N	2.77	0.47
1:J:689:GLU:O	1:J:689:GLU:HG2	2.14	0.47
1:J:838:ILE:C	1:J:840:PRO:HD2	2.35	0.47
4:4:213:LYS:O	4:4:217:CYS:HB2	2.13	0.47
4:7:120:THR:HG21	4:7:370:VAL:HG11	1.95	0.47
4:W:120:THR:HG21	4:W:370:VAL:HG11	1.95	0.47
4:X:162:ASN:OD1	4:X:277:THR:HG22	2.15	0.47
4:Y:162:ASN:OD1	4:Y:277:THR:HG22	2.15	0.47
4:Z:162:ASN:OD1	4:Z:277:THR:HG22	2.15	0.47
1:A:400:ALA:HB1	1:A:606:THR:CG2	2.45	0.47
1:A:505:MLY:HB2	1:A:761:GLY:HA2	1.96	0.47
1:A:732:ILE:CG2	1:A:747:LEU:CD1	0.65	0.47
1:D:214:MET:C	1:D:340:ILE:CD1	2.82	0.47
1:D:248:MLY:HE2	1:D:250:ILE:HD11	1.96	0.47
1:D:311:ASP:CB	1:D:312:TYR:CE1	2.98	0.47
1:D:524:GLU:HB3	1:D:528:MLY:HG2	1.97	0.47
1:D:642:LYS:HB2	4:5:24:ASP:O	1.88	0.47
1:D:675:ILE:CG2	1:D:676:ILE:N	2.74	0.47
1:D:724:TYR:HD1	1:D:727:LEU:CD1	2.27	0.47
1:D:783:LEU:HA	1:D:786:ILE:HB	1.97	0.47
2:E:139:ALA:C	2:E:141:PRO:HD3	2.33	0.47
3:F:53:PRO:O	3:F:55:LYS:HG3	2.14	0.47
1:G:84:MLY:HH11	1:G:719:ASP:C	2.33	0.47
1:G:84:MLY:NZ	1:G:719:ASP:O	2.18	0.47
1:G:214:MET:HA	1:G:340:ILE:CD1	2.41	0.47
1:G:215:GLN:H	1:G:340:ILE:CD1	2.20	0.47
1:G:406:VAL:CG1	1:G:407:GLY:N	2.77	0.47
1:G:418:THR:CB	1:G:421:GLU:HG3	2.37	0.47
1:G:595:TRP:N	1:G:595:TRP:CD1	2.80	0.47
1:G:689:GLU:O	1:G:689:GLU:HG2	2.14	0.47
1:G:695:LEU:HB3	1:G:701:LEU:HD22	1.97	0.47
1:G:765:VAL:CG1	1:G:766:PHE:N	2.77	0.47
2:H:121:LEU:HA	2:H:128:PHE:CD2	2.47	0.47
1:J:154:HIS:CE1	1:J:156:PHE:CE2	3.02	0.47
1:J:406:VAL:CG1	1:J:407:GLY:H	2.28	0.47
1:J:510:TRP:CD2	1:J:768:MLY:HH13	2.50	0.47
1:J:519:LEU:N	1:J:519:LEU:CD1	2.77	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:524:GLU:HB3	1:J:528:MLY:HG2	1.97	0.47
1:J:554:LEU:HD12	1:J:554:LEU:HA	1.77	0.47
1:J:568:PRO:HD3	1:J:579:PHE:HA	1.96	0.47
1:J:602:PRO:O	1:J:603:LEU:HD12	2.14	0.47
1:J:749:GLY:O	3:L:114:LEU:HD22	2.12	0.47
2:K:137:TRP:CZ3	2:K:145:ALA:N	2.81	0.47
2:K:139:ALA:C	2:K:141:PRO:HD3	2.33	0.47
4:0:162:ASN:OD1	4:0:277:THR:HG22	2.15	0.47
4:5:162:ASN:OD1	4:5:277:THR:HG22	2.15	0.47
4:6:253:GLU:HA	4:6:256:ARG:CG	2.42	0.47
4:X:120:THR:HG21	4:X:370:VAL:HG11	1.95	0.47
1:A:406:VAL:CG1	1:A:407:GLY:H	2.28	0.47
1:A:538:GLU:OE1	4:4:355:MET:HE3	2.15	0.47
1:A:564:ASN:HD22	1:A:582:VAL:HB	1.79	0.47
1:D:400:ALA:HB1	1:D:606:THR:CG2	2.45	0.47
1:D:496:PHE:CE2	1:D:514:ASP:HA	2.50	0.47
1:D:629:GLU:CB	1:D:645:SER:N	2.74	0.47
1:D:732:ILE:CG2	1:D:747:LEU:CD1	0.65	0.47
1:G:251:ARG:HB2	1:G:264:ASP:HB3	1.95	0.47
1:G:404:PRO:HD2	1:G:415:MLY:O	2.13	0.47
1:G:543:PRO:HD2	4:6:146:GLY:O	2.15	0.47
1:J:496:PHE:CE2	1:J:514:ASP:HA	2.50	0.47
1:J:499:GLU:OE1	1:J:499:GLU:HA	2.13	0.47
1:J:725:ARG:NE	1:J:733:PRO:CB	1.95	0.47
4:3:253:GLU:HA	4:3:256:ARG:CG	2.42	0.47
1:A:524:GLU:HB3	1:A:528:MLY:HG2	1.96	0.47
1:A:732:ILE:HG21	1:A:747:LEU:CD1	0.64	0.47
1:A:768:MLY:CA	1:A:771:LEU:HB2	2.43	0.47
1:A:839:MLY:NZ	2:B:159:HIS:CB	2.62	0.47
1:D:406:VAL:CG1	1:D:407:GLY:N	2.77	0.47
1:D:543:PRO:HD2	4:5:146:GLY:O	2.15	0.47
1:D:695:LEU:HB3	1:D:701:LEU:HD22	1.97	0.47
1:D:809:ARG:NH1	2:E:124:GLY:C	2.68	0.47
2:E:112:ILE:CG2	2:E:147:ASN:O	2.62	0.47
1:G:202:SER:HA	1:G:207:LYS:NZ	2.22	0.47
1:G:406:VAL:CG1	1:G:407:GLY:H	2.28	0.47
1:G:538:GLU:CD	4:6:355:MET:HE1	2.25	0.47
1:G:793:ARG:HB2	3:I:40:ASN:ND2	2.30	0.47
1:G:831:TRP:CZ2	2:H:67:MET:CB	2.98	0.47
1:J:84:MLY:HG2	1:J:719:ASP:OD2	2.14	0.47
1:J:311:ASP:CB	1:J:312:TYR:CE1	2.98	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:400:ALA:HB1	1:J:606:THR:CG2	2.45	0.47
1:J:578:HIS:HB3	1:J:592:ILE:CD1	2.38	0.47
4:2:162:ASN:OD1	4:2:277:THR:HG22	2.15	0.47
1:A:144:ARG:HA	1:A:144:ARG:HD2	1.78	0.47
1:A:202:SER:HA	1:A:207:LYS:NZ	2.22	0.47
1:A:265:ILE:CG2	1:A:266:GLU:N	2.78	0.47
1:A:292:MET:HE1	1:A:309:PRO:HD3	1.97	0.47
1:A:636:LYS:O	4:4:144:ALA:HB1	2.15	0.47
1:A:810:ARG:HG2	1:A:810:ARG:NH1	2.29	0.47
1:D:30:MLY:HB3	1:D:31:PRO:HD2	1.97	0.47
1:D:221:GLN:HG2	1:D:221:GLN:H	1.47	0.47
1:G:188:ASN:ND2	1:G:674:CYS:SG	2.88	0.47
1:J:106:LEU:HD12	1:J:117:THR:HG21	1.96	0.47
1:J:640:LYS:HD2	1:J:646:PHE:O	2.15	0.47
3:L:50:LEU:O	3:L:53:PRO:CD	2.63	0.47
4:4:162:ASN:OD1	4:4:277:THR:HG22	2.15	0.47
4:4:299:MET:HE2	4:4:331:ALA:HB2	1.96	0.47
4:4:324:THR:O	4:6:244:ASP:HA	2.08	0.47
4:V:120:THR:HG21	4:V:370:VAL:HG11	1.95	0.47
1:A:251:ARG:HB2	1:A:264:ASP:HB3	1.95	0.46
2:B:88:LEU:HB3	2:B:91:ALA:HB2	1.97	0.46
3:C:53:PRO:O	3:C:55:LYS:HG3	2.15	0.46
1:D:406:VAL:CG1	1:D:407:GLY:H	2.28	0.46
1:D:556:ASP:CA	4:7:49:GLN:O	2.52	0.46
1:G:214:MET:C	1:G:340:ILE:CD1	2.82	0.46
1:G:559:LEU:HD23	1:G:560:GLY:N	2.30	0.46
1:G:568:PRO:HD3	1:G:579:PHE:HA	1.97	0.46
1:G:640:LYS:HB3	1:G:645:SER:CB	2.42	0.46
1:G:823:PHE:CD1	2:H:157:ILE:HA	2.50	0.46
1:J:122:PHE:CE2	1:J:700:VAL:HA	2.50	0.46
1:J:248:MLY:HE2	1:J:250:ILE:HD11	1.95	0.46
1:J:374:GLN:NE2	1:J:403:TYR:CE1	2.84	0.46
1:J:640:LYS:C	4:7:23:GLY:C	2.74	0.46
1:J:800:ARG:HD2	3:L:149:VAL:CA	2.45	0.46
1:J:839:MLY:HH21	2:K:158:THR:HG22	1.97	0.46
4:2:299:MET:HE2	4:2:331:ALA:HB2	1.97	0.46
4:6:162:ASN:OD1	4:6:277:THR:HG22	2.15	0.46
1:A:188:ASN:ND2	1:A:674:CYS:SG	2.88	0.46
1:A:332:MET:O	1:A:336:SER:OG	2.27	0.46
1:A:640:LYS:HB3	1:A:645:SER:CB	2.42	0.46
1:A:836:PHE:CD2	2:B:160:GLY:C	2.88	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:LEU:O	2:B:128:PHE:CG	2.61	0.46
1:D:122:PHE:CE2	1:D:700:VAL:HA	2.50	0.46
1:D:732:ILE:HG23	1:D:747:LEU:CD1	1.04	0.46
1:D:809:ARG:CZ	2:E:124:GLY:HA2	2.35	0.46
1:D:831:TRP:CE3	2:E:34:ILE:HD13	2.50	0.46
1:G:646:PHE:HE2	1:G:652:LEU:CG	2.24	0.46
1:G:715:VAL:HG11	1:G:720:PHE:CD1	2.49	0.46
1:G:724:TYR:HD1	1:G:727:LEU:CD1	2.27	0.46
1:J:42:HIS:O	1:J:45:GLN:O	2.33	0.46
1:J:206:LYS:HD2	1:J:217:THR:CG2	2.17	0.46
1:J:529:PRO:HB2	4:7:354:GLN:HB3	1.98	0.46
1:J:629:GLU:HG2	1:J:643:GLY:C	2.35	0.46
1:J:714:ARG:HD3	1:J:766:PHE:CE2	2.50	0.46
4:1:162:ASN:OD1	4:1:277:THR:HG22	2.15	0.46
4:1:299:MET:HE2	4:1:331:ALA:HB2	1.96	0.46
4:6:299:MET:HE2	4:6:331:ALA:HB2	1.96	0.46
4:8:299:MET:HE2	4:8:331:ALA:HB2	1.95	0.46
4:Y:299:MET:HE2	4:Y:331:ALA:HB2	1.96	0.46
1:A:41:VAL:CG1	1:A:42:HIS:N	2.76	0.46
1:A:42:HIS:O	1:A:45:GLN:O	2.33	0.46
1:A:106:LEU:HD12	1:A:117:THR:HG21	1.96	0.46
1:A:292:MET:HE1	1:A:309:PRO:CG	2.46	0.46
1:A:714:ARG:HD3	1:A:766:PHE:CE2	2.50	0.46
1:A:800:ARG:CZ	3:C:149:VAL:O	2.63	0.46
1:D:42:HIS:O	1:D:45:GLN:O	2.33	0.46
1:D:530:MET:HE3	4:5:354:GLN:CB	2.44	0.46
1:D:540:CYS:N	4:5:349:LEU:HD11	2.31	0.46
1:D:643:GLY:N	4:5:23:GLY:C	2.55	0.46
1:D:715:VAL:CG1	1:D:720:PHE:HB2	2.46	0.46
1:D:809:ARG:NH1	2:E:124:GLY:O	2.48	0.46
1:D:815:CYS:O	2:E:90:GLY:C	2.53	0.46
1:D:831:TRP:CA	2:E:51:PHE:CZ	2.98	0.46
2:E:163:ALA:O	2:K:21:GLU:N	2.47	0.46
1:G:218:LEU:HA	1:G:221:GLN:H	1.79	0.46
1:G:715:VAL:CG1	1:G:720:PHE:HB2	2.45	0.46
3:I:53:PRO:O	3:I:55:LYS:HG3	2.15	0.46
1:J:559:LEU:HD23	1:J:560:GLY:N	2.30	0.46
1:J:715:VAL:CG1	1:J:720:PHE:HB2	2.45	0.46
1:J:800:ARG:CB	3:L:149:VAL:HG23	2.26	0.46
2:K:160:GLY:O	2:K:161:GLU:HG2	2.15	0.46
4:5:6:THR:HG22	4:5:101:HIS:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:6:THR:HG22	4:7:101:HIS:HA	1.98	0.46
4:V:6:THR:HG22	4:V:101:HIS:HA	1.97	0.46
1:A:559:LEU:HD23	1:A:560:GLY:N	2.30	0.46
1:A:715:VAL:CG1	1:A:720:PHE:HB2	2.45	0.46
1:A:724:TYR:HD1	1:A:727:LEU:CD1	2.27	0.46
1:D:218:LEU:HA	1:D:221:GLN:H	1.79	0.46
1:D:374:GLN:NE2	1:D:403:TYR:CE1	2.84	0.46
1:D:543:PRO:CD	4:5:143:TYR:O	2.64	0.46
1:D:595:TRP:N	1:D:595:TRP:CD1	2.80	0.46
1:D:640:LYS:HB3	1:D:645:SER:CB	2.42	0.46
1:D:714:ARG:HD3	1:D:766:PHE:CE2	2.50	0.46
1:D:769:ALA:C	1:D:771:LEU:HA	2.36	0.46
1:G:139:VAL:HG12	1:G:143:TYR:HD2	1.81	0.46
1:G:784:ALA:O	1:G:788:THR:CA	2.62	0.46
1:J:82:PRO:HG2	1:J:85:TYR:CE2	2.50	0.46
1:J:540:CYS:N	4:7:349:LEU:HD11	2.31	0.46
1:J:797:PHE:CD2	3:L:126:LEU:HD22	2.50	0.46
1:J:797:PHE:CE2	3:L:126:LEU:CD2	2.99	0.46
4:4:287:ILE:CB	4:6:204:ALA:H	2.13	0.46
1:A:87:MLY:HH12	1:A:87:MLY:HD3	1.61	0.46
1:A:136:ASN:HA	1:A:137:PRO:HD3	1.50	0.46
1:A:374:GLN:NE2	1:A:403:TYR:CE1	2.84	0.46
1:A:543:PRO:HD2	4:4:146:GLY:O	2.15	0.46
1:A:568:PRO:HD3	1:A:579:PHE:HA	1.97	0.46
1:A:834:LEU:CD1	2:B:54:MET:CG	2.49	0.46
1:A:836:PHE:CB	2:B:161:GLU:HG2	2.37	0.46
1:D:82:PRO:HG2	1:D:85:TYR:CE2	2.51	0.46
1:D:322:VAL:HB	1:D:325:ILE:HG13	1.97	0.46
1:D:332:MET:H	1:D:332:MET:HG2	1.52	0.46
1:D:529:PRO:HB2	4:5:354:GLN:HB3	1.98	0.46
1:D:629:GLU:HG2	1:D:643:GLY:C	2.35	0.46
1:D:797:PHE:CE2	3:F:126:LEU:HD22	2.50	0.46
1:G:311:ASP:CB	1:G:312:TYR:CE1	2.98	0.46
1:G:659:MLY:HD2	1:G:659:MLY:HH22	1.42	0.46
1:J:84:MLY:HH11	1:J:720:PHE:CA	2.45	0.46
1:J:218:LEU:HA	1:J:221:GLN:H	1.79	0.46
1:J:292:MET:HE1	1:J:309:PRO:CG	2.46	0.46
1:J:793:ARG:O	1:J:797:PHE:N	2.39	0.46
4:V:366:GLY:O	4:V:369:ILE:HG22	2.16	0.46
4:W:253:GLU:HA	4:W:256:ARG:CG	2.42	0.46
4:X:6:THR:HG22	4:X:101:HIS:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ASP:O	1:A:330:GLU:HG2	2.16	0.46
1:A:411:GLU:H	4:4:333:PRO:HB2	1.80	0.46
1:A:543:PRO:CD	4:4:143:TYR:O	2.63	0.46
1:A:783:LEU:N	1:A:783:LEU:CD1	2.79	0.46
1:D:206:LYS:HD3	1:D:217:THR:OG1	2.16	0.46
1:D:265:ILE:CG2	1:D:266:GLU:N	2.78	0.46
1:D:448:GLN:C	1:D:450:ASP:H	2.19	0.46
1:D:640:LYS:C	4:5:23:GLY:C	2.74	0.46
1:G:374:GLN:NE2	1:G:403:TYR:CE1	2.84	0.46
1:G:400:ALA:HB1	1:G:606:THR:CG2	2.45	0.46
1:G:524:GLU:HB3	1:G:528:MLY:HG2	1.96	0.46
1:G:636:LYS:O	4:6:144:ALA:HB1	2.14	0.46
1:G:835:PHE:O	1:G:839:MLY:N	2.49	0.46
4:7:366:GLY:O	4:7:369:ILE:HG22	2.16	0.46
1:A:93:MET:CE	1:A:715:VAL:HA	2.45	0.46
1:A:206:LYS:HD3	1:A:217:THR:OG1	2.16	0.46
1:A:311:ASP:CB	1:A:312:TYR:CE1	2.98	0.46
1:A:335:ASP:OD1	1:A:348:MLY:NZ	2.49	0.46
1:A:361:TYR:O	1:A:364:LEU:HB2	2.16	0.46
1:A:640:LYS:C	4:4:23:GLY:C	2.74	0.46
1:A:642:LYS:CB	4:4:24:ASP:O	2.59	0.46
1:A:817:GLN:NE2	2:B:127:ARG:HG2	2.30	0.46
1:D:335:ASP:OD1	1:D:348:MLY:NZ	2.49	0.46
2:E:114:LYS:CG	2:E:146:GLY:HA2	2.46	0.46
1:G:89:GLU:CD	1:G:153:PRO:HD2	2.36	0.46
1:G:136:ASN:HA	1:G:137:PRO:HD3	1.49	0.46
1:G:335:ASP:OD1	1:G:348:MLY:NZ	2.49	0.46
1:G:642:LYS:HA	4:6:21:PHE:C	2.36	0.46
1:G:714:ARG:HD3	1:G:766:PHE:CE2	2.51	0.46
1:G:725:ARG:NE	1:G:733:PRO:CB	1.95	0.46
2:H:88:LEU:HB3	2:H:91:ALA:HB2	1.98	0.46
1:J:30:MLY:HB3	1:J:31:PRO:HD2	1.97	0.46
1:J:194:GLN:HE21	1:J:194:GLN:HB3	1.43	0.46
1:J:206:LYS:HD3	1:J:217:THR:OG1	2.16	0.46
1:J:503:TYR:CZ	1:J:711:PHE:CD2	3.03	0.46
1:J:543:PRO:HD2	4:7:146:GLY:O	2.16	0.46
1:J:642:LYS:HA	4:7:21:PHE:C	2.36	0.46
4:X:299:MET:HE2	4:X:331:ALA:HB2	1.98	0.46
4:X:366:GLY:O	4:X:369:ILE:HG22	2.16	0.46
4:Z:366:GLY:O	4:Z:369:ILE:HG22	2.16	0.46
1:A:629:GLU:CA	1:A:643:GLY:C	2.73	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:LYS:HA	4:4:21:PHE:C	2.36	0.46
1:A:695:LEU:HB3	1:A:701:LEU:HD22	1.97	0.46
1:A:725:ARG:NE	1:A:733:PRO:CB	1.95	0.46
1:A:793:ARG:HE	3:C:147:MET:CB	2.29	0.46
2:B:149:ASP:CG	2:B:150:TYR:N	2.49	0.46
1:D:443:ILE:HG22	1:D:444:ARG:N	2.29	0.46
1:D:510:TRP:CZ3	1:D:711:PHE:CE2	3.04	0.46
1:D:767:PHE:C	1:D:771:LEU:HD11	2.36	0.46
1:D:831:TRP:CE2	2:E:47:LEU:HB3	2.50	0.46
1:G:42:HIS:O	1:G:45:GLN:O	2.33	0.46
1:G:278:GLN:HE21	1:G:278:GLN:HB3	1.42	0.46
1:G:361:TYR:O	1:G:364:LEU:HB2	2.16	0.46
1:J:322:VAL:HB	1:J:325:ILE:HG13	1.98	0.46
1:J:695:LEU:HB3	1:J:701:LEU:HD22	1.97	0.46
1:J:795:ARG:HH22	3:L:116:GLU:CD	2.19	0.46
1:J:797:PHE:HE2	3:L:126:LEU:HD23	1.81	0.46
2:K:88:LEU:HB3	2:K:91:ALA:HB2	1.98	0.46
4:O:190:MET:O	4:O:194:THR:HG23	2.16	0.46
4:3:6:THR:HG22	4:3:101:HIS:HA	1.98	0.46
4:3:299:MET:HE2	4:3:331:ALA:HB2	1.97	0.46
4:3:366:GLY:O	4:3:369:ILE:HG22	2.16	0.46
4:5:366:GLY:O	4:5:369:ILE:HG22	2.16	0.46
4:V:190:MET:O	4:V:194:THR:HG23	2.16	0.46
4:W:162:ASN:OD1	4:W:277:THR:HG22	2.15	0.46
1:A:464:ILE:CG2	1:A:465:ALA:N	2.79	0.46
2:B:137:TRP:CA	2:B:145:ALA:HB2	2.37	0.46
1:D:99:GLU:N	1:D:100:PRO:CD	2.79	0.46
1:D:642:LYS:HA	4:5:21:PHE:C	2.36	0.46
1:G:206:LYS:HD3	1:G:217:THR:OG1	2.16	0.46
1:G:326:ASP:O	1:G:330:GLU:HG2	2.16	0.46
1:G:411:GLU:H	4:6:333:PRO:HB2	1.80	0.46
1:J:769:ALA:HB2	1:J:770:GLY:N	2.30	0.46
1:J:798:LEU:HA	1:J:798:LEU:HD12	1.36	0.46
4:3:324:THR:N	4:5:245:GLY:CA	2.69	0.46
1:A:214:MET:HA	1:A:340:ILE:CD1	2.42	0.46
1:A:295:MLY:HG3	1:A:332:MET:HE2	1.95	0.46
1:A:332:MET:H	1:A:332:MET:HG2	1.52	0.46
1:A:418:THR:CG2	1:A:419:VAL:N	2.79	0.46
1:A:418:THR:CB	1:A:421:GLU:HG3	2.37	0.46
1:A:502:GLU:OE2	1:A:764:MLY:O	2.34	0.46
1:A:793:ARG:O	1:A:797:PHE:N	2.40	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:LEU:HD13	3:C:126:LEU:HD11	1.98	0.46
3:C:50:LEU:O	3:C:53:PRO:CD	2.63	0.46
1:D:89:GLU:CD	1:D:153:PRO:HD2	2.36	0.46
1:D:136:ASN:O	1:D:139:VAL:N	2.47	0.46
1:D:559:LEU:HD23	1:D:560:GLY:N	2.30	0.46
1:D:810:ARG:HG2	1:D:810:ARG:NH1	2.29	0.46
1:D:822:SER:HB3	2:E:88:LEU:CD2	2.40	0.46
3:F:50:LEU:O	3:F:53:PRO:CD	2.63	0.46
1:G:82:PRO:HG2	1:G:85:TYR:CE2	2.51	0.46
1:G:206:LYS:HD2	1:G:217:THR:CG2	2.17	0.46
1:G:354:LEU:HD12	1:G:354:LEU:HA	1.56	0.46
1:G:543:PRO:CD	4:6:143:TYR:O	2.64	0.46
1:G:821:ARG:NH2	2:H:127:ARG:CD	2.74	0.46
2:H:137:TRP:CZ3	2:H:145:ALA:N	2.81	0.46
1:J:218:LEU:HD22	1:J:222:ILE:HG13	1.95	0.46
1:J:361:TYR:O	1:J:364:LEU:HB2	2.16	0.46
1:J:715:VAL:HG11	1:J:720:PHE:CD1	2.49	0.46
2:K:112:ILE:O	2:K:148:VAL:HA	2.16	0.46
4:7:253:GLU:HA	4:7:256:ARG:CG	2.42	0.46
4:V:223:PHE:CD2	4:V:259:GLU:HG3	2.51	0.46
4:W:32:PRO:HB2	4:W:34:ILE:HD11	1.98	0.46
1:A:501:GLU:HG2	1:A:762:HIS:CE1	2.44	0.45
1:D:664:LEU:HD12	1:D:664:LEU:HA	1.53	0.45
1:D:818:TYR:HB3	2:E:89:LYS:HB2	1.99	0.45
1:G:332:MET:O	1:G:336:SER:OG	2.27	0.45
1:G:448:GLN:C	1:G:450:ASP:H	2.19	0.45
1:G:464:ILE:CG2	1:G:465:ALA:N	2.79	0.45
1:G:728:ASN:HD21	3:I:109:HIS:C	2.20	0.45
1:J:292:MET:HE1	1:J:309:PRO:HD3	1.98	0.45
1:J:330:GLU:O	1:J:333:ALA:HB3	2.16	0.45
1:J:783:LEU:N	1:J:783:LEU:CD1	2.78	0.45
3:L:52:ASN:CB	3:L:53:PRO:CD	2.92	0.45
4:1:190:MET:O	4:1:194:THR:HG23	2.16	0.45
4:4:253:GLU:HA	4:4:256:ARG:CG	2.42	0.45
4:7:223:PHE:CD2	4:7:259:GLU:HG3	2.51	0.45
4:8:324:THR:N	4:W:245:GLY:CA	2.69	0.45
4:V:288:ASP:CA	4:X:204:ALA:HB2	2.31	0.45
4:Y:32:PRO:HB2	4:Y:34:ILE:HD11	1.98	0.45
4:Z:6:THR:HG22	4:Z:101:HIS:HA	1.98	0.45
1:A:30:MLY:HB3	1:A:31:PRO:HD2	1.97	0.45
1:A:82:PRO:HG2	1:A:85:TYR:CE2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:GLU:HG2	1:A:643:GLY:C	2.35	0.45
1:A:637:LYS:HD2	4:4:144:ALA:HB3	1.21	0.45
1:D:724:TYR:N	1:D:782:MLY:CH2	2.80	0.45
1:D:726:VAL:H	1:D:782:MLY:HH21	1.80	0.45
1:D:818:TYR:CD2	2:E:89:LYS:CB	2.99	0.45
1:G:30:MLY:HB3	1:G:31:PRO:HD2	1.97	0.45
1:G:436:MLY:HE3	1:G:626:TYR:HE1	1.77	0.45
1:J:56:GLU:HB2	1:J:59:MLY:CB	2.30	0.45
1:J:84:MLY:HH23	1:J:716:LEU:O	2.12	0.45
1:J:265:ILE:CG2	1:J:266:GLU:N	2.79	0.45
1:J:335:ASP:OD1	1:J:348:MLY:NZ	2.49	0.45
1:J:642:LYS:NZ	4:7:340:TRP:O	2.50	0.45
1:J:815:CYS:SG	2:K:92:ASP:OD1	2.74	0.45
4:0:6:THR:HG22	4:0:101:HIS:HA	1.97	0.45
4:0:366:GLY:O	4:0:369:ILE:HG22	2.16	0.45
4:2:190:MET:O	4:2:194:THR:HG23	2.16	0.45
4:7:190:MET:O	4:7:194:THR:HG23	2.16	0.45
4:X:190:MET:O	4:X:194:THR:HG23	2.16	0.45
4:X:324:THR:N	4:Z:245:GLY:CA	2.69	0.45
1:A:17:LEU:HD12	1:A:17:LEU:HA	1.68	0.45
1:A:476:GLU:OE2	1:A:598:MLY:HH13	2.17	0.45
1:A:667:THR:O	1:A:669:PRO:HD3	2.16	0.45
1:A:723:ARG:CG	1:A:723:ARG:NH1	2.79	0.45
1:A:733:PRO:O	1:A:737:PHE:CE1	2.53	0.45
1:D:136:ASN:HA	1:D:137:PRO:HD3	1.50	0.45
1:D:410:ASN:HA	4:5:334:GLU:HB3	1.29	0.45
1:D:476:GLU:OE2	1:D:598:MLY:HH13	2.16	0.45
1:D:612:GLN:NE2	1:D:627:GLY:H	2.14	0.45
1:G:17:LEU:HA	1:G:17:LEU:HD12	1.67	0.45
1:G:55:MLY:HH23	1:G:60:VAL:HG22	1.99	0.45
1:G:93:MET:SD	1:G:763:THR:CG2	2.94	0.45
1:G:144:ARG:HA	1:G:144:ARG:HD2	1.78	0.45
1:G:186:THR:O	1:G:190:MLY:HG2	2.17	0.45
1:G:322:VAL:HB	1:G:325:ILE:HG13	1.98	0.45
1:G:637:LYS:HD2	4:6:144:ALA:HB3	1.20	0.45
1:G:639:GLY:CA	4:6:344:SER:O	2.40	0.45
2:H:112:ILE:O	2:H:148:VAL:HA	2.16	0.45
1:J:186:THR:O	1:J:190:MLY:HG2	2.17	0.45
1:J:202:SER:HA	1:J:207:LYS:NZ	2.22	0.45
1:J:332:MET:O	1:J:336:SER:OG	2.27	0.45
1:J:448:GLN:C	1:J:450:ASP:H	2.19	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:732:ILE:CG2	1:J:747:LEU:CD1	0.65	0.45
4:1:6:THR:HG22	4:1:101:HIS:HA	1.98	0.45
4:X:223:PHE:CD2	4:X:259:GLU:HG3	2.52	0.45
4:X:288:ASP:CA	4:Z:204:ALA:HB2	2.31	0.45
1:A:139:VAL:HG12	1:A:143:TYR:HD2	1.81	0.45
1:A:206:LYS:CE	1:A:217:THR:HG23	2.29	0.45
1:A:322:VAL:HB	1:A:325:ILE:HG13	1.98	0.45
1:A:496:PHE:CE2	1:A:514:ASP:HA	2.50	0.45
1:A:529:PRO:HB2	4:4:354:GLN:HB3	1.98	0.45
1:A:642:LYS:HB2	4:4:24:ASP:O	1.88	0.45
1:D:330:GLU:O	1:D:333:ALA:HB3	2.17	0.45
1:D:464:ILE:CG2	1:D:465:ALA:N	2.79	0.45
1:D:818:TYR:CD2	2:E:89:LYS:HB3	2.52	0.45
1:D:830:PRO:CB	2:E:51:PHE:CE2	2.95	0.45
1:G:265:ILE:CG2	1:G:266:GLU:N	2.79	0.45
1:G:540:CYS:C	4:6:349:LEU:HD21	2.36	0.45
1:G:540:CYS:N	4:6:349:LEU:HD11	2.31	0.45
1:G:629:GLU:CB	1:G:645:SER:N	2.74	0.45
1:G:823:PHE:HE1	2:H:156:VAL:O	1.89	0.45
2:H:114:LYS:CG	2:H:146:GLY:HA2	2.46	0.45
1:J:17:LEU:HA	1:J:17:LEU:HD12	1.67	0.45
1:J:534:SER:HB2	4:7:354:GLN:HE22	1.56	0.45
1:J:723:ARG:CG	1:J:723:ARG:NH1	2.79	0.45
4:1:32:PRO:HB2	4:1:34:ILE:HD11	1.98	0.45
4:1:366:GLY:O	4:1:369:ILE:HG22	2.16	0.45
4:5:299:MET:HE2	4:5:331:ALA:HB2	1.98	0.45
4:6:32:PRO:HB2	4:6:34:ILE:HD11	1.98	0.45
4:8:6:THR:HG22	4:8:101:HIS:HA	1.98	0.45
4:8:288:ASP:CA	4:W:204:ALA:HB2	2.31	0.45
1:A:89:GLU:CD	1:A:153:PRO:HD2	2.36	0.45
1:A:296:MLY:O	1:A:299:LEU:HB2	2.17	0.45
1:A:411:GLU:H	4:4:333:PRO:CB	2.30	0.45
1:D:97:LEU:HD12	1:D:97:LEU:HA	1.67	0.45
1:D:411:GLU:H	4:5:333:PRO:CB	2.29	0.45
1:D:449:LEU:HD12	1:D:449:LEU:HA	1.60	0.45
2:E:112:ILE:O	2:E:148:VAL:HA	2.17	0.45
1:G:757:GLN:NE2	1:G:772:LEU:CD2	2.80	0.45
1:G:757:GLN:HE22	1:G:772:LEU:HG	1.80	0.45
3:I:50:LEU:O	3:I:53:PRO:CD	2.63	0.45
1:J:89:GLU:CD	1:J:153:PRO:HD2	2.37	0.45
1:J:476:GLU:OE2	1:J:598:MLY:HH13	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:640:LYS:HB3	1:J:645:SER:CB	2.42	0.45
1:J:724:TYR:HD1	1:J:727:LEU:CD1	2.27	0.45
1:J:725:ARG:HA	1:J:732:ILE:HG22	1.99	0.45
4:5:223:PHE:CD2	4:5:259:GLU:HG3	2.51	0.45
4:8:32:PRO:HB2	4:8:34:ILE:HD11	1.98	0.45
4:X:287:ILE:HA	4:Z:202:THR:HG21	1.59	0.45
1:A:55:MLY:HH23	1:A:60:VAL:HG22	1.99	0.45
1:A:179:GLY:O	1:A:185:LYS:HE2	2.17	0.45
1:A:443:ILE:HG22	1:A:444:ARG:N	2.29	0.45
1:D:179:GLY:O	1:D:185:LYS:HE2	2.17	0.45
1:D:642:LYS:NZ	4:5:340:TRP:O	2.50	0.45
1:D:725:ARG:HH21	1:D:733:PRO:HB2	1.81	0.45
1:D:783:LEU:N	1:D:783:LEU:CD1	2.78	0.45
1:G:173:GLN:HG3	1:G:670:HIS:HD2	1.82	0.45
1:G:529:PRO:HB2	4:6:354:GLN:HB3	1.98	0.45
1:G:725:ARG:HH21	1:G:733:PRO:HB2	1.81	0.45
1:G:800:ARG:CD	3:I:149:VAL:HG22	2.41	0.45
1:J:173:GLN:HG3	1:J:670:HIS:HD2	1.82	0.45
1:J:530:MET:CE	4:7:354:GLN:HG3	2.35	0.45
1:J:707:CYS:C	1:J:714:ARG:NH2	2.70	0.45
1:J:797:PHE:HD2	3:L:126:LEU:CD2	2.27	0.45
4:0:223:PHE:CD2	4:0:259:GLU:HG3	2.51	0.45
4:0:287:ILE:HA	4:2:202:THR:HG21	1.59	0.45
4:2:6:THR:HG22	4:2:101:HIS:HA	1.98	0.45
4:2:253:GLU:HA	4:2:256:ARG:CG	2.42	0.45
4:2:366:GLY:O	4:2:369:ILE:HG22	2.16	0.45
4:3:32:PRO:HB2	4:3:34:ILE:HD11	1.98	0.45
4:3:190:MET:O	4:3:194:THR:HG23	2.16	0.45
4:5:290:ARG:HH22	4:7:202:THR:CG2	2.17	0.45
4:6:6:THR:HG22	4:6:101:HIS:HA	1.97	0.45
4:Z:223:PHE:CD2	4:Z:259:GLU:HG3	2.52	0.45
1:A:210:GLN:C	1:A:211:SER:HG	2.15	0.45
1:A:448:GLN:C	1:A:450:ASP:H	2.19	0.45
1:A:540:CYS:N	4:4:349:LEU:HD11	2.31	0.45
2:B:112:ILE:O	2:B:148:VAL:HA	2.17	0.45
1:D:103:LEU:HD22	1:D:692:LEU:HG	1.98	0.45
1:D:229:LEU:HD12	1:D:229:LEU:HA	1.75	0.45
1:D:295:MLY:CG	1:D:332:MET:HE1	2.46	0.45
1:D:296:MLY:O	1:D:299:LEU:HB2	2.17	0.45
1:D:326:ASP:O	1:D:330:GLU:HG2	2.16	0.45
1:D:361:TYR:O	1:D:364:LEU:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:822:SER:HB3	2:E:88:LEU:HD21	1.99	0.45
1:D:835:PHE:O	1:D:839:MLY:N	2.49	0.45
1:G:292:MET:HE1	1:G:309:PRO:CG	2.46	0.45
1:G:418:THR:CG2	1:G:419:VAL:N	2.79	0.45
1:G:496:PHE:CE2	1:G:514:ASP:HA	2.50	0.45
1:G:612:GLN:NE2	1:G:627:GLY:H	2.14	0.45
1:G:642:LYS:NZ	4:6:340:TRP:O	2.50	0.45
1:J:179:GLY:O	1:J:185:LYS:HE2	2.17	0.45
1:J:326:ASP:O	1:J:330:GLU:HG2	2.16	0.45
1:J:732:ILE:H	1:J:733:PRO:HD2	1.74	0.45
4:4:366:GLY:O	4:4:369:ILE:HG22	2.16	0.45
4:6:288:ASP:CA	4:8:204:ALA:HB2	2.31	0.45
4:W:6:THR:HG22	4:W:101:HIS:HA	1.98	0.45
4:Y:366:GLY:O	4:Y:369:ILE:HG22	2.16	0.45
1:A:206:LYS:HD2	1:A:217:THR:CG2	2.17	0.45
1:A:278:GLN:HE21	1:A:278:GLN:HB3	1.42	0.45
1:D:14:ALA:N	1:D:15:PRO:HD2	2.32	0.45
1:D:37:SER:O	1:D:38:VAL:HG23	2.17	0.45
1:D:202:SER:HA	1:D:207:LYS:NZ	2.23	0.45
1:D:226:ASN:N	1:D:227:PRO:HD2	2.32	0.45
1:D:725:ARG:CG	1:D:733:PRO:HA	2.43	0.45
1:D:767:PHE:C	1:D:771:LEU:CD1	2.85	0.45
1:G:99:GLU:N	1:G:100:PRO:CD	2.80	0.45
1:G:410:ASN:HA	4:6:334:GLU:HB3	1.28	0.45
1:G:476:GLU:OE2	1:G:598:MLY:HH13	2.17	0.45
1:G:485:GLU:OE1	1:G:583:HIS:ND1	2.49	0.45
1:G:597:GLU:O	1:G:600:MLY:N	2.50	0.45
1:G:747:LEU:C	1:G:749:GLY:H	2.20	0.45
2:K:137:TRP:CA	2:K:145:ALA:HB2	2.37	0.45
4:0:287:ILE:CB	4:2:204:ALA:H	2.13	0.45
4:1:288:ASP:CA	4:3:204:ALA:HB2	2.32	0.45
4:2:287:ILE:HA	4:4:202:THR:HG21	1.59	0.45
4:4:190:MET:O	4:4:194:THR:HG23	2.16	0.45
1:D:186:THR:O	1:D:190:MLY:HG2	2.17	0.45
1:D:597:GLU:O	1:D:600:MLY:N	2.50	0.45
1:D:769:ALA:HB1	1:D:771:LEU:N	2.25	0.45
1:G:176:LEU:N	1:G:176:LEU:CD1	2.75	0.45
1:G:642:LYS:HG3	4:6:23:GLY:CA	2.31	0.45
1:G:725:ARG:CG	1:G:733:PRO:CA	2.95	0.45
2:H:137:TRP:CA	2:H:145:ALA:HB2	2.37	0.45
1:J:408:VAL:HG22	1:J:636:LYS:HG2	1.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:794:CYS:O	1:J:797:PHE:HB3	2.17	0.45
4:0:32:PRO:HB2	4:0:34:ILE:HD11	1.98	0.45
4:2:223:PHE:CD2	4:2:259:GLU:HG3	2.52	0.45
4:4:6:THR:HG22	4:4:101:HIS:HA	1.98	0.45
4:8:223:PHE:CD2	4:8:259:GLU:HG3	2.51	0.45
4:Y:6:THR:HG22	4:Y:101:HIS:HA	1.98	0.45
1:A:106:LEU:HD12	1:A:106:LEU:HA	1.79	0.45
1:A:163:TYR:O	1:A:166:MET:HB3	2.16	0.45
1:A:195:TYR:CE2	1:A:199:ILE:HD12	2.52	0.45
1:A:224:SER:O	1:A:227:PRO:HD2	2.17	0.45
1:A:322:VAL:CG1	1:A:325:ILE:HD11	2.47	0.45
1:A:488:GLN:O	1:A:491:PHE:HB3	2.17	0.45
1:A:519:LEU:N	1:A:519:LEU:CD1	2.77	0.45
1:A:747:LEU:C	1:A:749:GLY:H	2.20	0.45
1:A:839:MLY:CE	2:B:159:HIS:HB3	2.47	0.45
1:D:64:THR:HB	1:D:68:GLU:N	2.33	0.45
1:D:106:LEU:HD12	1:D:106:LEU:HA	1.79	0.45
1:D:675:ILE:HG23	1:D:676:ILE:N	2.32	0.45
1:G:14:ALA:N	1:G:15:PRO:HD2	2.32	0.45
1:G:296:MLY:O	1:G:299:LEU:HB2	2.17	0.45
1:G:408:VAL:CG1	4:6:332:PRO:HB3	2.41	0.45
1:G:640:LYS:C	4:6:23:GLY:C	2.75	0.45
1:G:768:MLY:HD3	1:G:772:LEU:CB	2.47	0.45
1:G:794:CYS:O	1:G:797:PHE:HB3	2.17	0.45
1:J:14:ALA:N	1:J:15:PRO:HD2	2.32	0.45
1:J:37:SER:O	1:J:38:VAL:HG23	2.17	0.45
1:J:322:VAL:CG1	1:J:325:ILE:HD11	2.47	0.45
1:J:553:MLY:NZ	4:V:45:VAL:CA	2.58	0.45
1:J:597:GLU:O	1:J:600:MLY:N	2.50	0.45
1:J:642:LYS:CB	4:7:24:ASP:O	2.60	0.45
1:J:667:THR:O	1:J:669:PRO:HD3	2.16	0.45
1:J:797:PHE:CE2	3:L:126:LEU:HD23	2.52	0.45
1:J:831:TRP:CZ3	2:K:34:ILE:HD11	2.36	0.45
4:4:223:PHE:CD2	4:4:259:GLU:HG3	2.51	0.45
4:6:223:PHE:CD2	4:6:259:GLU:HG3	2.51	0.45
4:6:324:THR:O	4:8:244:ASP:HA	2.09	0.45
4:8:366:GLY:O	4:8:369:ILE:HG22	2.16	0.45
4:V:287:ILE:CB	4:X:204:ALA:H	2.13	0.45
4:W:223:PHE:CD2	4:W:259:GLU:HG3	2.51	0.45
4:W:287:ILE:HA	4:Y:202:THR:HG21	1.59	0.45
4:Z:32:PRO:HB2	4:Z:34:ILE:HD11	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:SER:O	1:A:38:VAL:HG23	2.17	0.44
1:A:99:GLU:N	1:A:100:PRO:CD	2.80	0.44
1:A:229:LEU:HD12	1:A:229:LEU:HA	1.75	0.44
1:A:346:ASP:O	1:A:350:ALA:N	2.46	0.44
1:A:597:GLU:O	1:A:600:MLY:N	2.50	0.44
1:A:642:LYS:NZ	4:4:340:TRP:O	2.50	0.44
1:D:41:VAL:CG1	1:D:42:HIS:N	2.75	0.44
1:D:139:VAL:HG12	1:D:143:TYR:HD2	1.81	0.44
1:D:486:MLY:HH22	1:D:527:GLU:CD	2.37	0.44
1:D:568:PRO:CG	1:D:578:HIS:H	2.30	0.44
2:E:137:TRP:CZ3	2:E:145:ALA:N	2.81	0.44
1:G:64:THR:HB	1:G:68:GLU:N	2.32	0.44
1:G:667:THR:O	1:G:669:PRO:HD3	2.16	0.44
1:J:226:ASN:N	1:J:227:PRO:HD2	2.32	0.44
1:J:464:ILE:CG2	1:J:465:ALA:N	2.80	0.44
1:J:673:ARG:HA	1:J:673:ARG:HD2	1.79	0.44
1:J:732:ILE:HG23	1:J:747:LEU:HD12	0.95	0.44
1:J:829:TRP:HA	1:J:830:PRO:HD2	1.86	0.44
4:0:223:PHE:HB3	4:0:259:GLU:OE2	2.18	0.44
4:0:299:MET:HE2	4:0:331:ALA:HB2	1.99	0.44
4:2:223:PHE:HB3	4:2:259:GLU:OE2	2.18	0.44
4:3:223:PHE:HB3	4:3:259:GLU:OE2	2.18	0.44
4:4:32:PRO:HB2	4:4:34:ILE:HD11	1.98	0.44
4:5:190:MET:O	4:5:194:THR:HG23	2.16	0.44
4:5:223:PHE:HB3	4:5:259:GLU:OE2	2.18	0.44
4:X:32:PRO:HB2	4:X:34:ILE:HD11	1.98	0.44
4:Z:223:PHE:HB3	4:Z:259:GLU:OE2	2.18	0.44
1:A:48:VAL:HA	1:A:104:TYR:OH	2.17	0.44
1:A:64:THR:HB	1:A:68:GLU:N	2.33	0.44
1:A:186:THR:O	1:A:190:MLY:HG2	2.17	0.44
1:A:711:PHE:HB3	1:A:766:PHE:HB3	1.99	0.44
1:A:794:CYS:O	1:A:797:PHE:HB3	2.17	0.44
1:D:163:TYR:O	1:D:166:MET:HB3	2.17	0.44
1:D:278:GLN:HE21	1:D:278:GLN:HB3	1.42	0.44
1:D:640:LYS:C	1:D:645:SER:HG	2.09	0.44
2:E:121:LEU:O	2:E:128:PHE:CG	2.61	0.44
1:G:155:ILE:HG22	1:G:156:PHE:N	2.33	0.44
1:G:411:GLU:H	4:6:333:PRO:CB	2.29	0.44
1:G:485:GLU:HA	1:G:584:TYR:HE2	1.83	0.44
1:G:488:GLN:O	1:G:491:PHE:HB3	2.17	0.44
1:G:519:LEU:N	1:G:519:LEU:CD1	2.77	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:823:PHE:CE2	2:H:140:PHE:CZ	3.05	0.44
1:J:64:THR:HB	1:J:68:GLU:N	2.33	0.44
1:J:689:GLU:HA	1:J:692:LEU:HB2	2.00	0.44
4:1:223:PHE:HB3	4:1:259:GLU:OE2	2.18	0.44
4:4:324:THR:N	4:6:245:GLY:CA	2.69	0.44
4:5:32:PRO:HB2	4:5:34:ILE:HD11	1.98	0.44
4:7:32:PRO:HB2	4:7:34:ILE:HD11	1.98	0.44
4:7:223:PHE:HB3	4:7:259:GLU:OE2	2.18	0.44
4:V:287:ILE:HA	4:X:202:THR:HG21	1.59	0.44
4:W:366:GLY:O	4:W:369:ILE:HG22	2.16	0.44
4:X:223:PHE:HB3	4:X:259:GLU:OE2	2.18	0.44
4:Z:190:MET:O	4:Z:194:THR:HG23	2.16	0.44
1:A:97:LEU:HD12	1:A:97:LEU:HA	1.67	0.44
1:A:725:ARG:HH21	1:A:733:PRO:HB2	1.81	0.44
1:D:488:GLN:O	1:D:491:PHE:HB3	2.17	0.44
1:D:689:GLU:HA	1:D:692:LEU:HB2	1.99	0.44
1:D:708:ARG:O	1:D:710:GLY:N	2.50	0.44
1:D:723:ARG:O	1:D:782:MLY:HD2	1.99	0.44
1:D:794:CYS:O	1:D:797:PHE:HB3	2.16	0.44
2:E:129:THR:HG23	2:E:132:GLU:OE1	2.17	0.44
1:G:179:GLY:O	1:G:185:LYS:HE2	2.17	0.44
1:G:530:MET:CB	4:6:354:GLN:CB	2.96	0.44
1:G:629:GLU:HG2	1:G:643:GLY:C	2.35	0.44
2:H:112:ILE:O	2:H:148:VAL:N	2.50	0.44
1:J:408:VAL:HA	1:J:636:LYS:HG3	1.03	0.44
1:J:486:MLY:HH22	1:J:527:GLU:CD	2.37	0.44
1:J:488:GLN:O	1:J:491:PHE:HB3	2.17	0.44
1:J:543:PRO:CD	4:7:143:TYR:O	2.64	0.44
1:J:639:GLY:H	4:7:344:SER:HB3	1.83	0.44
1:J:725:ARG:HH21	1:J:733:PRO:HB2	1.82	0.44
1:J:817:GLN:CB	2:K:127:ARG:HD2	2.47	0.44
4:1:223:PHE:CD2	4:1:259:GLU:HG3	2.52	0.44
4:3:288:ASP:CA	4:5:204:ALA:HB2	2.31	0.44
4:6:190:MET:O	4:6:194:THR:HG23	2.16	0.44
4:V:32:PRO:HB2	4:V:34:ILE:HD11	1.98	0.44
4:V:223:PHE:HB3	4:V:259:GLU:OE2	2.18	0.44
4:Y:223:PHE:CD2	4:Y:259:GLU:HG3	2.52	0.44
1:A:502:GLU:CD	1:A:763:THR:N	2.56	0.44
1:A:793:ARG:HH21	3:C:147:MET:CE	2.28	0.44
1:D:292:MET:HE3	1:D:309:PRO:CA	2.44	0.44
1:D:809:ARG:NH2	2:E:124:GLY:HA3	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:768:MLY:CD	1:G:772:LEU:HB2	2.47	0.44
1:J:296:MLY:O	1:J:299:LEU:HB2	2.17	0.44
1:J:410:ASN:HA	4:7:334:GLU:HB3	1.29	0.44
4:3:223:PHE:CD2	4:3:259:GLU:HG3	2.52	0.44
4:4:223:PHE:HB3	4:4:259:GLU:OE2	2.18	0.44
4:6:223:PHE:HB3	4:6:259:GLU:OE2	2.18	0.44
4:W:287:ILE:CB	4:Y:204:ALA:H	2.13	0.44
1:A:103:LEU:HD22	1:A:692:LEU:HG	1.98	0.44
1:A:193:ILE:HD11	1:A:250:ILE:CD1	2.48	0.44
1:A:485:GLU:HA	1:A:584:TYR:HE2	1.83	0.44
1:A:701:LEU:HA	1:A:701:LEU:HD12	1.55	0.44
1:D:292:MET:HE1	1:D:309:PRO:CG	2.48	0.44
1:D:322:VAL:CG1	1:D:325:ILE:HD11	2.47	0.44
1:D:725:ARG:CG	1:D:733:PRO:CA	2.95	0.44
1:D:747:LEU:C	1:D:749:GLY:H	2.21	0.44
1:G:37:SER:O	1:G:38:VAL:HG23	2.17	0.44
1:G:103:LEU:HD22	1:G:692:LEU:HG	1.98	0.44
1:G:136:ASN:O	1:G:139:VAL:N	2.47	0.44
1:G:214:MET:CA	1:G:340:ILE:HD11	2.45	0.44
1:G:320:ILE:O	1:G:320:ILE:HG22	2.18	0.44
1:G:723:ARG:CG	1:G:723:ARG:NH1	2.79	0.44
2:H:129:THR:HG23	2:H:132:GLU:OE1	2.17	0.44
1:J:99:GLU:N	1:J:100:PRO:CD	2.80	0.44
1:J:155:ILE:HG22	1:J:156:PHE:N	2.33	0.44
1:J:195:TYR:CE2	1:J:199:ILE:HD12	2.52	0.44
1:J:443:ILE:HG22	1:J:444:ARG:N	2.29	0.44
1:J:540:CYS:C	4:7:349:LEU:HD21	2.36	0.44
1:J:568:PRO:CG	1:J:578:HIS:H	2.30	0.44
1:J:692:LEU:O	1:J:696:ARG:HG3	2.18	0.44
1:J:725:ARG:CG	1:J:733:PRO:CA	2.95	0.44
1:J:795:ARG:HH22	3:L:43:ASN:HB2	1.82	0.44
2:K:129:THR:HG23	2:K:132:GLU:OE1	2.17	0.44
4:0:290:ARG:HH22	4:2:202:THR:CG2	2.17	0.44
4:Y:223:PHE:HB3	4:Y:259:GLU:OE2	2.18	0.44
4:Z:299:MET:HE2	4:Z:331:ALA:HB2	2.00	0.44
1:A:14:ALA:N	1:A:15:PRO:HD2	2.32	0.44
1:A:123:CYS:CB	1:A:158:ILE:HD13	2.48	0.44
1:A:173:GLN:HG3	1:A:670:HIS:HD2	1.82	0.44
1:A:485:GLU:OE2	1:A:584:TYR:N	2.50	0.44
1:A:516:GLY:O	1:A:518:ASP:N	2.51	0.44
1:A:641:LYS:CE	1:A:647:GLN:CB	2.74	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:LEU:O	1:A:696:ARG:HG3	2.18	0.44
1:A:835:PHE:O	1:A:839:MLY:N	2.49	0.44
1:D:541:MET:HB3	4:5:345:ILE:HG22	2.00	0.44
1:D:692:LEU:O	1:D:696:ARG:HG3	2.18	0.44
1:D:725:ARG:CZ	1:D:733:PRO:CB	2.83	0.44
1:D:768:MLY:O	1:D:771:LEU:HD12	0.62	0.44
1:G:195:TYR:CE2	1:G:199:ILE:HD12	2.52	0.44
1:G:692:LEU:O	1:G:696:ARG:HG3	2.18	0.44
1:G:725:ARG:CZ	1:G:733:PRO:CB	2.83	0.44
3:I:119:THR:O	3:I:123:VAL:HG23	2.18	0.44
1:J:163:TYR:O	1:J:166:MET:HB3	2.17	0.44
1:J:485:GLU:OE1	1:J:583:HIS:ND1	2.49	0.44
1:J:516:GLY:O	1:J:518:ASP:N	2.51	0.44
2:K:114:LYS:CG	2:K:146:GLY:HA2	2.46	0.44
3:L:122:GLU:HA	3:L:125:GLU:OE1	2.18	0.44
4:1:193:LEU:O	4:1:198:TYR:HD2	2.01	0.44
4:2:32:PRO:HB2	4:2:34:ILE:HD11	1.98	0.44
4:4:287:ILE:HA	4:6:202:THR:HG21	1.59	0.44
4:6:290:ARG:HH22	4:8:202:THR:CG2	2.17	0.44
4:7:299:MET:HE2	4:7:331:ALA:HB2	2.00	0.44
4:8:223:PHE:HB3	4:8:259:GLU:OE2	2.18	0.44
4:Y:190:MET:O	4:Y:194:THR:HG23	2.16	0.44
1:A:226:ASN:N	1:A:227:PRO:HD2	2.32	0.44
1:A:439:LEU:N	1:A:439:LEU:CD1	2.81	0.44
1:A:632:GLY:HA3	1:A:643:GLY:N	2.17	0.44
1:A:725:ARG:CG	1:A:733:PRO:CA	2.95	0.44
1:D:418:THR:CG2	1:D:419:VAL:N	2.79	0.44
1:D:642:LYS:HG3	4:5:23:GLY:CA	2.31	0.44
1:G:175:ILE:C	1:G:176:LEU:HD12	2.38	0.44
1:G:224:SER:O	1:G:227:PRO:HD2	2.17	0.44
1:G:322:VAL:CG1	1:G:325:ILE:HD11	2.47	0.44
1:G:493:HIS:O	1:G:496:PHE:HB3	2.18	0.44
1:G:675:ILE:HG23	1:G:676:ILE:N	2.32	0.44
1:G:728:ASN:ND2	3:I:109:HIS:C	2.71	0.44
1:G:732:ILE:HG21	1:G:747:LEU:CD1	0.64	0.44
3:I:69:LEU:HB3	3:I:70:PRO:HD3	1.99	0.44
3:I:122:GLU:HA	3:I:125:GLU:OE1	2.18	0.44
1:J:91:MET:CE	1:J:119:SER:HB2	2.48	0.44
1:J:139:VAL:HG12	1:J:143:TYR:HD2	1.81	0.44
1:J:439:LEU:N	1:J:439:LEU:CD1	2.81	0.44
1:J:476:GLU:CD	1:J:476:GLU:H	2.21	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:725:ARG:CG	1:J:733:PRO:HA	2.43	0.44
1:J:747:LEU:C	1:J:749:GLY:H	2.20	0.44
1:J:818:TYR:CB	2:K:90:GLY:HA3	2.37	0.44
3:L:50:LEU:O	3:L:53:PRO:HG2	2.18	0.44
4:4:193:LEU:O	4:4:198:TYR:HD2	2.01	0.44
4:6:366:GLY:O	4:6:369:ILE:HG22	2.16	0.44
4:8:190:MET:O	4:8:194:THR:HG23	2.16	0.44
4:W:190:MET:O	4:W:194:THR:HG23	2.16	0.44
4:W:223:PHE:HB3	4:W:259:GLU:OE2	2.18	0.44
1:A:504:MLY:CB	1:A:762:HIS:NE2	2.80	0.44
1:A:530:MET:CB	4:4:354:GLN:CB	2.95	0.44
1:A:675:ILE:HG23	1:A:676:ILE:N	2.32	0.44
1:A:715:VAL:HG12	1:A:720:PHE:HB2	2.00	0.44
1:A:793:ARG:HH21	3:C:147:MET:CG	2.31	0.44
1:D:123:CYS:CB	1:D:158:ILE:HD13	2.48	0.44
1:D:266:GLU:OE1	1:D:659:MLY:NZ	2.51	0.44
1:D:485:GLU:OE1	1:D:583:HIS:ND1	2.49	0.44
1:D:508:ILE:HG12	1:D:766:PHE:HE1	1.33	0.44
1:D:541:MET:HG2	4:5:345:ILE:HG22	2.00	0.44
1:D:667:THR:O	1:D:669:PRO:HD3	2.16	0.44
1:D:788:THR:HG22	3:F:81:GLN:HE22	1.83	0.44
1:D:813:ILE:CG2	2:E:127:ARG:NH1	2.76	0.44
1:G:163:TYR:O	1:G:166:MET:HB3	2.17	0.44
1:G:330:GLU:O	1:G:333:ALA:HB3	2.17	0.44
2:H:139:ALA:C	2:H:141:PRO:HD3	2.33	0.44
3:I:50:LEU:O	3:I:53:PRO:HG2	2.18	0.44
3:I:101:THR:HA	3:I:137:ILE:O	2.18	0.44
1:J:103:LEU:HD22	1:J:692:LEU:HG	1.98	0.44
1:J:123:CYS:CB	1:J:158:ILE:HD13	2.48	0.44
1:J:136:ASN:HA	1:J:137:PRO:HD3	1.50	0.44
1:J:411:GLU:H	4:7:333:PRO:CB	2.30	0.44
1:J:810:ARG:HG2	1:J:810:ARG:NH1	2.29	0.44
3:L:101:THR:HA	3:L:137:ILE:O	2.18	0.44
4:2:287:ILE:N	4:4:202:THR:CG2	2.77	0.44
4:6:220:ALA:HB3	4:6:223:PHE:CD1	2.53	0.44
4:6:287:ILE:HA	4:8:202:THR:HG21	1.59	0.44
4:Z:253:GLU:HA	4:Z:256:ARG:CG	2.42	0.44
1:A:123:CYS:HB2	1:A:158:ILE:HD13	2.00	0.44
1:A:174:SER:OG	1:A:669:PRO:HA	2.18	0.44
1:A:175:ILE:C	1:A:176:LEU:HD12	2.38	0.44
1:A:639:GLY:H	4:4:344:SER:HB3	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:VAL:HG12	1:A:775:LEU:CD1	2.47	0.44
1:A:831:TRP:CG	2:B:51:PHE:CZ	3.03	0.44
1:D:195:TYR:CE2	1:D:199:ILE:HD12	2.52	0.44
1:D:206:LYS:CE	1:D:217:THR:HG23	2.29	0.44
1:D:218:LEU:HD22	1:D:222:ILE:HG13	1.95	0.44
1:D:346:ASP:O	1:D:350:ALA:N	2.46	0.44
1:D:439:LEU:N	1:D:439:LEU:CD1	2.81	0.44
1:D:485:GLU:OE2	1:D:584:TYR:N	2.50	0.44
1:D:711:PHE:HB3	1:D:766:PHE:HB3	1.99	0.44
1:D:798:LEU:HA	1:D:798:LEU:HD12	1.36	0.44
2:E:137:TRP:CA	2:E:145:ALA:HB2	2.37	0.44
3:F:122:GLU:HA	3:F:125:GLU:OE1	2.18	0.44
1:G:14:ALA:N	1:G:15:PRO:CD	2.81	0.44
1:G:193:ILE:HD11	1:G:250:ILE:CD1	2.48	0.44
1:G:226:ASN:HB2	1:G:227:PRO:CD	2.48	0.44
1:G:439:LEU:N	1:G:439:LEU:CD1	2.81	0.44
1:G:798:LEU:HD22	3:I:126:LEU:CD1	2.41	0.44
1:J:55:MLY:HH23	1:J:60:VAL:HG22	1.99	0.44
1:J:84:MLY:HH11	1:J:719:ASP:C	2.39	0.44
1:J:144:ARG:HA	1:J:144:ARG:HD2	1.78	0.44
1:J:193:ILE:HD11	1:J:250:ILE:CD1	2.48	0.44
1:J:206:LYS:CE	1:J:217:THR:HG23	2.29	0.44
1:J:308:ASN:HA	1:J:309:PRO:HD2	1.88	0.44
1:J:493:HIS:O	1:J:496:PHE:HB3	2.18	0.44
1:J:599:ASN:CG	1:J:649:VAL:CB	2.80	0.44
1:J:675:ILE:HG23	1:J:676:ILE:N	2.33	0.44
1:J:836:PHE:CD2	2:K:160:GLY:C	2.87	0.44
4:7:205:GLU:O	4:7:208:ILE:HG22	2.18	0.44
4:8:220:ALA:HB3	4:8:223:PHE:CD1	2.53	0.44
4:8:287:ILE:HA	4:W:202:THR:HG21	1.59	0.44
4:W:220:ALA:HB3	4:W:223:PHE:CD1	2.53	0.44
4:X:205:GLU:O	4:X:208:ILE:HG22	2.18	0.44
4:Y:171:LEU:HA	4:Y:172:PRO:HD2	1.84	0.44
1:A:217:THR:HG22	1:A:218:LEU:N	2.33	0.43
1:A:391:GLY:HA3	1:A:616:VAL:HG23	2.00	0.43
1:A:787:ILE:HG23	1:A:791:GLN:HG3	2.00	0.43
2:B:137:TRP:CZ3	2:B:145:ALA:N	2.81	0.43
1:D:40:VAL:HG23	1:D:76:GLN:O	2.18	0.43
1:D:48:VAL:HA	1:D:104:TYR:OH	2.17	0.43
1:D:134:VAL:C	1:D:136:ASN:H	2.16	0.43
1:D:485:GLU:HA	1:D:584:TYR:HE2	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:516:GLY:O	1:D:518:ASP:N	2.51	0.43
1:D:530:MET:CB	4:5:354:GLN:CB	2.95	0.43
1:D:540:CYS:C	4:5:349:LEU:HD21	2.36	0.43
1:D:724:TYR:C	1:D:782:MLY:CH1	2.79	0.43
1:G:107:MLY:CB	1:G:686:MET:HE2	2.37	0.43
1:G:123:CYS:CB	1:G:158:ILE:HD13	2.48	0.43
1:G:309:PRO:C	1:G:311:ASP:H	2.22	0.43
1:G:578:HIS:HB3	1:G:592:ILE:CD1	2.38	0.43
1:G:639:GLY:H	4:6:344:SER:HB3	1.83	0.43
1:J:129:TYR:HD1	1:J:129:TYR:HA	1.65	0.43
1:J:576:GLU:CG	1:J:577:ALA:N	2.44	0.43
3:L:69:LEU:HB3	3:L:70:PRO:HD3	1.99	0.43
4:2:193:LEU:O	4:2:198:TYR:HD2	2.01	0.43
4:V:299:MET:HE2	4:V:331:ALA:HB2	2.00	0.43
4:W:193:LEU:O	4:W:198:TYR:HD2	2.01	0.43
1:A:201:ALA:O	1:A:202:SER:OG	2.36	0.43
1:A:534:SER:CB	4:4:351:THR:HA	2.48	0.43
1:A:753:VAL:HG12	1:A:775:LEU:CG	2.47	0.43
1:D:55:MLY:HH23	1:D:60:VAL:HG22	1.99	0.43
1:D:64:THR:CG2	1:D:65:GLU:H	2.32	0.43
1:D:123:CYS:HB2	1:D:158:ILE:HD13	2.00	0.43
1:D:173:GLN:HG3	1:D:670:HIS:HD2	1.82	0.43
1:D:400:ALA:CB	1:D:606:THR:HG22	2.48	0.43
1:D:639:GLY:H	4:5:344:SER:HB3	1.83	0.43
2:E:88:LEU:HB3	2:E:91:ALA:HB2	1.98	0.43
1:G:322:VAL:CG1	1:G:325:ILE:HG13	2.48	0.43
1:J:174:SER:OG	1:J:669:PRO:HA	2.18	0.43
1:J:246:PHE:HB3	1:J:270:LEU:HD12	2.01	0.43
1:J:391:GLY:HA3	1:J:616:VAL:HG23	2.00	0.43
1:J:541:MET:HB3	4:7:345:ILE:HG22	2.01	0.43
1:J:835:PHE:O	1:J:839:MLY:N	2.49	0.43
4:3:193:LEU:O	4:3:198:TYR:HD2	2.01	0.43
4:3:287:ILE:CB	4:5:204:ALA:H	2.13	0.43
4:4:220:ALA:HB3	4:4:223:PHE:CD1	2.53	0.43
4:5:253:GLU:HA	4:5:256:ARG:CG	2.42	0.43
1:A:348:MLY:HH12	1:A:348:MLY:HD2	1.82	0.43
1:A:436:MLY:HE3	1:A:626:TYR:HE1	1.77	0.43
1:A:496:PHE:HB2	1:A:515:PHE:CD2	2.53	0.43
1:A:549:SER:C	4:6:45:VAL:O	2.56	0.43
1:A:747:LEU:C	1:A:749:GLY:N	2.71	0.43
2:B:129:THR:HG23	2:B:132:GLU:OE1	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:LEU:O	3:C:53:PRO:HG2	2.18	0.43
3:C:119:THR:O	3:C:123:VAL:HG23	2.18	0.43
3:C:122:GLU:HA	3:C:125:GLU:OE1	2.18	0.43
1:D:193:ILE:HD11	1:D:250:ILE:CD1	2.48	0.43
1:D:322:VAL:CG1	1:D:325:ILE:HG13	2.48	0.43
1:D:747:LEU:C	1:D:749:GLY:N	2.72	0.43
2:E:112:ILE:O	2:E:148:VAL:N	2.50	0.43
3:F:101:THR:HA	3:F:137:ILE:O	2.18	0.43
1:G:48:VAL:HA	1:G:104:TYR:OH	2.18	0.43
1:G:266:GLU:OE1	1:G:659:MLY:NZ	2.51	0.43
1:G:391:GLY:HA3	1:G:616:VAL:HG23	2.01	0.43
1:G:486:MLY:HH22	1:G:527:GLU:CD	2.37	0.43
1:G:692:LEU:HD23	1:G:692:LEU:HA	1.84	0.43
1:G:725:ARG:CZ	1:G:737:PHE:CZ	3.01	0.43
1:G:787:ILE:HG23	1:G:791:GLN:HG3	2.00	0.43
1:G:834:LEU:HD11	2:H:51:PHE:CD1	2.52	0.43
1:J:48:VAL:HA	1:J:104:TYR:OH	2.18	0.43
1:J:322:VAL:HA	1:J:323:PRO:HD3	1.87	0.43
1:J:409:GLY:N	1:J:636:LYS:CD	2.70	0.43
1:J:496:PHE:HB2	1:J:515:PHE:CD2	2.53	0.43
1:J:711:PHE:HB3	1:J:766:PHE:HB3	2.00	0.43
1:J:813:ILE:HG23	2:K:128:PHE:CZ	2.53	0.43
4:O:205:GLU:O	4:O:208:ILE:HG22	2.18	0.43
4:6:193:LEU:O	4:6:198:TYR:HD2	2.01	0.43
4:V:193:LEU:O	4:V:198:TYR:HD2	2.01	0.43
4:Y:220:ALA:HB3	4:Y:223:PHE:CD1	2.53	0.43
1:A:14:ALA:N	1:A:15:PRO:CD	2.81	0.43
1:A:109:ARG:CD	1:A:117:THR:HB	2.48	0.43
1:A:322:VAL:CG1	1:A:325:ILE:HG13	2.49	0.43
1:A:642:LYS:HG3	4:4:23:GLY:CA	2.32	0.43
1:A:725:ARG:CZ	1:A:737:PHE:CZ	3.01	0.43
1:D:166:MET:CE	1:D:254:PHE:CD2	3.01	0.43
1:D:292:MET:CE	1:D:309:PRO:CA	2.97	0.43
1:D:530:MET:CE	4:5:354:GLN:HG3	2.35	0.43
1:D:726:VAL:CA	1:D:782:MLY:HH13	2.45	0.43
1:D:793:ARG:HE	3:F:147:MET:CG	2.31	0.43
1:G:201:ALA:O	1:G:202:SER:OG	2.36	0.43
1:G:568:PRO:CG	1:G:578:HIS:H	2.29	0.43
1:G:783:LEU:N	1:G:783:LEU:CD1	2.78	0.43
1:G:795:ARG:HE	3:I:118:MET:CE	2.31	0.43
1:J:266:GLU:OE1	1:J:659:MLY:NZ	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:541:MET:HG2	4:7:345:ILE:HG22	2.00	0.43
1:J:790:THR:N	3:L:87:PHE:HE2	2.12	0.43
4:2:220:ALA:HB3	4:2:223:PHE:CD1	2.53	0.43
4:3:149:THR:HA	4:3:165:ILE:O	2.19	0.43
4:4:149:THR:HA	4:4:165:ILE:O	2.19	0.43
4:7:149:THR:HA	4:7:165:ILE:O	2.19	0.43
1:A:40:VAL:HG23	1:A:76:GLN:O	2.19	0.43
1:A:86:ASP:OD2	1:A:87:MLY:HH22	2.19	0.43
1:A:129:TYR:HD1	1:A:129:TYR:HA	1.65	0.43
1:A:295:MLY:CE	1:A:332:MET:CE	2.96	0.43
1:A:320:ILE:O	1:A:320:ILE:HG22	2.18	0.43
1:A:476:GLU:H	1:A:476:GLU:CD	2.22	0.43
1:A:486:MLY:HH22	1:A:527:GLU:CD	2.37	0.43
1:A:529:PRO:HB3	4:4:354:GLN:HA	1.99	0.43
1:A:537:GLU:OE1	4:4:350:SER:HA	2.19	0.43
1:A:540:CYS:C	4:4:349:LEU:HD21	2.36	0.43
1:A:568:PRO:CG	1:A:578:HIS:H	2.30	0.43
3:C:101:THR:HA	3:C:137:ILE:O	2.18	0.43
1:D:155:ILE:HG22	1:D:156:PHE:N	2.33	0.43
1:D:224:SER:O	1:D:227:PRO:HD2	2.17	0.43
1:D:493:HIS:O	1:D:496:PHE:HB3	2.18	0.43
1:D:508:ILE:CG2	1:D:766:PHE:CD1	3.01	0.43
1:D:530:MET:HA	4:5:354:GLN:CD	2.11	0.43
1:D:541:MET:CE	4:5:346:LEU:HD12	2.48	0.43
1:G:92:ALA:HB3	1:G:764:MLY:HH13	1.31	0.43
1:G:174:SER:OG	1:G:669:PRO:HA	2.18	0.43
1:G:217:THR:HG22	1:G:218:LEU:N	2.34	0.43
1:G:218:LEU:HD22	1:G:222:ILE:HG13	1.95	0.43
1:G:226:ASN:N	1:G:227:PRO:HD2	2.32	0.43
1:G:292:MET:CE	1:G:309:PRO:CA	2.97	0.43
1:G:295:MLY:CE	1:G:332:MET:CE	2.97	0.43
1:G:496:PHE:HB2	1:G:515:PHE:CD2	2.53	0.43
1:G:643:GLY:CA	4:6:24:ASP:OD1	2.62	0.43
1:G:689:GLU:HA	1:G:692:LEU:HB2	1.99	0.43
1:G:708:ARG:HA	1:G:714:ARG:NH2	2.33	0.43
3:I:49:ILE:CA	3:I:52:ASN:ND2	2.53	0.43
1:J:166:MET:CE	1:J:254:PHE:HB2	2.47	0.43
1:J:217:THR:HG22	1:J:218:LEU:N	2.34	0.43
1:J:322:VAL:CG1	1:J:325:ILE:HG13	2.49	0.43
1:J:503:TYR:CZ	1:J:711:PHE:CE2	3.05	0.43
1:J:529:PRO:HB3	4:7:354:GLN:HA	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:541:MET:CE	4:7:346:LEU:HD12	2.47	0.43
1:J:757:GLN:OE1	1:J:773:GLY:CA	2.66	0.43
4:0:149:THR:HA	4:0:165:ILE:O	2.19	0.43
4:2:149:THR:HA	4:2:165:ILE:O	2.19	0.43
4:2:205:GLU:O	4:2:208:ILE:HG22	2.18	0.43
4:3:205:GLU:O	4:3:208:ILE:HG22	2.18	0.43
4:Z:205:GLU:O	4:Z:208:ILE:HG22	2.18	0.43
1:A:151:ALA:HB1	1:A:152:PRO:HD2	2.01	0.43
1:A:266:GLU:OE1	1:A:659:MLY:NZ	2.51	0.43
1:A:449:LEU:HD12	1:A:449:LEU:HA	1.60	0.43
1:A:612:GLN:NE2	1:A:627:GLY:H	2.14	0.43
1:A:639:GLY:CA	4:4:344:SER:O	2.40	0.43
1:D:226:ASN:HB2	1:D:227:PRO:CD	2.47	0.43
1:D:246:PHE:HB3	1:D:270:LEU:HD12	2.01	0.43
1:D:391:GLY:HA3	1:D:616:VAL:HG23	2.00	0.43
1:D:723:ARG:CG	1:D:723:ARG:NH1	2.80	0.43
1:D:789:ALA:C	3:F:87:PHE:HE2	2.11	0.43
2:E:163:ALA:CA	2:K:21:GLU:HB3	2.37	0.43
1:G:40:VAL:HG23	1:G:76:GLN:O	2.19	0.43
1:G:332:MET:H	1:G:332:MET:HG2	1.52	0.43
1:G:516:GLY:O	1:G:518:ASP:N	2.51	0.43
1:G:549:SER:C	4:8:45:VAL:O	2.57	0.43
1:G:711:PHE:HB3	1:G:766:PHE:HB3	2.00	0.43
1:J:14:ALA:N	1:J:15:PRO:CD	2.81	0.43
1:J:400:ALA:CB	1:J:606:THR:HG22	2.49	0.43
1:J:530:MET:HA	4:7:354:GLN:CD	2.11	0.43
1:J:537:GLU:OE1	4:7:350:SER:HA	2.19	0.43
1:J:725:ARG:CZ	1:J:737:PHE:CZ	3.01	0.43
1:J:747:LEU:C	1:J:749:GLY:N	2.71	0.43
3:L:119:THR:O	3:L:123:VAL:HG23	2.18	0.43
4:6:149:THR:HA	4:6:165:ILE:O	2.19	0.43
4:V:205:GLU:O	4:V:208:ILE:HG22	2.18	0.43
4:X:149:THR:HA	4:X:165:ILE:O	2.19	0.43
4:X:193:LEU:O	4:X:198:TYR:HD2	2.01	0.43
4:Z:149:THR:HA	4:Z:165:ILE:O	2.19	0.43
1:A:155:ILE:HG22	1:A:156:PHE:N	2.33	0.43
1:A:369:MLY:HH22	1:A:369:MLY:HD3	1.79	0.43
1:A:400:ALA:CB	1:A:606:THR:HG22	2.48	0.43
1:A:442:VAL:O	1:A:445:ILE:HB	2.19	0.43
1:A:541:MET:HB3	4:4:345:ILE:HG22	2.00	0.43
1:A:715:VAL:HG11	1:A:720:PHE:CD1	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:MLY:HG3	1:D:332:MET:HE2	2.00	0.43
1:D:541:MET:HG2	4:5:345:ILE:HG23	2.01	0.43
1:D:712:PRO:HB2	1:D:713:SER:H	1.61	0.43
1:D:725:ARG:CZ	1:D:737:PHE:CE1	3.01	0.43
1:D:789:ALA:O	3:F:87:PHE:HZ	1.98	0.43
1:D:818:TYR:CB	2:E:89:LYS:HB2	2.48	0.43
1:D:822:SER:OG	2:E:87:LYS:O	2.20	0.43
1:G:86:ASP:OD2	1:G:87:MLY:HH22	2.19	0.43
1:G:294:ASN:OD1	1:G:307:THR:HG21	2.19	0.43
1:G:541:MET:HG2	4:6:345:ILE:HG22	2.00	0.43
1:G:725:ARG:CZ	1:G:737:PHE:CE1	3.02	0.43
1:J:64:THR:CG2	1:J:65:GLU:H	2.32	0.43
1:J:123:CYS:HB2	1:J:158:ILE:HD13	2.00	0.43
1:J:224:SER:O	1:J:227:PRO:HD2	2.17	0.43
1:J:485:GLU:OE2	1:J:584:TYR:N	2.50	0.43
1:J:724:TYR:HB3	1:J:727:LEU:CD1	2.48	0.43
1:J:725:ARG:CZ	1:J:737:PHE:CE1	3.02	0.43
4:3:217:CYS:C	4:3:218:TYR:HD1	2.22	0.43
4:7:220:ALA:HB3	4:7:223:PHE:CD1	2.53	0.43
4:7:287:ILE:CB	4:V:204:ALA:H	2.13	0.43
4:8:149:THR:HA	4:8:165:ILE:O	2.19	0.43
1:A:330:GLU:HG2	1:A:330:GLU:H	1.55	0.43
1:A:500:GLN:HB2	1:A:512:PHE:CZ	2.54	0.43
1:A:533:PHE:HD1	1:A:533:PHE:HA	1.79	0.43
1:A:551:MLY:C	4:6:47:MET:HA	2.48	0.43
1:D:14:ALA:N	1:D:15:PRO:CD	2.81	0.43
1:D:17:LEU:HA	1:D:17:LEU:HD12	1.68	0.43
1:D:144:ARG:HA	1:D:144:ARG:HD2	1.78	0.43
1:D:725:ARG:HA	1:D:732:ILE:HG22	1.99	0.43
3:F:69:LEU:HB3	3:F:70:PRO:HD3	1.99	0.43
3:F:119:THR:O	3:F:123:VAL:HG23	2.18	0.43
1:G:500:GLN:HB2	1:G:512:PHE:CZ	2.54	0.43
1:J:169:ASP:O	1:J:170:ARG:HB2	2.19	0.43
1:J:195:TYR:CD2	1:J:199:ILE:HD13	2.54	0.43
1:J:201:ALA:O	1:J:202:SER:OG	2.36	0.43
1:J:292:MET:CE	1:J:309:PRO:CA	2.97	0.43
1:J:309:PRO:C	1:J:311:ASP:H	2.22	0.43
2:K:140:PHE:HA	2:K:141:PRO:HD2	1.57	0.43
4:8:193:LEU:O	4:8:198:TYR:HD2	2.01	0.43
4:V:220:ALA:HB3	4:V:223:PHE:CD1	2.53	0.43
4:Y:193:LEU:O	4:Y:198:TYR:HD2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASN:OD1	1:A:307:THR:HG21	2.19	0.43
1:A:330:GLU:O	1:A:333:ALA:HB3	2.17	0.43
1:A:408:VAL:HG22	1:A:636:LYS:HG2	1.51	0.43
1:A:485:GLU:OE1	1:A:583:HIS:ND1	2.49	0.43
1:A:502:GLU:HG2	1:A:766:PHE:CE1	2.54	0.43
1:A:578:HIS:HB3	1:A:592:ILE:CD1	2.38	0.43
3:C:69:LEU:HB3	3:C:70:PRO:HD3	1.99	0.43
1:D:174:SER:OG	1:D:669:PRO:HA	2.18	0.43
1:D:529:PRO:HB3	4:5:354:GLN:HA	2.00	0.43
1:G:109:ARG:CD	1:G:117:THR:HB	2.48	0.43
1:G:151:ALA:HB1	1:G:152:PRO:HD2	2.01	0.43
1:G:206:LYS:CE	1:G:217:THR:HG23	2.30	0.43
1:G:442:VAL:O	1:G:445:ILE:HB	2.19	0.43
1:G:445:ILE:HG22	1:G:449:LEU:HD22	2.01	0.43
1:G:725:ARG:HA	1:G:732:ILE:HG22	1.99	0.43
3:I:11:LYS:HE2	3:I:11:LYS:HB3	1.83	0.43
1:J:97:LEU:HA	1:J:97:LEU:HD12	1.67	0.43
1:J:109:ARG:CD	1:J:117:THR:HB	2.49	0.43
1:J:320:ILE:O	1:J:320:ILE:HG22	2.18	0.43
1:J:549:SER:C	4:V:45:VAL:O	2.56	0.43
1:J:783:LEU:HA	1:J:786:ILE:HB	2.00	0.43
4:1:180:LEU:HD11	4:1:261:LEU:HD23	2.01	0.43
4:1:220:ALA:HB3	4:1:223:PHE:CD1	2.53	0.43
4:7:193:LEU:O	4:7:198:TYR:HD2	2.01	0.43
4:V:287:ILE:HD11	4:X:202:THR:HA	1.66	0.43
4:W:149:THR:HA	4:W:165:ILE:O	2.19	0.43
4:X:290:ARG:HH22	4:Z:202:THR:CG2	2.17	0.43
1:A:91:MET:CE	1:A:119:SER:HB2	2.47	0.43
1:A:309:PRO:C	1:A:311:ASP:H	2.22	0.43
1:A:493:HIS:O	1:A:496:PHE:HB3	2.18	0.43
1:A:636:LYS:CB	4:4:334:GLU:OE1	2.67	0.43
1:A:725:ARG:HA	1:A:732:ILE:HG22	1.99	0.43
2:B:140:PHE:CD2	2:B:144:VAL:HG11	2.54	0.43
1:D:169:ASP:O	1:D:170:ARG:HB2	2.19	0.43
1:D:550:PHE:C	4:7:46:GLY:CA	2.87	0.43
1:D:599:ASN:CG	1:D:649:VAL:CB	2.80	0.43
1:D:715:VAL:HG12	1:D:720:PHE:HB2	2.00	0.43
1:D:829:TRP:O	1:D:832:MET:N	2.50	0.43
1:G:195:TYR:CD2	1:G:199:ILE:HD13	2.54	0.43
1:G:213:LYS:HA	1:G:220:ASP:OD2	2.19	0.43
1:G:246:PHE:HB3	1:G:270:LEU:HD12	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:476:GLU:H	1:G:476:GLU:CD	2.21	0.43
1:G:747:LEU:C	1:G:749:GLY:N	2.71	0.43
1:J:442:VAL:O	1:J:445:ILE:HB	2.19	0.43
1:J:568:PRO:O	1:J:570:PRO:HD3	2.19	0.43
4:0:193:LEU:O	4:0:198:TYR:HD2	2.01	0.43
4:1:217:CYS:C	4:1:218:TYR:HD1	2.22	0.43
4:8:324:THR:O	4:W:244:ASP:HA	2.08	0.43
4:W:222:ASP:OD1	4:W:224:GLU:HB3	2.19	0.43
4:Y:149:THR:HA	4:Y:165:ILE:O	2.19	0.43
4:Y:217:CYS:C	4:Y:218:TYR:HD1	2.23	0.43
4:Z:180:LEU:HD11	4:Z:261:LEU:HD23	2.01	0.43
1:A:64:THR:CG2	1:A:65:GLU:H	2.32	0.42
1:A:195:TYR:CD2	1:A:199:ILE:HD13	2.54	0.42
1:A:246:PHE:HB3	1:A:270:LEU:HD12	2.01	0.42
1:A:292:MET:CE	1:A:309:PRO:CA	2.97	0.42
1:A:689:GLU:HA	1:A:692:LEU:HB2	2.00	0.42
1:D:195:TYR:CD2	1:D:199:ILE:HD13	2.54	0.42
1:D:217:THR:HG22	1:D:218:LEU:N	2.34	0.42
1:D:442:VAL:O	1:D:445:ILE:HB	2.19	0.42
1:D:549:SER:C	4:7:45:VAL:O	2.57	0.42
1:D:725:ARG:CZ	1:D:737:PHE:CZ	3.01	0.42
1:D:787:ILE:HG23	1:D:791:GLN:HG3	2.00	0.42
1:G:129:TYR:HD1	1:G:129:TYR:HA	1.65	0.42
1:G:289:TYR:OH	1:G:315:VAL:O	2.27	0.42
1:G:443:ILE:HG22	1:G:444:ARG:N	2.29	0.42
1:G:568:PRO:O	1:G:570:PRO:HD3	2.19	0.42
1:G:715:VAL:HG12	1:G:720:PHE:HB2	2.00	0.42
1:G:829:TRP:O	1:G:832:MET:N	2.50	0.42
3:I:63:ILE:CG2	3:I:64:THR:H	2.32	0.42
1:J:294:ASN:OD1	1:J:307:THR:HG21	2.19	0.42
1:J:406:VAL:O	1:J:412:ALA:HA	2.19	0.42
1:J:530:MET:CB	4:7:354:GLN:CB	2.95	0.42
1:J:541:MET:HG2	4:7:345:ILE:HG23	2.01	0.42
1:J:787:ILE:HG23	1:J:791:GLN:HG3	2.00	0.42
4:0:180:LEU:HD11	4:0:261:LEU:HD23	2.02	0.42
4:0:220:ALA:HB3	4:0:223:PHE:CD1	2.53	0.42
4:2:180:LEU:HD11	4:2:261:LEU:HD23	2.01	0.42
4:4:180:LEU:HD11	4:4:261:LEU:HD23	2.01	0.42
4:4:205:GLU:O	4:4:208:ILE:HG22	2.18	0.42
4:5:180:LEU:HD11	4:5:261:LEU:HD23	2.01	0.42
4:5:220:ALA:HB3	4:5:223:PHE:CD1	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:220:ALA:HB3	4:X:223:PHE:CD1	2.53	0.42
4:Z:220:ALA:HB3	4:Z:223:PHE:CD1	2.53	0.42
1:A:62:VAL:O	1:A:69:THR:HA	2.19	0.42
1:A:445:ILE:HG22	1:A:449:LEU:HD22	2.01	0.42
1:A:692:LEU:HA	1:A:692:LEU:HD23	1.84	0.42
1:D:206:LYS:HD2	1:D:217:THR:CG2	2.17	0.42
1:D:496:PHE:HB2	1:D:515:PHE:CD2	2.54	0.42
1:D:673:ARG:HD2	1:D:673:ARG:HA	1.79	0.42
1:D:692:LEU:HD23	1:D:692:LEU:HA	1.84	0.42
1:D:701:LEU:HD12	1:D:701:LEU:HA	1.55	0.42
1:D:834:LEU:HD21	2:E:54:MET:HG2	1.96	0.42
2:E:149:ASP:CG	2:E:150:TYR:N	2.49	0.42
3:F:50:LEU:O	3:F:53:PRO:HG2	2.18	0.42
1:G:64:THR:CG2	1:G:65:GLU:H	2.32	0.42
1:G:141:LEU:HD12	1:G:141:LEU:N	2.32	0.42
1:J:40:VAL:HG23	1:J:76:GLN:O	2.19	0.42
1:J:62:VAL:HG12	1:J:63:MLY:N	2.34	0.42
1:J:84:MLY:CG	1:J:719:ASP:OD2	2.66	0.42
1:J:747:LEU:O	1:J:749:GLY:N	2.52	0.42
2:K:112:ILE:O	2:K:148:VAL:N	2.50	0.42
4:1:149:THR:HA	4:1:165:ILE:O	2.19	0.42
4:2:315:LYS:HD2	4:2:315:LYS:HA	1.92	0.42
4:3:180:LEU:HD11	4:3:261:LEU:HD23	2.02	0.42
4:5:217:CYS:C	4:5:218:TYR:HD1	2.22	0.42
4:6:287:ILE:CB	4:8:204:ALA:H	2.13	0.42
4:7:287:ILE:HA	4:V:202:THR:HG21	1.59	0.42
4:W:217:CYS:C	4:W:218:TYR:HD1	2.22	0.42
4:Y:222:ASP:OD1	4:Y:224:GLU:HB3	2.19	0.42
4:Z:193:LEU:O	4:Z:198:TYR:HD2	2.01	0.42
1:A:402:CYS:C	1:A:404:PRO:HD3	2.39	0.42
1:A:724:TYR:HB3	1:A:727:LEU:CD1	2.48	0.42
1:A:829:TRP:O	1:A:832:MET:N	2.50	0.42
3:C:96:LYS:H	3:C:96:LYS:HG3	1.66	0.42
1:D:62:VAL:HG12	1:D:63:MLY:N	2.35	0.42
1:D:109:ARG:CD	1:D:117:THR:HB	2.49	0.42
1:D:449:LEU:N	1:D:449:LEU:CD1	2.82	0.42
1:D:741:LYS:HG2	1:D:742:LYS:N	2.35	0.42
1:D:829:TRP:HE1	2:E:67:MET:CB	2.26	0.42
2:E:140:PHE:CD2	2:E:144:VAL:HG11	2.54	0.42
1:G:406:VAL:O	1:G:412:ALA:HA	2.19	0.42
1:G:529:PRO:HB3	4:6:354:GLN:HA	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:747:LEU:O	1:G:749:GLY:N	2.52	0.42
1:G:798:LEU:HA	1:G:798:LEU:HD12	1.36	0.42
2:H:144:VAL:HG12	2:H:153:ILE:HD13	1.92	0.42
1:J:278:GLN:HE21	1:J:278:GLN:HB3	1.42	0.42
1:J:445:ILE:HG22	1:J:449:LEU:HD22	2.01	0.42
1:J:449:LEU:N	1:J:449:LEU:CD1	2.81	0.42
4:O:217:CYS:C	4:O:218:TYR:HD1	2.22	0.42
4:4:206:ARG:O	4:4:209:VAL:HG12	2.20	0.42
4:5:324:THR:N	4:7:245:GLY:CA	2.69	0.42
4:6:205:GLU:O	4:6:208:ILE:HG22	2.18	0.42
4:W:315:LYS:HD2	4:W:315:LYS:HA	1.92	0.42
4:X:180:LEU:HD11	4:X:261:LEU:HD23	2.01	0.42
4:Y:180:LEU:HD11	4:Y:261:LEU:HD23	2.01	0.42
1:A:214:MET:CA	1:A:340:ILE:HD11	2.46	0.42
1:A:625:THR:H	1:A:625:THR:HG22	1.48	0.42
1:A:797:PHE:HE2	3:C:126:LEU:CD2	1.91	0.42
1:A:831:TRP:CZ2	2:B:51:PHE:CE1	3.07	0.42
2:B:114:LYS:CG	2:B:146:GLY:HA2	2.46	0.42
1:D:175:ILE:C	1:D:176:LEU:HD12	2.38	0.42
1:D:295:MLY:CE	1:D:332:MET:CE	2.97	0.42
1:D:320:ILE:O	1:D:320:ILE:HG22	2.17	0.42
1:D:445:ILE:HG22	1:D:449:LEU:HD22	2.01	0.42
1:D:733:PRO:CB	1:D:737:PHE:CE1	3.02	0.42
1:D:793:ARG:HG2	3:F:147:MET:HG2	2.01	0.42
1:G:62:VAL:O	1:G:69:THR:HA	2.19	0.42
1:G:123:CYS:HB2	1:G:158:ILE:HD13	2.00	0.42
1:G:173:GLN:HG3	1:G:670:HIS:CD2	2.55	0.42
1:G:551:MLY:C	4:8:47:MET:HA	2.48	0.42
1:G:741:LYS:HG2	1:G:742:LYS:N	2.35	0.42
1:J:86:ASP:OD2	1:J:87:MLY:HH22	2.19	0.42
1:J:173:GLN:HG3	1:J:670:HIS:CD2	2.54	0.42
1:J:485:GLU:HA	1:J:584:TYR:HE2	1.83	0.42
1:J:533:PHE:HD1	1:J:533:PHE:HA	1.79	0.42
1:J:831:TRP:CH2	2:K:34:ILE:CG2	2.95	0.42
3:L:63:ILE:CG2	3:L:64:THR:H	2.33	0.42
4:1:205:GLU:O	4:1:208:ILE:HG22	2.18	0.42
4:4:217:CYS:C	4:4:218:TYR:HD1	2.22	0.42
4:8:205:GLU:O	4:8:208:ILE:HG22	2.18	0.42
4:8:287:ILE:CB	4:W:204:ALA:H	2.13	0.42
4:V:149:THR:HA	4:V:165:ILE:O	2.19	0.42
4:V:222:ASP:OD1	4:V:224:GLU:HB3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:196:ARG:HH21	4:W:249:THR:HG23	1.85	0.42
4:Z:217:CYS:C	4:Z:218:TYR:HD1	2.22	0.42
1:A:38:VAL:HG13	1:A:39:PHE:N	2.35	0.42
1:A:501:GLU:HA	1:A:762:HIS:CE1	2.54	0.42
1:A:541:MET:CE	4:4:346:LEU:HD12	2.48	0.42
1:A:712:PRO:HB2	1:A:713:SER:H	1.61	0.42
1:A:744:SER:O	1:A:748:LEU:HD12	2.20	0.42
1:A:747:LEU:O	1:A:749:GLY:N	2.52	0.42
1:D:14:ALA:HB3	1:D:15:PRO:CD	2.45	0.42
1:D:354:LEU:HD12	1:D:354:LEU:HA	1.56	0.42
1:D:476:GLU:CD	1:D:476:GLU:H	2.22	0.42
1:D:519:LEU:HD12	1:D:519:LEU:H	1.83	0.42
1:D:534:SER:CB	4:5:351:THR:HA	2.49	0.42
1:D:723:ARG:HE	1:D:779:ARG:HA	1.84	0.42
2:E:140:PHE:HA	2:E:141:PRO:HD2	1.57	0.42
1:G:346:ASP:O	1:G:350:ALA:N	2.46	0.42
1:G:534:SER:CB	4:6:351:THR:HA	2.50	0.42
1:G:578:HIS:CD2	1:G:592:ILE:H	2.38	0.42
1:G:842:LEU:N	1:G:842:LEU:CD1	2.82	0.42
1:J:93:MET:CA	1:J:714:ARG:HG3	2.44	0.42
1:J:175:ILE:C	1:J:176:LEU:HD12	2.39	0.42
1:J:226:ASN:HB2	1:J:227:PRO:CD	2.47	0.42
1:J:271:GLU:OE1	1:J:274:ARG:NH1	2.53	0.42
1:J:295:MLY:CE	1:J:332:MET:CE	2.97	0.42
1:J:354:LEU:HD12	1:J:354:LEU:HA	1.56	0.42
1:J:534:SER:CB	4:7:351:THR:HA	2.49	0.42
1:J:578:HIS:CD2	1:J:592:ILE:H	2.38	0.42
4:1:196:ARG:HH21	4:1:249:THR:HG23	1.85	0.42
4:4:196:ARG:HH21	4:4:249:THR:HG23	1.85	0.42
4:4:222:ASP:OD1	4:4:224:GLU:HB3	2.20	0.42
4:5:193:LEU:O	4:5:198:TYR:HD2	2.01	0.42
4:5:205:GLU:O	4:5:208:ILE:HG22	2.18	0.42
4:6:217:CYS:C	4:6:218:TYR:HD1	2.22	0.42
4:7:180:LEU:HD11	4:7:261:LEU:HD23	2.01	0.42
4:8:217:CYS:C	4:8:218:TYR:HD1	2.22	0.42
4:V:206:ARG:O	4:V:209:VAL:HG12	2.20	0.42
4:W:205:GLU:O	4:W:208:ILE:HG22	2.18	0.42
4:W:206:ARG:O	4:W:209:VAL:HG12	2.20	0.42
4:X:222:ASP:OD1	4:X:224:GLU:HB3	2.19	0.42
4:Y:205:GLU:O	4:Y:208:ILE:HG22	2.18	0.42
1:A:166:MET:CE	1:A:254:PHE:HB2	2.46	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ASP:O	1:A:170:ARG:HB2	2.19	0.42
1:A:791:GLN:OE1	3:C:116:GLU:HB2	2.20	0.42
2:B:113:LYS:O	2:B:147:ASN:HB2	2.20	0.42
1:D:402:CYS:C	1:D:404:PRO:HD3	2.40	0.42
1:D:409:GLY:N	1:D:636:LYS:CD	2.71	0.42
1:D:725:ARG:HA	1:D:732:ILE:CG2	2.50	0.42
1:D:822:SER:HG	2:E:88:LEU:HA	1.84	0.42
1:D:842:LEU:N	1:D:842:LEU:CD1	2.83	0.42
1:J:62:VAL:O	1:J:69:THR:HA	2.20	0.42
1:J:151:ALA:HB1	1:J:152:PRO:HD2	2.01	0.42
1:J:174:SER:HA	1:J:460:GLY:O	2.20	0.42
1:J:462:LEU:HD11	1:J:464:ILE:CD1	2.50	0.42
4:2:222:ASP:OD1	4:2:224:GLU:HB3	2.20	0.42
4:2:324:THR:HG23	4:4:245:GLY:HA2	1.09	0.42
4:6:180:LEU:HD11	4:6:261:LEU:HD23	2.01	0.42
4:7:222:ASP:OD1	4:7:224:GLU:HB3	2.20	0.42
4:8:222:ASP:OD1	4:8:224:GLU:HB3	2.19	0.42
4:X:206:ARG:O	4:X:209:VAL:HG12	2.20	0.42
4:Z:196:ARG:HH21	4:Z:249:THR:HG23	1.85	0.42
1:A:60:VAL:O	1:A:72:VAL:N	2.51	0.42
1:A:141:LEU:HD12	1:A:141:LEU:N	2.32	0.42
1:A:213:LYS:HA	1:A:220:ASP:OD2	2.19	0.42
1:A:501:GLU:CB	1:A:762:HIS:ND1	2.82	0.42
1:A:568:PRO:O	1:A:570:PRO:HD3	2.19	0.42
1:A:642:LYS:HB3	4:4:24:ASP:HB2	1.37	0.42
1:D:204:GLU:N	1:D:207:LYS:HE3	2.23	0.42
1:D:279:LEU:CB	1:D:280:PRO:HD2	2.49	0.42
1:D:406:VAL:O	1:D:412:ALA:HA	2.20	0.42
1:D:537:GLU:OE1	4:5:350:SER:HA	2.19	0.42
1:D:636:LYS:CB	4:5:334:GLU:OE1	2.68	0.42
1:D:659:MLY:HH22	1:D:659:MLY:HD2	1.42	0.42
1:D:759:ALA:O	1:D:766:PHE:N	2.32	0.42
1:G:166:MET:CE	1:G:254:PHE:HB2	2.46	0.42
1:G:400:ALA:CB	1:G:606:THR:HG22	2.49	0.42
2:H:140:PHE:CD2	2:H:144:VAL:HG11	2.55	0.42
1:J:214:MET:CA	1:J:340:ILE:HD11	2.45	0.42
1:J:418:THR:CG2	1:J:419:VAL:N	2.79	0.42
1:J:795:ARG:HH21	3:L:116:GLU:HB3	1.84	0.42
1:J:826:VAL:O	1:J:828:HIS:N	2.53	0.42
4:3:220:ALA:HB3	4:3:223:PHE:CD1	2.53	0.42
4:5:149:THR:HA	4:5:165:ILE:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:217:CYS:C	4:7:218:TYR:HD1	2.22	0.42
4:8:369:ILE:HG23	4:8:370:VAL:N	2.35	0.42
4:V:180:LEU:HD11	4:V:261:LEU:HD23	2.02	0.42
4:V:217:CYS:C	4:V:218:TYR:HD1	2.23	0.42
4:Z:222:ASP:OD1	4:Z:224:GLU:HB3	2.19	0.42
1:A:173:GLN:HG3	1:A:670:HIS:CD2	2.54	0.42
1:A:195:TYR:CE2	1:A:199:ILE:HD13	2.55	0.42
1:A:553:MLY:HE2	4:6:45:VAL:CA	2.38	0.42
1:A:757:GLN:CD	1:A:771:LEU:CD1	2.86	0.42
1:D:174:SER:HA	1:D:460:GLY:O	2.20	0.42
1:D:294:ASN:OD1	1:D:307:THR:HG21	2.19	0.42
1:D:839:MLY:N	1:D:840:PRO:HD2	2.35	0.42
1:G:38:VAL:HG13	1:G:39:PHE:N	2.35	0.42
1:G:633:GLY:HA2	4:6:25:ASP:HA	1.26	0.42
1:G:733:PRO:CB	1:G:737:PHE:CE1	3.02	0.42
1:J:11:GLY:O	1:J:14:ALA:HB3	2.20	0.42
1:J:332:MET:H	1:J:332:MET:HG2	1.52	0.42
1:J:500:GLN:HB2	1:J:512:PHE:CZ	2.54	0.42
1:J:715:VAL:HG12	1:J:720:PHE:HB2	2.00	0.42
2:K:140:PHE:CD2	2:K:144:VAL:HG11	2.54	0.42
4:1:171:LEU:HA	4:1:172:PRO:HD2	1.84	0.42
4:1:206:ARG:O	4:1:209:VAL:HG12	2.20	0.42
4:1:369:ILE:HG23	4:1:370:VAL:N	2.35	0.42
4:2:193:LEU:HD11	4:2:250:ILE:HG13	2.02	0.42
4:5:222:ASP:OD1	4:5:224:GLU:HB3	2.19	0.42
4:6:222:ASP:OD1	4:6:224:GLU:HB3	2.19	0.42
4:W:180:LEU:HD11	4:W:261:LEU:HD23	2.02	0.42
4:W:369:ILE:HG23	4:W:370:VAL:N	2.35	0.42
4:Y:369:ILE:HG23	4:Y:370:VAL:N	2.35	0.42
1:A:406:VAL:O	1:A:412:ALA:HA	2.19	0.42
1:A:797:PHE:CD2	1:A:798:LEU:HD12	2.55	0.42
1:D:215:GLN:H	1:D:340:ILE:CD1	2.21	0.42
1:D:271:GLU:OE1	1:D:274:ARG:NH1	2.53	0.42
1:D:462:LEU:HD11	1:D:464:ILE:CD1	2.50	0.42
1:D:471:ASP:CB	1:D:573:GLY:O	2.68	0.42
1:D:541:MET:CG	4:5:345:ILE:C	2.87	0.42
1:D:578:HIS:CD2	1:D:592:ILE:H	2.38	0.42
1:D:690:LEU:O	1:D:694:GLN:HG3	2.20	0.42
1:D:744:SER:O	1:D:748:LEU:HD12	2.20	0.42
1:G:97:LEU:HD12	1:G:97:LEU:HA	1.67	0.42
1:G:732:ILE:HG23	1:G:747:LEU:HD12	0.95	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:195:TYR:CE2	1:J:199:ILE:HD13	2.55	0.42
4:0:196:ARG:HH21	4:0:249:THR:HG23	1.85	0.42
4:0:206:ARG:O	4:0:209:VAL:HG12	2.20	0.42
4:0:222:ASP:OD1	4:0:224:GLU:HB3	2.19	0.42
4:3:369:ILE:HG23	4:3:370:VAL:N	2.35	0.42
4:5:221:LEU:HA	4:5:312:ARG:HG2	2.02	0.42
4:8:180:LEU:HD11	4:8:261:LEU:HD23	2.01	0.42
4:X:193:LEU:HD11	4:X:250:ILE:HG13	2.02	0.42
4:X:324:THR:HG23	4:Z:245:GLY:HA2	1.09	0.42
4:Y:193:LEU:HD11	4:Y:250:ILE:HG13	2.02	0.42
1:A:110:TYR:O	1:A:113:TRP:N	2.42	0.42
1:A:322:VAL:HA	1:A:323:PRO:HD3	1.87	0.42
1:A:578:HIS:CD2	1:A:592:ILE:H	2.38	0.42
1:A:725:ARG:CZ	1:A:737:PHE:CE1	3.02	0.42
1:D:86:ASP:OD2	1:D:87:MLY:HH22	2.19	0.42
1:D:507:GLY:C	1:D:761:GLY:HA3	2.37	0.42
1:D:747:LEU:O	1:D:749:GLY:N	2.52	0.42
3:F:63:ILE:CG2	3:F:64:THR:H	2.32	0.42
1:G:62:VAL:HG12	1:G:63:MLY:N	2.35	0.42
1:G:568:PRO:CG	1:G:578:HIS:N	2.83	0.42
1:G:732:ILE:CG2	1:G:747:LEU:CD1	0.65	0.42
1:J:84:MLY:HH13	1:J:715:VAL:CG1	2.06	0.42
1:J:754:ASP:HB3	1:J:776:GLU:HG3	1.72	0.42
4:0:193:LEU:HD11	4:0:250:ILE:HG13	2.02	0.42
4:3:221:LEU:HA	4:3:312:ARG:HG2	2.02	0.42
4:5:369:ILE:HG23	4:5:370:VAL:N	2.35	0.42
4:6:196:ARG:HH21	4:6:249:THR:HG23	1.85	0.42
4:6:206:ARG:O	4:6:209:VAL:HG12	2.20	0.42
4:7:206:ARG:O	4:7:209:VAL:HG12	2.20	0.42
4:7:221:LEU:HA	4:7:312:ARG:HG2	2.02	0.42
4:7:369:ILE:HG23	4:7:370:VAL:N	2.35	0.42
4:8:206:ARG:O	4:8:209:VAL:HG12	2.20	0.42
1:A:11:GLY:O	1:A:14:ALA:HB3	2.20	0.41
1:A:462:LEU:HD11	1:A:464:ILE:CD1	2.50	0.41
1:A:659:MLY:HD2	1:A:659:MLY:HH22	1.42	0.41
1:A:826:VAL:O	1:A:828:HIS:N	2.53	0.41
1:A:842:LEU:N	1:A:842:LEU:CD1	2.83	0.41
1:D:151:ALA:HB1	1:D:152:PRO:HD2	2.01	0.41
1:D:466:GLY:CA	1:D:484:ASN:HD21	2.32	0.41
1:D:625:THR:H	1:D:625:THR:HG22	1.48	0.41
1:G:11:GLY:O	1:G:14:ALA:HB3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:60:VAL:O	1:G:72:VAL:N	2.51	0.41
1:G:166:MET:CE	1:G:254:PHE:CD2	3.01	0.41
1:G:169:ASP:O	1:G:170:ARG:HB2	2.19	0.41
1:G:369:MLY:HH22	1:G:369:MLY:HD3	1.79	0.41
1:G:725:ARG:HA	1:G:732:ILE:CG2	2.50	0.41
1:J:725:ARG:HA	1:J:732:ILE:CG2	2.50	0.41
4:2:217:CYS:C	4:2:218:TYR:HD1	2.23	0.41
4:3:193:LEU:HD11	4:3:250:ILE:HG13	2.02	0.41
4:4:315:LYS:HD2	4:4:315:LYS:HA	1.92	0.41
4:4:324:THR:HG23	4:6:245:GLY:HA2	1.09	0.41
4:4:369:ILE:HG23	4:4:370:VAL:N	2.35	0.41
4:7:193:LEU:HD11	4:7:250:ILE:HG13	2.02	0.41
4:8:226:GLU:HG3	4:8:255:PHE:CE2	2.55	0.41
4:V:221:LEU:HA	4:V:312:ARG:HG2	2.02	0.41
4:X:369:ILE:HG23	4:X:370:VAL:N	2.35	0.41
4:Y:206:ARG:O	4:Y:209:VAL:HG12	2.20	0.41
1:A:221:GLN:HG2	1:A:221:GLN:H	1.47	0.41
1:A:330:GLU:OE1	1:A:330:GLU:HA	2.20	0.41
1:A:541:MET:HG2	4:4:345:ILE:HG23	2.01	0.41
1:A:568:PRO:CG	1:A:578:HIS:N	2.84	0.41
1:A:725:ARG:HA	1:A:732:ILE:CG2	2.50	0.41
2:B:140:PHE:HA	2:B:141:PRO:HD2	1.56	0.41
3:C:95:ASP:OD1	3:C:139:TYR:HE1	2.03	0.41
1:D:356:GLY:HA2	1:D:359:MET:HG3	2.02	0.41
1:D:500:GLN:HB2	1:D:512:PHE:CZ	2.54	0.41
1:D:568:PRO:CG	1:D:578:HIS:N	2.83	0.41
1:D:787:ILE:HD13	1:D:787:ILE:HG21	1.67	0.41
1:G:462:LEU:HD11	1:G:464:ILE:CD1	2.50	0.41
1:G:730:SER:OG	3:I:109:HIS:ND1	2.49	0.41
1:G:797:PHE:CD2	1:G:798:LEU:HD12	2.55	0.41
1:G:826:VAL:O	1:G:828:HIS:N	2.53	0.41
3:I:25:ILE:O	3:I:63:ILE:CB	2.66	0.41
3:I:95:ASP:OD1	3:I:139:TYR:HE1	2.03	0.41
1:J:402:CYS:C	1:J:404:PRO:HD3	2.40	0.41
1:J:541:MET:CG	4:7:345:ILE:C	2.87	0.41
1:J:568:PRO:CG	1:J:578:HIS:N	2.83	0.41
1:J:636:LYS:CB	4:7:334:GLU:OE1	2.68	0.41
1:J:690:LEU:O	1:J:694:GLN:HG3	2.20	0.41
4:2:226:GLU:HG3	4:2:255:PHE:CE2	2.56	0.41
4:3:222:ASP:OD1	4:3:224:GLU:HB3	2.20	0.41
4:3:287:ILE:N	4:5:202:THR:CG2	2.77	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:193:LEU:HD11	4:4:250:ILE:HG13	2.02	0.41
4:6:193:LEU:HD11	4:6:250:ILE:HG13	2.02	0.41
4:6:315:LYS:HD2	4:6:315:LYS:HA	1.92	0.41
4:6:369:ILE:HG23	4:6:370:VAL:N	2.35	0.41
4:8:193:LEU:HD11	4:8:250:ILE:HG13	2.02	0.41
4:8:287:ILE:HD11	4:W:202:THR:HA	1.66	0.41
4:V:369:ILE:HG23	4:V:370:VAL:N	2.35	0.41
4:W:299:MET:HE2	4:W:331:ALA:HB2	2.01	0.41
4:Y:196:ARG:HH21	4:Y:249:THR:HG23	1.85	0.41
4:Z:193:LEU:HD11	4:Z:250:ILE:HG13	2.02	0.41
1:A:25:ILE:HG23	1:A:29:ASN:HD22	1.85	0.41
1:A:166:MET:CE	1:A:254:PHE:CD2	3.01	0.41
1:A:690:LEU:O	1:A:694:GLN:HG3	2.20	0.41
1:A:795:ARG:CG	3:C:118:MET:HE1	2.50	0.41
1:A:831:TRP:HZ2	2:B:47:LEU:HA	1.85	0.41
1:D:87:MLY:HH12	1:D:87:MLY:HD3	1.61	0.41
1:D:129:TYR:HD1	1:D:129:TYR:HA	1.65	0.41
1:D:135:TYR:CD2	1:D:191:ARG:HD3	2.55	0.41
1:D:554:LEU:HA	1:D:554:LEU:HD12	1.77	0.41
1:D:568:PRO:O	1:D:570:PRO:HD3	2.19	0.41
1:D:641:LYS:CE	1:D:647:GLN:CB	2.75	0.41
1:D:795:ARG:NE	3:F:43:ASN:OD1	2.53	0.41
1:D:799:MET:CE	3:F:32:ASP:CB	2.83	0.41
1:G:136:ASN:O	1:G:138:MLY:N	2.54	0.41
1:G:185:LYS:H	1:G:185:LYS:HG3	1.63	0.41
1:G:541:MET:HB3	4:6:345:ILE:HG22	2.01	0.41
1:G:641:LYS:CE	1:G:647:GLN:CB	2.75	0.41
1:G:775:LEU:HD12	1:G:775:LEU:HA	1.71	0.41
1:J:136:ASN:O	1:J:138:MLY:N	2.54	0.41
1:J:556:ASP:OD1	4:V:50:LYS:CG	2.69	0.41
1:J:797:PHE:CD2	1:J:798:LEU:HD12	2.55	0.41
1:J:821:ARG:CZ	2:K:127:ARG:HD3	2.51	0.41
4:0:226:GLU:HG3	4:0:255:PHE:CE2	2.55	0.41
4:0:369:ILE:HG23	4:0:370:VAL:N	2.35	0.41
4:1:193:LEU:HD11	4:1:250:ILE:HG13	2.02	0.41
4:1:221:LEU:HA	4:1:312:ARG:HG2	2.03	0.41
4:2:206:ARG:O	4:2:209:VAL:HG12	2.20	0.41
4:2:369:ILE:HG23	4:2:370:VAL:N	2.35	0.41
4:3:206:ARG:O	4:3:209:VAL:HG12	2.20	0.41
4:3:287:ILE:HA	4:5:202:THR:HG21	1.59	0.41
4:5:226:GLU:HG3	4:5:255:PHE:CE2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:287:ILE:CB	4:7:204:ALA:H	2.13	0.41
4:7:324:THR:HG23	4:V:245:GLY:HA2	1.09	0.41
4:8:315:LYS:HD2	4:8:315:LYS:HA	1.92	0.41
4:V:196:ARG:HH21	4:V:249:THR:HG23	1.85	0.41
4:V:324:THR:HG23	4:X:245:GLY:HA2	1.09	0.41
4:W:193:LEU:HD11	4:W:250:ILE:HG13	2.02	0.41
4:W:226:GLU:HG3	4:W:255:PHE:CE2	2.55	0.41
4:X:217:CYS:C	4:X:218:TYR:HD1	2.23	0.41
4:X:221:LEU:HA	4:X:312:ARG:HG2	2.02	0.41
4:Z:369:ILE:HG23	4:Z:370:VAL:N	2.35	0.41
1:A:62:VAL:HG12	1:A:63:MLY:N	2.35	0.41
1:A:741:LYS:HG2	1:A:742:LYS:N	2.35	0.41
1:D:11:GLY:O	1:D:14:ALA:HB3	2.20	0.41
1:D:812:SER:O	1:D:816:ILE:HG13	2.21	0.41
1:D:822:SER:CB	2:E:88:LEU:HD21	2.47	0.41
1:D:831:TRP:CE2	2:E:51:PHE:CZ	3.09	0.41
2:E:113:LYS:O	2:E:147:ASN:HB2	2.20	0.41
1:G:330:GLU:OE1	1:G:330:GLU:HA	2.20	0.41
1:G:402:CYS:C	1:G:404:PRO:HD3	2.40	0.41
1:G:471:ASP:CB	1:G:573:GLY:O	2.68	0.41
1:G:541:MET:HG2	4:6:345:ILE:HG23	2.01	0.41
1:G:541:MET:CE	4:6:346:LEU:HD12	2.48	0.41
1:G:744:SER:O	1:G:748:LEU:HD12	2.20	0.41
1:J:229:LEU:HD12	1:J:229:LEU:HA	1.76	0.41
1:J:335:ASP:O	1:J:338:ILE:HB	2.20	0.41
1:J:471:ASP:CB	1:J:573:GLY:O	2.68	0.41
4:3:226:GLU:HG3	4:3:255:PHE:CE2	2.55	0.41
4:5:196:ARG:HH21	4:5:249:THR:HG23	1.85	0.41
4:Y:221:LEU:HA	4:Y:312:ARG:HG2	2.02	0.41
1:A:135:TYR:HD2	1:A:191:ARG:CG	2.33	0.41
1:A:839:MLY:N	1:A:840:PRO:HD2	2.35	0.41
2:B:140:PHE:HB3	2:B:144:VAL:HG11	2.03	0.41
2:B:150:TYR:HB3	2:B:151:LYS:HG3	2.03	0.41
1:D:25:ILE:HG23	1:D:29:ASN:HD22	1.85	0.41
1:D:173:GLN:HG3	1:D:670:HIS:CD2	2.55	0.41
1:D:296:MLY:HH11	1:D:348:MLY:CH2	2.48	0.41
1:D:507:GLY:HA3	1:D:762:HIS:N	2.36	0.41
2:E:141:PRO:CB	2:E:142:PRO:HD3	2.48	0.41
1:G:135:TYR:HD2	1:G:191:ARG:CG	2.33	0.41
1:G:174:SER:HA	1:G:460:GLY:O	2.20	0.41
1:G:195:TYR:CE2	1:G:199:ILE:HD13	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:217:THR:CA	1:G:221:GLN:HE21	2.33	0.41
1:G:556:ASP:OD1	4:8:50:LYS:CG	2.68	0.41
1:G:642:LYS:HE2	4:6:344:SER:HA	1.56	0.41
1:G:690:LEU:O	1:G:694:GLN:HG3	2.20	0.41
1:G:810:ARG:HG2	1:G:810:ARG:NH1	2.28	0.41
1:J:14:ALA:HB3	1:J:15:PRO:CD	2.46	0.41
1:J:295:MLY:CE	1:J:332:MET:HE1	2.51	0.41
1:J:296:MLY:HH11	1:J:348:MLY:CH2	2.48	0.41
1:J:320:ILE:O	1:J:320:ILE:CG2	2.68	0.41
1:J:346:ASP:O	1:J:350:ALA:N	2.46	0.41
1:J:464:ILE:HD13	1:J:464:ILE:HG21	1.69	0.41
1:J:612:GLN:NE2	1:J:627:GLY:H	2.14	0.41
1:J:817:GLN:CB	2:K:127:ARG:HH11	2.24	0.41
1:J:829:TRP:O	1:J:832:MET:N	2.50	0.41
2:K:144:VAL:HG12	2:K:153:ILE:HD13	1.92	0.41
4:0:32:PRO:HB2	4:0:34:ILE:CD1	2.51	0.41
4:4:227:MET:O	4:4:230:ALA:HB3	2.21	0.41
4:5:206:ARG:O	4:5:209:VAL:HG12	2.20	0.41
4:7:226:GLU:HG3	4:7:255:PHE:CE2	2.55	0.41
4:8:196:ARG:HH21	4:8:249:THR:HG23	1.85	0.41
4:V:193:LEU:HD11	4:V:250:ILE:HG13	2.02	0.41
4:X:226:GLU:HG3	4:X:255:PHE:CE2	2.55	0.41
4:Z:144:ALA:HB2	4:Z:342:GLY:CA	2.51	0.41
4:Z:206:ARG:O	4:Z:209:VAL:HG12	2.20	0.41
4:Z:226:GLU:HG3	4:Z:255:PHE:CE2	2.55	0.41
1:A:134:VAL:C	1:A:136:ASN:H	2.16	0.41
2:B:144:VAL:HG12	2:B:153:ILE:HD11	1.75	0.41
1:D:62:VAL:O	1:D:69:THR:HA	2.19	0.41
1:D:408:VAL:HG22	1:D:636:LYS:HG2	1.51	0.41
1:D:723:ARG:HH21	1:D:783:LEU:CD1	2.33	0.41
1:D:797:PHE:CD2	1:D:798:LEU:HD12	2.55	0.41
1:D:826:VAL:O	1:D:828:HIS:N	2.53	0.41
1:G:550:PHE:C	4:8:46:GLY:CA	2.88	0.41
1:G:636:LYS:CB	4:6:334:GLU:OE1	2.68	0.41
1:G:839:MLY:N	1:G:840:PRO:HD2	2.35	0.41
1:J:204:GLU:N	1:J:207:LYS:HE3	2.23	0.41
1:J:797:PHE:HB2	3:L:149:VAL:HG13	1.96	0.41
4:0:144:ALA:HB2	4:0:342:GLY:CA	2.51	0.41
4:1:222:ASP:OD1	4:1:224:GLU:HB3	2.19	0.41
4:2:144:ALA:HB2	4:2:342:GLY:CA	2.51	0.41
4:3:290:ARG:HH22	4:5:202:THR:CG2	2.17	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:288:ASP:OD1	4:6:204:ALA:HA	2.21	0.41
4:5:193:LEU:HD11	4:5:250:ILE:HG13	2.02	0.41
4:7:227:MET:O	4:7:230:ALA:HB3	2.21	0.41
1:A:49:MLY:HH23	1:A:80:MET:CE	2.51	0.41
1:A:174:SER:HA	1:A:460:GLY:O	2.20	0.41
1:A:541:MET:HG2	4:4:345:ILE:HG22	2.00	0.41
2:B:149:ASP:OD2	2:B:150:TYR:CA	2.64	0.41
1:D:136:ASN:O	1:D:138:MLY:N	2.54	0.41
1:D:330:GLU:HA	1:D:330:GLU:OE1	2.21	0.41
1:D:534:SER:HB2	4:5:354:GLN:HE22	1.56	0.41
2:E:150:TYR:HB3	2:E:151:LYS:HG3	2.03	0.41
3:F:48:LYS:HA	3:F:48:LYS:HD3	1.17	0.41
1:G:56:GLU:HB2	1:G:59:MLY:CB	2.30	0.41
1:G:449:LEU:N	1:G:449:LEU:CD1	2.82	0.41
1:G:831:TRP:CE2	2:H:67:MET:CB	3.01	0.41
1:J:25:ILE:HG23	1:J:29:ASN:HD22	1.85	0.41
1:J:90:ASP:CB	1:J:764:MLY:HH11	2.42	0.41
1:J:610:LEU:N	1:J:610:LEU:CD1	2.84	0.41
1:J:821:ARG:HH12	2:K:127:ARG:CZ	2.33	0.41
1:J:838:ILE:CD1	2:K:54:MET:HE1	2.42	0.41
4:0:288:ASP:OD1	4:2:204:ALA:HA	2.21	0.41
4:1:32:PRO:HB2	4:1:34:ILE:CD1	2.51	0.41
4:2:288:ASP:OD1	4:4:204:ALA:HA	2.21	0.41
4:3:32:PRO:HB2	4:3:34:ILE:CD1	2.51	0.41
4:3:196:ARG:HH21	4:3:249:THR:HG23	1.85	0.41
4:4:226:GLU:HG3	4:4:255:PHE:CE2	2.55	0.41
4:6:226:GLU:HG3	4:6:255:PHE:CE2	2.55	0.41
4:8:144:ALA:HB2	4:8:342:GLY:CA	2.51	0.41
4:V:144:ALA:HB2	4:V:342:GLY:CA	2.51	0.41
4:V:226:GLU:HG3	4:V:255:PHE:CE2	2.55	0.41
4:W:144:ALA:HB2	4:W:342:GLY:CA	2.51	0.41
4:W:324:THR:O	4:Y:244:ASP:HA	2.09	0.41
4:X:144:ALA:HB2	4:X:342:GLY:CA	2.51	0.41
4:Z:221:LEU:HA	4:Z:312:ARG:HG2	2.02	0.41
1:A:107:MLY:CB	1:A:686:MET:HE2	2.40	0.41
1:A:136:ASN:O	1:A:138:MLY:N	2.54	0.41
1:A:193:ILE:HD11	1:A:250:ILE:HD12	2.03	0.41
1:A:711:PHE:O	1:A:714:ARG:NH2	2.54	0.41
1:A:812:SER:O	1:A:816:ILE:HG13	2.21	0.41
3:C:63:ILE:CG2	3:C:64:THR:H	2.33	0.41
1:D:38:VAL:HG13	1:D:39:PHE:N	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:MET:CE	1:D:119:SER:HB2	2.48	0.41
1:D:308:ASN:HA	1:D:309:PRO:HD2	1.88	0.41
1:D:322:VAL:HG12	1:D:325:ILE:HG13	2.03	0.41
1:D:629:GLU:HB3	1:D:643:GLY:C	2.41	0.41
1:D:799:MET:SD	3:F:32:ASP:HA	2.51	0.41
1:G:193:ILE:CD1	1:G:250:ILE:HD13	2.51	0.41
1:G:665:ARG:C	1:G:667:THR:N	2.74	0.41
1:G:797:PHE:CD1	3:I:149:VAL:CB	2.85	0.41
1:J:135:TYR:CD2	1:J:191:ARG:HD3	2.55	0.41
1:J:193:ILE:HD11	1:J:250:ILE:HD12	2.03	0.41
1:J:356:GLY:HA2	1:J:359:MET:HG3	2.02	0.41
1:J:629:GLU:HB3	1:J:643:GLY:C	2.41	0.41
1:J:657:LEU:HD12	1:J:657:LEU:O	2.21	0.41
1:J:741:LYS:HG2	1:J:742:LYS:N	2.35	0.41
1:J:744:SER:O	1:J:748:LEU:HD12	2.20	0.41
1:J:812:SER:O	1:J:816:ILE:HG13	2.21	0.41
4:1:226:GLU:HG3	4:1:255:PHE:CE2	2.56	0.41
4:1:288:ASP:OD1	4:3:204:ALA:HA	2.21	0.41
4:5:287:ILE:N	4:7:202:THR:CG2	2.77	0.41
4:6:144:ALA:HB2	4:6:342:GLY:CA	2.51	0.41
4:W:221:LEU:HA	4:W:312:ARG:HG2	2.02	0.41
4:Y:32:PRO:HB2	4:Y:34:ILE:CD1	2.51	0.41
1:A:72:VAL:O	1:A:73:LYS:O	2.39	0.41
1:A:172:ASN:OD1	1:A:457:TYR:HA	2.21	0.41
1:A:193:ILE:CD1	1:A:250:ILE:HD13	2.51	0.41
1:A:194:GLN:HE21	1:A:194:GLN:HB3	1.43	0.41
1:A:217:THR:CA	1:A:221:GLN:HE21	2.33	0.41
1:A:226:ASN:HB2	1:A:227:PRO:CD	2.47	0.41
1:A:303:LEU:O	1:A:304:LEU:HB2	2.21	0.41
1:A:356:GLY:HA2	1:A:359:MET:HG3	2.02	0.41
1:A:471:ASP:CB	1:A:573:GLY:O	2.68	0.41
1:A:732:ILE:HG23	1:A:747:LEU:HD13	1.37	0.41
1:A:793:ARG:HH21	3:C:147:MET:HE2	1.84	0.41
1:A:800:ARG:HD3	3:C:149:VAL:C	2.35	0.41
1:A:800:ARG:NE	3:C:149:VAL:C	2.73	0.41
2:B:111:SER:OG	2:B:148:VAL:CA	2.69	0.41
3:C:56:GLU:OE1	3:C:59:ASN:ND2	2.54	0.41
1:D:195:TYR:CE2	1:D:199:ILE:HD13	2.55	0.41
1:D:242:ASN:OD1	1:D:286:HIS:NE2	2.49	0.41
1:D:309:PRO:C	1:D:311:ASP:H	2.22	0.41
1:D:322:VAL:HB	1:D:325:ILE:HD12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:LEU:HA	1:D:398:LEU:HD12	1.84	0.41
1:D:407:GLY:HA2	1:D:411:GLU:O	2.21	0.41
1:D:493:HIS:O	1:D:496:PHE:N	2.54	0.41
1:G:14:ALA:HB3	1:G:15:PRO:CD	2.46	0.41
1:G:322:VAL:HA	1:G:323:PRO:HD3	1.87	0.41
1:G:335:ASP:O	1:G:338:ILE:HB	2.20	0.41
1:G:356:GLY:HA2	1:G:359:MET:HG3	2.02	0.41
1:G:384:ASP:HA	1:G:394:SER:OG	2.21	0.41
1:G:485:GLU:OE2	1:G:584:TYR:N	2.50	0.41
1:G:534:SER:HB2	4:6:354:GLN:HE22	1.56	0.41
1:G:537:GLU:OE1	4:6:350:SER:HA	2.20	0.41
1:G:717:TYR:OH	1:G:760:PHE:HB3	2.21	0.41
1:G:768:MLY:HG2	1:G:772:LEU:HD23	2.03	0.41
1:G:791:GLN:HB3	3:I:118:MET:CE	2.51	0.41
1:G:812:SER:O	1:G:816:ILE:HG13	2.21	0.41
1:G:832:MET:SD	2:H:84:PHE:CE2	3.06	0.41
2:H:140:PHE:HA	2:H:141:PRO:HD2	1.57	0.41
1:J:107:MLY:N	1:J:686:MET:HE1	2.35	0.41
1:J:322:VAL:HG12	1:J:325:ILE:HG13	2.03	0.41
1:J:330:GLU:HG2	1:J:330:GLU:H	1.54	0.41
1:J:550:PHE:C	4:V:46:GLY:CA	2.88	0.41
1:J:839:MLY:N	1:J:840:PRO:HD2	2.35	0.41
2:K:149:ASP:CG	2:K:150:TYR:N	2.49	0.41
4:0:221:LEU:HA	4:0:312:ARG:HG2	2.02	0.41
4:2:32:PRO:HB2	4:2:34:ILE:CD1	2.51	0.41
4:2:196:ARG:HH21	4:2:249:THR:HG23	1.85	0.41
4:2:227:MET:O	4:2:230:ALA:HB3	2.21	0.41
4:4:144:ALA:HB2	4:4:342:GLY:CA	2.51	0.41
4:5:32:PRO:HB2	4:5:34:ILE:CD1	2.51	0.41
4:5:144:ALA:HB2	4:5:342:GLY:CA	2.51	0.41
4:5:227:MET:O	4:5:230:ALA:HB3	2.21	0.41
4:6:227:MET:O	4:6:230:ALA:HB3	2.21	0.41
4:6:288:ASP:OD1	4:8:204:ALA:HA	2.21	0.41
4:7:144:ALA:HB2	4:7:342:GLY:CA	2.51	0.41
4:V:227:MET:O	4:V:230:ALA:HB3	2.21	0.41
4:W:32:PRO:HB2	4:W:34:ILE:CD1	2.51	0.41
4:Y:144:ALA:HB2	4:Y:342:GLY:CA	2.51	0.41
4:Z:227:MET:O	4:Z:230:ALA:HB3	2.21	0.41
1:A:502:GLU:HG2	1:A:766:PHE:HE1	1.85	0.41
1:A:817:GLN:HG3	2:B:127:ARG:HD3	1.03	0.41
1:D:47:PHE:HE1	1:D:78:PHE:CE1	2.40	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:THR:CA	1:D:221:GLN:HE21	2.33	0.41
1:D:335:ASP:O	1:D:338:ILE:HB	2.20	0.41
1:D:723:ARG:C	1:D:782:MLY:CH2	2.89	0.41
1:D:724:TYR:CA	1:D:782:MLY:HH11	2.48	0.41
1:G:91:MET:CE	1:G:119:SER:HB2	2.47	0.41
1:G:172:ASN:OD1	1:G:457:TYR:HA	2.21	0.41
1:G:193:ILE:HD11	1:G:250:ILE:HD12	2.03	0.41
1:G:657:LEU:HD12	1:G:657:LEU:O	2.21	0.41
1:G:712:PRO:HB2	1:G:713:SER:H	1.61	0.41
1:G:795:ARG:HH22	3:I:43:ASN:CB	2.33	0.41
1:G:798:LEU:CD2	3:I:126:LEU:HD11	2.44	0.41
2:H:113:LYS:O	2:H:147:ASN:HB2	2.20	0.41
3:I:56:GLU:OE1	3:I:59:ASN:ND2	2.54	0.41
1:J:193:ILE:CD1	1:J:250:ILE:HD13	2.51	0.41
1:J:322:VAL:HB	1:J:325:ILE:HD12	2.03	0.41
1:J:493:HIS:O	1:J:496:PHE:N	2.54	0.41
1:J:519:LEU:HD12	1:J:519:LEU:H	1.83	0.41
1:J:642:LYS:HE2	4:7:344:SER:HA	1.56	0.41
1:J:701:LEU:HD12	1:J:701:LEU:HA	1.55	0.41
1:J:733:PRO:CB	1:J:737:PHE:CE1	3.02	0.41
1:J:776:GLU:O	1:J:780:ASP:N	2.45	0.41
1:J:793:ARG:HD2	3:L:146:ILE:O	2.21	0.41
1:J:842:LEU:N	1:J:842:LEU:CD1	2.83	0.41
4:1:287:ILE:N	4:3:202:THR:CG2	2.77	0.41
4:3:227:MET:O	4:3:230:ALA:HB3	2.21	0.41
4:4:219:VAL:HG22	4:4:258:PRO:CB	2.52	0.41
4:6:219:VAL:HG22	4:6:258:PRO:CB	2.51	0.41
4:7:32:PRO:HB2	4:7:34:ILE:CD1	2.51	0.41
4:8:221:LEU:HA	4:8:312:ARG:HG2	2.02	0.41
4:X:288:ASP:OD1	4:Z:204:ALA:HA	2.21	0.41
1:A:295:MLY:CG	1:A:332:MET:HE1	2.50	0.40
1:A:335:ASP:O	1:A:338:ILE:HB	2.20	0.40
1:A:410:ASN:HA	4:4:334:GLU:HB3	1.30	0.40
1:A:757:GLN:OE1	1:A:771:LEU:CD1	2.69	0.40
2:B:139:ALA:O	2:B:141:PRO:CD	2.51	0.40
1:D:48:VAL:CG2	1:D:49:MLY:N	2.84	0.40
1:D:135:TYR:HD2	1:D:191:ARG:CG	2.33	0.40
1:D:193:ILE:HD11	1:D:250:ILE:HD12	2.03	0.40
1:D:556:ASP:OD1	4:7:50:LYS:CG	2.69	0.40
1:G:528:MLY:HB2	1:G:529:PRO:HD2	2.03	0.40
1:G:817:GLN:CG	2:H:128:PHE:CE1	3.01	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:835:PHE:CZ	2:H:27:PHE:CE1	3.09	0.40
1:J:330:GLU:OE1	1:J:330:GLU:HA	2.20	0.40
1:J:384:ASP:HA	1:J:394:SER:OG	2.21	0.40
1:J:508:ILE:HD13	1:J:759:ALA:HB2	1.79	0.40
2:K:113:LYS:O	2:K:147:ASN:HB2	2.20	0.40
3:L:48:LYS:HD3	3:L:48:LYS:HA	1.17	0.40
3:L:56:GLU:OE1	3:L:59:ASN:ND2	2.54	0.40
4:0:227:MET:O	4:0:230:ALA:HB3	2.21	0.40
4:1:144:ALA:HB2	4:1:342:GLY:CA	2.51	0.40
4:1:219:VAL:HG22	4:1:258:PRO:CB	2.52	0.40
4:3:144:ALA:HB2	4:3:342:GLY:CA	2.51	0.40
4:5:287:ILE:HA	4:7:202:THR:HG21	1.59	0.40
4:5:288:ASP:OD1	4:7:204:ALA:HA	2.21	0.40
4:6:32:PRO:HB2	4:6:34:ILE:CD1	2.51	0.40
4:8:32:PRO:HB2	4:8:34:ILE:CD1	2.51	0.40
4:W:219:VAL:HG22	4:W:258:PRO:CB	2.52	0.40
4:X:250:ILE:HG22	4:X:254:ARG:HB2	2.04	0.40
4:Z:219:VAL:HG22	4:Z:258:PRO:CB	2.51	0.40
1:A:384:ASP:HA	1:A:394:SER:OG	2.21	0.40
1:A:795:ARG:HH22	3:C:43:ASN:HB2	1.86	0.40
2:B:63:GLU:O	2:B:67:MET:HG3	2.22	0.40
1:D:193:ILE:CD1	1:D:250:ILE:HD13	2.51	0.40
1:D:213:LYS:HA	1:D:220:ASP:OD2	2.19	0.40
1:D:320:ILE:O	1:D:320:ILE:CG2	2.68	0.40
1:D:348:MLY:HH12	1:D:348:MLY:HD2	1.82	0.40
1:D:528:MLY:HB2	1:D:529:PRO:HD2	2.03	0.40
3:F:56:GLU:OE1	3:F:59:ASN:ND2	2.54	0.40
1:G:25:ILE:HG23	1:G:29:ASN:HD22	1.85	0.40
1:G:110:TYR:O	1:G:113:TRP:N	2.42	0.40
1:G:464:ILE:HG22	1:G:465:ALA:H	1.87	0.40
1:G:493:HIS:O	1:G:496:PHE:N	2.54	0.40
1:G:739:ASP:OD1	1:G:739:ASP:C	2.58	0.40
1:G:795:ARG:NH2	3:I:116:GLU:HB3	2.36	0.40
1:G:795:ARG:NH2	3:I:43:ASN:OD1	1.62	0.40
1:J:88:ILE:HG22	1:J:90:ASP:C	2.42	0.40
1:J:172:ASN:OD1	1:J:457:TYR:HA	2.21	0.40
1:J:303:LEU:O	1:J:304:LEU:HB2	2.21	0.40
4:1:120:THR:HG21	4:1:370:VAL:CG1	2.52	0.40
4:2:219:VAL:HG22	4:2:258:PRO:CB	2.51	0.40
4:4:221:LEU:HA	4:4:312:ARG:HG2	2.02	0.40
4:5:120:THR:HG21	4:5:370:VAL:CG1	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:120:THR:HG21	4:V:370:VAL:CG1	2.52	0.40
4:W:120:THR:HG21	4:W:370:VAL:CG1	2.51	0.40
4:Y:219:VAL:HG22	4:Y:258:PRO:CB	2.52	0.40
4:Y:226:GLU:HG3	4:Y:255:PHE:CE2	2.55	0.40
4:Y:227:MET:O	4:Y:230:ALA:HB3	2.21	0.40
1:A:464:ILE:HG22	1:A:465:ALA:H	1.87	0.40
1:A:798:LEU:HD12	1:A:798:LEU:HA	1.37	0.40
2:B:112:ILE:O	2:B:148:VAL:N	2.50	0.40
1:D:60:VAL:O	1:D:72:VAL:N	2.51	0.40
1:D:201:ALA:O	1:D:202:SER:OG	2.36	0.40
1:D:237:THR:CG2	1:D:238:VAL:N	2.85	0.40
1:D:657:LEU:O	1:D:657:LEU:HD12	2.21	0.40
1:G:303:LEU:O	1:G:304:LEU:HB2	2.21	0.40
1:G:407:GLY:HA2	1:G:411:GLU:O	2.21	0.40
1:G:768:MLY:HD3	1:G:772:LEU:HD23	1.87	0.40
1:J:38:VAL:HG13	1:J:39:PHE:N	2.35	0.40
1:J:528:MLY:HB2	1:J:529:PRO:HD2	2.03	0.40
1:J:544:LYS:N	4:7:146:GLY:O	2.55	0.40
1:J:659:MLY:HD2	1:J:659:MLY:HH22	1.42	0.40
3:L:95:ASP:OD1	3:L:139:TYR:HE1	2.04	0.40
4:2:221:LEU:HA	4:2:312:ARG:HG2	2.02	0.40
4:3:219:VAL:HG22	4:3:258:PRO:CB	2.51	0.40
4:6:221:LEU:HA	4:6:312:ARG:HG2	2.02	0.40
4:6:324:THR:HG23	4:8:245:GLY:HA2	1.09	0.40
4:7:196:ARG:HH21	4:7:249:THR:HG23	1.85	0.40
4:8:287:ILE:N	4:W:202:THR:CG2	2.77	0.40
4:X:196:ARG:HH21	4:X:249:THR:HG23	1.85	0.40
4:X:287:ILE:N	4:Z:202:THR:CG2	2.77	0.40
1:A:817:GLN:CB	2:B:127:ARG:CZ	2.69	0.40
3:C:84:PHE:HB3	3:C:147:MET:HE1	2.04	0.40
1:D:64:THR:OG1	1:D:68:GLU:HB3	2.22	0.40
1:D:88:ILE:HG22	1:D:90:ASP:C	2.42	0.40
1:D:172:ASN:OD1	1:D:457:TYR:HA	2.21	0.40
1:D:176:LEU:N	1:D:176:LEU:CD1	2.75	0.40
1:D:303:LEU:O	1:D:304:LEU:HB2	2.21	0.40
1:D:507:GLY:HA2	1:D:762:HIS:NE2	2.36	0.40
1:D:610:LEU:N	1:D:610:LEU:CD1	2.84	0.40
1:D:717:TYR:OH	1:D:760:PHE:HB3	2.21	0.40
1:D:813:ILE:HG22	2:E:127:ARG:NH1	2.08	0.40
1:G:93:MET:SD	1:G:764:MLY:HH23	2.61	0.40
1:G:305:ILE:HG22	1:G:312:TYR:OH	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:47:PHE:HE1	1:J:78:PHE:CE1	2.40	0.40
1:J:648:THR:CG2	1:J:651:ALA:CB	2.92	0.40
1:J:717:TYR:OH	1:J:760:PHE:HB3	2.21	0.40
3:L:62:ALA:O	3:L:63:ILE:CB	2.63	0.40
4:1:227:MET:O	4:1:230:ALA:HB3	2.21	0.40
4:6:120:THR:HG21	4:6:370:VAL:CG1	2.52	0.40
4:8:219:VAL:HG22	4:8:258:PRO:CB	2.52	0.40
4:8:227:MET:O	4:8:230:ALA:HB3	2.21	0.40
4:8:250:ILE:HG22	4:8:254:ARG:HB2	2.04	0.40
4:8:288:ASP:OD1	4:W:204:ALA:HA	2.21	0.40
4:W:250:ILE:HG22	4:W:254:ARG:HB2	2.04	0.40
4:X:32:PRO:HB2	4:X:34:ILE:CD1	2.51	0.40
1:A:237:THR:CG2	1:A:238:VAL:N	2.84	0.40
1:A:292:MET:CE	1:A:309:PRO:HD3	2.52	0.40
1:A:556:ASP:OD1	4:6:50:LYS:CG	2.69	0.40
2:B:137:TRP:CA	2:B:145:ALA:CB	2.82	0.40
1:D:89:GLU:HB3	1:D:153:PRO:HG3	2.03	0.40
1:D:400:ALA:CB	1:D:606:THR:CG2	3.00	0.40
2:E:163:ALA:O	2:K:20:ASP:OD2	2.39	0.40
1:G:193:ILE:HD13	1:G:252:ILE:HD11	2.04	0.40
2:H:63:GLU:O	2:H:67:MET:HG3	2.22	0.40
1:J:63:MLY:HD3	1:J:63:MLY:HH23	1.76	0.40
4:1:250:ILE:HG22	4:1:254:ARG:HB2	2.04	0.40
4:4:32:PRO:HB2	4:4:34:ILE:CD1	2.51	0.40
4:4:287:ILE:N	4:6:202:THR:CG2	2.77	0.40
4:8:88:HIS:HA	4:8:92:ASN:OD1	2.22	0.40
4:V:32:PRO:HB2	4:V:34:ILE:CD1	2.51	0.40
4:V:324:THR:N	4:X:245:GLY:CA	2.69	0.40
4:W:193:LEU:HD12	4:W:193:LEU:HA	1.96	0.40
4:W:288:ASP:OD1	4:Y:204:ALA:HA	2.21	0.40
4:X:227:MET:O	4:X:230:ALA:HB3	2.21	0.40
4:Y:120:THR:HG21	4:Y:370:VAL:CG1	2.52	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 PDB entries followed by that with respect to all EM

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	789/840 (94%)	650 (82%)	113 (14%)	26 (3%)	4	26
1	D	789/840 (94%)	651 (82%)	112 (14%)	26 (3%)	4	26
1	G	789/840 (94%)	649 (82%)	113 (14%)	27 (3%)	3	26
1	J	791/840 (94%)	651 (82%)	112 (14%)	28 (4%)	3	25
2	B	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	E	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	H	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
2	K	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	2	19
3	C	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	F	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	I	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	L	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
4	0	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	1	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	2	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	3	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	4	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	5	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	6	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	7	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	8	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
4	V	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	W	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	X	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	Y	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	9	44
4	Z	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	9	44
All	All	9482/9778 (97%)	8319 (88%)	940 (10%)	223 (2%)	9	33

All (223) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	LYS
1	A	202	SER
1	A	572	LYS
1	A	712	PRO
1	A	729	ALA
1	A	757	GLN
1	A	762	HIS
2	B	131	GLU
2	B	141	PRO
1	D	73	LYS
1	D	202	SER
1	D	572	LYS
1	D	712	PRO
1	D	729	ALA
1	D	757	GLN
1	D	762	HIS
2	E	131	GLU
2	E	141	PRO
1	G	73	LYS
1	G	202	SER
1	G	572	LYS
1	G	712	PRO
1	G	729	ALA
1	G	757	GLN
1	G	762	HIS
2	H	131	GLU
2	H	141	PRO
1	J	73	LYS
1	J	202	SER
1	J	572	LYS
1	J	712	PRO
1	J	729	ALA
1	J	757	GLN
1	J	762	HIS
1	J	785	GLU
2	K	131	GLU
2	K	141	PRO
4	0	246	GLN
4	1	246	GLN
4	2	246	GLN
4	3	246	GLN
4	4	246	GLN
4	5	246	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	6	246	GLN
4	7	246	GLN
4	8	246	GLN
4	V	246	GLN
4	W	246	GLN
4	X	246	GLN
4	Y	246	GLN
4	Z	246	GLN
1	A	11	GLY
1	A	21	GLU
1	A	219	GLU
1	A	517	MET
1	A	532	ILE
1	A	637	LYS
2	B	130	PRO
2	B	147	ASN
2	B	151	LYS
2	B	161	GLU
1	D	11	GLY
1	D	21	GLU
1	D	219	GLU
1	D	517	MET
1	D	532	ILE
1	D	637	LYS
2	E	130	PRO
2	E	147	ASN
2	E	151	LYS
2	E	161	GLU
1	G	11	GLY
1	G	21	GLU
1	G	219	GLU
1	G	517	MET
1	G	532	ILE
1	G	637	LYS
1	G	785	GLU
2	H	130	PRO
2	H	147	ASN
2	H	151	LYS
1	J	11	GLY
1	J	21	GLU
1	J	219	GLU
1	J	517	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	637	LYS
2	K	130	PRO
2	K	147	ASN
2	K	151	LYS
2	K	161	GLU
4	0	274	ILE
4	1	274	ILE
4	2	274	ILE
4	3	274	ILE
4	4	274	ILE
4	5	274	ILE
4	6	274	ILE
4	7	274	ILE
4	8	274	ILE
4	V	274	ILE
4	W	274	ILE
4	X	274	ILE
4	Y	274	ILE
4	Z	274	ILE
1	A	58	GLY
1	A	294	ASN
1	A	644	SER
1	D	58	GLY
1	D	294	ASN
1	D	644	SER
1	G	58	GLY
1	G	294	ASN
1	G	644	SER
2	H	161	GLU
1	J	58	GLY
1	J	294	ASN
1	J	532	ILE
1	J	644	SER
4	0	233	SER
4	1	233	SER
4	2	233	SER
4	3	233	SER
4	4	233	SER
4	5	233	SER
4	6	233	SER
4	7	233	SER
4	8	233	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	V	233	SER
4	W	233	SER
4	X	233	SER
4	Y	233	SER
4	Z	233	SER
1	A	435	GLU
1	A	817	GLN
1	D	269	LEU
1	D	435	GLU
1	D	817	GLN
1	G	269	LEU
1	G	435	GLU
1	G	817	GLN
1	J	435	GLU
1	J	817	GLN
4	0	2	GLU
4	0	253	GLU
4	1	2	GLU
4	1	253	GLU
4	2	2	GLU
4	2	253	GLU
4	3	2	GLU
4	3	253	GLU
4	4	2	GLU
4	4	253	GLU
4	5	2	GLU
4	6	2	GLU
4	6	253	GLU
4	7	2	GLU
4	7	253	GLU
4	8	2	GLU
4	V	2	GLU
4	V	253	GLU
4	W	2	GLU
4	X	2	GLU
4	X	253	GLU
4	Y	2	GLU
4	Y	253	GLU
4	Z	2	GLU
1	A	8	ALA
1	A	269	LEU
1	A	578	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	140	PHE
1	D	8	ALA
1	D	578	HIS
2	E	140	PHE
1	G	8	ALA
1	G	79	SER
1	G	578	HIS
2	H	140	PHE
1	J	8	ALA
1	J	269	LEU
1	J	578	HIS
2	K	140	PHE
4	5	253	GLU
4	8	253	GLU
4	W	253	GLU
4	Z	253	GLU
1	A	79	SER
1	A	199	ILE
1	A	556	ASP
2	B	142	PRO
1	D	79	SER
1	D	199	ILE
1	D	556	ASP
2	E	142	PRO
1	G	199	ILE
1	G	556	ASP
2	H	142	PRO
1	J	79	SER
1	J	199	ILE
1	J	556	ASP
1	J	822	SER
2	K	142	PRO
1	A	840	PRO
1	D	287	ILE
1	D	840	PRO
1	G	840	PRO
1	J	287	ILE
1	J	840	PRO
4	0	242	LEU
4	1	242	LEU
4	2	242	LEU
4	3	242	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	242	LEU
4	5	242	LEU
4	6	242	LEU
4	7	242	LEU
4	8	242	LEU
4	V	242	LEU
4	W	242	LEU
4	X	242	LEU
4	Y	242	LEU
4	Z	242	LEU
1	A	287	ILE
1	G	287	ILE

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	672/672 (100%)	512 (76%)	160 (24%)	0	4
1	D	672/672 (100%)	515 (77%)	157 (23%)	1	4
1	G	672/672 (100%)	514 (76%)	158 (24%)	1	4
1	J	672/672 (100%)	514 (76%)	158 (24%)	1	4
2	B	120/120 (100%)	119 (99%)	1 (1%)	81	89
2	E	120/120 (100%)	119 (99%)	1 (1%)	81	89
2	H	120/120 (100%)	119 (99%)	1 (1%)	81	89
2	K	120/120 (100%)	119 (99%)	1 (1%)	81	89
3	C	117/117 (100%)	112 (96%)	5 (4%)	29	53
3	F	117/117 (100%)	112 (96%)	5 (4%)	29	53
3	I	117/117 (100%)	112 (96%)	5 (4%)	29	53
3	L	117/117 (100%)	112 (96%)	5 (4%)	29	53
4	0	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	1	315/318 (99%)	268 (85%)	47 (15%)	3	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	2	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	3	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	4	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	5	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	6	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	7	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	8	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	V	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	W	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	X	315/318 (99%)	269 (85%)	46 (15%)	3	15
4	Y	315/318 (99%)	268 (85%)	47 (15%)	3	15
4	Z	315/318 (99%)	268 (85%)	47 (15%)	3	15
All	All	8046/8088 (100%)	6737 (84%)	1309 (16%)	5	13

All (1309) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	7	MET
1	A	12	GLU
1	A	15	PRO
1	A	17	LEU
1	A	20	SER
1	A	22	LYS
1	A	36	SER
1	A	37	SER
1	A	46	SER
1	A	61	THR
1	A	69	THR
1	A	70	LEU
1	A	72	VAL
1	A	73	LYS
1	A	75	ASP
1	A	76	GLN
1	A	97	LEU
1	A	106	LEU
1	A	109	ARG
1	A	114	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	117	THR
1	A	121	LEU
1	A	126	VAL
1	A	127	ASN
1	A	135	TYR
1	A	136	ASN
1	A	146	LYS
1	A	149	GLN
1	A	155	ILE
1	A	157	SER
1	A	158	ILE
1	A	159	SER
1	A	165	PHE
1	A	167	LEU
1	A	169	ASP
1	A	173	GLN
1	A	178	THR
1	A	185	LYS
1	A	186	THR
1	A	187	VAL
1	A	189	THR
1	A	191	ARG
1	A	193	ILE
1	A	194	GLN
1	A	198	THR
1	A	199	ILE
1	A	218	LEU
1	A	219	GLU
1	A	221	GLN
1	A	223	ILE
1	A	227	PRO
1	A	229	LEU
1	A	244	SER
1	A	245	ARG
1	A	251	ARG
1	A	264	ASP
1	A	273	SER
1	A	274	ARG
1	A	278	GLN
1	A	282	GLU
1	A	287	ILE
1	A	290	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	294	ASN
1	A	298	GLU
1	A	300	ILE
1	A	325	ILE
1	A	331	LEU
1	A	336	SER
1	A	351	ILE
1	A	354	LEU
1	A	364	LEU
1	A	365	LYS
1	A	372	GLU
1	A	376	GLU
1	A	381	GLU
1	A	389	LEU
1	A	392	LEU
1	A	394	SER
1	A	399	LYS
1	A	405	ARG
1	A	410	ASN
1	A	439	LEU
1	A	447	GLN
1	A	448	GLN
1	A	449	LEU
1	A	453	GLN
1	A	455	ARG
1	A	457	TYR
1	A	462	LEU
1	A	471	ASP
1	A	474	SER
1	A	480	ILE
1	A	487	LEU
1	A	495	MET
1	A	499	GLU
1	A	506	GLU
1	A	513	ILE
1	A	518	ASP
1	A	524	GLU
1	A	532	ILE
1	A	534	SER
1	A	537	GLU
1	A	543	PRO
1	A	549	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	561	LYS
1	A	562	SER
1	A	563	ASN
1	A	569	LYS
1	A	580	SER
1	A	593	SER
1	A	597	GLU
1	A	604	ASN
1	A	608	ILE
1	A	610	LEU
1	A	615	SER
1	A	621	LEU
1	A	625	THR
1	A	664	LEU
1	A	666	SER
1	A	673	ARG
1	A	675	ILE
1	A	676	ILE
1	A	686	MET
1	A	689	GLU
1	A	690	LEU
1	A	693	HIS
1	A	698	ASN
1	A	701	LEU
1	A	702	GLU
1	A	704	ILE
1	A	708	ARG
1	A	713	SER
1	A	714	ARG
1	A	716	LEU
1	A	719	ASP
1	A	722	GLN
1	A	723	ARG
1	A	727	LEU
1	A	728	ASN
1	A	745	GLU
1	A	752	ASP
1	A	753	VAL
1	A	754	ASP
1	A	762	HIS
1	A	774	LEU
1	A	785	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	787	ILE
1	A	793	ARG
1	A	799	MET
1	A	802	GLU
1	A	804	ARG
1	A	810	ARG
1	A	816	ILE
1	A	822	SER
1	A	832	MET
1	A	834	LEU
1	A	838	ILE
1	A	842	LEU
1	A	843	LYS
2	B	142	PRO
3	C	48	LYS
3	C	68	PHE
3	C	83	THR
3	C	95	ASP
3	C	96	LYS
1	D	4	ASP
1	D	7	MET
1	D	12	GLU
1	D	15	PRO
1	D	17	LEU
1	D	20	SER
1	D	22	LYS
1	D	36	SER
1	D	37	SER
1	D	46	SER
1	D	61	THR
1	D	69	THR
1	D	70	LEU
1	D	72	VAL
1	D	73	LYS
1	D	75	ASP
1	D	76	GLN
1	D	97	LEU
1	D	106	LEU
1	D	109	ARG
1	D	114	MET
1	D	117	THR
1	D	121	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	126	VAL
1	D	127	ASN
1	D	135	TYR
1	D	136	ASN
1	D	146	LYS
1	D	149	GLN
1	D	155	ILE
1	D	157	SER
1	D	158	ILE
1	D	159	SER
1	D	165	PHE
1	D	167	LEU
1	D	169	ASP
1	D	173	GLN
1	D	178	THR
1	D	185	LYS
1	D	186	THR
1	D	187	VAL
1	D	191	ARG
1	D	193	ILE
1	D	194	GLN
1	D	198	THR
1	D	199	ILE
1	D	218	LEU
1	D	219	GLU
1	D	221	GLN
1	D	223	ILE
1	D	229	LEU
1	D	244	SER
1	D	245	ARG
1	D	251	ARG
1	D	264	ASP
1	D	273	SER
1	D	274	ARG
1	D	278	GLN
1	D	282	GLU
1	D	287	ILE
1	D	290	GLN
1	D	294	ASN
1	D	298	GLU
1	D	300	ILE
1	D	325	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	331	LEU
1	D	336	SER
1	D	351	ILE
1	D	354	LEU
1	D	364	LEU
1	D	365	LYS
1	D	372	GLU
1	D	376	GLU
1	D	381	GLU
1	D	389	LEU
1	D	392	LEU
1	D	394	SER
1	D	399	LYS
1	D	405	ARG
1	D	410	ASN
1	D	439	LEU
1	D	447	GLN
1	D	448	GLN
1	D	449	LEU
1	D	453	GLN
1	D	455	ARG
1	D	457	TYR
1	D	462	LEU
1	D	471	ASP
1	D	474	SER
1	D	480	ILE
1	D	487	LEU
1	D	495	MET
1	D	499	GLU
1	D	506	GLU
1	D	513	ILE
1	D	518	ASP
1	D	524	GLU
1	D	532	ILE
1	D	534	SER
1	D	537	GLU
1	D	549	SER
1	D	561	LYS
1	D	562	SER
1	D	563	ASN
1	D	569	LYS
1	D	580	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	593	SER
1	D	597	GLU
1	D	604	ASN
1	D	608	ILE
1	D	610	LEU
1	D	615	SER
1	D	621	LEU
1	D	625	THR
1	D	664	LEU
1	D	666	SER
1	D	673	ARG
1	D	675	ILE
1	D	676	ILE
1	D	686	MET
1	D	689	GLU
1	D	690	LEU
1	D	693	HIS
1	D	698	ASN
1	D	701	LEU
1	D	702	GLU
1	D	704	ILE
1	D	708	ARG
1	D	713	SER
1	D	714	ARG
1	D	716	LEU
1	D	719	ASP
1	D	722	GLN
1	D	723	ARG
1	D	727	LEU
1	D	728	ASN
1	D	745	GLU
1	D	752	ASP
1	D	753	VAL
1	D	754	ASP
1	D	762	HIS
1	D	774	LEU
1	D	785	GLU
1	D	787	ILE
1	D	793	ARG
1	D	799	MET
1	D	802	GLU
1	D	804	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	810	ARG
1	D	816	ILE
1	D	822	SER
1	D	832	MET
1	D	834	LEU
1	D	838	ILE
1	D	842	LEU
1	D	843	LYS
2	E	142	PRO
3	F	48	LYS
3	F	68	PHE
3	F	83	THR
3	F	95	ASP
3	F	96	LYS
1	G	4	ASP
1	G	7	MET
1	G	12	GLU
1	G	15	PRO
1	G	17	LEU
1	G	20	SER
1	G	22	LYS
1	G	36	SER
1	G	37	SER
1	G	46	SER
1	G	61	THR
1	G	69	THR
1	G	70	LEU
1	G	72	VAL
1	G	73	LYS
1	G	75	ASP
1	G	76	GLN
1	G	97	LEU
1	G	106	LEU
1	G	109	ARG
1	G	114	MET
1	G	117	THR
1	G	121	LEU
1	G	126	VAL
1	G	127	ASN
1	G	135	TYR
1	G	136	ASN
1	G	146	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	149	GLN
1	G	155	ILE
1	G	157	SER
1	G	158	ILE
1	G	159	SER
1	G	165	PHE
1	G	167	LEU
1	G	169	ASP
1	G	173	GLN
1	G	178	THR
1	G	185	LYS
1	G	186	THR
1	G	187	VAL
1	G	189	THR
1	G	191	ARG
1	G	193	ILE
1	G	194	GLN
1	G	198	THR
1	G	199	ILE
1	G	218	LEU
1	G	219	GLU
1	G	221	GLN
1	G	223	ILE
1	G	229	LEU
1	G	244	SER
1	G	245	ARG
1	G	251	ARG
1	G	264	ASP
1	G	273	SER
1	G	274	ARG
1	G	278	GLN
1	G	282	GLU
1	G	287	ILE
1	G	290	GLN
1	G	294	ASN
1	G	298	GLU
1	G	300	ILE
1	G	325	ILE
1	G	331	LEU
1	G	336	SER
1	G	351	ILE
1	G	354	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	364	LEU
1	G	365	LYS
1	G	372	GLU
1	G	376	GLU
1	G	381	GLU
1	G	389	LEU
1	G	392	LEU
1	G	394	SER
1	G	399	LYS
1	G	405	ARG
1	G	410	ASN
1	G	439	LEU
1	G	447	GLN
1	G	448	GLN
1	G	449	LEU
1	G	453	GLN
1	G	455	ARG
1	G	457	TYR
1	G	462	LEU
1	G	471	ASP
1	G	474	SER
1	G	480	ILE
1	G	487	LEU
1	G	495	MET
1	G	499	GLU
1	G	506	GLU
1	G	513	ILE
1	G	518	ASP
1	G	524	GLU
1	G	532	ILE
1	G	534	SER
1	G	537	GLU
1	G	549	SER
1	G	561	LYS
1	G	562	SER
1	G	563	ASN
1	G	569	LYS
1	G	580	SER
1	G	593	SER
1	G	597	GLU
1	G	604	ASN
1	G	608	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	610	LEU
1	G	615	SER
1	G	621	LEU
1	G	625	THR
1	G	664	LEU
1	G	666	SER
1	G	673	ARG
1	G	675	ILE
1	G	676	ILE
1	G	686	MET
1	G	689	GLU
1	G	690	LEU
1	G	693	HIS
1	G	698	ASN
1	G	701	LEU
1	G	702	GLU
1	G	704	ILE
1	G	708	ARG
1	G	713	SER
1	G	714	ARG
1	G	716	LEU
1	G	719	ASP
1	G	722	GLN
1	G	723	ARG
1	G	727	LEU
1	G	728	ASN
1	G	745	GLU
1	G	752	ASP
1	G	753	VAL
1	G	754	ASP
1	G	762	HIS
1	G	774	LEU
1	G	785	GLU
1	G	787	ILE
1	G	793	ARG
1	G	799	MET
1	G	802	GLU
1	G	804	ARG
1	G	810	ARG
1	G	816	ILE
1	G	822	SER
1	G	832	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	834	LEU
1	G	838	ILE
1	G	842	LEU
1	G	843	LYS
2	H	142	PRO
3	I	48	LYS
3	I	68	PHE
3	I	83	THR
3	I	95	ASP
3	I	96	LYS
1	J	4	ASP
1	J	7	MET
1	J	12	GLU
1	J	15	PRO
1	J	17	LEU
1	J	20	SER
1	J	22	LYS
1	J	36	SER
1	J	37	SER
1	J	46	SER
1	J	61	THR
1	J	69	THR
1	J	70	LEU
1	J	72	VAL
1	J	73	LYS
1	J	75	ASP
1	J	76	GLN
1	J	97	LEU
1	J	106	LEU
1	J	109	ARG
1	J	114	MET
1	J	117	THR
1	J	121	LEU
1	J	126	VAL
1	J	127	ASN
1	J	135	TYR
1	J	136	ASN
1	J	146	LYS
1	J	149	GLN
1	J	155	ILE
1	J	157	SER
1	J	158	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	159	SER
1	J	165	PHE
1	J	167	LEU
1	J	169	ASP
1	J	173	GLN
1	J	178	THR
1	J	185	LYS
1	J	186	THR
1	J	187	VAL
1	J	189	THR
1	J	191	ARG
1	J	193	ILE
1	J	194	GLN
1	J	198	THR
1	J	199	ILE
1	J	218	LEU
1	J	219	GLU
1	J	221	GLN
1	J	223	ILE
1	J	229	LEU
1	J	244	SER
1	J	245	ARG
1	J	251	ARG
1	J	264	ASP
1	J	273	SER
1	J	274	ARG
1	J	278	GLN
1	J	282	GLU
1	J	287	ILE
1	J	290	GLN
1	J	294	ASN
1	J	298	GLU
1	J	300	ILE
1	J	325	ILE
1	J	331	LEU
1	J	336	SER
1	J	351	ILE
1	J	354	LEU
1	J	364	LEU
1	J	365	LYS
1	J	372	GLU
1	J	376	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	381	GLU
1	J	389	LEU
1	J	392	LEU
1	J	394	SER
1	J	399	LYS
1	J	405	ARG
1	J	410	ASN
1	J	439	LEU
1	J	447	GLN
1	J	448	GLN
1	J	449	LEU
1	J	453	GLN
1	J	455	ARG
1	J	457	TYR
1	J	462	LEU
1	J	471	ASP
1	J	474	SER
1	J	480	ILE
1	J	487	LEU
1	J	495	MET
1	J	499	GLU
1	J	506	GLU
1	J	513	ILE
1	J	518	ASP
1	J	524	GLU
1	J	532	ILE
1	J	534	SER
1	J	537	GLU
1	J	543	PRO
1	J	549	SER
1	J	561	LYS
1	J	562	SER
1	J	563	ASN
1	J	569	LYS
1	J	580	SER
1	J	593	SER
1	J	597	GLU
1	J	604	ASN
1	J	608	ILE
1	J	610	LEU
1	J	615	SER
1	J	621	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	625	THR
1	J	664	LEU
1	J	666	SER
1	J	673	ARG
1	J	675	ILE
1	J	676	ILE
1	J	686	MET
1	J	689	GLU
1	J	690	LEU
1	J	693	HIS
1	J	698	ASN
1	J	701	LEU
1	J	702	GLU
1	J	708	ARG
1	J	713	SER
1	J	714	ARG
1	J	716	LEU
1	J	719	ASP
1	J	722	GLN
1	J	723	ARG
1	J	727	LEU
1	J	728	ASN
1	J	745	GLU
1	J	752	ASP
1	J	753	VAL
1	J	754	ASP
1	J	762	HIS
1	J	774	LEU
1	J	785	GLU
1	J	787	ILE
1	J	793	ARG
1	J	799	MET
1	J	802	GLU
1	J	804	ARG
1	J	810	ARG
1	J	816	ILE
1	J	822	SER
1	J	832	MET
1	J	834	LEU
1	J	838	ILE
1	J	842	LEU
1	J	843	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	142	PRO
3	L	48	LYS
3	L	68	PHE
3	L	83	THR
3	L	95	ASP
3	L	96	LYS
4	0	33	SER
4	0	34	ILE
4	0	37	ARG
4	0	66	THR
4	0	72	GLU
4	0	80	ASP
4	0	100	GLU
4	0	109	PRO
4	0	116	ARG
4	0	145	SER
4	0	153	LEU
4	0	159	VAL
4	0	180	LEU
4	0	191	LYS
4	0	196	ARG
4	0	199	SER
4	0	201	VAL
4	0	206	ARG
4	0	221	LEU
4	0	223	PHE
4	0	229	THR
4	0	239	SER
4	0	242	LEU
4	0	246	GLN
4	0	263	GLN
4	0	281	SER
4	0	283	MET
4	0	287	ILE
4	0	291	LYS
4	0	293	LEU
4	0	297	ASN
4	0	299	MET
4	0	312	ARG
4	0	315	LYS
4	0	318	THR
4	0	320	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	0	327	ILE
4	0	334	GLU
4	0	349	LEU
4	0	350	SER
4	0	351	THR
4	0	354	GLN
4	0	359	LYS
4	0	360	GLN
4	0	361	GLU
4	0	368	SER
4	1	16	LEU
4	1	33	SER
4	1	34	ILE
4	1	37	ARG
4	1	66	THR
4	1	72	GLU
4	1	80	ASP
4	1	100	GLU
4	1	109	PRO
4	1	116	ARG
4	1	145	SER
4	1	153	LEU
4	1	159	VAL
4	1	180	LEU
4	1	191	LYS
4	1	196	ARG
4	1	199	SER
4	1	201	VAL
4	1	206	ARG
4	1	221	LEU
4	1	223	PHE
4	1	229	THR
4	1	239	SER
4	1	242	LEU
4	1	246	GLN
4	1	263	GLN
4	1	281	SER
4	1	283	MET
4	1	287	ILE
4	1	291	LYS
4	1	293	LEU
4	1	297	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	1	299	MET
4	1	312	ARG
4	1	315	LYS
4	1	318	THR
4	1	320	LEU
4	1	327	ILE
4	1	334	GLU
4	1	349	LEU
4	1	350	SER
4	1	351	THR
4	1	354	GLN
4	1	359	LYS
4	1	360	GLN
4	1	361	GLU
4	1	368	SER
4	2	16	LEU
4	2	33	SER
4	2	34	ILE
4	2	37	ARG
4	2	66	THR
4	2	72	GLU
4	2	80	ASP
4	2	100	GLU
4	2	109	PRO
4	2	116	ARG
4	2	145	SER
4	2	153	LEU
4	2	159	VAL
4	2	180	LEU
4	2	191	LYS
4	2	196	ARG
4	2	199	SER
4	2	201	VAL
4	2	206	ARG
4	2	221	LEU
4	2	223	PHE
4	2	229	THR
4	2	239	SER
4	2	242	LEU
4	2	246	GLN
4	2	263	GLN
4	2	281	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	2	283	MET
4	2	287	ILE
4	2	291	LYS
4	2	293	LEU
4	2	297	ASN
4	2	299	MET
4	2	312	ARG
4	2	315	LYS
4	2	318	THR
4	2	320	LEU
4	2	327	ILE
4	2	334	GLU
4	2	349	LEU
4	2	350	SER
4	2	351	THR
4	2	354	GLN
4	2	359	LYS
4	2	360	GLN
4	2	361	GLU
4	2	368	SER
4	3	16	LEU
4	3	33	SER
4	3	34	ILE
4	3	37	ARG
4	3	66	THR
4	3	72	GLU
4	3	80	ASP
4	3	100	GLU
4	3	109	PRO
4	3	116	ARG
4	3	145	SER
4	3	153	LEU
4	3	159	VAL
4	3	180	LEU
4	3	191	LYS
4	3	196	ARG
4	3	199	SER
4	3	201	VAL
4	3	206	ARG
4	3	221	LEU
4	3	223	PHE
4	3	229	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	3	239	SER
4	3	242	LEU
4	3	246	GLN
4	3	263	GLN
4	3	281	SER
4	3	283	MET
4	3	287	ILE
4	3	291	LYS
4	3	293	LEU
4	3	297	ASN
4	3	299	MET
4	3	312	ARG
4	3	315	LYS
4	3	318	THR
4	3	320	LEU
4	3	327	ILE
4	3	334	GLU
4	3	349	LEU
4	3	350	SER
4	3	351	THR
4	3	354	GLN
4	3	359	LYS
4	3	360	GLN
4	3	361	GLU
4	3	368	SER
4	4	16	LEU
4	4	33	SER
4	4	34	ILE
4	4	37	ARG
4	4	66	THR
4	4	72	GLU
4	4	80	ASP
4	4	100	GLU
4	4	109	PRO
4	4	116	ARG
4	4	145	SER
4	4	153	LEU
4	4	159	VAL
4	4	180	LEU
4	4	191	LYS
4	4	196	ARG
4	4	199	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	201	VAL
4	4	206	ARG
4	4	221	LEU
4	4	223	PHE
4	4	229	THR
4	4	239	SER
4	4	242	LEU
4	4	246	GLN
4	4	263	GLN
4	4	281	SER
4	4	283	MET
4	4	287	ILE
4	4	291	LYS
4	4	293	LEU
4	4	297	ASN
4	4	299	MET
4	4	312	ARG
4	4	315	LYS
4	4	318	THR
4	4	320	LEU
4	4	327	ILE
4	4	334	GLU
4	4	349	LEU
4	4	350	SER
4	4	351	THR
4	4	354	GLN
4	4	359	LYS
4	4	360	GLN
4	4	361	GLU
4	4	368	SER
4	5	33	SER
4	5	34	ILE
4	5	37	ARG
4	5	66	THR
4	5	72	GLU
4	5	80	ASP
4	5	100	GLU
4	5	109	PRO
4	5	116	ARG
4	5	145	SER
4	5	153	LEU
4	5	159	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	5	180	LEU
4	5	191	LYS
4	5	196	ARG
4	5	199	SER
4	5	201	VAL
4	5	206	ARG
4	5	221	LEU
4	5	223	PHE
4	5	229	THR
4	5	239	SER
4	5	242	LEU
4	5	246	GLN
4	5	263	GLN
4	5	281	SER
4	5	283	MET
4	5	287	ILE
4	5	291	LYS
4	5	293	LEU
4	5	297	ASN
4	5	299	MET
4	5	312	ARG
4	5	315	LYS
4	5	318	THR
4	5	320	LEU
4	5	327	ILE
4	5	334	GLU
4	5	349	LEU
4	5	350	SER
4	5	351	THR
4	5	354	GLN
4	5	359	LYS
4	5	360	GLN
4	5	361	GLU
4	5	368	SER
4	6	16	LEU
4	6	33	SER
4	6	34	ILE
4	6	37	ARG
4	6	66	THR
4	6	72	GLU
4	6	80	ASP
4	6	100	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	6	109	PRO
4	6	116	ARG
4	6	145	SER
4	6	153	LEU
4	6	159	VAL
4	6	180	LEU
4	6	191	LYS
4	6	196	ARG
4	6	199	SER
4	6	201	VAL
4	6	206	ARG
4	6	221	LEU
4	6	223	PHE
4	6	229	THR
4	6	239	SER
4	6	242	LEU
4	6	246	GLN
4	6	263	GLN
4	6	281	SER
4	6	283	MET
4	6	287	ILE
4	6	291	LYS
4	6	293	LEU
4	6	297	ASN
4	6	299	MET
4	6	312	ARG
4	6	315	LYS
4	6	318	THR
4	6	320	LEU
4	6	327	ILE
4	6	334	GLU
4	6	349	LEU
4	6	350	SER
4	6	351	THR
4	6	354	GLN
4	6	359	LYS
4	6	360	GLN
4	6	361	GLU
4	6	368	SER
4	7	33	SER
4	7	34	ILE
4	7	37	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	7	66	THR
4	7	72	GLU
4	7	80	ASP
4	7	100	GLU
4	7	109	PRO
4	7	116	ARG
4	7	145	SER
4	7	153	LEU
4	7	159	VAL
4	7	180	LEU
4	7	191	LYS
4	7	196	ARG
4	7	199	SER
4	7	201	VAL
4	7	206	ARG
4	7	221	LEU
4	7	223	PHE
4	7	229	THR
4	7	239	SER
4	7	242	LEU
4	7	246	GLN
4	7	263	GLN
4	7	281	SER
4	7	283	MET
4	7	287	ILE
4	7	291	LYS
4	7	293	LEU
4	7	297	ASN
4	7	299	MET
4	7	312	ARG
4	7	315	LYS
4	7	318	THR
4	7	320	LEU
4	7	327	ILE
4	7	334	GLU
4	7	349	LEU
4	7	350	SER
4	7	351	THR
4	7	354	GLN
4	7	359	LYS
4	7	360	GLN
4	7	361	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	7	368	SER
4	8	16	LEU
4	8	33	SER
4	8	34	ILE
4	8	37	ARG
4	8	66	THR
4	8	72	GLU
4	8	80	ASP
4	8	100	GLU
4	8	109	PRO
4	8	116	ARG
4	8	145	SER
4	8	153	LEU
4	8	159	VAL
4	8	180	LEU
4	8	191	LYS
4	8	196	ARG
4	8	199	SER
4	8	201	VAL
4	8	206	ARG
4	8	221	LEU
4	8	223	PHE
4	8	229	THR
4	8	239	SER
4	8	242	LEU
4	8	246	GLN
4	8	263	GLN
4	8	281	SER
4	8	283	MET
4	8	287	ILE
4	8	291	LYS
4	8	293	LEU
4	8	297	ASN
4	8	299	MET
4	8	312	ARG
4	8	315	LYS
4	8	318	THR
4	8	320	LEU
4	8	327	ILE
4	8	334	GLU
4	8	349	LEU
4	8	350	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	8	351	THR
4	8	354	GLN
4	8	359	LYS
4	8	360	GLN
4	8	361	GLU
4	8	368	SER
4	V	33	SER
4	V	34	ILE
4	V	37	ARG
4	V	66	THR
4	V	72	GLU
4	V	80	ASP
4	V	100	GLU
4	V	109	PRO
4	V	116	ARG
4	V	145	SER
4	V	153	LEU
4	V	159	VAL
4	V	180	LEU
4	V	191	LYS
4	V	196	ARG
4	V	199	SER
4	V	201	VAL
4	V	206	ARG
4	V	221	LEU
4	V	223	PHE
4	V	229	THR
4	V	239	SER
4	V	242	LEU
4	V	246	GLN
4	V	263	GLN
4	V	281	SER
4	V	283	MET
4	V	287	ILE
4	V	291	LYS
4	V	293	LEU
4	V	297	ASN
4	V	299	MET
4	V	312	ARG
4	V	315	LYS
4	V	318	THR
4	V	320	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	V	327	ILE
4	V	334	GLU
4	V	349	LEU
4	V	350	SER
4	V	351	THR
4	V	354	GLN
4	V	359	LYS
4	V	360	GLN
4	V	361	GLU
4	V	368	SER
4	W	33	SER
4	W	34	ILE
4	W	37	ARG
4	W	66	THR
4	W	72	GLU
4	W	80	ASP
4	W	100	GLU
4	W	109	PRO
4	W	116	ARG
4	W	145	SER
4	W	153	LEU
4	W	159	VAL
4	W	180	LEU
4	W	191	LYS
4	W	196	ARG
4	W	199	SER
4	W	201	VAL
4	W	206	ARG
4	W	221	LEU
4	W	223	PHE
4	W	229	THR
4	W	239	SER
4	W	242	LEU
4	W	246	GLN
4	W	263	GLN
4	W	281	SER
4	W	283	MET
4	W	287	ILE
4	W	291	LYS
4	W	293	LEU
4	W	297	ASN
4	W	299	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	W	312	ARG
4	W	315	LYS
4	W	318	THR
4	W	320	LEU
4	W	327	ILE
4	W	334	GLU
4	W	349	LEU
4	W	350	SER
4	W	351	THR
4	W	354	GLN
4	W	359	LYS
4	W	360	GLN
4	W	361	GLU
4	W	368	SER
4	X	33	SER
4	X	34	ILE
4	X	37	ARG
4	X	66	THR
4	X	72	GLU
4	X	80	ASP
4	X	100	GLU
4	X	109	PRO
4	X	116	ARG
4	X	145	SER
4	X	153	LEU
4	X	159	VAL
4	X	180	LEU
4	X	191	LYS
4	X	196	ARG
4	X	199	SER
4	X	201	VAL
4	X	206	ARG
4	X	221	LEU
4	X	223	PHE
4	X	229	THR
4	X	239	SER
4	X	242	LEU
4	X	246	GLN
4	X	263	GLN
4	X	281	SER
4	X	283	MET
4	X	287	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	X	291	LYS
4	X	293	LEU
4	X	297	ASN
4	X	299	MET
4	X	312	ARG
4	X	315	LYS
4	X	318	THR
4	X	320	LEU
4	X	327	ILE
4	X	334	GLU
4	X	349	LEU
4	X	350	SER
4	X	351	THR
4	X	354	GLN
4	X	359	LYS
4	X	360	GLN
4	X	361	GLU
4	X	368	SER
4	Y	16	LEU
4	Y	33	SER
4	Y	34	ILE
4	Y	37	ARG
4	Y	66	THR
4	Y	72	GLU
4	Y	80	ASP
4	Y	100	GLU
4	Y	109	PRO
4	Y	116	ARG
4	Y	145	SER
4	Y	153	LEU
4	Y	159	VAL
4	Y	180	LEU
4	Y	191	LYS
4	Y	196	ARG
4	Y	199	SER
4	Y	201	VAL
4	Y	206	ARG
4	Y	221	LEU
4	Y	223	PHE
4	Y	229	THR
4	Y	239	SER
4	Y	242	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	Y	246	GLN
4	Y	263	GLN
4	Y	281	SER
4	Y	283	MET
4	Y	287	ILE
4	Y	291	LYS
4	Y	293	LEU
4	Y	297	ASN
4	Y	299	MET
4	Y	312	ARG
4	Y	315	LYS
4	Y	318	THR
4	Y	320	LEU
4	Y	327	ILE
4	Y	334	GLU
4	Y	349	LEU
4	Y	350	SER
4	Y	351	THR
4	Y	354	GLN
4	Y	359	LYS
4	Y	360	GLN
4	Y	361	GLU
4	Y	368	SER
4	Z	16	LEU
4	Z	33	SER
4	Z	34	ILE
4	Z	37	ARG
4	Z	66	THR
4	Z	72	GLU
4	Z	80	ASP
4	Z	100	GLU
4	Z	109	PRO
4	Z	116	ARG
4	Z	145	SER
4	Z	153	LEU
4	Z	159	VAL
4	Z	180	LEU
4	Z	191	LYS
4	Z	196	ARG
4	Z	199	SER
4	Z	201	VAL
4	Z	206	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	Z	221	LEU
4	Z	223	PHE
4	Z	229	THR
4	Z	239	SER
4	Z	242	LEU
4	Z	246	GLN
4	Z	263	GLN
4	Z	281	SER
4	Z	283	MET
4	Z	287	ILE
4	Z	291	LYS
4	Z	293	LEU
4	Z	297	ASN
4	Z	299	MET
4	Z	312	ARG
4	Z	315	LYS
4	Z	318	THR
4	Z	320	LEU
4	Z	327	ILE
4	Z	334	GLU
4	Z	349	LEU
4	Z	350	SER
4	Z	351	THR
4	Z	354	GLN
4	Z	359	LYS
4	Z	360	GLN
4	Z	361	GLU
4	Z	368	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (184) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	127	ASN
1	A	149	GLN
1	A	164	GLN
1	A	188	ASN
1	A	194	GLN
1	A	221	GLN
1	A	253	HIS
1	A	290	GLN
1	A	368	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	424	ASN
1	A	453	GLN
1	A	481	ASN
1	A	484	ASN
1	A	563	ASN
1	A	564	ASN
1	A	578	HIS
1	A	612	GLN
1	A	656	ASN
1	A	670	HIS
1	A	762	HIS
2	B	159	HIS
3	C	52	ASN
1	D	29	ASN
1	D	127	ASN
1	D	149	GLN
1	D	164	GLN
1	D	188	ASN
1	D	194	GLN
1	D	221	GLN
1	D	253	HIS
1	D	290	GLN
1	D	368	GLN
1	D	424	ASN
1	D	447	GLN
1	D	453	GLN
1	D	481	ASN
1	D	484	ASN
1	D	563	ASN
1	D	564	ASN
1	D	578	HIS
1	D	612	GLN
1	D	656	ASN
1	D	670	HIS
1	D	698	ASN
1	D	757	GLN
1	D	762	HIS
1	D	817	GLN
2	E	159	HIS
3	F	39	GLN
3	F	52	ASN
3	F	81	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	29	ASN
1	G	127	ASN
1	G	164	GLN
1	G	188	ASN
1	G	194	GLN
1	G	221	GLN
1	G	253	HIS
1	G	290	GLN
1	G	368	GLN
1	G	424	ASN
1	G	447	GLN
1	G	453	GLN
1	G	481	ASN
1	G	484	ASN
1	G	563	ASN
1	G	564	ASN
1	G	578	HIS
1	G	612	GLN
1	G	656	ASN
1	G	670	HIS
1	G	728	ASN
1	G	762	HIS
3	I	39	GLN
3	I	40	ASN
3	I	52	ASN
3	I	81	GLN
3	I	109	HIS
1	J	29	ASN
1	J	127	ASN
1	J	164	GLN
1	J	188	ASN
1	J	194	GLN
1	J	221	GLN
1	J	253	HIS
1	J	290	GLN
1	J	368	GLN
1	J	424	ASN
1	J	447	GLN
1	J	453	GLN
1	J	481	ASN
1	J	484	ASN
1	J	563	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	564	ASN
1	J	578	HIS
1	J	612	GLN
1	J	656	ASN
1	J	670	HIS
1	J	698	ASN
1	J	762	HIS
2	K	159	HIS
3	L	39	GLN
3	L	52	ASN
4	0	41	GLN
4	0	92	ASN
4	0	137	GLN
4	0	252	ASN
4	0	263	GLN
4	0	354	GLN
4	1	41	GLN
4	1	92	ASN
4	1	137	GLN
4	1	252	ASN
4	1	263	GLN
4	1	354	GLN
4	2	41	GLN
4	2	92	ASN
4	2	137	GLN
4	2	252	ASN
4	2	263	GLN
4	2	354	GLN
4	3	41	GLN
4	3	92	ASN
4	3	137	GLN
4	3	252	ASN
4	3	263	GLN
4	3	354	GLN
4	4	41	GLN
4	4	92	ASN
4	4	137	GLN
4	4	252	ASN
4	4	263	GLN
4	5	41	GLN
4	5	92	ASN
4	5	137	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	5	252	ASN
4	5	263	GLN
4	6	41	GLN
4	6	92	ASN
4	6	137	GLN
4	6	252	ASN
4	6	263	GLN
4	7	41	GLN
4	7	92	ASN
4	7	137	GLN
4	7	252	ASN
4	7	263	GLN
4	8	41	GLN
4	8	92	ASN
4	8	137	GLN
4	8	252	ASN
4	8	263	GLN
4	8	354	GLN
4	V	41	GLN
4	V	92	ASN
4	V	137	GLN
4	V	252	ASN
4	V	263	GLN
4	V	354	GLN
4	W	41	GLN
4	W	92	ASN
4	W	137	GLN
4	W	252	ASN
4	W	263	GLN
4	W	354	GLN
4	X	41	GLN
4	X	92	ASN
4	X	137	GLN
4	X	252	ASN
4	X	263	GLN
4	X	354	GLN
4	Y	41	GLN
4	Y	92	ASN
4	Y	137	GLN
4	Y	252	ASN
4	Y	263	GLN
4	Y	354	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	Z	41	GLN
4	Z	92	ASN
4	Z	137	GLN
4	Z	252	ASN
4	Z	263	GLN
4	Z	354	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

180 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	MLY	A	551	1	9,10,11	0.51	0	6,11,13	0.19	0
1	MLY	D	505	1	9,10,11	0.85	1 (11%)	6,11,13	0.35	0
1	MLY	A	613	1	9,10,11	0.57	0	6,11,13	0.63	0
1	MLY	A	367	1	9,10,11	0.63	0	6,11,13	0.37	0
1	MLY	A	681	1	9,10,11	0.60	0	6,11,13	0.46	0
1	MLY	A	49	1	9,10,11	1.07	1 (11%)	6,11,13	0.75	0
1	MLY	D	551	1	9,10,11	0.53	0	6,11,13	0.20	0
1	MLY	G	782	1	9,10,11	0.76	0	6,11,13	0.35	0
1	MLY	A	369	1	9,10,11	0.71	0	6,11,13	0.45	0
1	MLY	D	837	1	9,10,11	0.61	0	6,11,13	0.56	0
1	MLY	A	782	1	9,10,11	0.78	0	6,11,13	0.35	0
1	MLY	A	35	1	9,10,11	0.71	0	6,11,13	0.38	0
1	MLY	D	84	1	9,10,11	0.51	0	6,11,13	0.80	0
1	MLY	D	369	1	9,10,11	0.70	0	6,11,13	0.44	0
1	MLY	G	553	1,4	9,10,11	0.67	0	6,11,13	0.55	0
1	MLY	J	782	1	9,10,11	0.79	0	6,11,13	0.36	0
1	MLY	J	296	1	9,10,11	0.67	0	6,11,13	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	G	30	1	9,10,11	0.89	0	6,11,13	0.30	0
1	MLY	J	107	1	9,10,11	0.47	0	6,11,13	0.34	0
1	MLY	D	659	1	9,10,11	0.83	0	6,11,13	0.60	0
1	MLY	D	598	1	9,10,11	0.93	1 (11%)	6,11,13	0.44	0
1	MLY	G	837	1	9,10,11	0.59	0	6,11,13	0.53	0
1	MLY	G	436	1	9,10,11	1.06	1 (11%)	6,11,13	0.48	0
1	MLY	D	272	1	9,10,11	0.99	1 (11%)	6,11,13	0.57	0
1	MLY	A	63	1	9,10,11	0.91	0	6,11,13	0.43	0
1	MLY	J	553	1,4	9,10,11	0.67	0	6,11,13	0.53	0
1	MLY	A	59	1	9,10,11	0.87	0	6,11,13	0.50	0
1	MLY	D	138	1	9,10,11	1.39	1 (11%)	6,11,13	0.85	0
1	MLY	A	236	1	9,10,11	0.80	1 (11%)	6,11,13	0.49	0
1	MLY	D	681	1	9,10,11	0.57	0	6,11,13	0.45	0
1	MLY	D	63	1	9,10,11	0.90	0	6,11,13	0.45	0
1	MLY	D	87	1	9,10,11	1.16	1 (11%)	6,11,13	0.44	0
1	MLY	D	833	1	9,10,11	1.14	2 (22%)	6,11,13	0.31	0
1	MLY	G	598	1	9,10,11	0.87	1 (11%)	6,11,13	0.42	0
1	MLY	J	431	1	9,10,11	0.53	0	6,11,13	0.44	0
1	MLY	J	59	1	9,10,11	0.88	0	6,11,13	0.49	0
1	MLY	G	19	1	9,10,11	1.15	1 (11%)	6,11,13	0.59	0
1	MLY	J	598	1	9,10,11	0.90	1 (11%)	6,11,13	0.43	0
1	MLY	G	138	1	9,10,11	1.31	1 (11%)	6,11,13	0.84	0
1	MLY	A	19	1	9,10,11	1.12	1 (11%)	6,11,13	0.57	0
1	MLY	J	295	1	9,10,11	0.78	0	6,11,13	0.35	0
1	MLY	D	486	1	9,10,11	0.66	0	6,11,13	0.39	0
1	MLY	J	764	1	9,10,11	0.84	0	6,11,13	0.38	0
1	MLY	D	415	1	9,10,11	0.77	0	6,11,13	0.19	0
1	MLY	G	505	1	9,10,11	0.87	1 (11%)	6,11,13	0.35	0
1	MLY	D	528	1	9,10,11	0.91	0	6,11,13	0.65	0
1	MLY	A	87	1	9,10,11	1.20	1 (11%)	6,11,13	0.43	0
1	MLY	A	348	1	9,10,11	0.85	0	6,11,13	0.48	0
1	MLY	G	504	1	9,10,11	0.88	0	6,11,13	0.23	0
1	MLY	J	190	1	9,10,11	1.25	1 (11%)	6,11,13	0.52	0
1	MLY	G	764	1	9,10,11	0.82	0	6,11,13	0.36	0
1	MLY	D	367	1	9,10,11	0.61	0	6,11,13	0.38	0
1	MLY	J	659	1	9,10,11	0.80	0	6,11,13	0.57	0
1	MLY	A	839	1,2	9,10,11	0.70	0	6,11,13	0.80	0
1	MLY	G	49	1	9,10,11	1.08	1 (11%)	6,11,13	0.75	0
1	MLY	J	236	1	9,10,11	0.79	1 (11%)	6,11,13	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	D	107	1	9,10,11	0.51	0	6,11,13	0.34	0
1	MLY	G	369	1	9,10,11	0.70	0	6,11,13	0.46	0
1	MLY	G	385	1	9,10,11	1.00	1 (11%)	6,11,13	0.43	0
1	MLY	D	385	1	9,10,11	0.99	1 (11%)	6,11,13	0.44	0
1	MLY	J	528	1	9,10,11	0.88	0	6,11,13	0.66	0
1	MLY	A	296	1	9,10,11	0.60	0	6,11,13	0.36	0
1	MLY	G	35	1	9,10,11	0.72	0	6,11,13	0.39	0
1	MLY	J	504	1	9,10,11	0.86	0	6,11,13	0.23	0
1	MLY	A	827	1	9,10,11	0.71	0	6,11,13	0.46	0
1	MLY	A	504	1	9,10,11	0.90	0	6,11,13	0.25	0
1	MLY	A	505	1	9,10,11	0.89	1 (11%)	6,11,13	0.34	0
1	MLY	G	659	1	9,10,11	0.84	0	6,11,13	0.59	0
1	MLY	J	49	1	9,10,11	1.08	1 (11%)	6,11,13	0.75	0
1	MLY	A	353	1	9,10,11	0.86	0	6,11,13	0.78	0
1	MLY	J	385	1	9,10,11	1.01	1 (11%)	6,11,13	0.44	0
1	MLY	J	35	1	9,10,11	0.72	0	6,11,13	0.39	0
1	MLY	D	353	1	9,10,11	0.84	0	6,11,13	0.79	0
1	MLY	A	553	1,4	9,10,11	0.68	0	6,11,13	0.54	0
1	MLY	D	553	1,4	9,10,11	0.68	0	6,11,13	0.56	0
1	MLY	J	30	1	9,10,11	0.89	0	6,11,13	0.32	0
1	MLY	A	415	1	9,10,11	0.76	0	6,11,13	0.19	0
1	MLY	D	236	1	9,10,11	0.79	1 (11%)	6,11,13	0.47	0
1	MLY	G	272	1	9,10,11	0.99	1 (11%)	6,11,13	0.55	0
1	MLY	A	431	1	9,10,11	0.53	0	6,11,13	0.45	0
1	MLY	A	436	1	9,10,11	1.04	1 (11%)	6,11,13	0.50	0
1	MLY	A	130	1	9,10,11	0.81	0	6,11,13	0.75	0
1	MLY	G	827	1	9,10,11	0.69	0	6,11,13	0.49	0
1	MLY	D	431	1	9,10,11	0.52	0	6,11,13	0.46	0
1	MLY	A	768	1	9,10,11	0.75	0	6,11,13	0.40	0
1	MLY	D	35	1	9,10,11	0.74	0	6,11,13	0.37	0
1	MLY	G	63	1	9,10,11	0.92	1 (11%)	6,11,13	0.43	0
1	MLY	G	617	1	9,10,11	0.95	1 (11%)	6,11,13	0.34	0
1	MLY	J	369	1	9,10,11	0.70	0	6,11,13	0.45	0
1	MLY	G	59	1	9,10,11	0.85	0	6,11,13	0.49	0
1	MLY	J	681	1	9,10,11	0.59	0	6,11,13	0.46	0
1	MLY	J	600	1	9,10,11	0.53	0	6,11,13	0.36	0
1	MLY	D	295	1	9,10,11	0.79	0	6,11,13	0.35	0
1	MLY	J	617	1	9,10,11	0.96	1 (11%)	6,11,13	0.33	0
1	MLY	D	613	1	9,10,11	0.56	0	6,11,13	0.64	0
1	MLY	G	681	1	9,10,11	0.64	0	6,11,13	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	D	49	1	9,10,11	1.08	1 (11%)	6,11,13	0.73	0
1	MLY	G	600	1	9,10,11	0.51	0	6,11,13	0.37	0
1	MLY	J	138	1	9,10,11	1.34	1 (11%)	6,11,13	0.83	0
1	MLY	J	827	1	9,10,11	0.74	0	6,11,13	0.48	0
1	MLY	G	296	1	9,10,11	0.64	0	6,11,13	0.37	0
1	MLY	J	87	1	9,10,11	1.23	1 (11%)	6,11,13	0.43	0
1	MLY	A	486	1	9,10,11	0.65	0	6,11,13	0.39	0
1	MLY	D	436	1	9,10,11	1.12	1 (11%)	6,11,13	0.49	0
1	MLY	J	367	1	9,10,11	0.62	0	6,11,13	0.37	0
1	MLY	A	659	1	9,10,11	0.83	0	6,11,13	0.60	0
1	MLY	A	764	1	9,10,11	0.86	0	6,11,13	0.36	0
1	MLY	A	600	1	9,10,11	0.51	0	6,11,13	0.38	0
1	MLY	G	295	1	9,10,11	0.81	0	6,11,13	0.33	0
1	MLY	J	63	1	9,10,11	0.90	0	6,11,13	0.43	0
1	MLY	G	367	1	9,10,11	0.66	0	6,11,13	0.38	0
1	MLY	G	768	1	9,10,11	0.74	0	6,11,13	0.42	0
1	MLY	A	295	1	9,10,11	0.84	0	6,11,13	0.33	0
1	MLY	D	839	1	9,10,11	0.70	0	6,11,13	0.79	0
1	MLY	J	833	1	9,10,11	1.19	1 (11%)	6,11,13	0.31	0
1	MLY	D	248	1	9,10,11	0.83	0	6,11,13	0.62	0
1	MLY	D	600	1	9,10,11	0.50	0	6,11,13	0.38	0
1	MLY	G	107	1	9,10,11	0.47	0	6,11,13	0.34	0
1	MLY	D	296	1	9,10,11	0.64	0	6,11,13	0.37	0
1	MLY	A	248	1	9,10,11	0.84	0	6,11,13	0.60	0
1	MLY	G	833	1	9,10,11	1.17	2 (22%)	6,11,13	0.33	0
1	MLY	J	272	1	9,10,11	1.02	1 (11%)	6,11,13	0.55	0
1	MLY	A	55	1	9,10,11	0.71	0	6,11,13	0.78	0
1	MLY	J	415	1	9,10,11	0.79	0	6,11,13	0.19	0
1	MLY	J	19	1	9,10,11	1.18	1 (11%)	6,11,13	0.57	0
1	MLY	D	348	1	9,10,11	0.81	0	6,11,13	0.47	0
1	MLY	J	436	1	9,10,11	1.06	1 (11%)	6,11,13	0.49	0
1	MLY	D	55	1	9,10,11	0.72	0	6,11,13	0.79	0
1	MLY	G	55	1	9,10,11	0.74	0	6,11,13	0.79	0
1	MLY	G	415	1	9,10,11	0.75	0	6,11,13	0.19	0
1	MLY	J	248	1	9,10,11	0.82	0	6,11,13	0.62	0
1	MLY	J	348	1	9,10,11	0.82	0	6,11,13	0.47	0
1	MLY	G	839	1	9,10,11	0.70	0	6,11,13	0.80	0
1	MLY	J	353	1	9,10,11	0.84	0	6,11,13	0.79	0
1	MLY	D	30	1	9,10,11	0.91	0	6,11,13	0.32	0
1	MLY	G	348	1	9,10,11	0.86	1 (11%)	6,11,13	0.48	0
1	MLY	A	837	1	9,10,11	0.61	0	6,11,13	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	G	353	1	9,10,11	0.86	0	6,11,13	0.80	0
1	MLY	A	84	1	9,10,11	0.48	0	6,11,13	0.79	0
1	MLY	A	107	1	9,10,11	0.45	0	6,11,13	0.34	0
1	MLY	J	837	1	9,10,11	0.58	0	6,11,13	0.55	0
1	MLY	G	613	1	9,10,11	0.59	0	6,11,13	0.64	0
1	MLY	D	764	1	9,10,11	0.84	0	6,11,13	0.35	0
1	MLY	D	59	1	9,10,11	0.87	0	6,11,13	0.49	0
1	MLY	D	130	1	9,10,11	0.80	0	6,11,13	0.74	0
1	MLY	J	55	1	9,10,11	0.72	0	6,11,13	0.78	0
1	MLY	A	598	1	9,10,11	0.91	1 (11%)	6,11,13	0.44	0
1	MLY	D	768	1	9,10,11	0.74	0	6,11,13	0.41	0
1	MLY	J	839	1	9,10,11	0.71	0	6,11,13	0.76	0
1	MLY	G	486	1	9,10,11	0.64	0	6,11,13	0.38	0
1	MLY	A	138	1	9,10,11	1.32	1 (11%)	6,11,13	0.84	0
1	MLY	J	768	1	9,10,11	0.77	0	6,11,13	0.42	0
1	MLY	G	431	1	9,10,11	0.54	0	6,11,13	0.46	0
1	MLY	G	87	1	9,10,11	1.21	1 (11%)	6,11,13	0.43	0
1	MLY	G	130	1	9,10,11	0.79	0	6,11,13	0.75	0
1	MLY	A	833	1	9,10,11	1.15	1 (11%)	6,11,13	0.32	0
1	MLY	G	248	1	9,10,11	0.81	0	6,11,13	0.63	0
1	MLY	J	130	1	9,10,11	0.78	0	6,11,13	0.75	0
1	MLY	G	190	1	9,10,11	1.26	1 (11%)	6,11,13	0.52	0
1	MLY	J	84	1	9,10,11	0.49	0	6,11,13	0.80	0
1	MLY	D	504	1	9,10,11	0.88	0	6,11,13	0.22	0
1	MLY	G	84	1	9,10,11	0.49	0	6,11,13	0.80	0
1	MLY	J	486	1	9,10,11	0.63	0	6,11,13	0.39	0
1	MLY	A	190	1	9,10,11	1.26	1 (11%)	6,11,13	0.51	0
1	MLY	A	385	1	9,10,11	1.00	1 (11%)	6,11,13	0.43	0
1	MLY	A	528	1	9,10,11	0.89	0	6,11,13	0.66	0
1	MLY	J	505	1	9,10,11	0.92	1 (11%)	6,11,13	0.34	0
1	MLY	A	30	1	9,10,11	0.89	0	6,11,13	0.32	0
1	MLY	A	617	1	9,10,11	0.94	1 (11%)	6,11,13	0.34	0
1	MLY	G	236	1	9,10,11	0.78	1 (11%)	6,11,13	0.47	0
1	MLY	A	272	1	9,10,11	1.01	1 (11%)	6,11,13	0.56	0
1	MLY	J	551	1	9,10,11	0.52	0	6,11,13	0.18	0
1	MLY	D	190	1	9,10,11	1.22	1 (11%)	6,11,13	0.54	0
1	MLY	D	617	1	9,10,11	0.97	1 (11%)	6,11,13	0.34	0
1	MLY	G	551	1	9,10,11	0.52	0	6,11,13	0.20	0
1	MLY	D	19	1	9,10,11	1.20	1 (11%)	6,11,13	0.57	0
1	MLY	G	528	1	9,10,11	0.89	0	6,11,13	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	D	782	1	9,10,11	0.79	0	6,11,13	0.34	0
1	MLY	J	613	1	9,10,11	0.56	0	6,11,13	0.64	0
1	MLY	D	827	1	9,10,11	0.69	0	6,11,13	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	551	1	-	3/8/9/11	-
1	MLY	D	505	1	-	5/8/9/11	-
1	MLY	A	613	1	-	4/8/9/11	-
1	MLY	A	367	1	-	2/8/9/11	-
1	MLY	A	681	1	-	4/8/9/11	-
1	MLY	A	49	1	-	3/8/9/11	-
1	MLY	D	551	1	-	3/8/9/11	-
1	MLY	G	782	1	-	6/8/9/11	-
1	MLY	A	369	1	-	2/8/9/11	-
1	MLY	D	837	1	-	5/8/9/11	-
1	MLY	A	782	1	-	6/8/9/11	-
1	MLY	A	35	1	-	3/8/9/11	-
1	MLY	D	84	1	-	4/8/9/11	-
1	MLY	D	369	1	-	2/8/9/11	-
1	MLY	G	553	1,4	-	4/8/9/11	-
1	MLY	J	782	1	-	6/8/9/11	-
1	MLY	J	296	1	-	4/8/9/11	-
1	MLY	G	30	1	-	2/8/9/11	-
1	MLY	J	107	1	-	2/8/9/11	-
1	MLY	D	659	1	-	3/8/9/11	-
1	MLY	D	598	1	-	5/8/9/11	-
1	MLY	G	837	1	-	5/8/9/11	-
1	MLY	G	436	1	-	4/8/9/11	-
1	MLY	D	272	1	-	3/8/9/11	-
1	MLY	A	63	1	-	4/8/9/11	-
1	MLY	J	553	1,4	-	4/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	59	1	-	3/8/9/11	-
1	MLY	D	138	1	-	4/8/9/11	-
1	MLY	A	236	1	-	3/8/9/11	-
1	MLY	D	681	1	-	4/8/9/11	-
1	MLY	D	63	1	-	4/8/9/11	-
1	MLY	D	87	1	-	2/8/9/11	-
1	MLY	D	833	1	-	6/8/9/11	-
1	MLY	G	598	1	-	5/8/9/11	-
1	MLY	J	431	1	-	4/8/9/11	-
1	MLY	J	59	1	-	3/8/9/11	-
1	MLY	G	19	1	-	4/8/9/11	-
1	MLY	J	598	1	-	5/8/9/11	-
1	MLY	G	138	1	-	4/8/9/11	-
1	MLY	A	19	1	-	4/8/9/11	-
1	MLY	J	295	1	-	2/8/9/11	-
1	MLY	D	486	1	-	2/8/9/11	-
1	MLY	J	764	1	-	2/8/9/11	-
1	MLY	D	415	1	-	3/8/9/11	-
1	MLY	G	505	1	-	5/8/9/11	-
1	MLY	D	528	1	-	4/8/9/11	-
1	MLY	A	87	1	-	2/8/9/11	-
1	MLY	A	348	1	-	5/8/9/11	-
1	MLY	G	504	1	-	4/8/9/11	-
1	MLY	J	190	1	-	5/8/9/11	-
1	MLY	G	764	1	-	2/8/9/11	-
1	MLY	D	367	1	-	2/8/9/11	-
1	MLY	J	659	1	-	3/8/9/11	-
1	MLY	A	839	1,2	-	3/8/9/11	-
1	MLY	G	49	1	-	3/8/9/11	-
1	MLY	J	236	1	-	3/8/9/11	-
1	MLY	D	107	1	-	2/8/9/11	-
1	MLY	G	369	1	-	2/8/9/11	-
1	MLY	G	385	1	-	2/8/9/11	-
1	MLY	D	385	1	-	2/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	528	1	-	4/8/9/11	-
1	MLY	A	296	1	-	4/8/9/11	-
1	MLY	G	35	1	-	3/8/9/11	-
1	MLY	J	504	1	-	4/8/9/11	-
1	MLY	A	827	1	-	0/8/9/11	-
1	MLY	A	504	1	-	4/8/9/11	-
1	MLY	A	505	1	-	5/8/9/11	-
1	MLY	G	659	1	-	3/8/9/11	-
1	MLY	J	49	1	-	3/8/9/11	-
1	MLY	A	353	1	-	4/8/9/11	-
1	MLY	J	385	1	-	2/8/9/11	-
1	MLY	J	35	1	-	3/8/9/11	-
1	MLY	D	353	1	-	4/8/9/11	-
1	MLY	A	553	1,4	-	4/8/9/11	-
1	MLY	D	553	1,4	-	4/8/9/11	-
1	MLY	J	30	1	-	2/8/9/11	-
1	MLY	A	415	1	-	3/8/9/11	-
1	MLY	D	236	1	-	3/8/9/11	-
1	MLY	G	272	1	-	3/8/9/11	-
1	MLY	A	431	1	-	4/8/9/11	-
1	MLY	A	436	1	-	4/8/9/11	-
1	MLY	A	130	1	-	5/8/9/11	-
1	MLY	G	827	1	-	0/8/9/11	-
1	MLY	D	431	1	-	4/8/9/11	-
1	MLY	A	768	1	-	4/8/9/11	-
1	MLY	D	35	1	-	3/8/9/11	-
1	MLY	G	63	1	-	4/8/9/11	-
1	MLY	G	617	1	-	1/8/9/11	-
1	MLY	J	369	1	-	2/8/9/11	-
1	MLY	G	59	1	-	3/8/9/11	-
1	MLY	J	681	1	-	4/8/9/11	-
1	MLY	J	600	1	-	3/8/9/11	-
1	MLY	D	295	1	-	2/8/9/11	-
1	MLY	J	617	1	-	1/8/9/11	-
1	MLY	D	613	1	-	4/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	G	681	1	-	4/8/9/11	-
1	MLY	D	49	1	-	3/8/9/11	-
1	MLY	G	600	1	-	3/8/9/11	-
1	MLY	J	138	1	-	4/8/9/11	-
1	MLY	J	827	1	-	0/8/9/11	-
1	MLY	G	296	1	-	4/8/9/11	-
1	MLY	J	87	1	-	2/8/9/11	-
1	MLY	A	486	1	-	2/8/9/11	-
1	MLY	D	436	1	-	4/8/9/11	-
1	MLY	J	367	1	-	2/8/9/11	-
1	MLY	A	659	1	-	3/8/9/11	-
1	MLY	A	764	1	-	2/8/9/11	-
1	MLY	A	600	1	-	3/8/9/11	-
1	MLY	G	295	1	-	2/8/9/11	-
1	MLY	J	63	1	-	4/8/9/11	-
1	MLY	G	367	1	-	2/8/9/11	-
1	MLY	G	768	1	-	4/8/9/11	-
1	MLY	A	295	1	-	2/8/9/11	-
1	MLY	D	839	1	-	3/8/9/11	-
1	MLY	J	833	1	-	6/8/9/11	-
1	MLY	D	248	1	-	6/8/9/11	-
1	MLY	D	600	1	-	3/8/9/11	-
1	MLY	G	107	1	-	2/8/9/11	-
1	MLY	D	296	1	-	4/8/9/11	-
1	MLY	A	248	1	-	6/8/9/11	-
1	MLY	G	833	1	-	6/8/9/11	-
1	MLY	J	272	1	-	3/8/9/11	-
1	MLY	A	55	1	-	6/8/9/11	-
1	MLY	J	415	1	-	3/8/9/11	-
1	MLY	J	19	1	-	4/8/9/11	-
1	MLY	D	348	1	-	5/8/9/11	-
1	MLY	J	436	1	-	4/8/9/11	-
1	MLY	D	55	1	-	6/8/9/11	-
1	MLY	G	55	1	-	6/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	G	415	1	-	3/8/9/11	-
1	MLY	J	248	1	-	6/8/9/11	-
1	MLY	J	348	1	-	5/8/9/11	-
1	MLY	G	839	1	-	3/8/9/11	-
1	MLY	J	353	1	-	4/8/9/11	-
1	MLY	D	30	1	-	2/8/9/11	-
1	MLY	G	348	1	-	5/8/9/11	-
1	MLY	A	837	1	-	5/8/9/11	-
1	MLY	G	353	1	-	4/8/9/11	-
1	MLY	A	84	1	-	4/8/9/11	-
1	MLY	A	107	1	-	2/8/9/11	-
1	MLY	J	837	1	-	5/8/9/11	-
1	MLY	G	613	1	-	4/8/9/11	-
1	MLY	D	764	1	-	2/8/9/11	-
1	MLY	D	59	1	-	3/8/9/11	-
1	MLY	D	130	1	-	5/8/9/11	-
1	MLY	J	55	1	-	6/8/9/11	-
1	MLY	A	598	1	-	5/8/9/11	-
1	MLY	D	768	1	-	4/8/9/11	-
1	MLY	J	839	1	-	3/8/9/11	-
1	MLY	G	486	1	-	2/8/9/11	-
1	MLY	A	138	1	-	4/8/9/11	-
1	MLY	J	768	1	-	4/8/9/11	-
1	MLY	G	431	1	-	4/8/9/11	-
1	MLY	G	87	1	-	2/8/9/11	-
1	MLY	G	130	1	-	5/8/9/11	-
1	MLY	A	833	1	-	6/8/9/11	-
1	MLY	G	248	1	-	6/8/9/11	-
1	MLY	J	130	1	-	5/8/9/11	-
1	MLY	G	190	1	-	5/8/9/11	-
1	MLY	J	84	1	-	4/8/9/11	-
1	MLY	D	504	1	-	4/8/9/11	-
1	MLY	G	84	1	-	4/8/9/11	-
1	MLY	J	486	1	-	2/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	190	1	-	5/8/9/11	-
1	MLY	A	385	1	-	2/8/9/11	-
1	MLY	A	528	1	-	5/8/9/11	-
1	MLY	J	505	1	-	5/8/9/11	-
1	MLY	A	30	1	-	2/8/9/11	-
1	MLY	A	617	1	-	1/8/9/11	-
1	MLY	G	236	1	-	3/8/9/11	-
1	MLY	A	272	1	-	3/8/9/11	-
1	MLY	J	551	1	-	3/8/9/11	-
1	MLY	D	190	1	-	5/8/9/11	-
1	MLY	D	617	1	-	1/8/9/11	-
1	MLY	G	551	1	-	3/8/9/11	-
1	MLY	D	19	1	-	4/8/9/11	-
1	MLY	G	528	1	-	4/8/9/11	-
1	MLY	D	782	1	-	6/8/9/11	-
1	MLY	J	613	1	-	4/8/9/11	-
1	MLY	D	827	1	-	0/8/9/11	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	MLY	CB-CA	-3.80	1.48	1.53
1	J	138	MLY	CB-CA	-3.66	1.48	1.53
1	A	138	MLY	CB-CA	-3.60	1.48	1.53
1	G	138	MLY	CB-CA	-3.55	1.48	1.53
1	D	19	MLY	CB-CA	-3.23	1.49	1.53
1	J	19	MLY	CB-CA	-3.15	1.49	1.53
1	G	87	MLY	CB-CA	-3.14	1.49	1.53
1	J	87	MLY	CB-CA	-3.13	1.49	1.53
1	D	436	MLY	CB-CA	-3.09	1.49	1.53
1	G	19	MLY	CB-CA	-3.06	1.49	1.53
1	A	87	MLY	CB-CA	-3.06	1.49	1.53
1	A	19	MLY	CB-CA	-2.98	1.49	1.53
1	D	87	MLY	CB-CA	-2.98	1.49	1.53
1	G	436	MLY	CB-CA	-2.92	1.49	1.53
1	J	436	MLY	CB-CA	-2.90	1.49	1.53
1	A	436	MLY	CB-CA	-2.85	1.49	1.53
1	D	49	MLY	CB-CA	-2.83	1.49	1.53
1	J	49	MLY	CB-CA	-2.82	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	272	MLY	CB-CA	-2.82	1.49	1.53
1	G	49	MLY	CB-CA	-2.81	1.49	1.53
1	A	49	MLY	CB-CA	-2.78	1.49	1.53
1	A	272	MLY	CB-CA	-2.77	1.49	1.53
1	G	272	MLY	CB-CA	-2.70	1.50	1.53
1	D	272	MLY	CB-CA	-2.70	1.50	1.53
1	G	190	MLY	CB-CA	-2.59	1.50	1.53
1	J	190	MLY	CB-CA	-2.56	1.50	1.53
1	A	190	MLY	CB-CA	-2.55	1.50	1.53
1	J	833	MLY	CB-CA	-2.50	1.50	1.53
1	J	385	MLY	CB-CA	-2.48	1.50	1.53
1	D	190	MLY	CB-CA	-2.47	1.50	1.53
1	A	385	MLY	CB-CA	-2.45	1.50	1.53
1	G	385	MLY	CB-CA	-2.43	1.50	1.53
1	D	385	MLY	CB-CA	-2.38	1.50	1.53
1	D	598	MLY	CB-CA	-2.35	1.50	1.53
1	A	833	MLY	CB-CA	-2.30	1.50	1.53
1	J	505	MLY	CB-CA	-2.30	1.50	1.53
1	A	598	MLY	CB-CA	-2.28	1.50	1.53
1	D	617	MLY	CB-CA	-2.28	1.50	1.53
1	J	598	MLY	CB-CA	-2.25	1.50	1.53
1	G	833	MLY	CB-CA	-2.24	1.50	1.53
1	J	617	MLY	CB-CA	-2.24	1.50	1.53
1	A	505	MLY	CB-CA	-2.21	1.50	1.53
1	G	598	MLY	CB-CA	-2.18	1.50	1.53
1	D	833	MLY	CB-CA	-2.18	1.50	1.53
1	G	505	MLY	CB-CA	-2.17	1.50	1.53
1	A	617	MLY	CB-CA	-2.16	1.50	1.53
1	A	236	MLY	CA-N	-2.14	1.41	1.48
1	G	617	MLY	CB-CA	-2.14	1.50	1.53
1	D	236	MLY	CA-N	-2.13	1.41	1.48
1	J	236	MLY	CA-N	-2.10	1.41	1.48
1	G	236	MLY	CA-N	-2.09	1.41	1.48
1	D	505	MLY	CB-CA	-2.08	1.50	1.53
1	G	833	MLY	CA-N	-2.04	1.42	1.48
1	G	348	MLY	CB-CA	-2.04	1.50	1.53
1	G	63	MLY	CB-CA	-2.04	1.50	1.53
1	D	833	MLY	CA-N	-2.03	1.42	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (637) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	19	MLY	C-CA-CB-CG
1	A	49	MLY	N-CA-CB-CG
1	A	49	MLY	C-CA-CB-CG
1	A	55	MLY	N-CA-CB-CG
1	A	55	MLY	C-CA-CB-CG
1	A	84	MLY	C-CA-CB-CG
1	A	130	MLY	C-CA-CB-CG
1	A	248	MLY	N-CA-CB-CG
1	A	248	MLY	C-CA-CB-CG
1	A	348	MLY	N-CA-CB-CG
1	A	436	MLY	C-CA-CB-CG
1	A	486	MLY	C-CA-CB-CG
1	A	505	MLY	N-CA-CB-CG
1	A	505	MLY	C-CA-CB-CG
1	A	528	MLY	C-CA-CB-CG
1	A	551	MLY	C-CA-CB-CG
1	A	553	MLY	C-CA-CB-CG
1	A	598	MLY	N-CA-CB-CG
1	A	598	MLY	C-CA-CB-CG
1	A	613	MLY	N-CA-CB-CG
1	A	613	MLY	C-CA-CB-CG
1	A	681	MLY	C-CA-CB-CG
1	A	782	MLY	C-CA-CB-CG
1	A	782	MLY	O-C-CA-CB
1	D	19	MLY	C-CA-CB-CG
1	D	49	MLY	N-CA-CB-CG
1	D	49	MLY	C-CA-CB-CG
1	D	55	MLY	N-CA-CB-CG
1	D	55	MLY	C-CA-CB-CG
1	D	84	MLY	C-CA-CB-CG
1	D	130	MLY	C-CA-CB-CG
1	D	248	MLY	N-CA-CB-CG
1	D	248	MLY	C-CA-CB-CG
1	D	436	MLY	C-CA-CB-CG
1	D	486	MLY	C-CA-CB-CG
1	D	505	MLY	N-CA-CB-CG
1	D	505	MLY	C-CA-CB-CG
1	D	528	MLY	C-CA-CB-CG
1	D	551	MLY	C-CA-CB-CG
1	D	553	MLY	C-CA-CB-CG
1	D	598	MLY	N-CA-CB-CG
1	D	598	MLY	C-CA-CB-CG
1	D	613	MLY	N-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	D	613	MLY	C-CA-CB-CG
1	D	681	MLY	C-CA-CB-CG
1	D	782	MLY	C-CA-CB-CG
1	D	782	MLY	O-C-CA-CB
1	G	19	MLY	C-CA-CB-CG
1	G	49	MLY	N-CA-CB-CG
1	G	49	MLY	C-CA-CB-CG
1	G	55	MLY	N-CA-CB-CG
1	G	55	MLY	C-CA-CB-CG
1	G	84	MLY	C-CA-CB-CG
1	G	130	MLY	C-CA-CB-CG
1	G	248	MLY	N-CA-CB-CG
1	G	248	MLY	C-CA-CB-CG
1	G	348	MLY	N-CA-CB-CG
1	G	436	MLY	C-CA-CB-CG
1	G	486	MLY	C-CA-CB-CG
1	G	505	MLY	N-CA-CB-CG
1	G	505	MLY	C-CA-CB-CG
1	G	528	MLY	C-CA-CB-CG
1	G	551	MLY	C-CA-CB-CG
1	G	553	MLY	C-CA-CB-CG
1	G	598	MLY	N-CA-CB-CG
1	G	598	MLY	C-CA-CB-CG
1	G	613	MLY	N-CA-CB-CG
1	G	613	MLY	C-CA-CB-CG
1	G	681	MLY	C-CA-CB-CG
1	G	782	MLY	C-CA-CB-CG
1	G	782	MLY	O-C-CA-CB
1	J	19	MLY	C-CA-CB-CG
1	J	49	MLY	N-CA-CB-CG
1	J	49	MLY	C-CA-CB-CG
1	J	55	MLY	N-CA-CB-CG
1	J	55	MLY	C-CA-CB-CG
1	J	84	MLY	C-CA-CB-CG
1	J	130	MLY	C-CA-CB-CG
1	J	248	MLY	N-CA-CB-CG
1	J	248	MLY	C-CA-CB-CG
1	J	348	MLY	N-CA-CB-CG
1	J	436	MLY	C-CA-CB-CG
1	J	486	MLY	C-CA-CB-CG
1	J	505	MLY	N-CA-CB-CG
1	J	505	MLY	C-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	J	528	MLY	C-CA-CB-CG
1	J	551	MLY	C-CA-CB-CG
1	J	553	MLY	C-CA-CB-CG
1	J	598	MLY	N-CA-CB-CG
1	J	598	MLY	C-CA-CB-CG
1	J	613	MLY	N-CA-CB-CG
1	J	613	MLY	C-CA-CB-CG
1	J	681	MLY	C-CA-CB-CG
1	J	782	MLY	C-CA-CB-CG
1	J	782	MLY	O-C-CA-CB
1	A	84	MLY	CD-CE-NZ-CH1
1	D	84	MLY	CD-CE-NZ-CH1
1	G	84	MLY	CD-CE-NZ-CH1
1	J	84	MLY	CD-CE-NZ-CH1
1	A	59	MLY	CD-CE-NZ-CH1
1	A	59	MLY	CD-CE-NZ-CH2
1	A	63	MLY	CD-CE-NZ-CH1
1	A	84	MLY	CD-CE-NZ-CH2
1	A	130	MLY	CD-CE-NZ-CH1
1	A	130	MLY	CD-CE-NZ-CH2
1	A	138	MLY	CD-CE-NZ-CH1
1	A	138	MLY	CD-CE-NZ-CH2
1	A	190	MLY	CD-CE-NZ-CH1
1	A	190	MLY	CD-CE-NZ-CH2
1	A	248	MLY	CD-CE-NZ-CH1
1	A	272	MLY	CD-CE-NZ-CH1
1	A	296	MLY	CD-CE-NZ-CH1
1	A	296	MLY	CD-CE-NZ-CH2
1	A	353	MLY	CD-CE-NZ-CH1
1	A	353	MLY	CD-CE-NZ-CH2
1	A	367	MLY	CD-CE-NZ-CH2
1	A	385	MLY	CD-CE-NZ-CH1
1	A	385	MLY	CD-CE-NZ-CH2
1	A	431	MLY	CD-CE-NZ-CH2
1	A	504	MLY	CD-CE-NZ-CH2
1	A	505	MLY	CD-CE-NZ-CH2
1	A	528	MLY	CD-CE-NZ-CH1
1	A	528	MLY	CD-CE-NZ-CH2
1	A	553	MLY	CD-CE-NZ-CH2
1	A	600	MLY	CD-CE-NZ-CH2
1	A	764	MLY	CD-CE-NZ-CH1
1	A	764	MLY	CD-CE-NZ-CH2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	768	MLY	CD-CE-NZ-CH1
1	A	782	MLY	CD-CE-NZ-CH1
1	A	782	MLY	CD-CE-NZ-CH2
1	A	833	MLY	CD-CE-NZ-CH1
1	A	833	MLY	CD-CE-NZ-CH2
1	A	837	MLY	CD-CE-NZ-CH1
1	A	837	MLY	CD-CE-NZ-CH2
1	A	839	MLY	CD-CE-NZ-CH2
1	D	55	MLY	CD-CE-NZ-CH2
1	D	59	MLY	CD-CE-NZ-CH1
1	D	59	MLY	CD-CE-NZ-CH2
1	D	63	MLY	CD-CE-NZ-CH1
1	D	84	MLY	CD-CE-NZ-CH2
1	D	130	MLY	CD-CE-NZ-CH1
1	D	130	MLY	CD-CE-NZ-CH2
1	D	138	MLY	CD-CE-NZ-CH1
1	D	138	MLY	CD-CE-NZ-CH2
1	D	190	MLY	CD-CE-NZ-CH2
1	D	248	MLY	CD-CE-NZ-CH1
1	D	272	MLY	CD-CE-NZ-CH1
1	D	296	MLY	CD-CE-NZ-CH1
1	D	296	MLY	CD-CE-NZ-CH2
1	D	353	MLY	CD-CE-NZ-CH1
1	D	353	MLY	CD-CE-NZ-CH2
1	D	367	MLY	CD-CE-NZ-CH2
1	D	385	MLY	CD-CE-NZ-CH1
1	D	385	MLY	CD-CE-NZ-CH2
1	D	431	MLY	CD-CE-NZ-CH2
1	D	505	MLY	CD-CE-NZ-CH2
1	D	528	MLY	CD-CE-NZ-CH1
1	D	528	MLY	CD-CE-NZ-CH2
1	D	553	MLY	CD-CE-NZ-CH2
1	D	600	MLY	CD-CE-NZ-CH2
1	D	764	MLY	CD-CE-NZ-CH1
1	D	764	MLY	CD-CE-NZ-CH2
1	D	768	MLY	CD-CE-NZ-CH1
1	D	782	MLY	CD-CE-NZ-CH1
1	D	782	MLY	CD-CE-NZ-CH2
1	D	833	MLY	CD-CE-NZ-CH1
1	D	833	MLY	CD-CE-NZ-CH2
1	D	837	MLY	CD-CE-NZ-CH1
1	D	837	MLY	CD-CE-NZ-CH2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	D	839	MLY	CD-CE-NZ-CH2
1	G	59	MLY	CD-CE-NZ-CH1
1	G	59	MLY	CD-CE-NZ-CH2
1	G	63	MLY	CD-CE-NZ-CH1
1	G	84	MLY	CD-CE-NZ-CH2
1	G	130	MLY	CD-CE-NZ-CH1
1	G	130	MLY	CD-CE-NZ-CH2
1	G	138	MLY	CD-CE-NZ-CH1
1	G	138	MLY	CD-CE-NZ-CH2
1	G	190	MLY	CD-CE-NZ-CH2
1	G	248	MLY	CD-CE-NZ-CH1
1	G	272	MLY	CD-CE-NZ-CH1
1	G	296	MLY	CD-CE-NZ-CH1
1	G	296	MLY	CD-CE-NZ-CH2
1	G	353	MLY	CD-CE-NZ-CH1
1	G	353	MLY	CD-CE-NZ-CH2
1	G	385	MLY	CD-CE-NZ-CH1
1	G	385	MLY	CD-CE-NZ-CH2
1	G	431	MLY	CD-CE-NZ-CH2
1	G	505	MLY	CD-CE-NZ-CH2
1	G	528	MLY	CD-CE-NZ-CH1
1	G	528	MLY	CD-CE-NZ-CH2
1	G	553	MLY	CD-CE-NZ-CH2
1	G	600	MLY	CD-CE-NZ-CH2
1	G	764	MLY	CD-CE-NZ-CH1
1	G	764	MLY	CD-CE-NZ-CH2
1	G	768	MLY	CD-CE-NZ-CH1
1	G	782	MLY	CD-CE-NZ-CH1
1	G	782	MLY	CD-CE-NZ-CH2
1	G	833	MLY	CD-CE-NZ-CH1
1	G	833	MLY	CD-CE-NZ-CH2
1	G	837	MLY	CD-CE-NZ-CH1
1	G	837	MLY	CD-CE-NZ-CH2
1	G	839	MLY	CD-CE-NZ-CH2
1	J	59	MLY	CD-CE-NZ-CH1
1	J	59	MLY	CD-CE-NZ-CH2
1	J	63	MLY	CD-CE-NZ-CH1
1	J	84	MLY	CD-CE-NZ-CH2
1	J	130	MLY	CD-CE-NZ-CH1
1	J	130	MLY	CD-CE-NZ-CH2
1	J	138	MLY	CD-CE-NZ-CH1
1	J	138	MLY	CD-CE-NZ-CH2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	J	190	MLY	CD-CE-NZ-CH2
1	J	248	MLY	CD-CE-NZ-CH1
1	J	272	MLY	CD-CE-NZ-CH1
1	J	296	MLY	CD-CE-NZ-CH1
1	J	296	MLY	CD-CE-NZ-CH2
1	J	353	MLY	CD-CE-NZ-CH1
1	J	353	MLY	CD-CE-NZ-CH2
1	J	367	MLY	CD-CE-NZ-CH2
1	J	385	MLY	CD-CE-NZ-CH1
1	J	385	MLY	CD-CE-NZ-CH2
1	J	431	MLY	CD-CE-NZ-CH2
1	J	505	MLY	CD-CE-NZ-CH2
1	J	528	MLY	CD-CE-NZ-CH1
1	J	528	MLY	CD-CE-NZ-CH2
1	J	553	MLY	CD-CE-NZ-CH2
1	J	600	MLY	CD-CE-NZ-CH2
1	J	764	MLY	CD-CE-NZ-CH1
1	J	764	MLY	CD-CE-NZ-CH2
1	J	768	MLY	CD-CE-NZ-CH1
1	J	782	MLY	CD-CE-NZ-CH1
1	J	782	MLY	CD-CE-NZ-CH2
1	J	833	MLY	CD-CE-NZ-CH1
1	J	833	MLY	CD-CE-NZ-CH2
1	J	837	MLY	CD-CE-NZ-CH1
1	J	837	MLY	CD-CE-NZ-CH2
1	J	839	MLY	CD-CE-NZ-CH2
1	A	659	MLY	CG-CD-CE-NZ
1	D	659	MLY	CG-CD-CE-NZ
1	G	659	MLY	CG-CD-CE-NZ
1	J	659	MLY	CG-CD-CE-NZ
1	A	87	MLY	CG-CD-CE-NZ
1	G	87	MLY	CG-CD-CE-NZ
1	J	87	MLY	CG-CD-CE-NZ
1	A	35	MLY	CG-CD-CE-NZ
1	D	35	MLY	CG-CD-CE-NZ
1	D	87	MLY	CG-CD-CE-NZ
1	G	35	MLY	CG-CD-CE-NZ
1	J	35	MLY	CG-CD-CE-NZ
1	A	295	MLY	CG-CD-CE-NZ
1	D	295	MLY	CG-CD-CE-NZ
1	G	295	MLY	CG-CD-CE-NZ
1	J	295	MLY	CG-CD-CE-NZ

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	138	MLY	CG-CD-CE-NZ
1	A	782	MLY	CG-CD-CE-NZ
1	D	782	MLY	CG-CD-CE-NZ
1	G	782	MLY	CG-CD-CE-NZ
1	J	782	MLY	CG-CD-CE-NZ
1	D	138	MLY	CG-CD-CE-NZ
1	J	138	MLY	CG-CD-CE-NZ
1	G	138	MLY	CG-CD-CE-NZ
1	A	55	MLY	CD-CE-NZ-CH2
1	A	248	MLY	CD-CE-NZ-CH2
1	A	272	MLY	CD-CE-NZ-CH2
1	A	348	MLY	CD-CE-NZ-CH1
1	A	348	MLY	CD-CE-NZ-CH2
1	A	367	MLY	CD-CE-NZ-CH1
1	A	431	MLY	CD-CE-NZ-CH1
1	A	504	MLY	CD-CE-NZ-CH1
1	A	505	MLY	CD-CE-NZ-CH1
1	A	600	MLY	CD-CE-NZ-CH1
1	A	659	MLY	CD-CE-NZ-CH2
1	D	190	MLY	CD-CE-NZ-CH1
1	D	248	MLY	CD-CE-NZ-CH2
1	D	272	MLY	CD-CE-NZ-CH2
1	D	348	MLY	CD-CE-NZ-CH1
1	D	348	MLY	CD-CE-NZ-CH2
1	D	367	MLY	CD-CE-NZ-CH1
1	D	431	MLY	CD-CE-NZ-CH1
1	D	504	MLY	CD-CE-NZ-CH1
1	D	504	MLY	CD-CE-NZ-CH2
1	D	505	MLY	CD-CE-NZ-CH1
1	D	600	MLY	CD-CE-NZ-CH1
1	D	659	MLY	CD-CE-NZ-CH2
1	G	55	MLY	CD-CE-NZ-CH2
1	G	190	MLY	CD-CE-NZ-CH1
1	G	248	MLY	CD-CE-NZ-CH2
1	G	272	MLY	CD-CE-NZ-CH2
1	G	348	MLY	CD-CE-NZ-CH1
1	G	348	MLY	CD-CE-NZ-CH2
1	G	367	MLY	CD-CE-NZ-CH1
1	G	367	MLY	CD-CE-NZ-CH2
1	G	431	MLY	CD-CE-NZ-CH1
1	G	504	MLY	CD-CE-NZ-CH1
1	G	504	MLY	CD-CE-NZ-CH2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	G	505	MLY	CD-CE-NZ-CH1
1	G	600	MLY	CD-CE-NZ-CH1
1	G	659	MLY	CD-CE-NZ-CH2
1	J	55	MLY	CD-CE-NZ-CH2
1	J	190	MLY	CD-CE-NZ-CH1
1	J	248	MLY	CD-CE-NZ-CH2
1	J	348	MLY	CD-CE-NZ-CH1
1	J	348	MLY	CD-CE-NZ-CH2
1	J	367	MLY	CD-CE-NZ-CH1
1	J	431	MLY	CD-CE-NZ-CH1
1	J	504	MLY	CD-CE-NZ-CH1
1	J	504	MLY	CD-CE-NZ-CH2
1	J	505	MLY	CD-CE-NZ-CH1
1	J	600	MLY	CD-CE-NZ-CH1
1	J	659	MLY	CD-CE-NZ-CH2
1	A	84	MLY	CG-CD-CE-NZ
1	A	130	MLY	CG-CD-CE-NZ
1	D	130	MLY	CG-CD-CE-NZ
1	G	84	MLY	CG-CD-CE-NZ
1	G	130	MLY	CG-CD-CE-NZ
1	J	84	MLY	CG-CD-CE-NZ
1	J	130	MLY	CG-CD-CE-NZ
1	G	504	MLY	CG-CD-CE-NZ
1	A	504	MLY	CG-CD-CE-NZ
1	A	681	MLY	CG-CD-CE-NZ
1	D	84	MLY	CG-CD-CE-NZ
1	D	681	MLY	CG-CD-CE-NZ
1	G	681	MLY	CG-CD-CE-NZ
1	J	504	MLY	CG-CD-CE-NZ
1	A	295	MLY	CA-CB-CG-CD
1	D	295	MLY	CA-CB-CG-CD
1	G	295	MLY	CA-CB-CG-CD
1	J	295	MLY	CA-CB-CG-CD
1	D	504	MLY	CG-CD-CE-NZ
1	J	681	MLY	CG-CD-CE-NZ
1	A	107	MLY	CD-CE-NZ-CH1
1	A	369	MLY	CD-CE-NZ-CH2
1	A	768	MLY	CD-CE-NZ-CH2
1	D	87	MLY	CD-CE-NZ-CH1
1	D	107	MLY	CD-CE-NZ-CH1
1	D	369	MLY	CD-CE-NZ-CH2
1	D	768	MLY	CD-CE-NZ-CH2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	G	63	MLY	CD-CE-NZ-CH2
1	G	107	MLY	CD-CE-NZ-CH1
1	G	369	MLY	CD-CE-NZ-CH2
1	G	768	MLY	CD-CE-NZ-CH2
1	J	107	MLY	CD-CE-NZ-CH1
1	J	369	MLY	CD-CE-NZ-CH2
1	J	768	MLY	CD-CE-NZ-CH2
1	A	598	MLY	CG-CD-CE-NZ
1	G	598	MLY	CG-CD-CE-NZ
1	J	598	MLY	CG-CD-CE-NZ
1	D	598	MLY	CG-CD-CE-NZ
1	A	504	MLY	CA-CB-CG-CD
1	A	768	MLY	CA-CB-CG-CD
1	D	504	MLY	CA-CB-CG-CD
1	D	768	MLY	CA-CB-CG-CD
1	G	504	MLY	CA-CB-CG-CD
1	G	768	MLY	CA-CB-CG-CD
1	J	504	MLY	CA-CB-CG-CD
1	J	768	MLY	CA-CB-CG-CD
1	A	63	MLY	CD-CE-NZ-CH2
1	A	415	MLY	CD-CE-NZ-CH1
1	A	415	MLY	CD-CE-NZ-CH2
1	A	553	MLY	CD-CE-NZ-CH1
1	A	659	MLY	CD-CE-NZ-CH1
1	D	55	MLY	CD-CE-NZ-CH1
1	D	63	MLY	CD-CE-NZ-CH2
1	D	415	MLY	CD-CE-NZ-CH1
1	D	415	MLY	CD-CE-NZ-CH2
1	D	553	MLY	CD-CE-NZ-CH1
1	D	659	MLY	CD-CE-NZ-CH1
1	G	415	MLY	CD-CE-NZ-CH1
1	G	415	MLY	CD-CE-NZ-CH2
1	G	553	MLY	CD-CE-NZ-CH1
1	J	55	MLY	CD-CE-NZ-CH1
1	J	63	MLY	CD-CE-NZ-CH2
1	J	87	MLY	CD-CE-NZ-CH1
1	J	272	MLY	CD-CE-NZ-CH2
1	J	415	MLY	CD-CE-NZ-CH1
1	J	415	MLY	CD-CE-NZ-CH2
1	J	553	MLY	CD-CE-NZ-CH1
1	J	659	MLY	CD-CE-NZ-CH1
1	A	415	MLY	CA-CB-CG-CD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	G	415	MLY	CA-CB-CG-CD
1	A	19	MLY	CD-CE-NZ-CH2
1	A	55	MLY	CD-CE-NZ-CH1
1	A	87	MLY	CD-CE-NZ-CH1
1	D	19	MLY	CD-CE-NZ-CH2
1	G	19	MLY	CD-CE-NZ-CH2
1	G	55	MLY	CD-CE-NZ-CH1
1	G	87	MLY	CD-CE-NZ-CH1
1	G	659	MLY	CD-CE-NZ-CH1
1	J	19	MLY	CD-CE-NZ-CH2
1	D	551	MLY	CG-CD-CE-NZ
1	G	551	MLY	CG-CD-CE-NZ
1	J	551	MLY	CG-CD-CE-NZ
1	A	551	MLY	CG-CD-CE-NZ
1	D	415	MLY	CA-CB-CG-CD
1	J	415	MLY	CA-CB-CG-CD
1	A	272	MLY	CE-CD-CG-CB
1	D	272	MLY	CE-CD-CG-CB
1	J	272	MLY	CE-CD-CG-CB
1	G	272	MLY	CE-CD-CG-CB
1	A	30	MLY	CE-CD-CG-CB
1	A	296	MLY	CE-CD-CG-CB
1	D	30	MLY	CE-CD-CG-CB
1	D	296	MLY	CE-CD-CG-CB
1	G	30	MLY	CE-CD-CG-CB
1	G	296	MLY	CE-CD-CG-CB
1	J	296	MLY	CE-CD-CG-CB
1	A	505	MLY	CE-CD-CG-CB
1	D	505	MLY	CE-CD-CG-CB
1	G	505	MLY	CE-CD-CG-CB
1	J	30	MLY	CE-CD-CG-CB
1	J	505	MLY	CE-CD-CG-CB
1	A	107	MLY	CD-CE-NZ-CH2
1	A	839	MLY	CD-CE-NZ-CH1
1	D	839	MLY	CD-CE-NZ-CH1
1	G	839	MLY	CD-CE-NZ-CH1
1	J	107	MLY	CD-CE-NZ-CH2
1	J	839	MLY	CD-CE-NZ-CH1
1	D	681	MLY	CE-CD-CG-CB
1	G	681	MLY	CE-CD-CG-CB
1	J	681	MLY	CE-CD-CG-CB
1	A	681	MLY	CE-CD-CG-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	D	49	MLY	CE-CD-CG-CB
1	G	49	MLY	CE-CD-CG-CB
1	J	49	MLY	CE-CD-CG-CB
1	A	49	MLY	CE-CD-CG-CB
1	D	353	MLY	CE-CD-CG-CB
1	D	768	MLY	CE-CD-CG-CB
1	J	353	MLY	CE-CD-CG-CB
1	A	353	MLY	CE-CD-CG-CB
1	G	353	MLY	CE-CD-CG-CB
1	A	190	MLY	CE-CD-CG-CB
1	A	768	MLY	CE-CD-CG-CB
1	D	190	MLY	CE-CD-CG-CB
1	G	768	MLY	CE-CD-CG-CB
1	J	190	MLY	CE-CD-CG-CB
1	J	768	MLY	CE-CD-CG-CB
1	G	190	MLY	CE-CD-CG-CB
1	A	782	MLY	CE-CD-CG-CB
1	D	782	MLY	CE-CD-CG-CB
1	A	369	MLY	CE-CD-CG-CB
1	D	369	MLY	CE-CD-CG-CB
1	G	369	MLY	CE-CD-CG-CB
1	G	782	MLY	CE-CD-CG-CB
1	J	369	MLY	CE-CD-CG-CB
1	J	782	MLY	CE-CD-CG-CB
1	A	236	MLY	CD-CE-NZ-CH1
1	D	107	MLY	CD-CE-NZ-CH2
1	D	236	MLY	CD-CE-NZ-CH1
1	G	107	MLY	CD-CE-NZ-CH2
1	G	236	MLY	CD-CE-NZ-CH1
1	J	236	MLY	CD-CE-NZ-CH1
1	D	190	MLY	CG-CD-CE-NZ
1	A	436	MLY	CA-CB-CG-CD
1	A	837	MLY	CA-CB-CG-CD
1	D	436	MLY	CA-CB-CG-CD
1	D	837	MLY	CA-CB-CG-CD
1	G	436	MLY	CA-CB-CG-CD
1	G	837	MLY	CA-CB-CG-CD
1	J	436	MLY	CA-CB-CG-CD
1	J	837	MLY	CA-CB-CG-CD
1	G	190	MLY	CG-CD-CE-NZ
1	J	190	MLY	CG-CD-CE-NZ
1	A	190	MLY	CG-CD-CE-NZ

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	D	833	MLY	CE-CD-CG-CB
1	A	833	MLY	CE-CD-CG-CB
1	G	833	MLY	CE-CD-CG-CB
1	J	833	MLY	CE-CD-CG-CB
1	A	431	MLY	CA-CB-CG-CD
1	D	236	MLY	CA-CB-CG-CD
1	D	431	MLY	CA-CB-CG-CD
1	G	431	MLY	CA-CB-CG-CD
1	J	236	MLY	CA-CB-CG-CD
1	J	431	MLY	CA-CB-CG-CD
1	A	55	MLY	CG-CD-CE-NZ
1	G	55	MLY	CG-CD-CE-NZ
1	D	55	MLY	CG-CD-CE-NZ
1	D	551	MLY	CE-CD-CG-CB
1	J	55	MLY	CG-CD-CE-NZ
1	J	617	MLY	CE-CD-CG-CB
1	A	617	MLY	CE-CD-CG-CB
1	D	617	MLY	CE-CD-CG-CB
1	G	617	MLY	CE-CD-CG-CB
1	A	236	MLY	CA-CB-CG-CD
1	A	833	MLY	CA-CB-CG-CD
1	D	833	MLY	CA-CB-CG-CD
1	G	236	MLY	CA-CB-CG-CD
1	G	833	MLY	CA-CB-CG-CD
1	J	833	MLY	CA-CB-CG-CD
1	A	348	MLY	C-CA-CB-CG
1	D	348	MLY	C-CA-CB-CG
1	G	348	MLY	C-CA-CB-CG
1	J	348	MLY	C-CA-CB-CG
1	A	551	MLY	CE-CD-CG-CB
1	J	551	MLY	CE-CD-CG-CB
1	G	551	MLY	CE-CD-CG-CB
1	G	59	MLY	CE-CD-CG-CB
1	J	59	MLY	CE-CD-CG-CB
1	A	55	MLY	CE-CD-CG-CB
1	A	59	MLY	CE-CD-CG-CB
1	D	55	MLY	CE-CD-CG-CB
1	D	59	MLY	CE-CD-CG-CB
1	D	553	MLY	CE-CD-CG-CB
1	G	55	MLY	CE-CD-CG-CB
1	G	553	MLY	CE-CD-CG-CB
1	J	55	MLY	CE-CD-CG-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	J	553	MLY	CE-CD-CG-CB
1	A	553	MLY	CE-CD-CG-CB
1	J	431	MLY	CE-CD-CG-CB
1	A	431	MLY	CE-CD-CG-CB
1	G	248	MLY	CE-CD-CG-CB
1	A	248	MLY	CE-CD-CG-CB
1	D	248	MLY	CE-CD-CG-CB
1	J	248	MLY	CE-CD-CG-CB
1	D	431	MLY	CE-CD-CG-CB
1	G	431	MLY	CE-CD-CG-CB
1	D	35	MLY	CE-CD-CG-CB
1	A	35	MLY	CE-CD-CG-CB
1	G	35	MLY	CE-CD-CG-CB
1	J	35	MLY	CE-CD-CG-CB
1	D	528	MLY	CG-CD-CE-NZ
1	G	528	MLY	CG-CD-CE-NZ
1	A	528	MLY	CG-CD-CE-NZ
1	J	528	MLY	CG-CD-CE-NZ
1	G	248	MLY	CG-CD-CE-NZ
1	A	138	MLY	CA-CB-CG-CD
1	A	296	MLY	CA-CB-CG-CD
1	D	138	MLY	CA-CB-CG-CD
1	G	138	MLY	CA-CB-CG-CD
1	J	138	MLY	CA-CB-CG-CD
1	J	296	MLY	CA-CB-CG-CD
1	A	248	MLY	CG-CD-CE-NZ
1	J	248	MLY	CG-CD-CE-NZ
1	D	248	MLY	CG-CD-CE-NZ
1	D	296	MLY	CA-CB-CG-CD
1	G	296	MLY	CA-CB-CG-CD
1	A	436	MLY	CE-CD-CG-CB
1	A	598	MLY	CE-CD-CG-CB
1	A	600	MLY	CE-CD-CG-CB
1	D	436	MLY	CE-CD-CG-CB
1	D	598	MLY	CE-CD-CG-CB
1	D	600	MLY	CE-CD-CG-CB
1	G	436	MLY	CE-CD-CG-CB
1	G	598	MLY	CE-CD-CG-CB
1	G	600	MLY	CE-CD-CG-CB
1	J	436	MLY	CE-CD-CG-CB
1	J	598	MLY	CE-CD-CG-CB
1	J	600	MLY	CE-CD-CG-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	486	MLY	CE-CD-CG-CB
1	G	486	MLY	CE-CD-CG-CB
1	J	486	MLY	CE-CD-CG-CB
1	D	486	MLY	CE-CD-CG-CB
1	G	839	MLY	CE-CD-CG-CB
1	J	839	MLY	CE-CD-CG-CB
1	D	839	MLY	CE-CD-CG-CB
1	A	839	MLY	CE-CD-CG-CB
1	A	236	MLY	CD-CE-NZ-CH2
1	D	236	MLY	CD-CE-NZ-CH2
1	G	236	MLY	CD-CE-NZ-CH2
1	J	236	MLY	CD-CE-NZ-CH2
1	A	35	MLY	N-CA-CB-CG
1	A	63	MLY	N-CA-CB-CG
1	A	130	MLY	N-CA-CB-CG
1	A	436	MLY	N-CA-CB-CG
1	A	681	MLY	N-CA-CB-CG
1	A	833	MLY	N-CA-CB-CG
1	A	837	MLY	N-CA-CB-CG
1	D	35	MLY	N-CA-CB-CG
1	D	63	MLY	N-CA-CB-CG
1	D	130	MLY	N-CA-CB-CG
1	D	348	MLY	N-CA-CB-CG
1	D	436	MLY	N-CA-CB-CG
1	D	681	MLY	N-CA-CB-CG
1	D	833	MLY	N-CA-CB-CG
1	D	837	MLY	N-CA-CB-CG
1	G	35	MLY	N-CA-CB-CG
1	G	63	MLY	N-CA-CB-CG
1	G	130	MLY	N-CA-CB-CG
1	G	436	MLY	N-CA-CB-CG
1	G	681	MLY	N-CA-CB-CG
1	G	833	MLY	N-CA-CB-CG
1	G	837	MLY	N-CA-CB-CG
1	J	35	MLY	N-CA-CB-CG
1	J	63	MLY	N-CA-CB-CG
1	J	130	MLY	N-CA-CB-CG
1	J	436	MLY	N-CA-CB-CG
1	J	681	MLY	N-CA-CB-CG
1	J	833	MLY	N-CA-CB-CG
1	J	837	MLY	N-CA-CB-CG
1	D	833	MLY	C-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	J	833	MLY	C-CA-CB-CG
1	A	19	MLY	CA-CB-CG-CD
1	D	19	MLY	CA-CB-CG-CD
1	G	19	MLY	CA-CB-CG-CD
1	J	19	MLY	CA-CB-CG-CD
1	D	837	MLY	CE-CD-CG-CB
1	G	837	MLY	CE-CD-CG-CB
1	A	19	MLY	CE-CD-CG-CB
1	A	837	MLY	CE-CD-CG-CB
1	J	837	MLY	CE-CD-CG-CB
1	D	19	MLY	CE-CD-CG-CB
1	J	19	MLY	CE-CD-CG-CB
1	G	19	MLY	CE-CD-CG-CB
1	G	613	MLY	CE-CD-CG-CB
1	J	613	MLY	CE-CD-CG-CB
1	A	613	MLY	CE-CD-CG-CB
1	D	613	MLY	CE-CD-CG-CB
1	A	598	MLY	CD-CE-NZ-CH2
1	D	598	MLY	CD-CE-NZ-CH2
1	G	598	MLY	CD-CE-NZ-CH2
1	J	598	MLY	CD-CE-NZ-CH2
1	A	63	MLY	C-CA-CB-CG
1	A	353	MLY	C-CA-CB-CG
1	A	833	MLY	C-CA-CB-CG
1	D	63	MLY	C-CA-CB-CG
1	D	353	MLY	C-CA-CB-CG
1	G	63	MLY	C-CA-CB-CG
1	G	353	MLY	C-CA-CB-CG
1	G	833	MLY	C-CA-CB-CG
1	J	63	MLY	C-CA-CB-CG
1	J	353	MLY	C-CA-CB-CG
1	A	30	MLY	CA-CB-CG-CD
1	D	30	MLY	CA-CB-CG-CD
1	G	30	MLY	CA-CB-CG-CD
1	J	30	MLY	CA-CB-CG-CD
1	J	348	MLY	CE-CD-CG-CB
1	A	348	MLY	CE-CD-CG-CB
1	D	348	MLY	CE-CD-CG-CB
1	G	348	MLY	CE-CD-CG-CB
1	A	613	MLY	CA-CB-CG-CD
1	J	613	MLY	CA-CB-CG-CD
1	D	613	MLY	CA-CB-CG-CD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	G	613	MLY	CA-CB-CG-CD
1	A	190	MLY	CA-CB-CG-CD
1	A	528	MLY	CA-CB-CG-CD
1	D	190	MLY	CA-CB-CG-CD
1	G	190	MLY	CA-CB-CG-CD
1	J	190	MLY	CA-CB-CG-CD

There are no ring outliers.

124 monomers are involved in 525 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	551	MLY	2	0
1	A	49	MLY	3	0
1	D	551	MLY	1	0
1	G	782	MLY	1	0
1	A	369	MLY	1	0
1	D	837	MLY	1	0
1	A	782	MLY	1	0
1	G	553	MLY	16	0
1	J	782	MLY	1	0
1	J	296	MLY	3	0
1	G	30	MLY	1	0
1	J	107	MLY	3	0
1	D	659	MLY	2	0
1	D	598	MLY	1	0
1	G	837	MLY	1	0
1	G	436	MLY	2	0
1	D	272	MLY	1	0
1	A	63	MLY	3	0
1	J	553	MLY	17	0
1	A	59	MLY	2	0
1	D	138	MLY	1	0
1	D	63	MLY	3	0
1	D	87	MLY	3	0
1	G	598	MLY	1	0
1	J	59	MLY	3	0
1	J	598	MLY	1	0
1	G	138	MLY	1	0
1	J	295	MLY	6	0
1	D	486	MLY	3	0
1	J	764	MLY	26	0
1	D	415	MLY	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	528	MLY	3	0
1	A	87	MLY	3	0
1	A	348	MLY	5	0
1	J	190	MLY	2	0
1	G	764	MLY	12	0
1	J	659	MLY	2	0
1	A	839	MLY	15	0
1	G	49	MLY	2	0
1	D	107	MLY	2	0
1	G	369	MLY	1	0
1	J	528	MLY	3	0
1	A	296	MLY	2	0
1	A	504	MLY	4	0
1	A	505	MLY	11	0
1	G	659	MLY	2	0
1	J	49	MLY	2	0
1	A	553	MLY	17	0
1	D	553	MLY	16	0
1	J	30	MLY	1	0
1	A	415	MLY	1	0
1	G	272	MLY	1	0
1	A	436	MLY	2	0
1	G	827	MLY	1	0
1	A	768	MLY	14	0
1	G	63	MLY	3	0
1	G	617	MLY	1	0
1	G	59	MLY	3	0
1	J	600	MLY	1	0
1	D	295	MLY	6	0
1	J	617	MLY	1	0
1	D	49	MLY	3	0
1	G	600	MLY	1	0
1	J	138	MLY	1	0
1	J	827	MLY	1	0
1	G	296	MLY	2	0
1	J	87	MLY	3	0
1	A	486	MLY	3	0
1	D	436	MLY	2	0
1	A	659	MLY	2	0
1	A	764	MLY	7	0
1	A	600	MLY	1	0
1	G	295	MLY	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	63	MLY	4	0
1	G	768	MLY	15	0
1	A	295	MLY	6	0
1	D	839	MLY	16	0
1	D	248	MLY	2	0
1	D	600	MLY	1	0
1	G	107	MLY	3	0
1	D	296	MLY	3	0
1	A	248	MLY	2	0
1	J	272	MLY	1	0
1	A	55	MLY	1	0
1	J	415	MLY	1	0
1	D	348	MLY	6	0
1	J	436	MLY	2	0
1	D	55	MLY	1	0
1	G	55	MLY	1	0
1	G	415	MLY	1	0
1	J	248	MLY	2	0
1	J	348	MLY	5	0
1	G	839	MLY	4	0
1	D	30	MLY	1	0
1	G	348	MLY	4	0
1	A	837	MLY	1	0
1	A	107	MLY	3	0
1	J	837	MLY	1	0
1	D	764	MLY	2	0
1	D	59	MLY	2	0
1	J	55	MLY	1	0
1	A	598	MLY	1	0
1	D	768	MLY	6	0
1	J	839	MLY	5	0
1	G	486	MLY	3	0
1	A	138	MLY	1	0
1	J	768	MLY	41	0
1	G	87	MLY	2	0
1	G	248	MLY	2	0
1	G	190	MLY	2	0
1	J	84	MLY	25	0
1	G	84	MLY	18	0
1	J	486	MLY	3	0
1	A	190	MLY	2	0
1	A	528	MLY	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	30	MLY	1	0
1	A	617	MLY	1	0
1	A	272	MLY	1	0
1	J	551	MLY	1	0
1	D	190	MLY	2	0
1	D	617	MLY	1	0
1	G	551	MLY	2	0
1	G	528	MLY	3	0
1	D	782	MLY	32	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	4
1	J	4
1	D	4
1	A	4
3	C	1
3	F	1
3	I	1
3	L	1
2	B	1
2	E	1
2	H	1
2	K	1

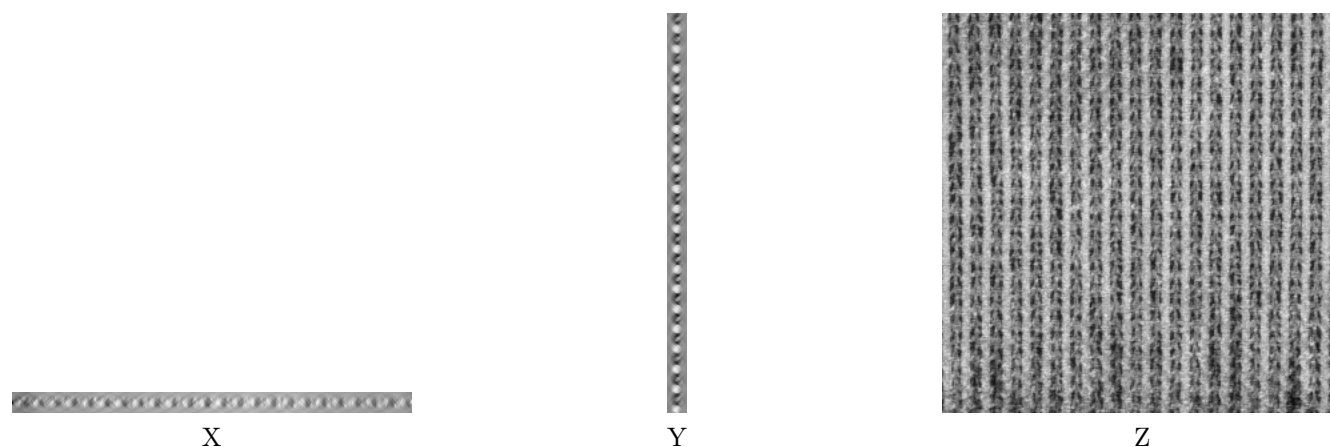
All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	769:ALA	C	770:GLY	N	4.89
1	J	769:ALA	C	770:GLY	N	4.67
1	D	769:ALA	C	770:GLY	N	4.54
1	D	709:LYS	C	710:GLY	N	3.32
1	A	709:LYS	C	710:GLY	N	3.28
1	A	769:ALA	C	770:GLY	N	2.79
1	C	4:LYS	C	5:ALA	N	2.61
1	F	4:LYS	C	5:ALA	N	2.61
1	I	4:LYS	C	5:ALA	N	2.61
1	L	4:LYS	C	5:ALA	N	2.61
1	G	709:LYS	C	710:GLY	N	2.16
1	B	140:PHE	C	141:PRO	N	1.09
1	E	140:PHE	C	141:PRO	N	1.09
1	H	140:PHE	C	141:PRO	N	1.09
1	K	140:PHE	C	141:PRO	N	1.09
1	A	637:LYS	C	638:GLY	N	1.06
1	G	637:LYS	C	638:GLY	N	1.06
1	J	637:LYS	C	638:GLY	N	1.06
1	D	637:LYS	C	638:GLY	N	1.05
1	A	649:VAL	C	650:SER	N	1.03
1	D	649:VAL	C	650:SER	N	1.03
1	G	649:VAL	C	650:SER	N	1.03
1	J	649:VAL	C	650:SER	N	1.03
1	J	709:LYS	C	710:GLY	N	0.33

6 Tomogram visualisation [i](#)

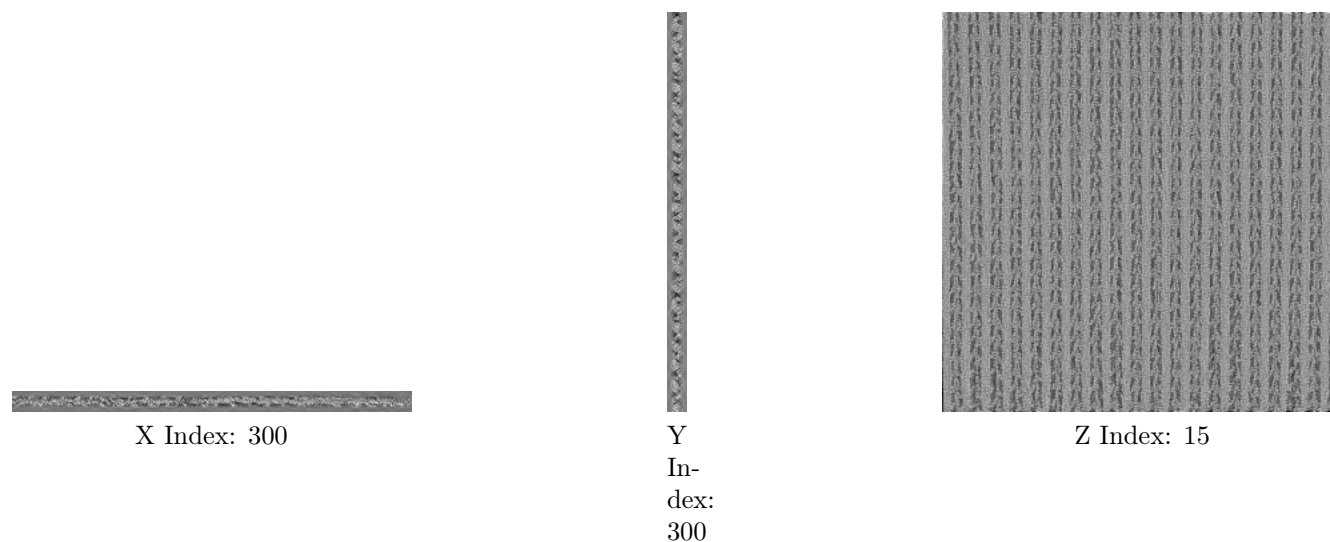
This section contains visualisations of the EMDB entry EMD-1001. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



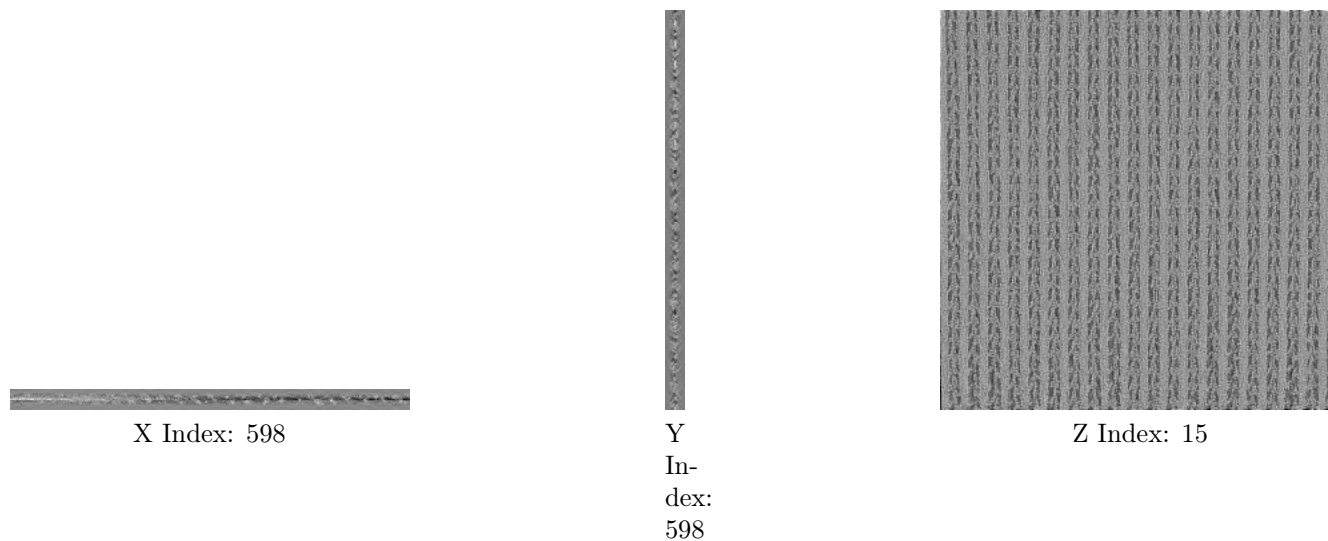
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices [i](#)



The images above show central slices of the tomogram in three orthogonal directions.

6.3 Largest variance slices [i](#)



The images above show the largest variance slices of the tomogram in three orthogonal directions.

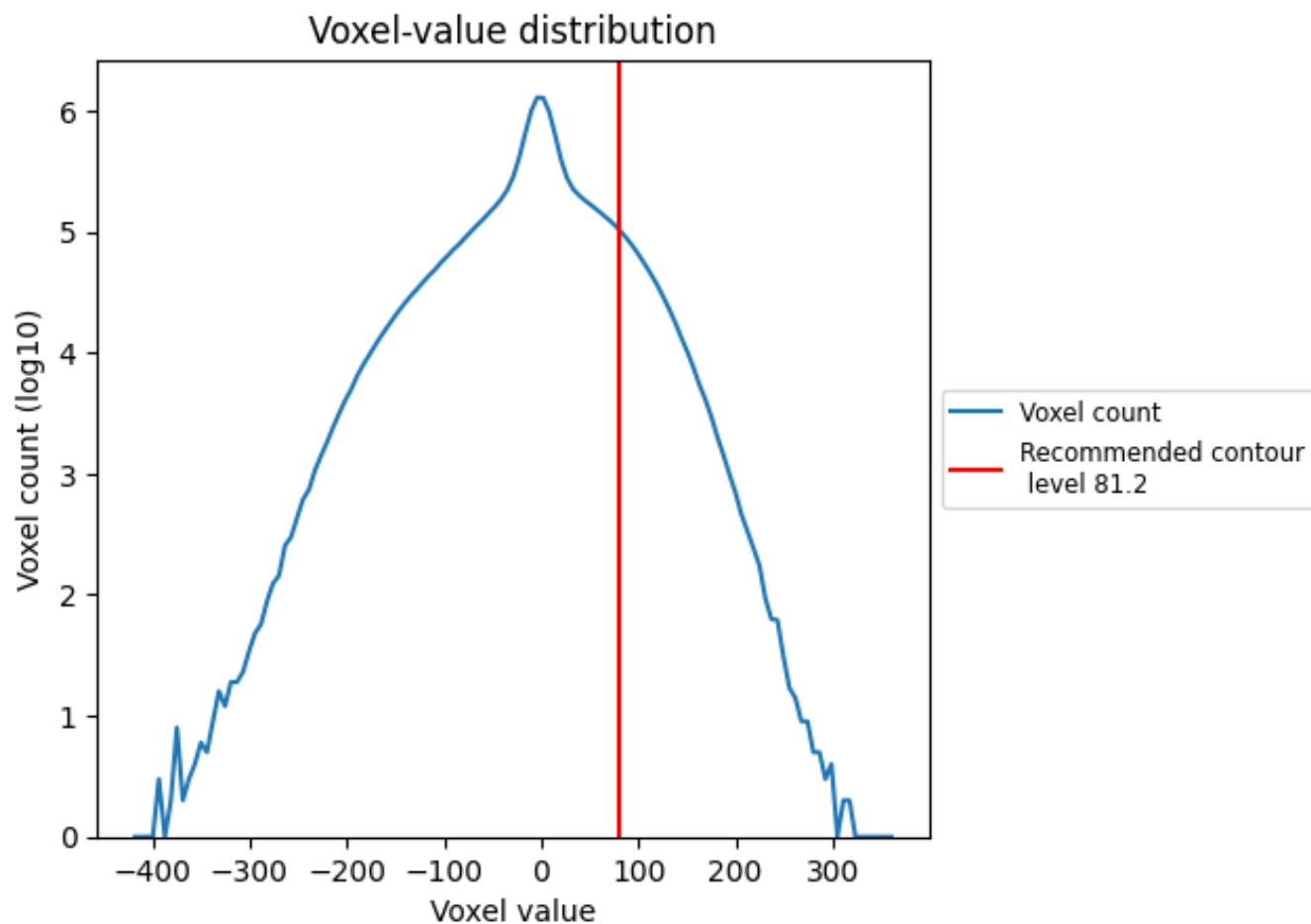
6.4 Mask visualisation [i](#)

This section was not generated.

7 Tomogram analysis [i](#)

This section contains the results of statistical analysis of the tomogram.

7.1 Voxel-value distribution [i](#)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

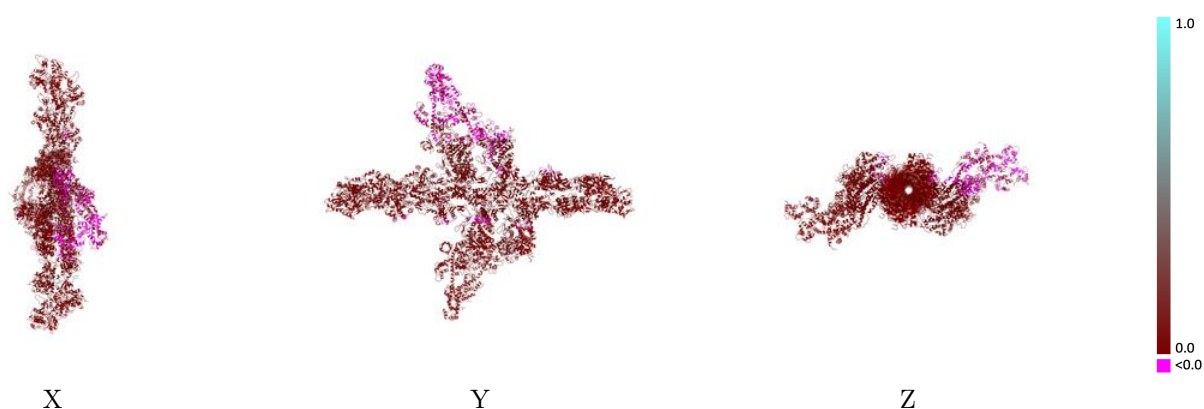
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1001 and PDB model 1O1F. Per-residue inclusion information can be found in section 3 on page 7.

8.1 Map-model overlay [i](#)

This section was not generated.

8.2 Q-score mapped to coordinate model [i](#)

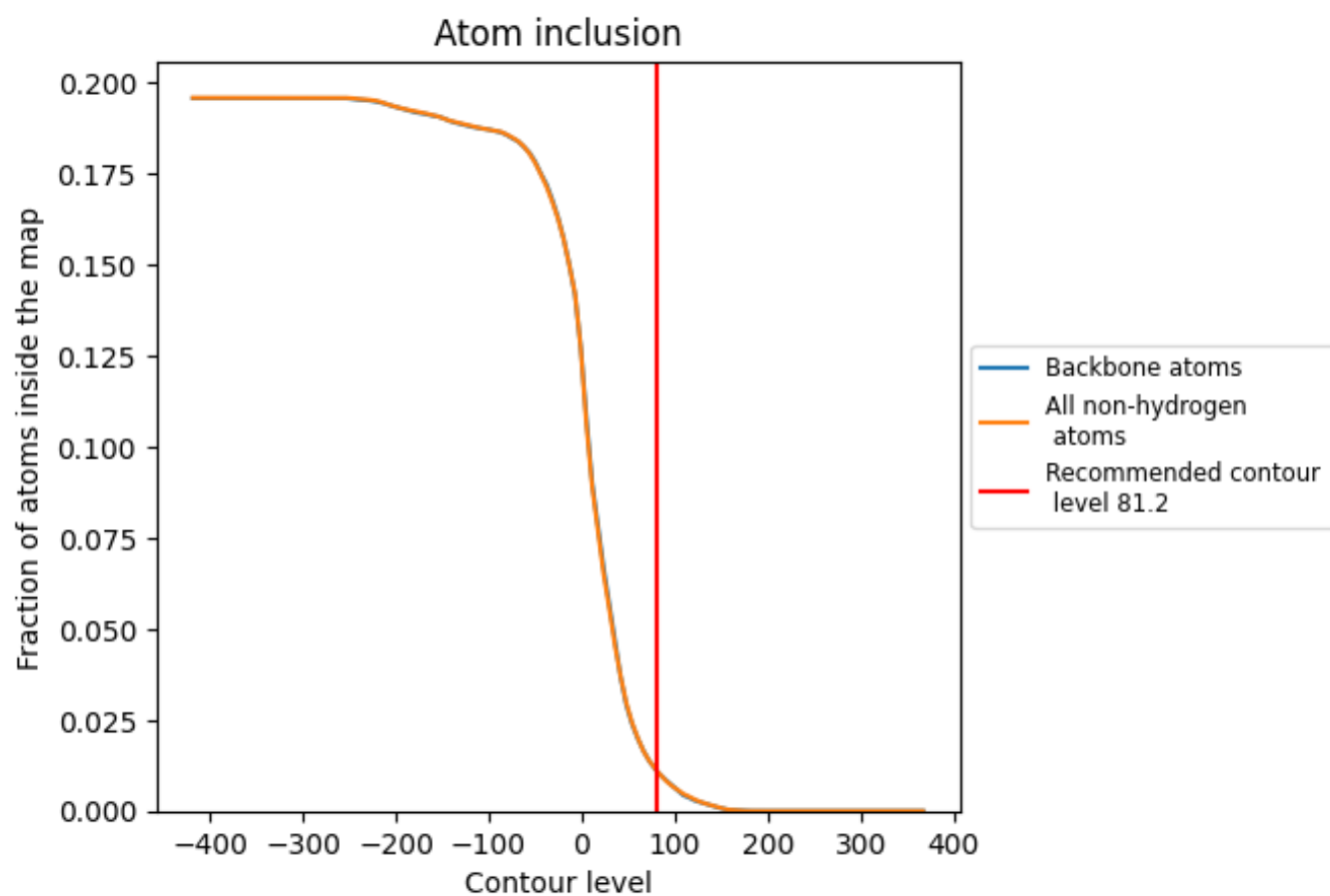


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.























































8.4 Atom inclusion [i](#)



At the recommended contour level, 1% of all backbone atoms, 1% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (81.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.0108	 0.0000
0	 0.0000	 0.0000
1	 0.0000	 -0.0000
2	 0.0000	 0.0000
3	 0.0004	 0.0000
4	 0.0375	 0.0000
5	 0.0000	 0.0020
6	 0.0077	 0.0010
7	 0.0000	 0.0000
8	 0.0635	 -0.0010
A	 0.0000	 -0.0010
B	 0.0000	 0.0000
C	 0.0000	 0.0000
D	 0.0080	 -0.0030
E	 0.0000	 -0.0260
F	 0.0961	 0.0180
G	 0.0000	 0.0030
H	 0.0000	 0.0000
I	 0.0000	 0.0000
J	 0.0092	 0.0010
K	 0.0000	 0.0000
L	 0.2549	 0.0230
V	 0.0000	 0.0000
W	 0.0000	 -0.0010
X	 0.0000	 0.0000
Y	 0.0000	 0.0000
Z	 0.0000	 0.0000

