



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:05 AM UTC

PDB ID : 4LNN / pdb_00004lnn
Title : B. subtilis glutamine synthetase structures reveal large active site conformational changes and basis for isoenzyme specific regulation: structure of apo form of GS
Authors : Schumacher, M.A.; Chinnam, N.; Tonthat, N.; Fisher, S.; Wray, L.
Deposited on : 2013-07-11
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

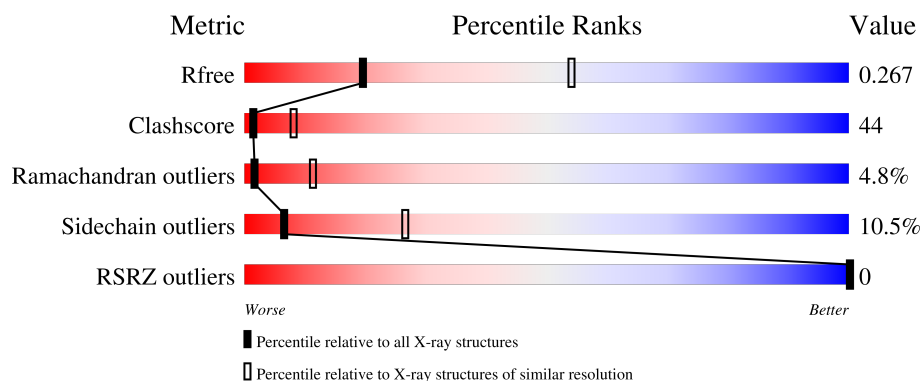
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



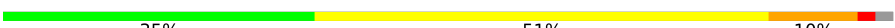
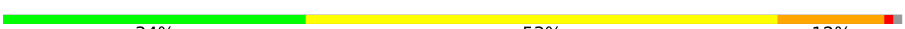
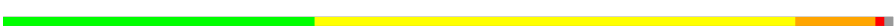
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	443	 34% 56% 9% ..
1	B	443	 37% 55% 7% .
1	C	443	 36% 51% 12% ..
1	D	443	 33% 55% 11% ..
1	E	443	 35% 50% 13% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	443	 31% 57% 10% .
1	G	443	 38% 48% 12% ..
1	H	443	 37% 51% 10% ..
1	I	443	 35% 51% 10% . .
1	J	443	 34% 53% 12% ..
1	K	443	 35% 54% 9% ..
1	L	443	 35% 53% 12% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 42284 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3505	2240	586	663	16			
1	B	439	Total	C	N	O	S	0	0	0
			3505	2240	586	663	16			
1	C	438	Total	C	N	O	S	0	0	0
			3498	2235	585	662	16			
1	D	439	Total	C	N	O	S	0	0	0
			3505	2240	586	663	16			
1	E	438	Total	C	N	O	S	0	0	0
			3498	2235	585	662	16			
1	F	437	Total	C	N	O	S	0	0	0
			3491	2230	584	661	16			
1	G	438	Total	C	N	O	S	0	0	0
			3498	2235	585	662	16			
1	H	437	Total	C	N	O	S	0	0	0
			3491	2230	584	661	16			
1	I	436	Total	C	N	O	S	0	0	0
			3485	2227	583	660	15			
1	J	438	Total	C	N	O	S	0	0	0
			3498	2235	585	662	16			
1	K	438	Total	C	N	O	S	0	0	0
			3498	2235	585	662	16			
1	L	440	Total	C	N	O	S	0	0	0
			3509	2242	587	664	16			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

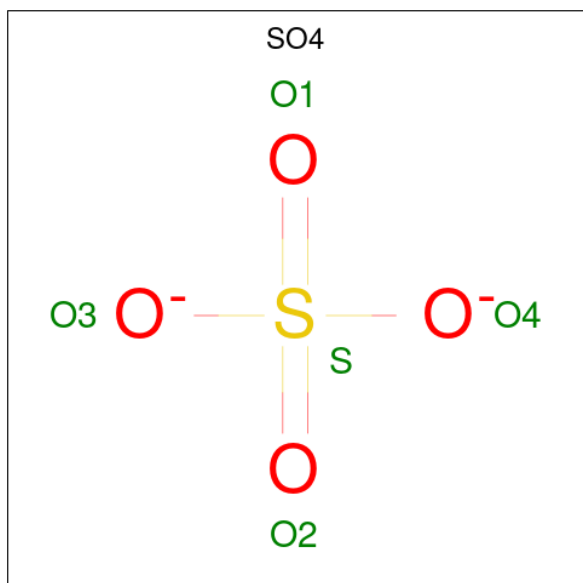
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	3	Total	Mg	0	0
			3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	2	Total	Mg	0	0
			2	2		
2	D	2	Total	Mg	0	0
			2	2		
2	E	2	Total	Mg	0	0
			2	2		
2	F	2	Total	Mg	0	0
			2	2		
2	G	2	Total	Mg	0	0
			2	2		
2	H	2	Total	Mg	0	0
			2	2		
2	I	2	Total	Mg	0	0
			2	2		
2	J	2	Total	Mg	0	0
			2	2		
2	K	2	Total	Mg	0	0
			2	2		
2	L	2	Total	Mg	0	0
			2	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

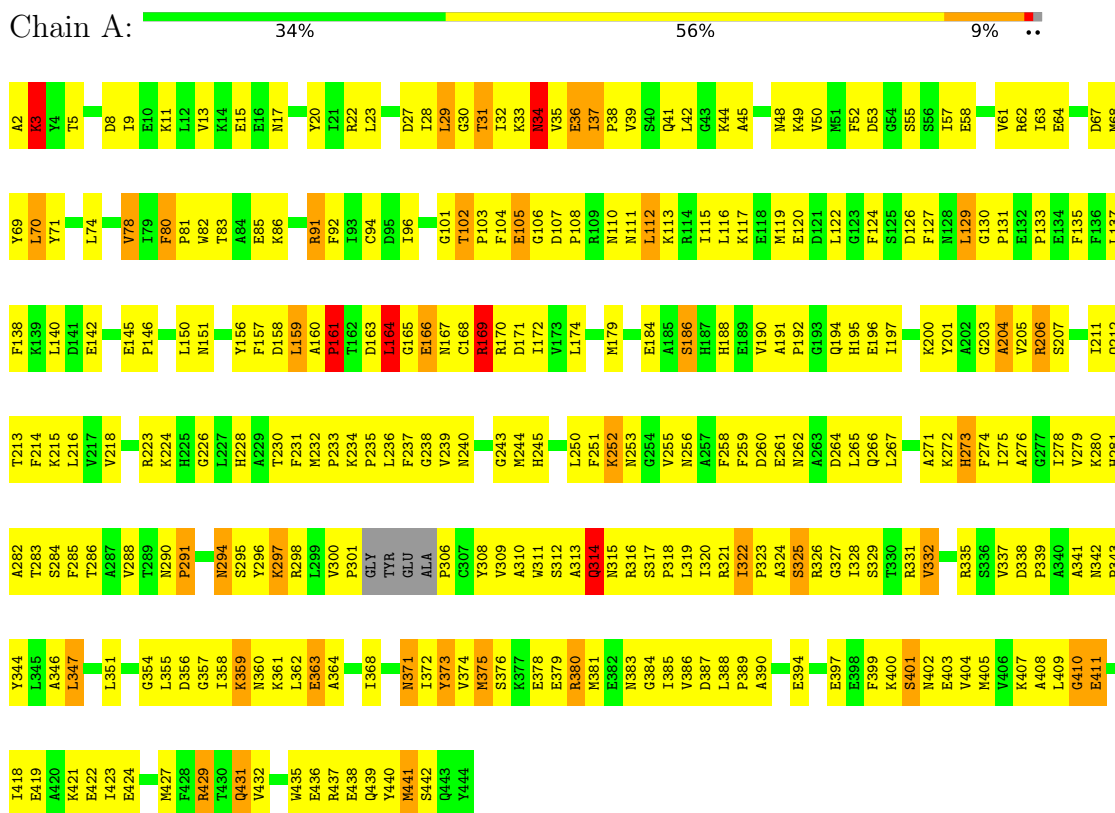
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		
4	B	27	Total	O	0	0
			27	27		
4	C	28	Total	O	0	0
			28	28		
4	D	20	Total	O	0	0
			20	20		
4	E	17	Total	O	0	0
			17	17		
4	F	24	Total	O	0	0
			24	24		
4	G	21	Total	O	0	0
			21	21		
4	H	20	Total	O	0	0
			20	20		
4	I	23	Total	O	0	0
			23	23		
4	J	12	Total	O	0	0
			12	12		
4	K	22	Total	O	0	0
			22	22		
4	L	22	Total	O	0	0
			22	22		

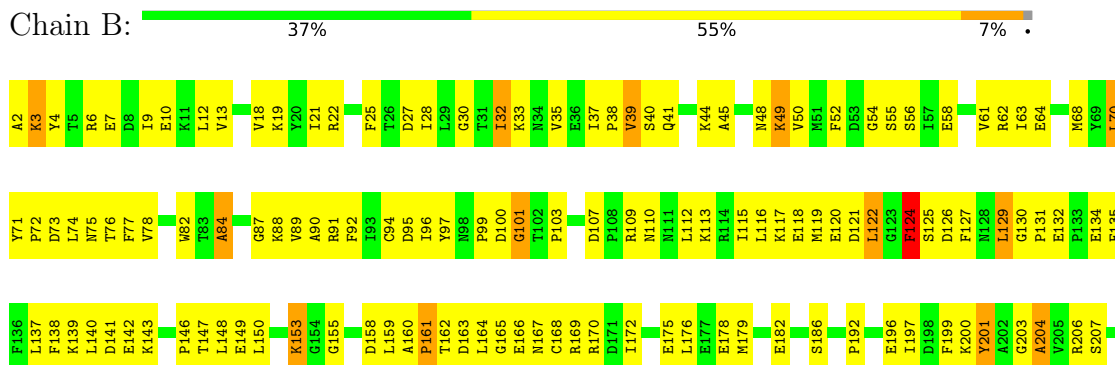
3 Residue-property plots [i](#)

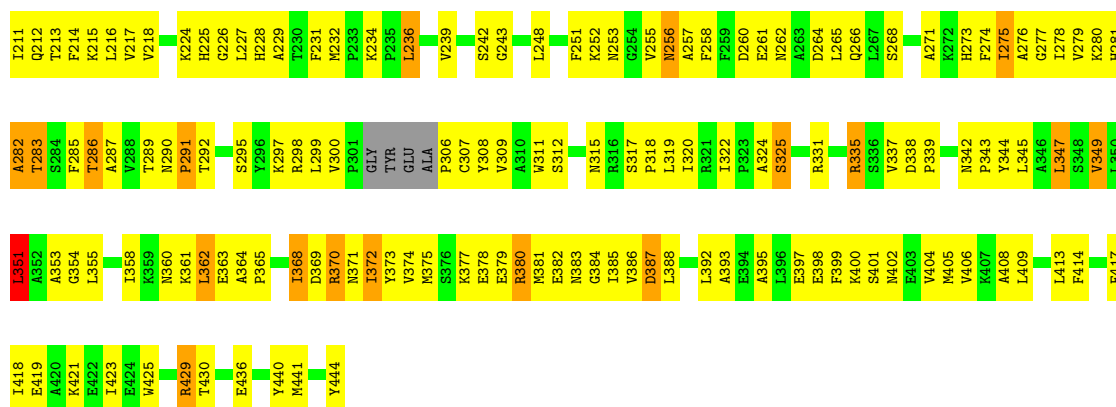
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Glutamine synthetase



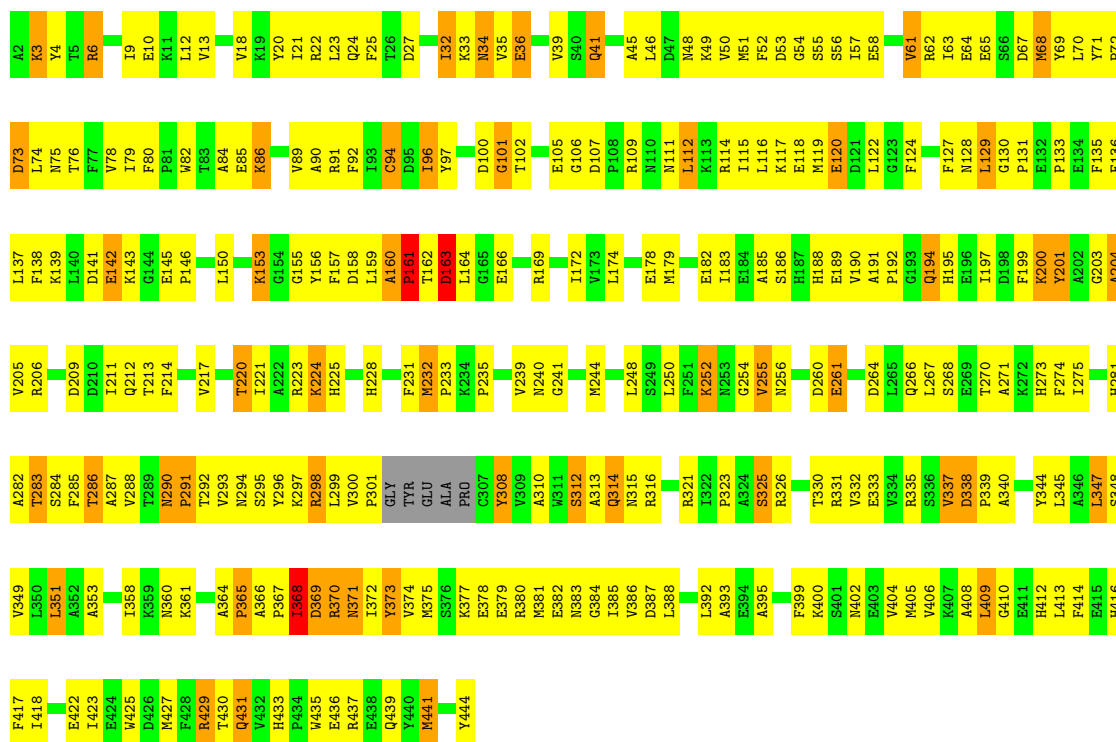
• Molecule 1: Glutamine synthetase





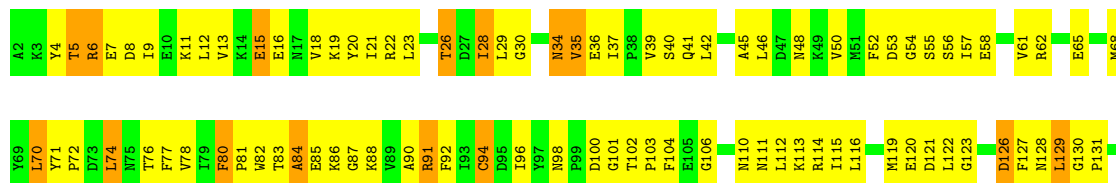
• Molecule 1: Glutamine synthetase

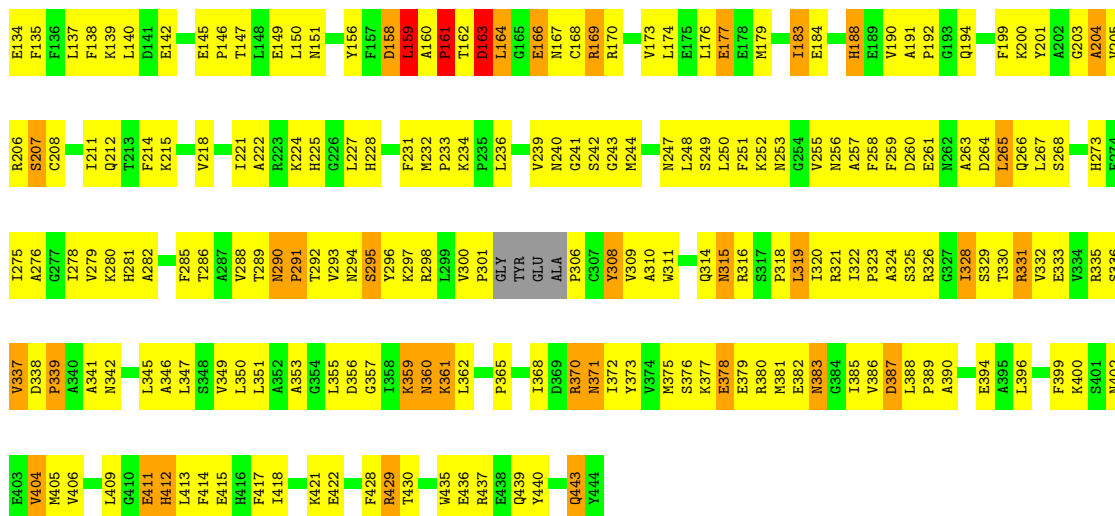
Chain C: 36% 51% 12% ..



• Molecule 1: Glutamine synthetase

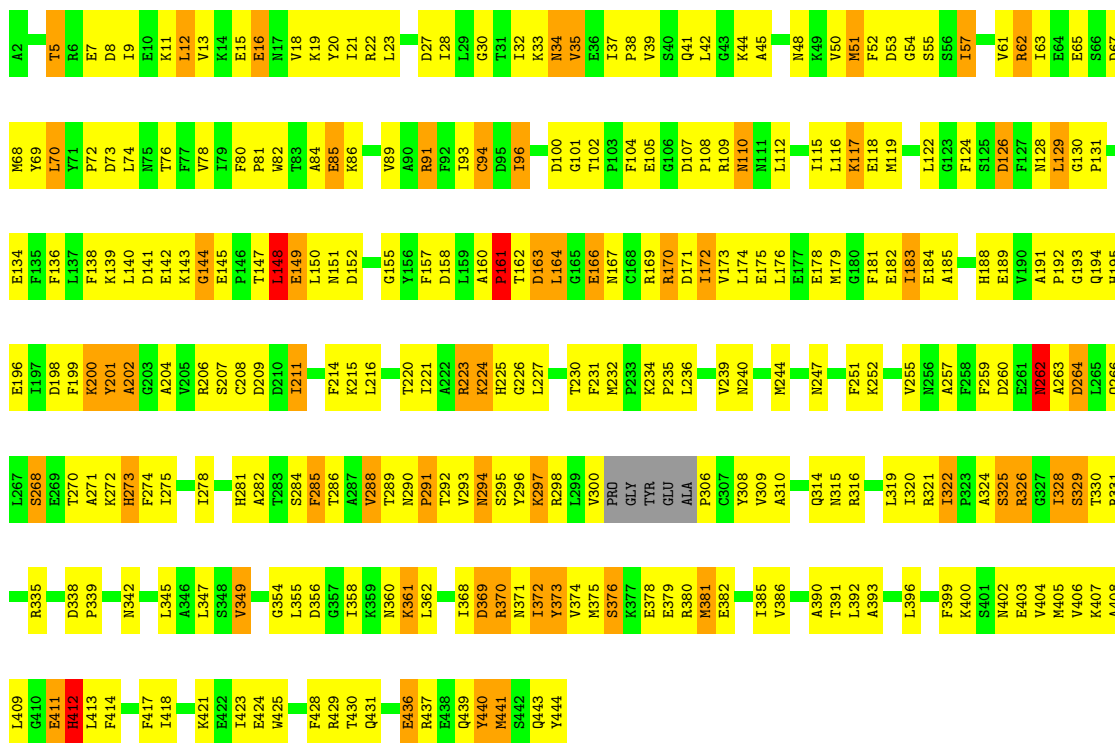
Chain D: 33% 55% 11% ..





• Molecule 1: Glutamine synthetase

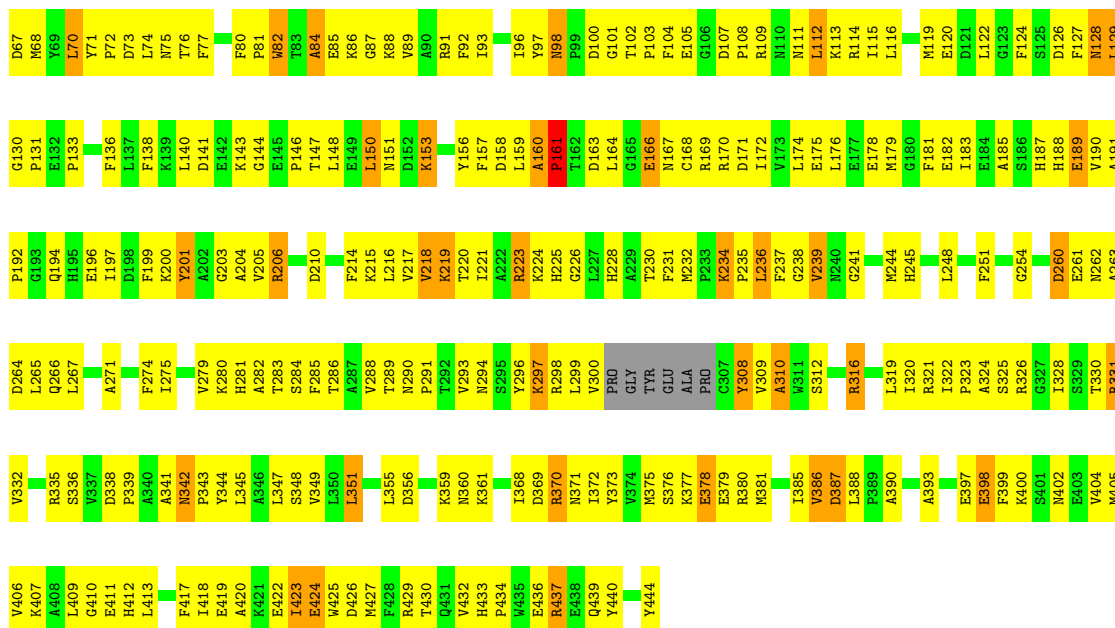
Chain E: 35% 50% 13% ..



• Molecule 1: Glutamine synthetase

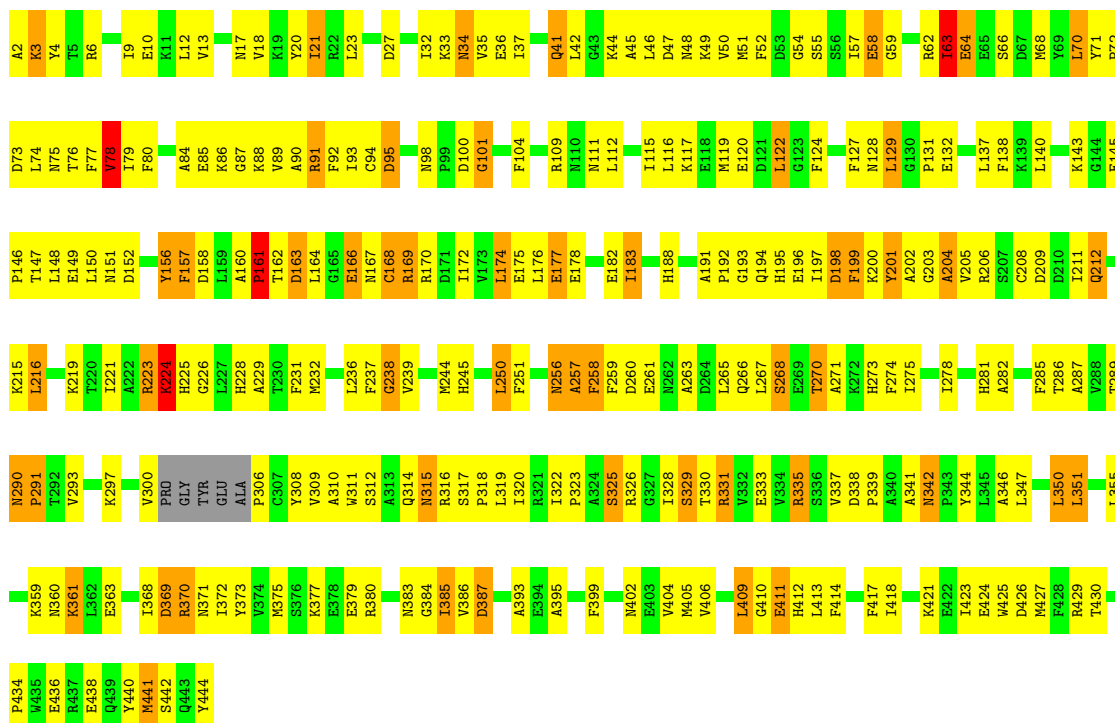
Chain F: 31% 57% 10% .





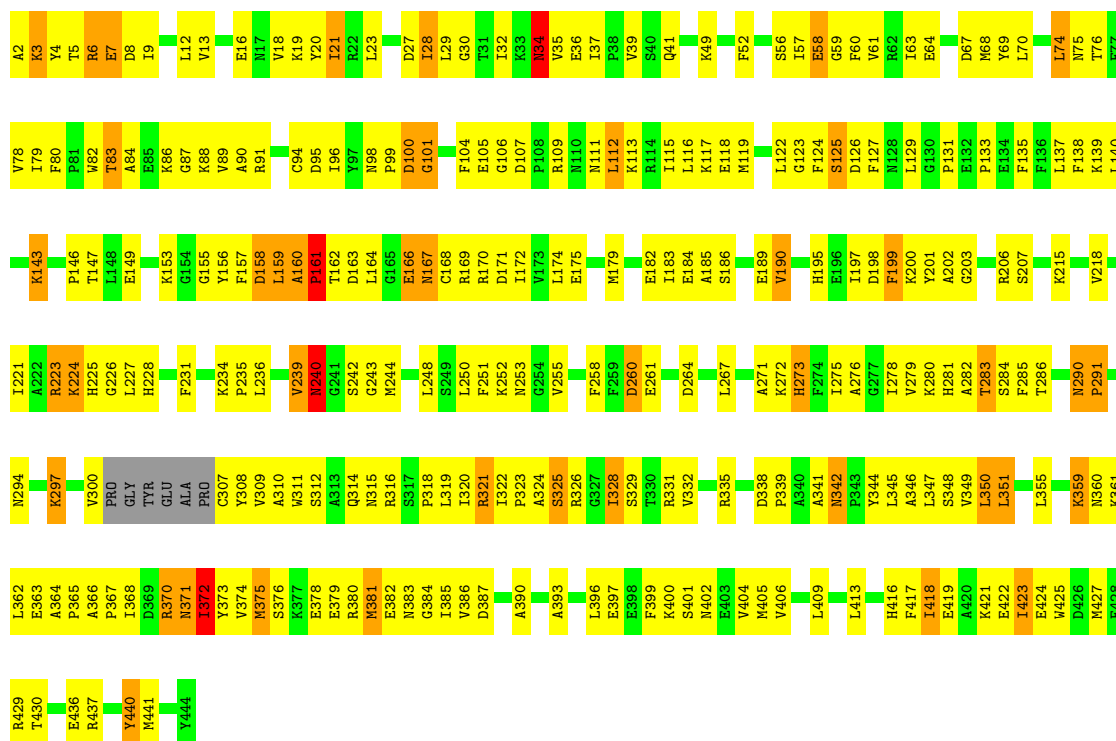
• Molecule 1: Glutamine synthetase

Chain G: 38% 48% 12% ..



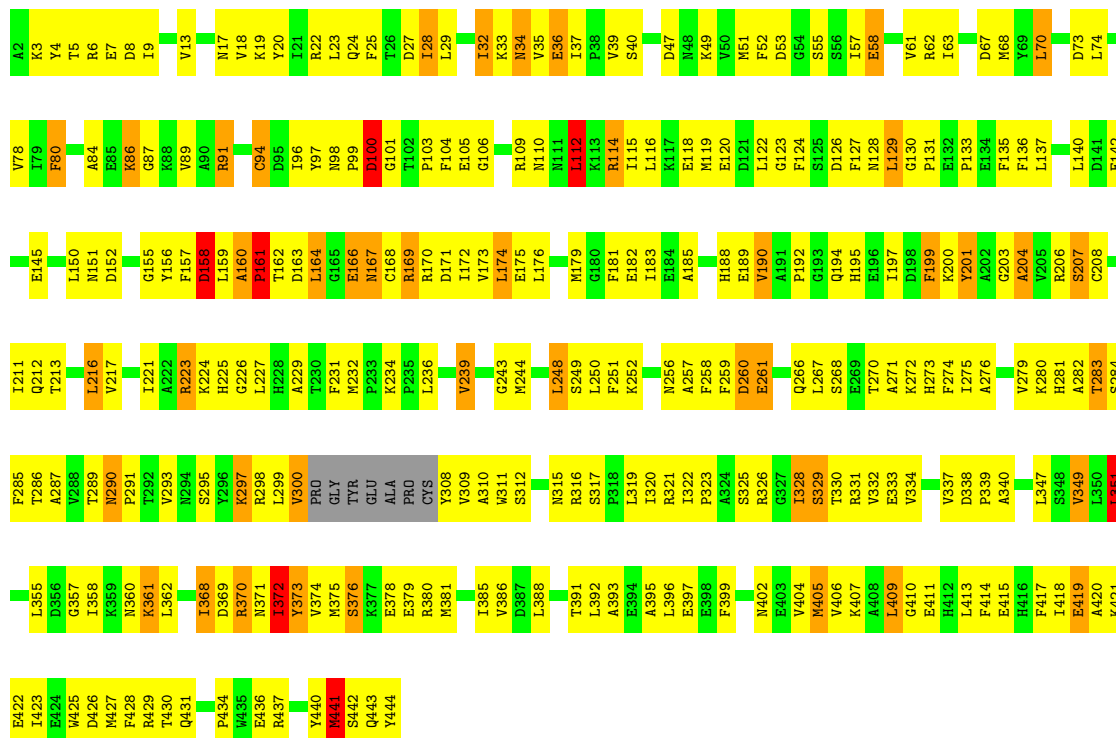
• Molecule 1: Glutamine synthetase

Chain H: 37% 51% 10% ..

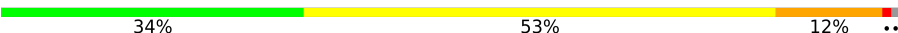


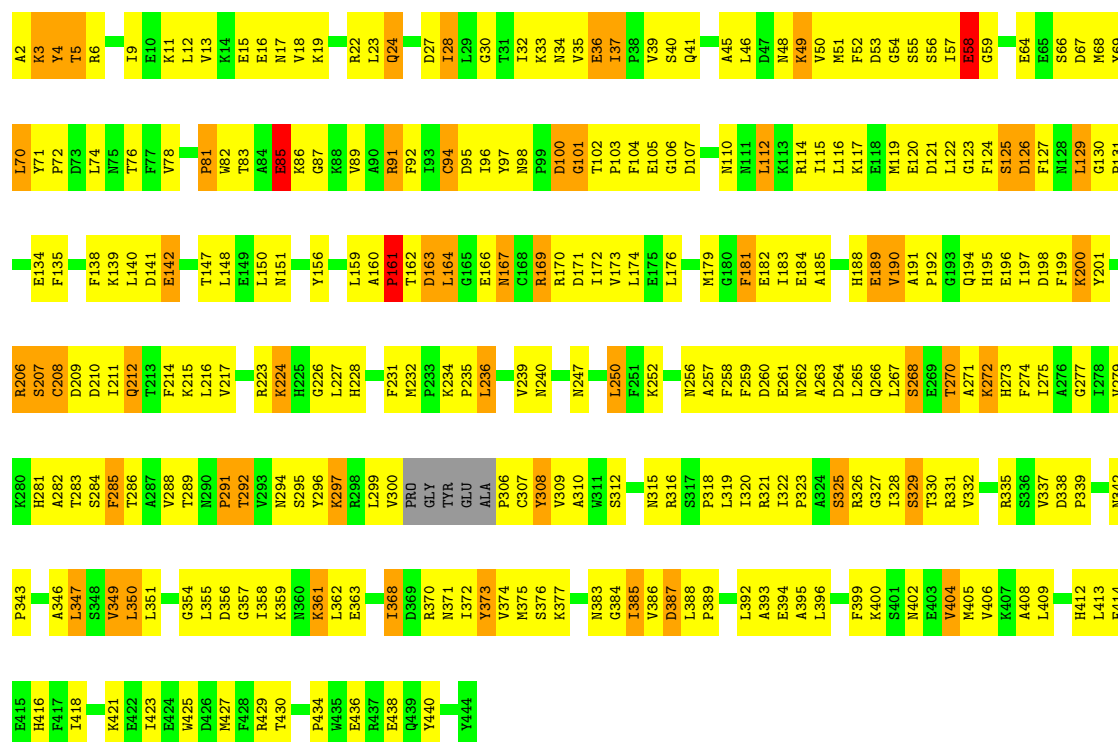
• Molecule 1: Glutamine synthetase

Chain I: 35% 51% 10% . .



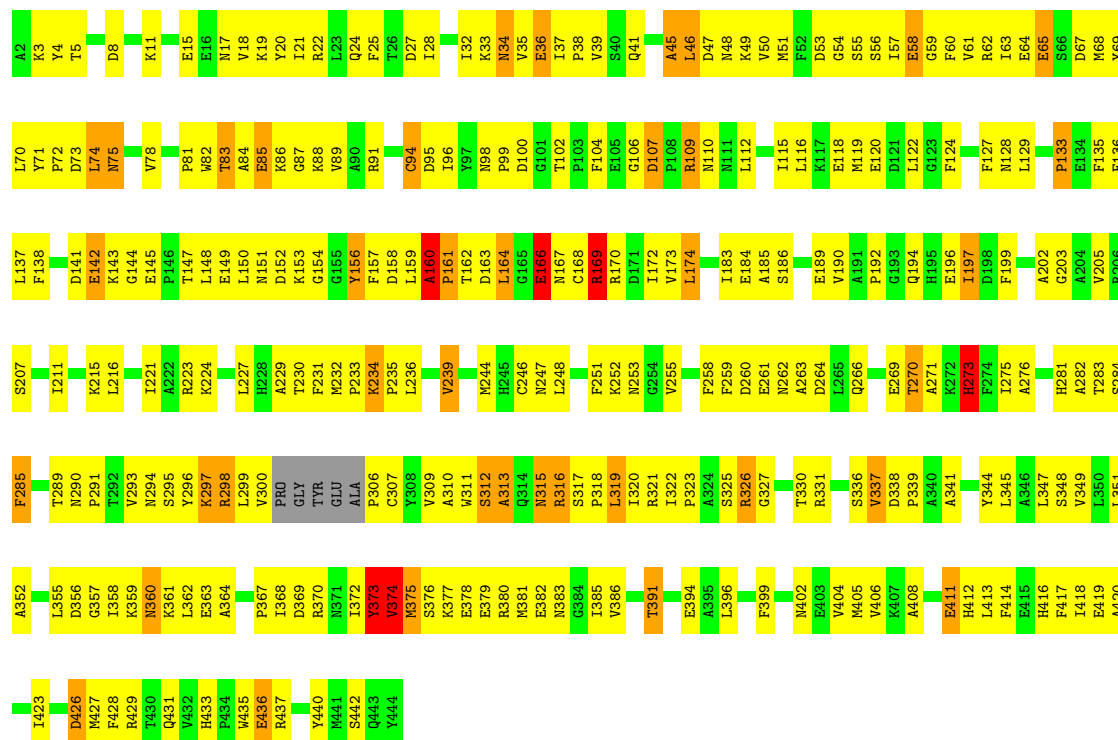
• Molecule 1: Glutamine synthetase

Chain J:  34% 53% 12% ..

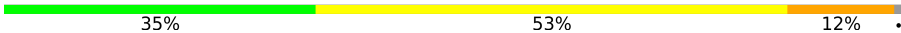


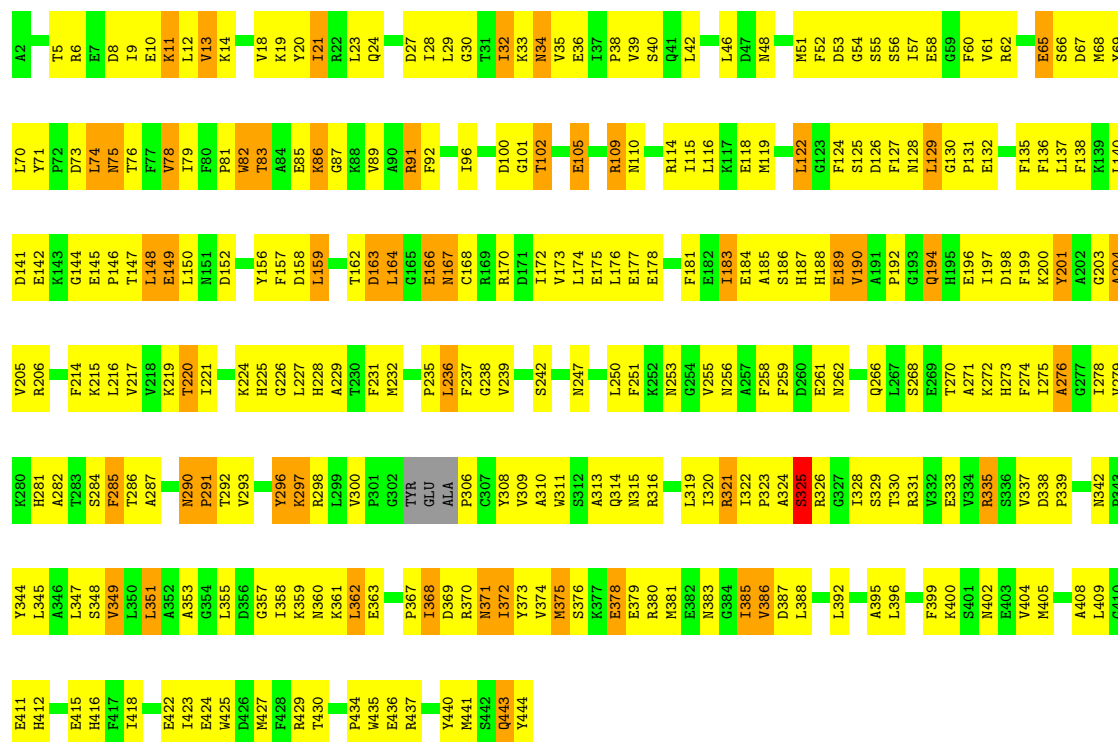
● Molecule 1: Glutamine synthetase

Chain K:  35% 54% 9% ..



● Molecule 1: Glutamine synthetase

Chain L:  35% 53% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	109.99Å 138.38Å 138.74Å 119.80° 90.19° 93.85°	Depositor
Resolution (Å)	84.25 – 3.10 84.25 – 3.10	Depositor EDS
% Data completeness (in resolution range)	85.7 (84.25-3.10) 84.4 (84.25-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.13Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.217 , 0.267 0.217 , 0.267	Depositor DCC
R_{free} test set	8289 reflections (7.53%)	wwPDB-VP
Wilson B-factor (Å ²)	70.3	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.327 for -h,-k-l,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	42284	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.47	0/3586	0.94	11/4849 (0.2%)
1	B	0.48	0/3586	0.94	9/4849 (0.2%)
1	C	0.49	0/3578	0.96	18/4838 (0.4%)
1	D	0.48	0/3586	0.94	12/4849 (0.2%)
1	E	0.49	0/3578	0.91	9/4837 (0.2%)
1	F	0.49	0/3570	0.94	10/4826 (0.2%)
1	G	0.48	0/3578	0.94	12/4837 (0.2%)
1	H	0.49	0/3570	0.97	16/4826 (0.3%)
1	I	0.48	0/3564	0.98	17/4818 (0.4%)
1	J	0.53	2/3578 (0.1%)	0.94	12/4837 (0.2%)
1	K	0.47	0/3578	0.97	21/4837 (0.4%)
1	L	0.51	0/3590	0.96	7/4854 (0.1%)
All	All	0.49	2/42942 (0.0%)	0.95	154/58057 (0.3%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	3	LYS	C-N	7.96	1.43	1.33
1	J	4	TYR	N-CA	6.35	1.54	1.46

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	86	LYS	N-CA-C	-9.22	103.19	112.97
1	A	374	VAL	N-CA-C	-8.27	105.12	113.47
1	K	86	LYS	N-CA-C	-8.25	103.41	113.97
1	E	297	LYS	N-CA-C	-8.15	103.34	113.20
1	A	291	PRO	N-CA-C	7.61	123.39	114.03
1	I	190	VAL	N-CA-C	7.37	118.14	110.62
1	A	290	ASN	CA-C-N	7.28	127.45	119.87
1	A	290	ASN	C-N-CA	7.28	127.45	119.87
1	G	84	ALA	N-CA-C	-7.28	98.74	110.32
1	C	128	ASN	N-CA-C	7.18	120.24	110.55
1	E	440	TYR	N-CA-C	7.07	119.84	111.71
1	K	184	GLU	N-CA-C	-7.02	103.24	111.03
1	I	36	GLU	N-CA-C	6.90	120.31	109.96
1	K	46	LEU	N-CA-C	-6.81	101.74	110.19
1	B	351	LEU	N-CA-C	-6.78	103.82	111.14
1	C	84	ALA	N-CA-C	-6.73	101.19	110.35
1	G	290	ASN	CA-C-N	6.68	126.13	118.85
1	G	290	ASN	C-N-CA	6.68	126.13	118.85
1	D	290	ASN	CA-C-N	6.66	128.16	119.84
1	D	290	ASN	C-N-CA	6.66	128.16	119.84
1	E	117	LYS	N-CA-C	-6.65	104.11	111.36
1	F	93	ILE	N-CA-C	-6.53	100.27	108.89
1	A	80	PHE	CA-C-N	6.48	126.61	119.87
1	A	80	PHE	C-N-CA	6.48	126.61	119.87
1	J	404	VAL	N-CA-C	6.45	117.20	110.62
1	K	107	ASP	CA-C-N	6.44	126.67	119.32
1	K	107	ASP	C-N-CA	6.44	126.67	119.32
1	H	382	GLU	N-CA-C	-6.41	105.28	113.23
1	G	21	ILE	N-CA-C	6.41	117.10	107.80
1	H	290	ASN	CA-C-N	6.41	126.10	119.82
1	H	290	ASN	C-N-CA	6.41	126.10	119.82
1	H	423	ILE	N-CA-C	-6.39	104.52	110.53
1	E	84	ALA	N-CA-C	-6.37	100.77	110.14
1	L	128	ASN	N-CA-C	6.35	119.12	110.55
1	C	232	MET	CA-C-N	6.31	126.22	119.28
1	C	232	MET	C-N-CA	6.31	126.22	119.28
1	A	373	TYR	N-CA-C	6.30	120.31	111.30
1	H	342	ASN	CA-C-N	6.28	125.77	119.24
1	H	342	ASN	C-N-CA	6.28	125.77	119.24
1	C	298	ARG	N-CA-C	-6.16	105.81	113.38
1	L	297	LYS	N-CA-C	-6.14	105.89	113.19
1	G	331	ARG	N-CA-C	6.12	117.88	109.18
1	H	223	ARG	N-CA-C	-6.12	104.24	111.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	80	PHE	N-CA-C	6.12	117.09	109.57
1	F	128	ASN	N-CA-C	6.09	118.38	110.53
1	I	223	ARG	N-CA-C	-6.07	104.58	111.14
1	C	290	ASN	CA-C-N	6.04	127.39	119.84
1	C	290	ASN	C-N-CA	6.04	127.39	119.84
1	J	412	HIS	N-CA-C	6.02	117.51	111.07
1	K	273	HIS	N-CA-C	-6.02	104.65	112.23
1	J	4	TYR	N-CA-C	6.01	117.95	107.49
1	C	211	ILE	N-CA-C	-6.01	104.65	110.72
1	K	122	LEU	N-CA-C	-5.96	105.66	113.17
1	F	297	LYS	N-CA-C	-5.95	105.98	113.18
1	I	243	GLY	N-CA-C	-5.95	102.19	112.06
1	C	338	ASP	CA-C-N	5.93	125.80	119.28
1	C	338	ASP	C-N-CA	5.93	125.80	119.28
1	F	331	ARG	N-CA-C	5.92	117.85	108.79
1	H	83	THR	N-CA-C	5.91	118.36	108.73
1	K	160	ALA	CA-C-N	5.90	127.21	119.84
1	K	160	ALA	C-N-CA	5.90	127.21	119.84
1	E	34	ASN	N-CA-C	5.87	117.45	108.52
1	D	404	VAL	N-CA-C	5.87	116.52	110.36
1	D	188	HIS	N-CA-C	-5.82	101.91	110.52
1	C	107	ASP	CA-C-N	5.81	125.50	119.05
1	C	107	ASP	C-N-CA	5.81	125.50	119.05
1	G	47	ASP	N-CA-C	-5.79	105.80	112.92
1	B	234	LYS	CA-C-N	5.77	125.14	118.85
1	B	234	LYS	C-N-CA	5.77	125.14	118.85
1	A	322	ILE	CA-C-N	5.76	126.57	120.11
1	A	322	ILE	C-N-CA	5.76	126.57	120.11
1	I	94	CYS	N-CA-C	5.74	117.47	110.41
1	I	112	LEU	N-CA-C	-5.74	104.94	111.14
1	I	297	LYS	N-CA-C	-5.74	106.28	113.28
1	D	84	ALA	N-CA-C	-5.73	102.42	110.50
1	F	424	GLU	N-CA-C	-5.73	104.94	111.07
1	C	200	LYS	N-CA-C	-5.72	102.01	110.48
1	I	298	ARG	N-CA-C	-5.72	106.47	113.50
1	C	288	VAL	N-CA-C	-5.71	107.33	112.12
1	E	211	ILE	N-CA-C	-5.69	104.96	110.42
1	E	335	ARG	N-CA-C	5.66	119.89	113.15
1	D	291	PRO	N-CA-C	5.66	124.12	112.47
1	F	24	GLN	N-CA-C	5.65	119.31	110.32
1	E	94	CYS	N-CA-C	5.64	118.15	109.07
1	K	128	ASN	N-CA-C	5.64	119.16	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	290	ASN	CA-C-N	5.63	124.83	118.97
1	I	290	ASN	C-N-CA	5.63	124.83	118.97
1	D	159	LEU	N-CA-C	-5.62	101.78	109.71
1	G	291	PRO	N-CA-C	5.61	120.92	113.40
1	J	24	GLN	N-CA-C	5.61	119.19	110.17
1	F	234	LYS	CA-C-N	5.60	126.84	119.84
1	F	234	LYS	C-N-CA	5.60	126.84	119.84
1	K	234	LYS	CA-C-N	5.59	125.06	119.24
1	K	234	LYS	C-N-CA	5.59	125.06	119.24
1	H	240	ASN	N-CA-C	5.58	117.11	110.19
1	G	278	ILE	N-CA-C	-5.58	105.66	110.74
1	L	290	ASN	CA-C-N	5.57	126.80	119.84
1	L	290	ASN	C-N-CA	5.57	126.80	119.84
1	J	100	ASP	N-CA-C	5.56	118.41	111.24
1	B	117	LYS	N-CA-C	-5.53	105.34	111.36
1	L	335	ARG	N-CA-C	5.53	119.65	113.02
1	H	199	PHE	CB-CA-C	-5.52	107.50	114.40
1	A	297	LYS	N-CA-C	-5.52	106.50	113.18
1	H	34	ASN	N-CA-C	5.50	116.59	107.73
1	H	297	LYS	N-CA-C	-5.48	105.85	112.54
1	B	94	CYS	N-CA-C	5.46	117.56	109.69
1	J	2	ALA	CA-C-N	5.45	131.96	121.54
1	J	2	ALA	C-N-CA	5.45	131.96	121.54
1	B	74	LEU	N-CA-C	5.43	119.40	112.34
1	K	133	PRO	N-CA-C	5.43	119.00	110.80
1	I	397	GLU	N-CA-C	-5.43	105.47	111.71
1	H	440	TYR	N-CA-C	5.42	120.91	113.97
1	A	34	ASN	N-CA-C	5.42	116.77	108.42
1	C	441	MET	N-CA-C	5.40	117.92	111.71
1	D	191	ALA	CA-C-N	5.40	125.57	119.90
1	D	191	ALA	C-N-CA	5.40	125.57	119.90
1	K	269	GLU	N-CA-C	-5.39	106.66	113.18
1	F	34	ASN	N-CA-C	5.39	116.33	108.14
1	I	24	GLN	N-CA-C	5.38	118.44	110.48
1	I	351	LEU	N-CA-C	-5.38	105.50	111.36
1	D	278	ILE	N-CA-C	-5.36	105.49	110.53
1	D	339	PRO	N-CA-C	5.36	120.56	113.86
1	E	288	VAL	N-CA-C	-5.36	106.58	111.67
1	J	297	LYS	N-CA-C	-5.34	106.72	113.18
1	J	28	ILE	N-CA-C	5.31	115.51	110.42
1	I	80	PHE	CA-C-N	5.29	124.92	119.05
1	I	80	PHE	C-N-CA	5.29	124.92	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	443	GLN	N-CA-C	-5.28	105.93	112.38
1	H	234	LYS	CA-C-N	5.28	125.08	119.28
1	H	234	LYS	C-N-CA	5.28	125.08	119.28
1	G	80	PHE	CA-C-N	5.27	124.94	119.56
1	G	80	PHE	C-N-CA	5.27	124.94	119.56
1	B	324	ALA	N-CA-C	-5.26	105.23	110.97
1	L	441	MET	N-CA-C	5.22	117.88	111.82
1	H	291	PRO	N-CA-C	5.22	120.72	113.98
1	B	335	ARG	N-CA-C	5.14	119.42	113.20
1	F	223	ARG	N-CA-C	-5.13	105.77	111.36
1	G	270	THR	N-CA-C	-5.13	105.60	111.14
1	J	4	TYR	CB-CA-C	-5.13	104.38	110.94
1	K	319	LEU	N-CA-C	-5.08	106.25	112.90
1	J	189	GLU	N-CA-C	5.07	117.22	110.53
1	B	84	ALA	N-CA-C	-5.07	102.11	109.31
1	K	336	SER	N-CA-C	5.06	117.58	111.40
1	G	212	GLN	N-CA-C	-5.04	105.43	111.03
1	J	416	HIS	N-CA-C	5.04	116.47	111.07
1	K	297	LYS	N-CA-C	-5.04	107.11	113.20
1	K	45	ALA	N-CA-C	-5.03	105.44	111.03
1	C	80	PHE	CA-C-N	5.02	124.74	119.82
1	C	80	PHE	C-N-CA	5.02	124.74	119.82
1	C	387	ASP	N-CA-C	5.01	116.93	108.96
1	K	154	GLY	N-CA-C	5.01	118.61	112.14
1	K	433	HIS	CA-C-N	5.00	125.02	119.32
1	K	433	HIS	C-N-CA	5.00	125.02	119.32
1	I	405	MET	N-CA-C	-5.00	105.91	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	296	TYR	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	3505	0	3443	332	0
1	B	3505	0	3443	305	0
1	C	3498	0	3435	313	0
1	D	3505	0	3443	329	0
1	E	3498	0	3436	351	0
1	F	3491	0	3428	357	0
1	G	3498	0	3436	320	0
1	H	3491	0	3428	316	0
1	I	3485	0	3423	320	0
1	J	3498	0	3436	338	0
1	K	3498	0	3436	333	0
1	L	3509	0	3446	318	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	D	10	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	H	5	0	0	0	0
4	A	17	0	0	4	0
4	B	27	0	0	1	0
4	C	28	0	0	1	0
4	D	20	0	0	3	0
4	E	17	0	0	1	0
4	F	24	0	0	1	0
4	G	21	0	0	4	0
4	H	20	0	0	2	0
4	I	23	0	0	2	0
4	J	12	0	0	1	0
4	K	22	0	0	1	0
4	L	22	0	0	2	0
All	All	42284	0	41233	3660	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 44.

All (3660) 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:F:232:MET:HE3	1:L:440:TYR:HB2	1.24	1.20
1:K:83:THR:HG21	1:K:89:VAL:H	1.13	1.09
1:F:286:THR:HG23	1:F:290:ASN:HD22	1.19	1.07
1:B:232:MET:HE3	1:H:440:TYR:HB2	1.34	1.07
1:I:173:VAL:HG13	1:I:183:ILE:HD12	1.31	1.07
1:I:372:ILE:HG22	1:I:385:ILE:HD13	1.37	1.05
1:G:371:ASN:HD22	1:G:375:MET:HB3	1.18	1.04
1:E:9:ILE:HG13	1:E:74:LEU:HD12	1.39	1.04
1:E:440:TYR:HB2	1:K:232:MET:HE3	1.33	1.03
1:C:372:ILE:HG22	1:C:385:ILE:HD13	1.40	1.02
1:E:232:MET:HE3	1:K:440:TYR:HB2	1.42	1.02
1:E:319:LEU:HG	1:E:320:ILE:HD12	1.40	1.02
1:G:27:ASP:HA	1:G:57:ILE:HG23	1.41	1.02
1:I:261:GLU:HA	1:I:266:GLN:HG2	1.37	1.02
1:B:126:ASP:HB2	1:B:251:PHE:HB2	1.37	1.02
1:J:98:ASN:HD22	1:J:102:THR:HG23	1.24	1.02
1:G:258:PHE:HB2	1:G:271:ALA:HB2	1.40	1.01
1:J:272:LYS:HA	1:J:275:ILE:HD12	1.42	1.01
1:F:13:VAL:HG13	1:F:18:VAL:HB	1.43	1.00
1:F:440:TYR:HB2	1:L:232:MET:HE3	1.38	1.00
1:B:153:LYS:H	1:B:153:LYS:HE2	1.23	0.99
1:J:182:GLU:HB3	1:J:200:LYS:HE2	1.44	0.99
1:H:182:GLU:HB3	1:H:200:LYS:HD2	1.42	0.98
1:A:380:ARG:HH11	1:A:380:ARG:HB2	1.28	0.97
1:A:160:ALA:HB1	1:A:161:PRO:HD2	1.45	0.97
1:H:321:ARG:HG2	1:H:335:ARG:HD2	1.45	0.97
1:K:315:ASN:HD21	1:K:370:ARG:H	1.10	0.95
1:H:140:LEU:HD21	1:H:223:ARG:NH2	1.81	0.95
1:E:232:MET:HE1	1:K:437:ARG:HA	1.48	0.94
1:H:129:LEU:HD13	1:H:131:PRO:HD3	1.46	0.94
1:I:328:ILE:HD13	1:I:328:ILE:H	1.32	0.94
1:I:129:LEU:HD22	1:I:131:PRO:HG3	1.49	0.94
1:K:160:ALA:HB1	1:K:161:PRO:HD2	1.50	0.93
1:K:370:ARG:HH21	1:K:374:VAL:HG22	1.32	0.93
1:D:129:LEU:HD13	1:D:131:PRO:HD3	1.51	0.92
1:H:5:THR:H	1:H:8:ASP:HB2	1.34	0.92
1:F:371:ASN:HD21	1:F:373:TYR:HB2	1.32	0.92
1:J:386:VAL:HG12	1:J:387:ASP:H	1.31	0.92
1:B:325:SER:HB2	1:B:331:ARG:NH2	1.85	0.92
1:F:146:PRO:HG3	1:F:228:HIS:CD2	2.04	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:281:HIS:CD2	1:J:402:ASN:HD21	1.88	0.92
1:G:182:GLU:HB3	1:G:200:LYS:HD2	1.52	0.91
1:K:33:LYS:HA	1:L:158:ASP:HA	1.53	0.91
1:L:315:ASN:HD21	1:L:370:ARG:HA	1.36	0.91
1:F:429:ARG:HH21	1:L:300:VAL:HG22	1.33	0.91
1:H:74:LEU:HD22	1:H:74:LEU:H	1.35	0.91
1:I:57:ILE:HD11	1:I:96:ILE:HG12	1.53	0.91
1:E:325:SER:HB2	1:E:331:ARG:HH22	1.34	0.90
1:K:316:ARG:HH11	1:K:316:ARG:H	1.16	0.90
1:J:281:HIS:HD2	1:J:402:ASN:HD21	1.20	0.90
1:J:371:ASN:HD22	1:J:374:VAL:HG22	1.34	0.90
1:C:51:MET:HE3	1:C:67:ASP:HB3	1.52	0.90
1:H:13:VAL:HG13	1:H:18:VAL:HB	1.51	0.90
1:B:370:ARG:HH22	1:B:375:MET:HG3	1.36	0.90
1:C:404:VAL:HG13	1:C:405:MET:HE3	1.53	0.89
1:I:63:ILE:HG22	1:J:316:ARG:HD3	1.55	0.89
1:G:370:ARG:HD3	1:G:370:ARG:H	1.35	0.89
1:F:300:VAL:HG22	1:L:429:ARG:NH2	1.88	0.89
1:J:377:LYS:H	1:J:377:LYS:HD2	1.37	0.88
1:I:86:LYS:HB3	1:J:174:LEU:HD13	1.55	0.88
1:J:160:ALA:HB3	1:J:169:ARG:HH12	1.38	0.88
1:I:248:LEU:HD11	1:I:334:VAL:HG23	1.54	0.88
1:J:13:VAL:HG13	1:J:18:VAL:HB	1.52	0.88
1:L:55:SER:HB2	1:L:62:ARG:HG3	1.56	0.88
1:G:281:HIS:NE2	1:G:404:VAL:HG11	1.88	0.87
1:B:201:TYR:HB2	4:B:602:HOH:O	1.73	0.87
1:A:306:PRO:HB3	1:A:319:LEU:HA	1.53	0.87
1:F:300:VAL:HG22	1:L:429:ARG:HH22	1.39	0.87
1:B:429:ARG:HH21	1:H:390:ALA:HB1	1.37	0.87
1:D:150:LEU:HD13	1:D:192:PRO:HB2	1.56	0.87
1:E:57:ILE:HD11	1:E:96:ILE:HG12	1.55	0.86
1:F:286:THR:HG23	1:F:290:ASN:ND2	1.89	0.86
1:G:310:ALA:HB1	1:G:368:ILE:HG12	1.55	0.86
1:E:13:VAL:HG13	1:E:18:VAL:HB	1.56	0.86
1:E:281:HIS:HD2	1:E:402:ASN:HD21	1.20	0.86
1:A:200:LYS:HZ1	1:B:41:GLN:HE22	1.19	0.86
1:K:313:ALA:HA	1:K:321:ARG:HG3	1.56	0.86
1:E:319:LEU:HG	1:E:320:ILE:CD1	2.05	0.85
1:G:32:ILE:HD13	1:G:216:LEU:HD12	1.56	0.85
1:H:404:VAL:HG13	1:H:405:MET:HE2	1.57	0.85
1:D:319:LEU:HD23	1:D:320:ILE:HG12	1.59	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:LYS:HB3	1:B:75:ASN:OD1	1.77	0.84
1:E:129:LEU:HD23	1:E:347:LEU:HD21	1.59	0.84
1:G:160:ALA:HB1	1:G:161:PRO:HD2	1.57	0.84
1:B:182:GLU:HB3	1:B:200:LYS:HD2	1.59	0.84
1:G:115:ILE:HG22	1:G:351:LEU:HD13	1.59	0.84
1:B:153:LYS:HE2	1:B:153:LYS:N	1.92	0.84
1:H:370:ARG:HH22	1:H:375:MET:HE3	1.40	0.84
1:E:316:ARG:HB3	1:E:372:ILE:HD11	1.60	0.84
1:J:236:LEU:HB2	1:J:239:VAL:HG21	1.60	0.84
1:F:368:ILE:HG23	1:F:372:ILE:HD11	1.57	0.84
1:J:54:GLY:O	1:J:57:ILE:HG12	1.77	0.83
1:F:3:LYS:HB3	1:F:75:ASN:OD1	1.77	0.83
1:J:9:ILE:HG13	1:J:74:LEU:HD12	1.58	0.83
1:J:236:LEU:HB2	1:J:239:VAL:CG2	2.06	0.83
1:L:57:ILE:HD11	1:L:96:ILE:HG12	1.60	0.83
1:E:140:LEU:HD12	1:E:226:GLY:C	2.03	0.83
1:F:45:ALA:HA	1:F:50:VAL:HG23	1.59	0.83
1:G:371:ASN:HB3	1:G:375:MET:HG2	1.60	0.83
1:I:280:LYS:HE3	1:I:281:HIS:HE2	1.43	0.83
1:J:231:PHE:HB3	1:J:339:PRO:HB2	1.61	0.83
1:B:236:LEU:HD12	1:B:239:VAL:HG21	1.61	0.83
1:B:27:ASP:OD1	1:B:33:LYS:HE3	1.79	0.83
1:H:129:LEU:CD1	1:H:131:PRO:HD3	2.09	0.83
1:L:27:ASP:HA	1:L:57:ILE:HG23	1.60	0.82
1:F:182:GLU:HB3	1:F:200:LYS:HD2	1.60	0.82
1:G:236:LEU:HB2	1:G:239:VAL:CG2	2.09	0.82
1:D:160:ALA:HB1	1:D:161:PRO:HD2	1.59	0.82
1:L:386:VAL:HG12	1:L:387:ASP:H	1.43	0.82
1:J:275:ILE:O	1:J:279:VAL:HG23	1.80	0.82
1:E:91:ARG:HD2	1:E:91:ARG:C	2.05	0.82
1:F:300:VAL:HG21	1:L:430:THR:HG22	1.60	0.82
1:A:338:ASP:HB2	1:A:339:PRO:HD2	1.61	0.82
1:G:54:GLY:HA3	1:G:68:MET:HE3	1.59	0.82
1:L:375:MET:HG3	1:L:379:GLU:HG3	1.60	0.82
1:F:404:VAL:HG13	1:F:405:MET:HE2	1.60	0.81
1:F:136:PHE:CD1	1:F:235:PRO:HG2	2.14	0.81
1:B:150:LEU:HD13	1:B:192:PRO:O	1.80	0.81
1:D:91:ARG:HD2	1:D:91:ARG:C	2.05	0.81
1:K:83:THR:HG21	1:K:89:VAL:N	1.94	0.81
1:J:306:PRO:HG2	1:J:335:ARG:HB2	1.61	0.81
1:L:52:PHE:CZ	1:L:54:GLY:HA2	2.14	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:127:PHE:CE2	1:L:351:LEU:HG	2.15	0.81
1:G:325:SER:HB2	1:G:331:ARG:NH2	1.94	0.81
1:F:297:LYS:HD3	1:L:429:ARG:O	1.79	0.81
1:A:252:LYS:HB2	1:A:252:LYS:NZ	1.96	0.81
1:E:310:ALA:HB1	1:E:368:ILE:HG12	1.63	0.81
1:G:236:LEU:HB2	1:G:239:VAL:HG21	1.62	0.81
1:B:132:GLU:HB3	1:B:196:GLU:OE1	1.80	0.81
1:G:129:LEU:HD13	1:G:131:PRO:HD3	1.63	0.81
1:B:370:ARG:HH22	1:B:375:MET:CG	1.95	0.80
1:C:402:ASN:O	1:C:406:VAL:HG23	1.82	0.80
1:L:404:VAL:HG13	1:L:405:MET:HE2	1.63	0.80
1:B:325:SER:HB2	1:B:331:ARG:HH22	1.46	0.80
1:B:281:HIS:NE2	1:B:404:VAL:HG21	1.97	0.80
1:H:41:GLN:HE22	1:I:200:LYS:NZ	1.78	0.80
1:E:286:THR:HG23	1:E:290:ASN:HD22	1.47	0.80
1:L:166:GLU:O	1:L:168:CYS:N	2.14	0.80
1:J:212:GLN:OE1	1:J:212:GLN:HA	1.81	0.80
1:E:314:GLN:HE22	1:E:321:ARG:HH21	1.30	0.80
1:H:160:ALA:HB1	1:H:161:PRO:HD2	1.63	0.80
1:C:310:ALA:HB2	1:C:385:ILE:HG23	1.64	0.79
1:F:16:GLU:O	1:F:88:LYS:HE2	1.82	0.79
1:I:5:THR:HG23	1:I:8:ASP:H	1.47	0.79
1:K:152:ASP:HB3	1:K:161:PRO:HG3	1.64	0.79
1:D:273:HIS:O	1:D:276:ALA:HB3	1.82	0.79
1:E:406:VAL:HG22	1:E:414:PHE:CE1	2.18	0.79
1:E:314:GLN:NE2	1:E:321:ARG:HH21	1.81	0.79
1:G:371:ASN:ND2	1:G:375:MET:HB3	1.97	0.79
1:J:389:PRO:HB2	1:J:394:GLU:HB3	1.64	0.79
1:I:27:ASP:HA	1:I:57:ILE:HG23	1.63	0.79
1:L:83:THR:HG21	1:L:89:VAL:HB	1.65	0.79
1:A:310:ALA:HB3	1:A:372:ILE:HD13	1.62	0.78
1:A:355:LEU:O	1:A:359:LYS:HG2	1.83	0.78
1:B:345:LEU:HD22	1:B:409:LEU:HD21	1.64	0.78
1:C:281:HIS:CE1	1:C:404:VAL:HG11	2.18	0.78
1:F:57:ILE:HD11	1:F:96:ILE:HG12	1.64	0.78
1:J:190:VAL:HG13	1:J:191:ALA:H	1.47	0.78
1:K:270:THR:HG22	1:K:358:ILE:HD12	1.63	0.78
1:E:285:PHE:HB2	1:E:349:VAL:CG1	2.14	0.78
1:K:404:VAL:HG23	1:K:405:MET:HE3	1.65	0.78
1:J:98:ASN:ND2	1:J:102:THR:HG23	1.98	0.78
1:F:286:THR:CG2	1:F:290:ASN:HD22	1.95	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:368:ILE:CG2	1:F:372:ILE:HD11	2.12	0.78
1:H:98:ASN:HD21	1:H:104:PHE:HA	1.46	0.78
1:H:272:LYS:HE3	1:H:363:GLU:HA	1.64	0.78
1:J:156:TYR:HB2	1:J:190:VAL:HA	1.65	0.78
1:K:357:GLY:HA2	1:K:362:LEU:HD13	1.64	0.78
1:L:67:ASP:O	1:L:68:MET:HG3	1.83	0.78
1:L:291:PRO:O	1:L:392:LEU:HD13	1.84	0.78
1:E:372:ILE:HD12	1:E:373:TYR:N	1.99	0.78
1:G:250:LEU:HB2	1:G:258:PHE:CZ	2.19	0.78
1:I:150:LEU:HD13	1:I:192:PRO:O	1.83	0.78
1:G:132:GLU:HA	1:G:198:ASP:HB3	1.64	0.77
1:H:380:ARG:NH1	1:H:380:ARG:HB2	1.98	0.77
1:C:436:GLU:OE2	1:I:297:LYS:HE3	1.85	0.77
1:G:160:ALA:HB2	1:G:188:HIS:HD2	1.50	0.77
1:A:135:PHE:HB3	1:A:231:PHE:CE1	2.19	0.77
1:D:111:ASN:HD21	1:D:409:LEU:HA	1.50	0.77
1:E:257:ALA:O	1:E:270:THR:HB	1.84	0.77
1:G:13:VAL:HG13	1:G:18:VAL:HB	1.65	0.77
1:A:41:GLN:HE22	1:F:200:LYS:HE2	1.48	0.77
1:D:68:MET:HE1	1:D:104:PHE:HB2	1.66	0.77
1:E:136:PHE:CD1	1:E:235:PRO:HG2	2.20	0.77
1:F:309:VAL:HB	1:F:386:VAL:HG23	1.65	0.77
1:K:115:ILE:HG22	1:K:351:LEU:HD12	1.64	0.77
1:D:241:GLY:HA3	1:D:298:ARG:HG3	1.66	0.77
1:L:78:VAL:HG13	1:L:91:ARG:HG3	1.66	0.77
1:E:160:ALA:HB1	1:E:161:PRO:HD2	1.67	0.77
1:F:81:PRO:HD3	1:F:179:MET:HE3	1.67	0.77
1:G:86:LYS:HG3	1:H:174:LEU:HB3	1.66	0.77
1:K:316:ARG:HH12	1:K:372:ILE:HG13	1.49	0.77
1:A:440:TYR:HB2	1:G:232:MET:HE3	1.66	0.77
1:B:271:ALA:O	1:B:275:ILE:HD12	1.85	0.77
1:C:164:LEU:HD11	1:D:224:LYS:HD3	1.65	0.77
1:I:406:VAL:HG22	1:I:414:PHE:CE1	2.20	0.77
1:K:127:PHE:CZ	1:K:248:LEU:HD22	2.19	0.77
1:E:273:HIS:CD2	1:E:361:LYS:HA	2.20	0.76
1:F:160:ALA:HB1	1:F:161:PRO:HD2	1.65	0.76
1:J:328:ILE:HD12	1:J:329:SER:N	2.00	0.76
1:H:273:HIS:CD2	1:H:361:LYS:HA	2.20	0.76
1:A:232:MET:HE2	1:A:235:PRO:HA	1.67	0.76
1:A:372:ILE:HG23	1:A:385:ILE:HD13	1.67	0.76
1:C:429:ARG:HH22	1:I:300:VAL:HA	1.49	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:9:ILE:O	1:I:13:VAL:HG23	1.85	0.76
1:B:159:LEU:CD1	1:C:22:ARG:HH11	1.99	0.76
1:G:91:ARG:HD2	1:G:91:ARG:C	2.11	0.76
1:G:399:PHE:HZ	1:G:409:LEU:HD22	1.49	0.76
1:G:21:ILE:HD13	1:G:42:LEU:HD13	1.66	0.76
1:J:30:GLY:HA2	1:J:342:ASN:ND2	2.01	0.76
1:D:371:ASN:ND2	1:D:375:MET:HE3	2.01	0.75
1:H:309:VAL:HG23	1:H:386:VAL:O	1.86	0.75
1:L:109:ARG:HD2	1:L:344:TYR:CE2	2.21	0.75
1:A:273:HIS:CD2	1:A:361:LYS:HA	2.21	0.75
1:B:429:ARG:HH12	1:H:300:VAL:HG23	1.51	0.75
1:C:136:PHE:HB3	1:C:138:PHE:HE1	1.52	0.75
1:E:96:ILE:H	1:E:96:ILE:HD12	1.50	0.75
1:G:34:ASN:HD22	1:G:34:ASN:C	1.93	0.75
1:H:98:ASN:ND2	1:H:104:PHE:HA	2.00	0.75
1:A:129:LEU:HG	1:A:347:LEU:HD21	1.69	0.75
1:J:176:LEU:HB2	1:J:183:ILE:HD11	1.68	0.75
1:J:83:THR:HG21	1:J:89:VAL:HB	1.66	0.75
1:H:372:ILE:H	1:H:372:ILE:HD13	1.50	0.75
1:C:105:GLU:OE1	1:C:412:HIS:HB2	1.86	0.75
1:E:281:HIS:CD2	1:E:402:ASN:HD21	2.04	0.75
1:F:434:PRO:HA	1:F:437:ARG:HH12	1.51	0.75
1:J:160:ALA:HB3	1:J:169:ARG:NH1	2.02	0.75
1:G:4:TYR:HB3	1:G:9:ILE:HD11	1.69	0.75
1:H:242:SER:O	1:H:339:PRO:HD2	1.87	0.75
1:K:11:LYS:HG3	1:K:15:GLU:OE2	1.87	0.75
1:A:34:ASN:HD22	1:A:34:ASN:C	1.94	0.74
1:E:21:ILE:HD13	1:E:39:VAL:HA	1.68	0.74
1:L:91:ARG:HD2	1:L:91:ARG:C	2.11	0.74
1:F:232:MET:CE	1:L:440:TYR:HB2	2.13	0.74
1:F:98:ASN:HD22	1:F:98:ASN:N	1.83	0.74
1:B:338:ASP:HB2	1:B:339:PRO:HD2	1.69	0.74
1:K:273:HIS:CD2	1:K:361:LYS:HA	2.21	0.74
1:B:232:MET:HE1	1:H:437:ARG:HA	1.70	0.74
1:D:129:LEU:HD22	1:D:130:GLY:N	2.03	0.74
1:F:312:SER:HB2	1:F:368:ILE:HB	1.69	0.74
1:I:225:HIS:O	1:I:227:LEU:HG	1.88	0.74
1:A:380:ARG:HB2	1:A:380:ARG:NH1	2.03	0.73
1:B:129:LEU:HG	1:B:347:LEU:HD21	1.70	0.73
1:F:232:MET:HE1	1:L:437:ARG:HA	1.69	0.73
1:H:106:GLY:O	1:H:413:LEU:HD21	1.86	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:272:LYS:C	1:H:272:LYS:HD3	2.13	0.73
1:E:100:ASP:O	1:E:102:THR:HG23	1.88	0.73
1:E:136:PHE:HD1	1:E:235:PRO:HG2	1.52	0.73
1:A:206:ARG:HG2	1:A:206:ARG:HH11	1.52	0.73
1:D:309:VAL:HG13	1:D:319:LEU:HD22	1.70	0.73
1:H:41:GLN:HE22	1:I:200:LYS:HZ2	1.34	0.73
1:I:260:ASP:O	1:I:266:GLN:HA	1.88	0.73
1:J:70:LEU:O	1:J:72:PRO:HD3	1.88	0.73
1:E:76:THR:O	1:E:78:VAL:HG23	1.89	0.73
1:F:380:ARG:HA	1:F:385:ILE:HB	1.71	0.73
1:L:150:LEU:HD13	1:L:192:PRO:O	1.86	0.73
1:K:3:LYS:H	1:K:75:ASN:HB3	1.53	0.73
1:C:129:LEU:HD22	1:C:131:PRO:HD3	1.69	0.73
1:D:252:LYS:O	1:D:255:VAL:HG22	1.88	0.73
1:J:121:ASP:O	1:J:122:LEU:HD22	1.89	0.73
1:J:125:SER:H	1:J:252:LYS:HA	1.53	0.73
1:K:129:LEU:HD22	1:K:347:LEU:HD21	1.70	0.73
1:D:142:GLU:H	1:D:142:GLU:CD	1.95	0.73
1:D:328:ILE:HD12	1:D:329:SER:H	1.52	0.73
1:F:98:ASN:HD21	1:F:104:PHE:HA	1.54	0.73
1:B:148:LEU:HD21	1:H:437:ARG:HD3	1.71	0.72
1:E:158:ASP:OD1	1:F:33:LYS:HE2	1.89	0.72
1:J:282:ALA:HA	1:J:285:PHE:CZ	2.23	0.72
1:A:363:GLU:H	1:A:363:GLU:CD	1.96	0.72
1:D:243:GLY:HA3	1:D:298:ARG:HH12	1.55	0.72
1:K:247:ASN:HB3	1:K:331:ARG:HG3	1.70	0.72
1:D:310:ALA:HB1	1:D:368:ILE:HG21	1.71	0.72
1:E:371:ASN:HB3	1:E:375:MET:SD	2.28	0.72
1:J:404:VAL:HG13	1:J:405:MET:HE2	1.70	0.72
1:B:377:LYS:O	1:B:381:MET:HG2	1.88	0.72
1:G:34:ASN:C	1:G:34:ASN:ND2	2.47	0.72
1:K:233:PRO:C	1:K:235:PRO:HD3	2.14	0.72
1:D:259:PHE:CE2	1:D:326:ARG:HB3	2.24	0.72
1:F:308:TYR:HA	1:F:387:ASP:HA	1.70	0.72
1:F:423:ILE:HD12	1:F:423:ILE:C	2.13	0.72
1:H:172:ILE:HD12	1:H:218:VAL:HA	1.72	0.72
1:J:310:ALA:HB1	1:J:368:ILE:HG21	1.71	0.72
1:D:378:GLU:OE2	1:D:381:MET:HE3	1.90	0.72
1:D:390:ALA:HB1	1:J:429:ARG:HE	1.55	0.72
1:L:116:LEU:O	1:L:119:MET:HG2	1.89	0.72
1:L:287:ALA:HB2	1:L:395:ALA:HB1	1.70	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:VAL:HG22	1:B:405:MET:SD	2.30	0.72
1:E:191:ALA:HB2	1:E:240:ASN:HB3	1.70	0.72
1:F:22:ARG:HD2	1:F:80:PHE:HE1	1.53	0.72
1:G:128:ASN:HA	1:G:202:ALA:O	1.89	0.72
1:H:57:ILE:HD11	1:H:96:ILE:HG12	1.70	0.72
1:I:355:LEU:HD23	1:I:358:ILE:HD12	1.71	0.72
1:A:3:LYS:NZ	1:A:3:LYS:HB3	2.05	0.72
1:A:404:VAL:HG13	1:A:405:MET:HE2	1.72	0.72
1:C:182:GLU:HG3	1:C:200:LYS:HD2	1.69	0.72
1:I:267:LEU:HD11	1:I:322:ILE:HD13	1.70	0.72
1:A:429:ARG:NH2	1:G:300:VAL:HG22	2.05	0.72
1:I:96:ILE:H	1:I:96:ILE:HD12	1.54	0.72
1:K:67:ASP:O	1:K:68:MET:HG3	1.90	0.72
1:K:291:PRO:HG3	1:K:341:ALA:HA	1.71	0.72
1:C:55:SER:HB2	1:C:62:ARG:HG2	1.72	0.71
1:H:112:LEU:O	1:H:116:LEU:HG	1.90	0.71
1:L:51:MET:CE	1:L:67:ASP:HB3	2.20	0.71
1:L:375:MET:HG2	1:L:380:ARG:HG2	1.71	0.71
1:C:366:ALA:HB1	1:C:367:PRO:HD2	1.70	0.71
1:D:140:LEU:HD21	1:D:228:HIS:HB2	1.72	0.71
1:A:429:ARG:HH22	1:G:300:VAL:HG22	1.56	0.71
1:K:310:ALA:HB2	1:K:372:ILE:HG21	1.71	0.71
1:G:183:ILE:H	1:G:183:ILE:HD12	1.55	0.71
1:D:236:LEU:HB2	1:D:239:VAL:CG2	2.20	0.71
1:G:338:ASP:HB2	1:G:339:PRO:HD2	1.73	0.71
1:H:272:LYS:HZ1	1:H:364:ALA:H	1.38	0.71
1:L:82:TRP:HH2	1:L:217:VAL:HG22	1.55	0.71
1:G:23:LEU:HB2	1:G:35:VAL:HG13	1.73	0.71
1:J:72:PRO:HA	1:J:94:CYS:HB3	1.71	0.71
1:A:294:ASN:HB2	1:G:436:GLU:OE2	1.91	0.71
1:A:300:VAL:HG22	1:G:429:ARG:HH22	1.56	0.71
1:B:211:ILE:HG22	1:B:215:LYS:HE3	1.73	0.71
1:B:160:ALA:HB1	1:B:161:PRO:HD2	1.72	0.71
1:G:375:MET:HB2	1:G:379:GLU:HB2	1.73	0.71
1:I:248:LEU:O	1:I:331:ARG:HB2	1.91	0.71
1:J:52:PHE:CE2	1:J:54:GLY:HA2	2.26	0.71
1:K:316:ARG:H	1:K:316:ARG:NH1	1.88	0.71
1:L:189:GLU:HB2	1:L:194:GLN:HB3	1.72	0.71
1:C:150:LEU:CD1	1:C:192:PRO:HG2	2.21	0.70
1:D:345:LEU:HD22	1:D:409:LEU:HD22	1.73	0.70
1:F:437:ARG:HH11	1:F:437:ARG:HB2	1.56	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:142:GLU:H	1:J:142:GLU:CD	1.97	0.70
1:A:45:ALA:HA	1:A:50:VAL:HG23	1.72	0.70
1:E:236:LEU:O	1:E:239:VAL:HG22	1.91	0.70
1:G:402:ASN:O	1:G:406:VAL:HG23	1.91	0.70
1:A:252:LYS:HE3	1:A:253:ASN:HD22	1.56	0.70
1:C:267:LEU:HD21	1:C:326:ARG:NH1	2.07	0.70
1:J:231:PHE:HB3	1:J:339:PRO:CB	2.20	0.70
1:J:371:ASN:ND2	1:J:374:VAL:HG22	2.05	0.70
1:L:51:MET:HE3	1:L:69:TYR:CE1	2.26	0.70
1:L:402:ASN:ND2	1:L:404:VAL:HG12	2.07	0.70
1:C:380:ARG:HH11	1:C:380:ARG:HB2	1.55	0.70
1:A:224:LYS:HB2	1:F:164:LEU:HD11	1.73	0.70
1:F:129:LEU:HD22	1:F:131:PRO:HD3	1.73	0.70
1:G:375:MET:SD	1:G:380:ARG:HG2	2.31	0.70
1:I:375:MET:HE2	1:I:379:GLU:OE2	1.90	0.70
1:B:201:TYR:HD1	1:B:201:TYR:H	1.39	0.70
1:C:182:GLU:CG	1:C:200:LYS:HD2	2.22	0.70
1:A:112:LEU:O	1:A:116:LEU:HG	1.92	0.70
1:A:372:ILE:HG22	1:A:380:ARG:HH21	1.56	0.70
1:E:320:ILE:HG22	1:E:321:ARG:N	2.07	0.70
1:F:437:ARG:HA	1:L:232:MET:HE1	1.72	0.70
1:I:338:ASP:HB2	1:I:339:PRO:HD2	1.74	0.70
1:L:323:PRO:HD2	1:L:331:ARG:O	1.92	0.70
1:J:414:PHE:O	1:J:418:ILE:HG12	1.91	0.70
1:B:368:ILE:HG21	1:B:385:ILE:HD11	1.73	0.70
1:C:58:GLU:O	1:C:61:VAL:HG23	1.91	0.70
1:D:289:THR:O	1:D:341:ALA:HB2	1.92	0.70
1:F:59:GLY:O	1:F:62:ARG:HG3	1.91	0.70
1:J:310:ALA:HA	1:J:368:ILE:HG13	1.74	0.70
1:A:252:LYS:O	1:A:252:LYS:HG3	1.90	0.69
1:C:73:ASP:OD2	1:C:76:THR:HG23	1.90	0.69
1:H:279:VAL:HG13	1:H:309:VAL:HG12	1.72	0.69
1:I:328:ILE:H	1:I:328:ILE:CD1	2.05	0.69
1:B:281:HIS:CD2	1:B:402:ASN:HD21	2.09	0.69
1:C:314:GLN:HE22	1:D:65:GLU:C	2.01	0.69
1:J:119:MET:SD	1:J:127:PHE:HB2	2.32	0.69
1:L:378:GLU:OE1	1:L:381:MET:HG3	1.92	0.69
1:A:127:PHE:CD2	1:A:351:LEU:HD13	2.28	0.69
1:B:261:GLU:C	1:B:262:ASN:HD22	2.00	0.69
1:K:85:GLU:HG2	1:L:170:ARG:HH12	1.58	0.69
1:K:325:SER:HB2	1:K:331:ARG:NH2	2.06	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:325:SER:HB2	1:K:331:ARG:HH22	1.57	0.69
1:G:368:ILE:HD13	1:G:372:ILE:HD11	1.72	0.69
1:H:310:ALA:HB1	1:H:368:ILE:HG12	1.72	0.69
1:E:285:PHE:HB2	1:E:349:VAL:HG11	1.73	0.69
1:F:136:PHE:HB3	1:F:138:PHE:CE1	2.26	0.69
1:I:375:MET:HB3	1:I:379:GLU:HB3	1.75	0.69
1:F:34:ASN:C	1:F:34:ASN:HD22	2.00	0.69
1:J:281:HIS:HD2	1:J:402:ASN:ND2	1.91	0.69
1:A:231:PHE:HB3	1:A:339:PRO:HB2	1.73	0.69
1:C:293:VAL:HG23	1:I:440:TYR:OH	1.92	0.69
1:D:231:PHE:HB3	1:D:339:PRO:HB2	1.74	0.69
1:G:377:LYS:HA	1:G:380:ARG:NH1	2.08	0.69
1:J:129:LEU:HD23	1:J:130:GLY:N	2.07	0.69
1:K:293:VAL:HG11	1:K:428:PHE:CD2	2.28	0.69
1:B:236:LEU:HB2	1:B:239:VAL:CG2	2.23	0.69
1:D:21:ILE:HD13	1:D:42:LEU:HD13	1.74	0.69
1:D:119:MET:SD	1:D:127:PHE:HB2	2.33	0.69
1:D:437:ARG:HA	1:J:232:MET:HE1	1.74	0.69
1:E:325:SER:HB3	1:E:329:SER:HB2	1.75	0.69
1:G:111:ASN:O	1:G:115:ILE:HD13	1.93	0.69
1:B:429:ARG:HH21	1:H:390:ALA:CB	2.06	0.68
1:C:287:ALA:HB2	1:C:395:ALA:HB1	1.75	0.68
1:E:96:ILE:HD12	1:E:96:ILE:N	2.08	0.68
1:G:55:SER:O	1:G:62:ARG:HG2	1.91	0.68
1:C:48:ASN:HB3	1:C:71:TYR:CD1	2.28	0.68
1:D:236:LEU:O	1:D:239:VAL:HG22	1.92	0.68
1:D:247:ASN:HB3	1:D:331:ARG:HG3	1.75	0.68
1:H:437:ARG:NH1	4:H:602:HOH:O	2.26	0.68
1:A:34:ASN:C	1:A:34:ASN:ND2	2.51	0.68
1:D:13:VAL:HG13	1:D:18:VAL:HB	1.75	0.68
1:I:80:PHE:HE1	1:I:91:ARG:HG2	1.57	0.68
1:J:91:ARG:HD2	1:J:91:ARG:C	2.18	0.68
1:L:368:ILE:H	1:L:368:ILE:HD12	1.59	0.68
1:G:375:MET:HE1	1:G:385:ILE:HG13	1.74	0.68
1:L:125:SER:HB3	1:L:251:PHE:O	1.93	0.68
1:L:129:LEU:HG	1:L:347:LEU:HD21	1.76	0.68
1:G:370:ARG:HD3	1:G:370:ARG:N	2.08	0.68
1:L:386:VAL:HG12	1:L:387:ASP:N	2.08	0.68
1:B:178:GLU:OE1	1:C:86:LYS:HD3	1.93	0.68
1:I:281:HIS:CE1	1:I:404:VAL:HG11	2.28	0.68
1:C:372:ILE:CG2	1:C:385:ILE:HD13	2.22	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:129:LEU:HD13	1:E:130:GLY:N	2.08	0.68
1:K:315:ASN:ND2	1:K:370:ARG:H	1.86	0.68
1:I:167:ASN:OD1	1:I:170:ARG:HB3	1.93	0.68
1:J:182:GLU:O	1:J:200:LYS:HB2	1.92	0.68
1:B:441:MET:O	1:H:228:HIS:HE1	1.77	0.68
1:G:323:PRO:HG3	1:G:331:ARG:HG2	1.75	0.68
1:J:67:ASP:O	1:J:68:MET:HG3	1.93	0.68
1:K:316:ARG:HH11	1:K:316:ARG:N	1.90	0.68
1:C:402:ASN:OD1	1:C:404:VAL:HG12	1.94	0.68
1:E:314:GLN:HE22	1:E:321:ARG:NH2	1.91	0.68
1:C:129:LEU:O	1:C:201:TYR:HA	1.94	0.67
1:C:169:ARG:HH22	1:C:188:HIS:HB2	1.59	0.67
1:C:377:LYS:HG3	1:C:381:MET:HE2	1.75	0.67
1:D:83:THR:HG22	1:D:88:LYS:HD3	1.76	0.67
1:D:300:VAL:HG13	1:D:301:PRO:HD2	1.73	0.67
1:D:440:TYR:HB2	1:J:232:MET:HE3	1.76	0.67
1:G:260:ASP:O	1:G:266:GLN:HA	1.94	0.67
1:K:404:VAL:HG23	1:K:405:MET:CE	2.22	0.67
1:E:52:PHE:CE2	1:E:54:GLY:HA2	2.30	0.67
1:E:264:ASP:C	1:E:266:GLN:H	2.02	0.67
1:G:160:ALA:HB1	1:G:161:PRO:CD	2.24	0.67
1:I:114:ARG:HB3	1:I:114:ARG:HH11	1.58	0.67
1:K:316:ARG:NH1	1:K:316:ARG:HB2	2.08	0.67
1:E:178:GLU:OE2	1:F:86:LYS:HD2	1.95	0.67
1:E:309:VAL:HG21	1:E:386:VAL:HG23	1.75	0.67
1:H:312:SER:HB2	1:H:368:ILE:HG22	1.74	0.67
1:J:295:SER:O	1:J:299:LEU:HD13	1.94	0.67
1:A:381:MET:HA	1:A:381:MET:HE3	1.77	0.67
1:A:419:GLU:O	1:A:423:ILE:HD13	1.93	0.67
1:C:232:MET:HE3	1:C:235:PRO:HB3	1.75	0.67
1:K:109:ARG:HD2	1:K:344:TYR:CE2	2.30	0.67
1:K:316:ARG:HH11	1:K:316:ARG:HB2	1.59	0.67
1:C:13:VAL:HG13	1:C:18:VAL:HB	1.76	0.67
1:D:116:LEU:O	1:D:120:GLU:HG3	1.95	0.67
1:E:320:ILE:CG2	1:E:321:ARG:N	2.58	0.67
1:I:280:LYS:HE3	1:I:281:HIS:NE2	2.09	0.67
1:K:259:PHE:HD1	1:K:326:ARG:HD2	1.58	0.67
1:K:58:GLU:O	1:K:61:VAL:HG22	1.95	0.67
1:C:423:ILE:O	1:C:427:MET:HG3	1.93	0.67
1:F:40:SER:O	1:F:41:GLN:HG2	1.93	0.67
1:F:423:ILE:HD12	1:F:424:GLU:N	2.09	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:ALA:HB2	1:G:188:HIS:CD2	2.29	0.67
1:I:23:LEU:HB2	1:I:35:VAL:HG13	1.77	0.67
1:K:282:ALA:HA	1:K:285:PHE:CZ	2.30	0.67
1:A:30:GLY:HA2	1:A:342:ASN:ND2	2.10	0.67
1:B:319:LEU:HG	1:B:320:ILE:HG13	1.77	0.67
1:H:30:GLY:HA2	1:H:342:ASN:ND2	2.09	0.67
1:I:127:PHE:CD2	1:I:351:LEU:HG	2.29	0.67
1:L:21:ILE:HG12	1:L:42:LEU:HD13	1.76	0.67
1:I:310:ALA:HB2	1:I:368:ILE:HD12	1.75	0.67
1:K:112:LEU:O	1:K:116:LEU:HG	1.95	0.67
1:E:155:GLY:HA3	4:E:616:HOH:O	1.94	0.66
1:G:267:LEU:HD21	1:G:326:ARG:HH12	1.61	0.66
1:I:97:TYR:CZ	1:I:103:PRO:HG3	2.30	0.66
1:K:309:VAL:HG13	1:K:319:LEU:HD23	1.76	0.66
1:A:431:GLN:HE21	1:A:432:VAL:N	1.93	0.66
1:D:402:ASN:O	1:D:406:VAL:HG23	1.96	0.66
1:F:321:ARG:C	1:F:322:ILE:HD12	2.20	0.66
1:H:260:ASP:HB3	1:H:267:LEU:O	1.96	0.66
1:L:129:LEU:HD12	1:L:347:LEU:HD11	1.76	0.66
1:A:200:LYS:NZ	1:B:41:GLN:HE22	1.93	0.66
1:C:32:ILE:HD12	1:C:32:ILE:N	2.10	0.66
1:C:282:ALA:C	1:C:284:SER:H	2.03	0.66
1:D:289:THR:C	1:D:290:ASN:HD22	2.03	0.66
1:E:444:TYR:OXT	1:K:231:PHE:HB2	1.95	0.66
1:C:160:ALA:HB1	1:C:161:PRO:HD2	1.77	0.66
1:F:319:LEU:HD12	1:F:336:SER:HB3	1.78	0.66
1:K:323:PRO:HD2	1:K:331:ARG:O	1.96	0.66
1:K:402:ASN:OD1	1:K:404:VAL:HG22	1.96	0.66
1:A:32:ILE:HD13	1:A:216:LEU:HD13	1.77	0.66
1:D:265:LEU:O	1:D:267:LEU:HD13	1.94	0.66
1:E:57:ILE:CD1	1:E:96:ILE:HG12	2.24	0.66
1:G:224:LYS:HD2	1:H:164:LEU:HD11	1.78	0.66
1:L:349:VAL:HG22	1:L:405:MET:SD	2.34	0.66
1:B:414:PHE:O	1:B:418:ILE:HD13	1.95	0.66
1:D:183:ILE:HD11	1:E:38:PRO:HG3	1.77	0.66
1:F:189:GLU:OE1	1:F:189:GLU:HA	1.96	0.66
1:H:244:MET:H	1:H:338:ASP:HA	1.61	0.66
1:H:322:ILE:HD13	1:H:332:VAL:HA	1.77	0.66
1:I:105:GLU:HB3	4:I:608:HOH:O	1.96	0.66
1:K:295:SER:O	1:K:299:LEU:HD13	1.95	0.66
1:A:131:PRO:CB	1:A:211:ILE:HD11	2.25	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:LEU:HD22	1:B:409:LEU:CD2	2.25	0.66
1:B:372:ILE:HG21	1:B:385:ILE:HG21	1.77	0.66
1:D:264:ASP:C	1:D:266:GLN:H	2.03	0.66
1:D:411:GLU:O	1:D:415:GLU:HG2	1.96	0.66
1:E:331:ARG:HH21	1:E:331:ARG:HG2	1.60	0.66
1:H:5:THR:OG1	1:H:7:GLU:HG3	1.96	0.66
1:E:234:LYS:HE3	1:E:239:VAL:O	1.96	0.66
1:E:378:GLU:HA	1:E:381:MET:HB3	1.77	0.66
1:I:182:GLU:HB3	1:I:200:LYS:HE2	1.76	0.66
1:J:160:ALA:CB	1:J:169:ARG:HH12	2.08	0.66
1:B:129:LEU:HD22	1:B:130:GLY:N	2.10	0.65
1:G:314:GLN:HE22	1:L:66:SER:HA	1.59	0.65
1:L:82:TRP:HE1	1:L:221:ILE:CD1	2.09	0.65
1:A:310:ALA:HB2	1:A:385:ILE:HG23	1.77	0.65
1:B:84:ALA:HB3	1:B:87:GLY:O	1.95	0.65
1:B:120:GLU:C	1:B:122:LEU:H	2.02	0.65
1:E:300:VAL:HG22	1:K:429:ARG:NH2	2.11	0.65
1:I:368:ILE:HG21	1:I:372:ILE:HG23	1.78	0.65
1:J:236:LEU:O	1:J:239:VAL:HG22	1.95	0.65
1:L:189:GLU:OE1	1:L:189:GLU:HA	1.93	0.65
1:B:68:MET:HG2	1:B:99:PRO:HD3	1.79	0.65
1:D:18:VAL:HA	1:D:88:LYS:HB2	1.78	0.65
1:D:236:LEU:HB2	1:D:239:VAL:HG22	1.77	0.65
1:K:78:VAL:HB	1:K:91:ARG:HG3	1.77	0.65
1:L:313:ALA:HA	1:L:322:ILE:H	1.60	0.65
1:C:119:MET:SD	1:C:127:PHE:HB2	2.37	0.65
1:E:264:ASP:OD2	1:E:264:ASP:N	2.29	0.65
1:F:4:TYR:HB3	1:F:9:ILE:HD11	1.78	0.65
1:L:135:PHE:HB3	1:L:231:PHE:CE1	2.31	0.65
1:B:129:LEU:HD12	1:B:207:SER:HB3	1.79	0.65
1:B:200:LYS:HE2	1:C:41:GLN:OE1	1.96	0.65
1:C:331:ARG:HG2	1:C:331:ARG:HH21	1.61	0.65
1:F:168:CYS:O	1:F:172:ILE:HG12	1.97	0.65
1:A:37:ILE:HG22	1:F:185:ALA:HA	1.77	0.65
1:A:191:ALA:HB2	1:A:240:ASN:HB3	1.79	0.65
1:C:52:PHE:CE1	1:C:70:LEU:HD13	2.31	0.65
1:E:129:LEU:CD2	1:E:347:LEU:HD21	2.26	0.65
1:I:248:LEU:CD1	1:I:334:VAL:HG23	2.26	0.65
1:I:274:PHE:CE2	1:I:332:VAL:HG21	2.32	0.65
1:K:315:ASN:HB3	1:K:318:PRO:HG3	1.78	0.65
1:A:357:GLY:HA2	1:A:362:LEU:HB2	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:429:ARG:HH22	1:K:300:VAL:HG12	1.61	0.65
1:G:383:ASN:HB2	1:G:385:ILE:HG12	1.78	0.65
1:A:400:LYS:HE2	1:A:418:ILE:HD13	1.79	0.65
1:C:273:HIS:NE2	1:C:361:LYS:HE3	2.10	0.65
1:D:205:VAL:HG23	1:D:206:ARG:H	1.61	0.65
1:F:205:VAL:HG13	1:F:206:ARG:N	2.12	0.65
1:K:261:GLU:HA	1:K:266:GLN:NE2	2.12	0.65
1:G:267:LEU:HD21	1:G:326:ARG:NH1	2.11	0.65
1:G:421:LYS:HD3	1:G:424:GLU:OE2	1.96	0.65
1:H:328:ILE:H	1:H:328:ILE:HD13	1.61	0.65
1:K:136:PHE:HB2	1:K:230:THR:HG23	1.78	0.65
1:L:271:ALA:O	1:L:275:ILE:HG12	1.96	0.65
1:A:22:ARG:HH22	1:F:167:ASN:HD21	1.44	0.65
1:F:282:ALA:CB	1:F:319:LEU:HD21	2.27	0.65
1:H:37:ILE:HG22	1:I:185:ALA:HB2	1.79	0.65
1:H:315:ASN:HD22	1:H:373:TYR:HE1	1.45	0.65
1:K:33:LYS:HG2	1:L:158:ASP:HB3	1.78	0.65
1:B:159:LEU:HD12	1:C:22:ARG:HH11	1.62	0.64
1:I:68:MET:HE1	1:I:104:PHE:HB2	1.79	0.64
1:I:114:ARG:HB3	1:I:114:ARG:NH1	2.12	0.64
1:A:244:MET:H	1:A:338:ASP:HA	1.61	0.64
1:A:431:GLN:NE2	1:A:432:VAL:H	1.94	0.64
1:B:289:THR:HB	1:B:337:VAL:HG22	1.78	0.64
1:L:351:LEU:HD22	1:L:355:LEU:HG	1.78	0.64
1:A:131:PRO:CG	1:A:211:ILE:HD11	2.28	0.64
1:G:91:ARG:HD2	1:G:92:PHE:N	2.12	0.64
1:H:250:LEU:HB2	1:H:258:PHE:CE2	2.32	0.64
1:I:176:LEU:O	1:I:181:PHE:HB2	1.95	0.64
1:B:370:ARG:NH2	1:B:375:MET:HG3	2.10	0.64
1:C:160:ALA:HB2	1:C:169:ARG:HH22	1.61	0.64
1:C:297:LYS:HG2	1:I:431:GLN:O	1.96	0.64
1:K:5:THR:HG22	1:K:8:ASP:CG	2.23	0.64
1:L:399:PHE:HD2	1:L:418:ILE:HD11	1.62	0.64
1:A:161:PRO:HD3	4:A:616:HOH:O	1.96	0.64
1:C:116:LEU:O	1:C:119:MET:HB3	1.97	0.64
1:C:160:ALA:HB2	1:C:169:ARG:NH2	2.12	0.64
1:F:19:LYS:HG3	1:F:86:LYS:O	1.97	0.64
1:F:338:ASP:HB2	1:F:339:PRO:HD2	1.80	0.64
1:G:122:LEU:HD11	1:G:359:LYS:HG3	1.79	0.64
1:C:24:GLN:NE2	1:C:91:ARG:HH11	1.95	0.64
1:D:127:PHE:CE2	1:D:351:LEU:HD23	2.33	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:MET:HE2	1:D:234:LYS:O	1.98	0.64
1:E:158:ASP:HA	1:F:33:LYS:HG2	1.78	0.64
1:K:293:VAL:HG11	1:K:428:PHE:CE2	2.32	0.64
1:A:23:LEU:HB2	1:A:35:VAL:HG13	1.78	0.64
1:A:150:LEU:HD13	1:A:192:PRO:O	1.98	0.64
1:D:48:ASN:HB3	1:D:71:TYR:CE1	2.33	0.64
1:G:129:LEU:CD1	1:G:131:PRO:HD3	2.27	0.64
1:J:11:LYS:HG3	1:J:15:GLU:CD	2.22	0.64
1:K:251:PHE:HA	1:K:255:VAL:O	1.97	0.64
1:L:306:PRO:HG2	1:L:335:ARG:O	1.98	0.64
1:C:261:GLU:HA	1:C:266:GLN:HE21	1.62	0.64
1:C:409:LEU:O	1:C:413:LEU:HB2	1.98	0.64
1:H:396:LEU:O	1:H:400:LYS:HG2	1.97	0.64
1:J:160:ALA:HB1	1:J:161:PRO:HD2	1.79	0.64
1:C:136:PHE:HB3	1:C:138:PHE:CE1	2.31	0.64
1:D:45:ALA:HA	1:D:50:VAL:HG23	1.80	0.64
1:D:281:HIS:HD2	1:D:402:ASN:HD21	1.45	0.64
1:D:396:LEU:HD11	1:D:421:LYS:HB3	1.77	0.64
1:E:322:ILE:HD12	1:E:322:ILE:N	2.13	0.64
1:F:187:HIS:HE1	1:F:196:GLU:OE1	1.81	0.64
1:L:9:ILE:HA	1:L:12:LEU:HD12	1.80	0.64
1:L:306:PRO:HG2	1:L:335:ARG:C	2.23	0.64
1:B:236:LEU:HB2	1:B:239:VAL:HG22	1.78	0.64
1:E:300:VAL:HG22	1:K:429:ARG:HH22	1.63	0.64
1:F:73:ASP:OD1	1:F:76:THR:HG23	1.97	0.64
1:G:57:ILE:C	1:G:59:GLY:H	2.06	0.64
1:H:236:LEU:HB2	1:H:239:VAL:CG2	2.27	0.64
1:K:46:LEU:O	1:K:47:ASP:HB2	1.98	0.64
1:A:311:TRP:HB3	1:A:320:ILE:HB	1.80	0.63
1:B:147:THR:CG2	1:B:149:GLU:HG3	2.28	0.63
1:C:241:GLY:HA3	1:C:298:ARG:HG3	1.81	0.63
1:F:377:LYS:HA	1:F:380:ARG:HG3	1.80	0.63
1:I:135:PHE:HB3	1:I:231:PHE:CE1	2.33	0.63
1:L:315:ASN:ND2	1:L:370:ARG:HA	2.11	0.63
1:K:309:VAL:HB	1:K:386:VAL:O	1.99	0.63
1:L:48:ASN:HB3	1:L:71:TYR:CE1	2.33	0.63
1:A:37:ILE:HG22	1:F:185:ALA:CB	2.29	0.63
1:A:281:HIS:HB3	1:A:405:MET:HE3	1.80	0.63
1:A:306:PRO:HG2	1:A:335:ARG:C	2.23	0.63
1:D:291:PRO:HG3	1:D:341:ALA:HA	1.78	0.63
1:F:402:ASN:O	1:F:406:VAL:HG23	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:98:ASN:HB3	1:I:100:ASP:OD1	1.98	0.63
1:I:279:VAL:HG13	1:I:309:VAL:HG12	1.81	0.63
1:I:295:SER:O	1:I:299:LEU:HD23	1.99	0.63
1:J:72:PRO:CA	1:J:94:CYS:HB3	2.27	0.63
1:K:307:CYS:H	1:K:317:SER:HB2	1.63	0.63
1:B:19:LYS:HA	1:B:39:VAL:HG11	1.80	0.63
1:C:150:LEU:HD13	1:C:192:PRO:HG2	1.80	0.63
1:G:160:ALA:HB3	1:G:169:ARG:NH1	2.14	0.63
1:I:282:ALA:C	1:I:284:SER:H	2.05	0.63
1:J:386:VAL:HG12	1:J:387:ASP:N	2.07	0.63
1:H:397:GLU:CD	1:H:400:LYS:HZ1	2.06	0.63
1:K:35:VAL:HG11	1:K:70:LEU:HD11	1.79	0.63
1:A:78:VAL:HG12	1:A:91:ARG:HG3	1.80	0.63
1:B:58:GLU:HB3	1:B:61:VAL:HG23	1.81	0.63
1:C:178:GLU:OE1	1:D:86:LYS:HD3	1.99	0.63
1:E:9:ILE:O	1:E:13:VAL:HG23	1.99	0.63
1:E:232:MET:HE2	1:E:294:ASN:OD1	1.98	0.63
1:E:368:ILE:HG21	1:E:372:ILE:HG23	1.81	0.63
1:F:96:ILE:HD13	1:F:107:ASP:CG	2.23	0.63
1:B:13:VAL:HG13	1:B:18:VAL:HB	1.80	0.63
1:G:160:ALA:O	1:G:161:PRO:C	2.42	0.63
1:K:310:ALA:HB3	1:K:372:ILE:HD13	1.80	0.63
1:K:316:ARG:HE	1:K:370:ARG:CZ	2.11	0.63
1:E:402:ASN:O	1:E:406:VAL:HG23	1.99	0.63
1:F:150:LEU:HD13	1:F:192:PRO:HB2	1.80	0.63
1:H:21:ILE:HG22	1:H:90:ALA:HB3	1.80	0.63
1:I:129:LEU:HD22	1:I:131:PRO:CG	2.27	0.63
1:A:22:ARG:NH2	1:F:167:ASN:HD21	1.97	0.63
1:A:418:ILE:O	1:A:422:GLU:HG3	1.99	0.63
1:E:430:THR:HG22	1:K:300:VAL:HG11	1.80	0.63
1:G:306:PRO:HG2	1:G:335:ARG:HH21	1.64	0.63
1:G:406:VAL:HG22	1:G:414:PHE:CE1	2.33	0.63
1:I:55:SER:O	1:I:58:GLU:HB2	1.97	0.63
1:J:399:PHE:CE1	1:J:405:MET:HB3	2.34	0.63
1:A:207:SER:O	1:A:211:ILE:HG12	1.99	0.62
1:B:19:LYS:HA	1:B:39:VAL:CG1	2.29	0.62
1:D:183:ILE:CD1	1:E:38:PRO:HG3	2.29	0.62
1:D:300:VAL:CG1	1:D:301:PRO:HD2	2.28	0.62
1:E:290:ASN:HB3	1:E:295:SER:HB3	1.81	0.62
1:F:129:LEU:HD23	1:F:130:GLY:N	2.14	0.62
1:J:234:LYS:HB3	1:J:294:ASN:HD21	1.63	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:98:ASN:ND2	1:K:104:PHE:HA	2.14	0.62
1:K:298:ARG:HG3	1:K:298:ARG:O	1.97	0.62
1:L:250:LEU:C	1:L:251:PHE:HD1	2.07	0.62
1:A:159:LEU:HD21	1:B:22:ARG:HE	1.64	0.62
1:A:184:GLU:HG2	4:A:604:HOH:O	1.97	0.62
1:B:311:TRP:CE3	1:B:322:ILE:HD13	2.34	0.62
1:E:129:LEU:HD12	1:E:131:PRO:HD3	1.81	0.62
1:G:37:ILE:O	1:G:37:ILE:HG13	1.99	0.62
1:G:48:ASN:OD1	1:G:71:TYR:HA	1.98	0.62
1:I:189:GLU:HB3	1:I:194:GLN:NE2	2.14	0.62
1:C:169:ARG:HD2	1:D:36:GLU:OE1	1.99	0.62
1:E:9:ILE:CG1	1:E:74:LEU:HD12	2.24	0.62
1:F:434:PRO:HA	1:F:437:ARG:NH1	2.14	0.62
1:H:5:THR:C	1:H:7:GLU:H	2.07	0.62
1:H:20:TYR:HB3	1:H:89:VAL:HG22	1.80	0.62
1:H:316:ARG:HB3	1:H:373:TYR:CD1	2.33	0.62
1:I:274:PHE:HE2	1:I:332:VAL:HG21	1.64	0.62
1:C:112:LEU:HD12	1:C:344:TYR:HD2	1.64	0.62
1:D:162:THR:O	1:D:164:LEU:N	2.29	0.62
1:F:282:ALA:HB1	1:F:319:LEU:HD21	1.81	0.62
1:L:114:ARG:NH2	1:L:115:ILE:HD11	2.14	0.62
1:E:285:PHE:HB2	1:E:349:VAL:HG13	1.81	0.62
1:F:24:GLN:NE2	1:F:91:ARG:HH11	1.98	0.62
1:F:33:LYS:NZ	1:F:56:SER:O	2.33	0.62
1:H:52:PHE:HE2	1:H:56:SER:HG	1.48	0.62
1:A:283:THR:HG22	1:A:388:LEU:HA	1.80	0.62
1:A:431:GLN:HE21	1:A:432:VAL:H	1.48	0.62
1:C:201:TYR:CD1	1:C:201:TYR:C	2.77	0.62
1:H:370:ARG:HH11	1:H:370:ARG:HG3	1.65	0.62
1:J:95:ASP:HB3	1:J:110:ASN:HD21	1.63	0.62
1:J:104:PHE:CZ	1:J:106:GLY:HA3	2.35	0.62
1:J:402:ASN:O	1:J:406:VAL:HG23	1.99	0.62
1:D:104:PHE:CZ	1:D:106:GLY:HA3	2.34	0.62
1:E:169:ARG:HH11	1:E:195:HIS:HD2	1.46	0.62
1:J:115:ILE:HD11	1:J:408:ALA:O	2.00	0.62
1:J:325:SER:HB3	1:J:329:SER:HB3	1.80	0.62
1:K:253:ASN:O	1:K:255:VAL:HG23	1.99	0.62
1:E:282:ALA:HA	1:E:285:PHE:CZ	2.35	0.62
1:F:21:ILE:HG13	1:F:42:LEU:HD13	1.81	0.62
1:F:371:ASN:ND2	1:F:373:TYR:HB2	2.10	0.62
1:H:380:ARG:HB2	1:H:380:ARG:HH11	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:372:ILE:CG2	1:L:385:ILE:HG21	2.30	0.62
1:A:312:SER:HB3	1:A:315:ASN:HD22	1.64	0.62
1:B:197:ILE:HD12	1:B:214:PHE:CZ	2.35	0.62
1:D:34:ASN:C	1:D:34:ASN:ND2	2.56	0.62
1:D:273:HIS:CE1	1:D:361:LYS:HA	2.35	0.62
1:F:183:ILE:HD12	1:F:197:ILE:HG22	1.80	0.62
1:H:138:PHE:HB3	1:H:147:THR:O	2.00	0.62
1:L:355:LEU:HD23	1:L:358:ILE:HD12	1.82	0.62
1:D:243:GLY:HA3	1:D:298:ARG:NH1	2.14	0.62
1:G:342:ASN:HD22	1:G:342:ASN:C	2.08	0.62
1:L:54:GLY:HA3	1:L:68:MET:HE3	1.82	0.62
1:L:74:LEU:H	1:L:74:LEU:HD22	1.64	0.62
1:C:267:LEU:HD21	1:C:326:ARG:HH12	1.64	0.61
1:C:380:ARG:HB2	1:C:380:ARG:NH1	2.15	0.61
1:H:86:LYS:HA	1:H:86:LYS:HE2	1.81	0.61
1:A:142:GLU:H	1:A:142:GLU:CD	2.08	0.61
1:C:96:ILE:HD12	1:C:96:ILE:N	2.14	0.61
1:E:161:PRO:O	1:E:167:ASN:ND2	2.33	0.61
1:H:4:TYR:HB3	1:H:9:ILE:HG13	1.82	0.61
1:H:308:TYR:HB3	1:H:385:ILE:HG23	1.81	0.61
1:H:370:ARG:NH2	1:H:375:MET:HE3	2.13	0.61
1:L:9:ILE:HG21	1:L:92:PHE:HZ	1.64	0.61
1:A:252:LYS:HE3	1:A:253:ASN:ND2	2.15	0.61
1:B:77:PHE:HB2	1:B:92:PHE:HE2	1.65	0.61
1:D:396:LEU:O	1:D:400:LYS:HG3	2.00	0.61
1:G:267:LEU:HD11	1:G:322:ILE:HG21	1.83	0.61
1:H:160:ALA:HB1	1:H:161:PRO:CD	2.31	0.61
1:I:57:ILE:CD1	1:I:96:ILE:HG12	2.27	0.61
1:I:287:ALA:HB2	1:I:395:ALA:HB1	1.82	0.61
1:L:236:LEU:HD12	1:L:239:VAL:HG21	1.83	0.61
1:D:338:ASP:HB2	1:D:339:PRO:HD2	1.82	0.61
1:E:264:ASP:C	1:E:266:GLN:N	2.59	0.61
1:H:202:ALA:HB3	1:H:207:SER:HB2	1.81	0.61
1:L:273:HIS:HB3	1:L:357:GLY:O	2.00	0.61
1:L:316:ARG:HD3	1:L:370:ARG:HH22	1.66	0.61
1:B:164:LEU:HD11	1:C:224:LYS:HG3	1.83	0.61
1:E:20:TYR:O	1:E:89:VAL:HG13	2.01	0.61
1:F:244:MET:H	1:F:338:ASP:HA	1.65	0.61
1:F:399:PHE:CE1	1:F:405:MET:HB3	2.35	0.61
1:I:35:VAL:HG11	1:I:70:LEU:CD2	2.30	0.61
1:J:156:TYR:HA	1:J:188:HIS:O	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ILE:HG21	1:A:343:PRO:HG3	1.82	0.61
1:B:281:HIS:HD2	1:B:402:ASN:HD21	1.46	0.61
1:B:315:ASN:HB3	1:B:318:PRO:HD3	1.83	0.61
1:E:136:PHE:CE2	1:E:194:GLN:HB2	2.35	0.61
1:F:16:GLU:O	1:F:17:ASN:HB3	2.01	0.61
1:F:34:ASN:C	1:F:34:ASN:ND2	2.57	0.61
1:F:436:GLU:OE2	1:L:297:LYS:HE3	2.01	0.61
1:G:236:LEU:HB2	1:G:239:VAL:HG22	1.83	0.61
1:I:127:PHE:CE2	1:I:351:LEU:HG	2.35	0.61
1:I:129:LEU:O	1:I:201:TYR:HA	2.00	0.61
1:K:45:ALA:HA	1:K:50:VAL:HG21	1.82	0.61
1:B:282:ALA:HA	1:B:285:PHE:CZ	2.36	0.61
1:E:139:LYS:HA	1:E:227:LEU:HD23	1.83	0.61
1:F:119:MET:HA	1:F:355:LEU:HD11	1.82	0.61
1:I:289:THR:HB	1:I:337:VAL:HG22	1.83	0.61
1:I:320:ILE:HD12	1:I:320:ILE:N	2.16	0.61
1:J:176:LEU:O	1:J:181:PHE:HB2	1.99	0.61
1:K:236:LEU:HB2	1:K:239:VAL:CG2	2.30	0.61
1:K:281:HIS:CD2	1:K:402:ASN:HD21	2.19	0.61
1:L:372:ILE:HG21	1:L:385:ILE:HG21	1.82	0.61
1:A:5:THR:H	1:A:8:ASP:HB2	1.66	0.61
1:A:45:ALA:HA	1:A:50:VAL:CG2	2.30	0.61
1:C:337:VAL:HG12	1:C:338:ASP:N	2.16	0.61
1:E:148:LEU:H	1:E:148:LEU:HD22	1.64	0.61
1:E:306:PRO:HB3	1:E:319:LEU:HA	1.81	0.61
1:G:311:TRP:CB	1:G:320:ILE:HB	2.31	0.61
1:H:311:TRP:CZ2	1:H:367:PRO:HB3	2.36	0.61
1:I:310:ALA:CB	1:I:368:ILE:HD12	2.31	0.61
1:A:131:PRO:HB3	1:A:211:ILE:HD11	1.83	0.61
1:A:400:LYS:HB3	1:A:418:ILE:CD1	2.30	0.61
1:H:183:ILE:HD12	1:H:183:ILE:N	2.15	0.61
1:B:163:ASP:OD1	1:C:89:VAL:HG21	2.01	0.60
1:B:436:GLU:OE2	1:H:297:LYS:HE3	2.01	0.60
1:C:375:MET:HE3	1:C:379:GLU:HB3	1.83	0.60
1:D:248:LEU:O	1:D:331:ARG:HB2	2.00	0.60
1:F:236:LEU:HD12	1:F:239:VAL:HG22	1.82	0.60
1:G:312:SER:HB3	1:G:315:ASN:HB2	1.82	0.60
1:I:32:ILE:HG21	1:I:216:LEU:HD12	1.82	0.60
1:K:160:ALA:HB1	1:K:161:PRO:CD	2.26	0.60
1:A:127:PHE:CE2	1:A:351:LEU:HD13	2.37	0.60
1:A:252:LYS:HB2	1:A:252:LYS:HZ2	1.64	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:GLY:HA3	1:B:68:MET:HE3	1.83	0.60
1:C:231:PHE:HB2	1:I:444:TYR:OXT	2.01	0.60
1:D:249:SER:HB3	1:D:331:ARG:HB3	1.84	0.60
1:D:260:ASP:O	1:D:266:GLN:HA	2.01	0.60
1:H:57:ILE:CD1	1:H:96:ILE:HG12	2.31	0.60
1:K:380:ARG:HA	1:K:383:ASN:HD22	1.65	0.60
1:A:9:ILE:HG13	1:A:74:LEU:HD12	1.82	0.60
1:B:197:ILE:HD12	1:B:214:PHE:CE1	2.36	0.60
1:C:159:LEU:HD11	1:D:22:ARG:HD3	1.83	0.60
1:D:259:PHE:CD2	1:D:326:ARG:HB3	2.36	0.60
1:D:316:ARG:NH1	1:E:63:ILE:HA	2.16	0.60
1:G:20:TYR:CZ	1:G:36:GLU:HB3	2.36	0.60
1:G:169:ARG:HG3	1:G:195:HIS:ND1	2.16	0.60
1:H:166:GLU:OE2	1:H:227:LEU:HD11	2.01	0.60
1:I:118:GLU:O	1:I:122:LEU:HD13	2.02	0.60
1:I:150:LEU:CD1	1:I:192:PRO:HB2	2.32	0.60
1:I:349:VAL:HG22	1:I:405:MET:SD	2.41	0.60
1:J:129:LEU:HD23	1:J:130:GLY:H	1.67	0.60
1:K:150:LEU:CD1	1:K:192:PRO:HG2	2.31	0.60
1:L:51:MET:HE2	1:L:67:ASP:HB3	1.83	0.60
1:L:323:PRO:HG3	1:L:331:ARG:HG3	1.82	0.60
1:D:111:ASN:O	1:D:115:ILE:HD13	2.00	0.60
1:D:377:LYS:HG3	1:D:380:ARG:NH2	2.15	0.60
1:F:27:ASP:HB2	1:F:57:ILE:O	2.01	0.60
1:F:120:GLU:C	1:F:122:LEU:H	2.09	0.60
1:H:84:ALA:HB3	1:H:87:GLY:O	2.02	0.60
1:K:248:LEU:O	1:K:331:ARG:HB2	2.02	0.60
1:B:96:ILE:H	1:B:96:ILE:HD12	1.65	0.60
1:D:129:LEU:HD12	1:D:207:SER:HB3	1.82	0.60
1:E:297:LYS:HE3	1:K:436:GLU:OE1	2.02	0.60
1:F:283:THR:O	1:F:398:GLU:HG2	2.01	0.60
1:H:2:ALA:N	4:H:613:HOH:O	2.34	0.60
1:I:319:LEU:C	1:I:320:ILE:HD12	2.27	0.60
1:J:236:LEU:HB2	1:J:239:VAL:HG22	1.80	0.60
1:K:37:ILE:HD13	1:K:41:GLN:HB2	1.82	0.60
1:K:163:ASP:C	1:K:164:LEU:HD23	2.26	0.60
1:A:329:SER:O	1:A:331:ARG:HG2	2.02	0.60
1:B:264:ASP:C	1:B:266:GLN:H	2.09	0.60
1:F:232:MET:HE3	1:L:440:TYR:CB	2.17	0.60
1:F:440:TYR:OH	1:L:293:VAL:HB	2.02	0.60
1:I:316:ARG:HB3	1:I:373:TYR:CE1	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:57:ILE:HG13	1:J:96:ILE:HD13	1.84	0.60
1:K:338:ASP:HB2	1:K:339:PRO:HD2	1.83	0.60
1:L:145:GLU:OE2	1:L:146:PRO:HD2	2.01	0.60
1:A:206:ARG:HH11	1:A:206:ARG:CG	2.13	0.60
1:B:430:THR:HG22	1:H:300:VAL:HG21	1.83	0.60
1:D:6:ARG:HH11	1:D:6:ARG:HG3	1.67	0.60
1:D:282:ALA:HA	1:D:285:PHE:CE2	2.35	0.60
1:E:232:MET:HE1	1:K:437:ARG:CA	2.26	0.60
1:F:32:ILE:HD13	1:F:216:LEU:HD13	1.83	0.60
1:G:224:LYS:CD	1:H:164:LEU:HD11	2.32	0.60
1:I:136:PHE:CE2	1:I:194:GLN:HB2	2.36	0.60
1:K:55:SER:O	1:K:62:ARG:HG2	2.02	0.60
1:K:83:THR:HB	1:K:88:LYS:HA	1.84	0.60
1:K:316:ARG:C	1:K:318:PRO:HD3	2.27	0.60
1:L:286:THR:HG23	1:L:290:ASN:ND2	2.17	0.60
1:E:19:LYS:HD3	1:E:39:VAL:HG11	1.83	0.60
1:E:326:ARG:NH1	1:E:326:ARG:HG2	2.17	0.60
1:F:100:ASP:O	1:F:102:THR:N	2.34	0.60
1:J:206:ARG:HH11	1:J:206:ARG:HG3	1.65	0.60
1:L:48:ASN:HB3	1:L:71:TYR:CD1	2.36	0.60
1:A:319:LEU:HD22	1:A:320:ILE:CD1	2.31	0.60
1:B:159:LEU:HD11	1:C:22:ARG:HH11	1.65	0.60
1:E:271:ALA:O	1:E:275:ILE:HG12	2.02	0.60
1:I:285:PHE:HB2	1:I:349:VAL:CG1	2.32	0.60
1:K:119:MET:HG2	1:K:124:PHE:HB2	1.84	0.60
1:D:325:SER:HB3	1:D:331:ARG:HH21	1.66	0.60
1:H:21:ILE:HD13	1:H:21:ILE:H	1.66	0.60
1:H:96:ILE:HD12	1:H:96:ILE:N	2.17	0.60
1:B:139:LYS:O	1:B:147:THR:HB	2.02	0.59
1:C:197:ILE:HD12	1:C:214:PHE:CE1	2.37	0.59
1:D:183:ILE:HD13	1:D:183:ILE:H	1.66	0.59
1:E:176:LEU:O	1:E:181:PHE:HB2	2.01	0.59
1:F:40:SER:C	1:F:41:GLN:HG2	2.27	0.59
1:G:282:ALA:HA	1:G:285:PHE:CZ	2.37	0.59
1:A:168:CYS:O	1:A:169:ARG:C	2.45	0.59
1:C:105:GLU:CD	1:C:412:HIS:HB2	2.27	0.59
1:C:260:ASP:HB2	1:C:268:SER:HB3	1.84	0.59
1:C:402:ASN:HD21	1:C:404:VAL:CG1	2.15	0.59
1:D:91:ARG:HD2	1:D:92:PHE:N	2.17	0.59
1:D:162:THR:C	1:D:164:LEU:H	2.10	0.59
1:D:325:SER:HB3	1:D:331:ARG:NH2	2.16	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:127:PHE:HE2	1:H:347:LEU:HD12	1.67	0.59
1:H:146:PRO:HG3	1:H:228:HIS:CD2	2.36	0.59
1:H:328:ILE:HD13	1:H:328:ILE:N	2.17	0.59
1:A:300:VAL:HG22	1:G:429:ARG:HH12	1.66	0.59
1:D:372:ILE:HG13	1:D:373:TYR:HD1	1.66	0.59
1:I:160:ALA:HB1	1:I:161:PRO:HD2	1.83	0.59
1:I:372:ILE:HG13	1:I:373:TYR:CE1	2.38	0.59
1:K:306:PRO:HB3	1:K:319:LEU:HA	1.85	0.59
1:K:383:ASN:HB2	1:K:385:ILE:HG13	1.83	0.59
1:E:314:GLN:NE2	1:F:65:GLU:HB3	2.16	0.59
1:F:96:ILE:N	1:F:96:ILE:HD12	2.17	0.59
1:F:437:ARG:HD3	1:L:148:LEU:HD21	1.84	0.59
1:G:258:PHE:HB3	1:G:270:THR:HB	1.83	0.59
1:H:127:PHE:CE2	1:H:347:LEU:HD12	2.38	0.59
1:I:163:ASP:HA	1:I:167:ASN:HD22	1.67	0.59
1:A:122:LEU:HD21	1:A:359:LYS:HB3	1.84	0.59
1:C:200:LYS:HE2	1:D:41:GLN:OE1	2.01	0.59
1:D:316:ARG:HH11	1:E:63:ILE:HA	1.66	0.59
1:E:161:PRO:HB3	1:F:223:ARG:HH12	1.67	0.59
1:G:325:SER:HB2	1:G:331:ARG:HH22	1.67	0.59
1:G:371:ASN:HB2	1:G:375:MET:HE3	1.84	0.59
1:K:315:ASN:HD21	1:K:370:ARG:N	1.91	0.59
1:D:83:THR:CG2	1:D:88:LYS:HD3	2.32	0.59
1:G:368:ILE:HD13	1:G:372:ILE:CD1	2.31	0.59
1:A:3:LYS:HB3	1:A:3:LYS:HZ3	1.66	0.59
1:C:85:GLU:O	1:C:86:LYS:HB2	2.01	0.59
1:E:273:HIS:NE2	1:E:361:LYS:HA	2.18	0.59
1:E:293:VAL:HG23	1:K:440:TYR:OH	2.02	0.59
1:F:380:ARG:HH11	1:F:385:ILE:CG2	2.15	0.59
1:G:4:TYR:HB3	1:G:9:ILE:CD1	2.32	0.59
1:J:368:ILE:HD12	1:J:385:ILE:HG23	1.83	0.59
1:K:17:ASN:HD22	1:K:87:GLY:HA2	1.67	0.59
1:K:316:ARG:N	1:K:316:ARG:HD3	2.18	0.59
1:L:168:CYS:O	1:L:172:ILE:HG13	2.02	0.59
1:A:41:GLN:HE22	1:F:200:LYS:CE	2.15	0.59
1:C:201:TYR:C	1:C:201:TYR:HD1	2.11	0.59
1:H:63:ILE:HD12	1:H:63:ILE:N	2.18	0.59
1:J:357:GLY:HA2	1:J:362:LEU:HG	1.85	0.59
1:K:260:ASP:O	1:K:266:GLN:HA	2.02	0.59
1:A:244:MET:N	1:A:338:ASP:HA	2.17	0.59
1:E:131:PRO:HG2	1:E:199:PHE:HD1	1.68	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:ILE:HG22	1:F:351:LEU:HD13	1.84	0.59
1:I:376:SER:O	1:I:380:ARG:HG3	2.03	0.59
1:J:371:ASN:ND2	1:J:374:VAL:H	2.01	0.59
1:L:136:PHE:HB3	1:L:138:PHE:HE1	1.68	0.59
1:A:191:ALA:HB3	1:A:194:GLN:HE21	1.68	0.59
1:B:370:ARG:NH2	1:B:375:MET:SD	2.76	0.59
1:E:207:SER:O	1:E:211:ILE:HG12	2.03	0.59
1:H:280:LYS:HG2	1:H:281:HIS:CD2	2.38	0.59
1:H:402:ASN:O	1:H:406:VAL:HG23	2.03	0.59
1:L:55:SER:CB	1:L:62:ARG:HG3	2.30	0.59
1:A:172:ILE:HD13	1:A:218:VAL:HG22	1.85	0.58
1:A:319:LEU:HB3	1:A:320:ILE:HD12	1.84	0.58
1:D:68:MET:CE	1:D:98:ASN:HA	2.33	0.58
1:E:140:LEU:HD12	1:E:226:GLY:CA	2.33	0.58
1:E:273:HIS:NE2	1:E:361:LYS:HG2	2.16	0.58
1:L:443:GLN:HG2	1:L:444:TYR:CE2	2.38	0.58
1:A:138:PHE:CZ	1:A:236:LEU:HD11	2.38	0.58
1:D:139:LYS:HE3	1:D:149:GLU:HB3	1.84	0.58
1:F:218:VAL:HG12	1:F:219:LYS:N	2.16	0.58
1:J:184:GLU:OE1	1:J:200:LYS:HG3	2.03	0.58
1:K:360:ASN:HD22	1:K:360:ASN:N	2.00	0.58
1:L:425:TRP:CZ3	1:L:429:ARG:HD2	2.38	0.58
1:B:129:LEU:HD13	1:B:131:PRO:HD3	1.86	0.58
1:C:6:ARG:O	1:C:10:GLU:HG3	2.03	0.58
1:C:9:ILE:HA	1:C:12:LEU:HD12	1.84	0.58
1:C:189:GLU:HB2	1:C:194:GLN:HB3	1.83	0.58
1:E:96:ILE:HD13	1:E:107:ASP:CG	2.28	0.58
1:J:299:LEU:HD12	1:J:299:LEU:N	2.17	0.58
1:K:54:GLY:C	1:K:56:SER:H	2.10	0.58
1:K:169:ARG:HH21	1:K:169:ARG:HG3	1.68	0.58
1:K:380:ARG:HA	1:K:383:ASN:ND2	2.18	0.58
1:D:310:ALA:O	1:D:318:PRO:HB2	2.03	0.58
1:E:152:ASP:OD1	1:E:193:GLY:HA2	2.03	0.58
1:E:247:ASN:HD22	1:E:331:ARG:HE	1.51	0.58
1:E:396:LEU:HD11	1:E:421:LYS:HB3	1.84	0.58
1:F:141:ASP:O	1:F:144:GLY:N	2.28	0.58
1:H:267:LEU:CD2	1:H:326:ARG:HH12	2.14	0.58
1:I:9:ILE:HG13	1:I:74:LEU:HD12	1.84	0.58
1:J:9:ILE:HG21	1:J:92:PHE:HZ	1.68	0.58
1:J:140:LEU:HD21	1:J:228:HIS:HB2	1.84	0.58
4:K:620:HOH:O	1:L:177:GLU:HG2	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:127:PHE:CD2	1:L:351:LEU:HG	2.38	0.58
1:L:423:ILE:C	1:L:423:ILE:HD12	2.27	0.58
1:B:134:GLU:O	1:B:242:SER:HB3	2.04	0.58
1:B:429:ARG:NH1	1:H:300:VAL:HG23	2.16	0.58
1:D:52:PHE:HZ	1:D:57:ILE:HD11	1.68	0.58
1:D:114:ARG:HH21	1:D:115:ILE:HD11	1.68	0.58
1:D:146:PRO:HG3	1:D:228:HIS:CD2	2.38	0.58
1:F:109:ARG:HG2	1:F:109:ARG:HH21	1.68	0.58
1:F:370:ARG:NH1	1:F:375:MET:HE3	2.19	0.58
1:F:437:ARG:CD	1:L:148:LEU:HD21	2.34	0.58
1:J:100:ASP:OD1	1:J:102:THR:HG22	2.03	0.58
1:J:123:GLY:O	1:J:252:LYS:HG3	2.03	0.58
1:J:346:ALA:O	1:J:350:LEU:HB2	2.03	0.58
1:L:201:TYR:CD1	1:L:201:TYR:C	2.81	0.58
1:E:160:ALA:O	1:E:161:PRO:C	2.46	0.58
1:G:77:PHE:CZ	1:G:79:ILE:HD11	2.38	0.58
1:G:371:ASN:HB3	1:G:375:MET:CG	2.33	0.58
1:I:27:ASP:OD1	1:I:33:LYS:HE3	2.04	0.58
1:I:189:GLU:OE1	1:I:190:VAL:HG23	2.03	0.58
1:K:85:GLU:H	1:K:85:GLU:CD	2.10	0.58
1:L:231:PHE:HB3	1:L:339:PRO:HB2	1.84	0.58
1:B:178:GLU:CD	1:C:86:LYS:HD3	2.29	0.58
1:C:191:ALA:HB2	1:C:240:ASN:HB3	1.85	0.58
1:E:282:ALA:HA	1:E:285:PHE:CE1	2.38	0.58
1:F:160:ALA:O	1:F:161:PRO:C	2.47	0.58
1:K:380:ARG:HB3	1:K:385:ILE:HD12	1.85	0.58
1:B:429:ARG:NH2	1:H:390:ALA:HB1	2.15	0.58
1:C:3:LYS:HG2	1:C:4:TYR:CD1	2.39	0.58
1:E:122:LEU:HD12	1:E:355:LEU:HD22	1.85	0.58
1:E:429:ARG:HH12	1:K:300:VAL:HG12	1.69	0.58
1:G:281:HIS:HD2	1:G:402:ASN:HD21	1.50	0.58
1:I:261:GLU:HA	1:I:266:GLN:CG	2.24	0.58
1:D:48:ASN:HB3	1:D:71:TYR:CD1	2.39	0.58
1:E:12:LEU:O	1:E:16:GLU:HB2	2.04	0.58
1:E:140:LEU:HD22	1:E:144:GLY:O	2.04	0.58
1:E:325:SER:HB2	1:E:331:ARG:NH2	2.14	0.58
1:G:177:GLU:HB2	1:G:183:ILE:HD11	1.85	0.58
1:G:308:TYR:HD2	1:G:380:ARG:HD3	1.68	0.58
1:H:122:LEU:HD21	1:H:359:LYS:HD3	1.86	0.58
1:I:156:TYR:C	1:I:158:ASP:H	2.11	0.58
1:L:201:TYR:C	1:L:201:TYR:HD1	2.12	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:287:ALA:HB2	1:L:395:ALA:CB	2.33	0.58
1:C:404:VAL:CG1	1:C:405:MET:HE3	2.32	0.58
1:E:5:THR:HG23	1:E:8:ASP:CG	2.29	0.58
1:G:156:TYR:C	1:G:158:ASP:H	2.12	0.58
1:G:265:LEU:HD12	1:G:265:LEU:N	2.19	0.58
1:H:279:VAL:HG13	1:H:309:VAL:CG1	2.32	0.58
1:L:291:PRO:HG2	1:L:292:THR:H	1.69	0.58
1:B:48:ASN:OD1	1:B:72:PRO:HD2	2.04	0.57
1:C:118:GLU:O	1:C:122:LEU:HD23	2.04	0.57
1:C:150:LEU:HD13	1:C:192:PRO:O	2.04	0.57
1:D:22:ARG:O	1:D:91:ARG:HB2	2.04	0.57
1:E:381:MET:O	1:E:381:MET:HE2	2.03	0.57
1:G:380:ARG:HD2	1:G:387:ASP:OD2	2.04	0.57
1:J:119:MET:O	1:J:124:PHE:HB2	2.03	0.57
1:K:325:SER:CB	1:K:331:ARG:HH22	2.17	0.57
1:L:402:ASN:HD21	1:L:404:VAL:HG12	1.67	0.57
1:C:124:PHE:CD2	1:C:250:LEU:HD13	2.39	0.57
1:D:52:PHE:CZ	1:D:54:GLY:HA2	2.38	0.57
1:E:429:ARG:O	1:K:297:LYS:HD3	2.04	0.57
1:F:151:ASN:HD22	1:F:166:GLU:CD	2.12	0.57
1:H:140:LEU:HD21	1:H:223:ARG:HH22	1.67	0.57
1:I:399:PHE:CE1	1:I:405:MET:HB3	2.39	0.57
1:L:118:GLU:O	1:L:122:LEU:HD23	2.03	0.57
1:A:52:PHE:CE1	1:A:70:LEU:HD13	2.38	0.57
1:A:63:ILE:O	1:F:316:ARG:HD2	2.03	0.57
1:E:13:VAL:CG1	1:E:18:VAL:HB	2.32	0.57
1:F:298:ARG:NH2	1:F:338:ASP:HB3	2.20	0.57
1:G:370:ARG:H	1:G:370:ARG:CD	2.11	0.57
1:H:215:LYS:HG2	1:H:231:PHE:CE2	2.39	0.57
1:J:81:PRO:HG2	1:J:82:TRP:H	1.69	0.57
1:K:150:LEU:HD13	1:K:192:PRO:HG2	1.87	0.57
1:K:323:PRO:HG3	1:K:331:ARG:NE	2.18	0.57
1:B:360:ASN:O	1:B:361:LYS:C	2.47	0.57
1:D:129:LEU:CD1	1:D:131:PRO:HD3	2.31	0.57
1:E:32:ILE:HD12	1:E:216:LEU:HD13	1.84	0.57
1:E:68:MET:HE1	1:E:104:PHE:CD1	2.39	0.57
1:E:440:TYR:HB2	1:K:232:MET:CE	2.22	0.57
1:F:98:ASN:N	1:F:98:ASN:ND2	2.47	0.57
1:H:155:GLY:O	1:H:158:ASP:HB2	2.05	0.57
1:I:112:LEU:HD21	1:I:347:LEU:HD12	1.86	0.57
1:K:45:ALA:HA	1:K:50:VAL:CG2	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:319:LEU:O	1:K:320:ILE:HD13	2.03	0.57
1:A:274:PHE:CE1	1:A:354:GLY:HA3	2.39	0.57
1:B:116:LEU:O	1:B:119:MET:HB3	2.04	0.57
1:C:65:GLU:HG3	1:C:65:GLU:O	2.04	0.57
1:F:98:ASN:HD21	1:F:104:PHE:CA	2.17	0.57
1:H:166:GLU:O	1:H:168:CYS:N	2.37	0.57
1:H:351:LEU:HD22	1:H:355:LEU:HG	1.87	0.57
1:I:323:PRO:HD2	1:I:331:ARG:O	2.05	0.57
1:J:273:HIS:CE1	1:J:361:LYS:HA	2.39	0.57
1:K:28:ILE:HD11	1:K:417:PHE:CA	2.34	0.57
1:A:55:SER:O	1:A:58:GLU:HG2	2.05	0.57
1:A:233:PRO:HG2	1:A:295:SER:OG	2.04	0.57
1:B:381:MET:N	1:B:381:MET:HE2	2.19	0.57
1:C:63:ILE:HG22	1:C:64:GLU:HG3	1.87	0.57
1:D:212:GLN:OE1	1:D:212:GLN:HA	2.05	0.57
1:H:123:GLY:O	1:H:252:LYS:HG3	2.05	0.57
1:I:347:LEU:O	1:I:347:LEU:HD13	2.04	0.57
1:A:205:VAL:HG23	4:A:602:HOH:O	2.04	0.57
1:B:142:GLU:HG3	1:B:143:LYS:N	2.20	0.57
1:B:164:LEU:HB2	1:C:82:TRP:CD1	2.38	0.57
1:D:160:ALA:O	1:D:161:PRO:O	2.23	0.57
1:D:243:GLY:CA	1:D:298:ARG:NH1	2.68	0.57
1:I:22:ARG:NH1	1:J:159:LEU:HD21	2.20	0.57
1:K:310:ALA:CB	1:K:372:ILE:HG21	2.34	0.57
1:A:223:ARG:HG3	1:A:223:ARG:HH11	1.69	0.57
1:D:214:PHE:O	1:D:218:VAL:HG23	2.04	0.57
1:E:440:TYR:OH	1:K:293:VAL:HG23	2.05	0.57
1:F:91:ARG:HD2	1:F:92:PHE:N	2.20	0.57
1:F:114:ARG:HH21	1:F:115:ILE:HD11	1.68	0.57
1:F:429:ARG:NH2	1:L:300:VAL:HG22	2.13	0.57
1:G:169:ARG:NE	1:L:36:GLU:OE1	2.38	0.57
1:G:371:ASN:CB	1:G:375:MET:HE3	2.35	0.57
1:K:316:ARG:HH11	1:K:316:ARG:CB	2.18	0.57
1:B:147:THR:HG21	1:B:149:GLU:HG3	1.85	0.57
1:B:160:ALA:O	1:B:161:PRO:C	2.47	0.57
1:E:170:ARG:NH1	1:E:171:ASP:OD2	2.38	0.57
1:G:375:MET:HB2	1:G:379:GLU:CB	2.33	0.57
1:I:309:VAL:HG23	1:I:386:VAL:O	2.04	0.57
1:K:370:ARG:NH2	1:K:374:VAL:HG22	2.13	0.57
1:A:135:PHE:HB3	1:A:231:PHE:CD1	2.40	0.57
1:A:311:TRP:CB	1:A:320:ILE:HB	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:GLU:HA	1:C:381:MET:HE3	1.86	0.57
1:F:5:THR:HG23	1:F:8:ASP:OD1	2.04	0.57
1:F:324:ALA:O	1:F:326:ARG:NE	2.38	0.57
1:F:380:ARG:HH11	1:F:380:ARG:HG2	1.69	0.57
1:H:223:ARG:HA	1:H:223:ARG:HE	1.70	0.57
1:I:114:ARG:HH12	1:I:115:ILE:HD11	1.69	0.57
1:J:96:ILE:HD12	1:J:107:ASP:HB2	1.86	0.57
1:C:52:PHE:CE2	1:C:54:GLY:HA2	2.40	0.56
1:C:68:MET:HG2	1:C:97:TYR:O	2.05	0.56
1:D:111:ASN:ND2	1:D:409:LEU:HA	2.17	0.56
1:G:383:ASN:HB2	1:G:385:ILE:CG1	2.35	0.56
1:I:34:ASN:ND2	1:I:34:ASN:C	2.62	0.56
1:I:58:GLU:HB3	1:I:62:ARG:HB2	1.86	0.56
1:J:282:ALA:HA	1:J:285:PHE:CE2	2.39	0.56
1:K:83:THR:CB	1:K:88:LYS:HA	2.34	0.56
1:E:74:LEU:H	1:E:74:LEU:HD22	1.70	0.56
1:F:23:LEU:HB2	1:F:35:VAL:HG13	1.86	0.56
1:F:437:ARG:HB2	1:F:437:ARG:NH1	2.20	0.56
1:G:209:ASP:OD2	1:G:344:TYR:OH	2.20	0.56
1:H:116:LEU:HD22	1:H:119:MET:HE1	1.85	0.56
1:H:119:MET:SD	1:H:127:PHE:HB2	2.44	0.56
1:I:4:TYR:HB3	1:I:9:ILE:HD11	1.87	0.56
1:K:53:ASP:CG	1:K:65:GLU:HG2	2.30	0.56
1:L:136:PHE:HB3	1:L:138:PHE:CE1	2.41	0.56
1:L:357:GLY:HA2	1:L:362:LEU:HD22	1.86	0.56
1:A:115:ILE:HD11	1:A:408:ALA:O	2.05	0.56
1:B:127:PHE:CE2	1:B:351:LEU:HG	2.41	0.56
1:C:146:PRO:HG3	1:C:228:HIS:CD2	2.40	0.56
1:E:117:LYS:O	1:E:117:LYS:HD3	2.05	0.56
1:F:380:ARG:HH11	1:F:385:ILE:HG21	1.70	0.56
1:G:6:ARG:HG3	1:G:10:GLU:OE2	2.04	0.56
1:H:64:GLU:OE2	1:I:315:ASN:HA	2.06	0.56
1:H:169:ARG:NH2	1:H:195:HIS:ND1	2.53	0.56
1:I:100:ASP:OD1	1:I:100:ASP:N	2.37	0.56
1:I:140:LEU:HD12	1:I:226:GLY:C	2.30	0.56
1:I:173:VAL:HG13	1:I:183:ILE:CD1	2.22	0.56
1:J:129:LEU:HD22	1:J:131:PRO:HG3	1.87	0.56
1:J:131:PRO:HG2	1:J:211:ILE:HD11	1.87	0.56
1:J:320:ILE:HG22	1:J:321:ARG:N	2.20	0.56
1:L:34:ASN:C	1:L:34:ASN:ND2	2.63	0.56
1:L:60:PHE:CE1	1:L:423:ILE:HD11	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ASP:OD1	1:B:101:GLY:N	2.39	0.56
1:B:402:ASN:O	1:B:406:VAL:HG23	2.05	0.56
1:C:282:ALA:O	1:C:284:SER:N	2.39	0.56
1:D:319:LEU:HD12	1:D:336:SER:HB3	1.86	0.56
1:E:293:VAL:HG11	1:E:428:PHE:CD2	2.40	0.56
1:G:62:ARG:O	1:G:63:ILE:HG23	2.05	0.56
1:I:169:ARG:NH2	1:I:195:HIS:ND1	2.53	0.56
1:K:345:LEU:O	1:K:348:SER:HB2	2.05	0.56
1:L:57:ILE:CD1	1:L:96:ILE:HG12	2.34	0.56
1:L:78:VAL:CG1	1:L:91:ARG:HG3	2.36	0.56
1:L:156:TYR:HE1	1:L:189:GLU:OE1	1.88	0.56
1:L:285:PHE:HD1	1:L:285:PHE:C	2.12	0.56
1:A:64:GLU:HG2	1:F:316:ARG:HA	1.87	0.56
1:B:58:GLU:O	1:B:61:VAL:HG22	2.05	0.56
1:J:46:LEU:HD21	1:J:74:LEU:HD11	1.87	0.56
1:J:116:LEU:O	1:J:120:GLU:HG3	2.06	0.56
1:K:147:THR:C	1:K:149:GLU:H	2.13	0.56
1:K:276:ALA:HB2	1:K:364:ALA:HB2	1.86	0.56
1:A:37:ILE:HG22	1:F:185:ALA:CA	2.35	0.56
1:A:186:SER:HB2	1:A:197:ILE:HD13	1.86	0.56
1:A:380:ARG:HA	1:A:383:ASN:HB2	1.86	0.56
1:A:442:SER:HB3	1:H:153:LYS:HD2	1.87	0.56
1:D:6:ARG:HG3	1:D:6:ARG:NH1	2.21	0.56
1:D:100:ASP:OD2	1:D:101:GLY:N	2.39	0.56
1:D:309:VAL:HG23	1:D:386:VAL:O	2.06	0.56
1:D:418:ILE:O	1:D:422:GLU:HG3	2.06	0.56
1:E:52:PHE:CD1	1:E:70:LEU:HD13	2.40	0.56
1:E:140:LEU:HD12	1:E:226:GLY:HA2	1.88	0.56
1:H:74:LEU:H	1:H:74:LEU:CD2	2.14	0.56
1:H:167:ASN:HB3	1:H:170:ARG:NH2	2.20	0.56
1:J:319:LEU:HD23	1:J:320:ILE:CD1	2.35	0.56
1:L:23:LEU:HB2	1:L:35:VAL:CG2	2.35	0.56
1:A:200:LYS:HZ1	1:B:41:GLN:NE2	1.98	0.56
1:C:313:ALA:O	1:C:314:GLN:HB2	2.06	0.56
1:E:138:PHE:CD2	1:E:148:LEU:HA	2.41	0.56
1:E:244:MET:HE2	1:E:338:ASP:O	2.05	0.56
1:F:160:ALA:CB	1:F:169:ARG:HH21	2.19	0.56
1:F:319:LEU:HG	1:F:320:ILE:HD12	1.87	0.56
1:H:129:LEU:HD13	1:H:129:LEU:C	2.29	0.56
1:I:234:LYS:HE3	1:I:239:VAL:O	2.05	0.56
1:K:38:PRO:HD2	1:K:41:GLN:HG3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:252:LYS:O	1:K:253:ASN:HB2	2.04	0.56
1:L:85:GLU:C	1:L:87:GLY:H	2.14	0.56
1:E:204:ALA:HB1	1:E:347:LEU:HD13	1.86	0.56
1:E:372:ILE:HD12	1:E:373:TYR:H	1.71	0.56
1:F:379:GLU:HG3	1:F:385:ILE:HD12	1.88	0.56
1:G:183:ILE:HD13	1:L:38:PRO:HG2	1.87	0.56
1:H:28:ILE:HG22	1:H:57:ILE:O	2.05	0.56
1:H:328:ILE:H	1:H:328:ILE:CD1	2.18	0.56
1:K:32:ILE:HD13	1:K:216:LEU:HD13	1.88	0.56
1:K:135:PHE:HB3	1:K:231:PHE:CE1	2.41	0.56
1:A:319:LEU:O	1:A:319:LEU:HD23	2.06	0.56
1:C:377:LYS:O	1:C:381:MET:HG3	2.06	0.56
1:D:377:LYS:HG3	1:D:380:ARG:HH21	1.69	0.56
1:G:203:GLY:O	1:G:204:ALA:C	2.48	0.56
1:G:308:TYR:HE2	1:G:380:ARG:HE	1.54	0.56
1:G:325:SER:CB	1:G:331:ARG:HH22	2.17	0.56
1:I:160:ALA:O	1:I:161:PRO:C	2.49	0.56
1:I:175:GLU:HG3	1:I:221:ILE:HD11	1.88	0.56
1:K:49:LYS:HD3	1:K:69:TYR:CE2	2.41	0.56
1:K:137:LEU:HD23	1:K:229:ALA:HA	1.88	0.56
1:K:167:ASN:OD1	1:K:170:ARG:HB3	2.05	0.56
1:B:91:ARG:HD2	1:B:91:ARG:C	2.32	0.56
1:B:164:LEU:C	1:B:164:LEU:HD23	2.31	0.56
1:B:372:ILE:CG2	1:B:385:ILE:HG21	2.36	0.56
1:D:323:PRO:HG2	1:D:331:ARG:NH2	2.21	0.56
1:D:429:ARG:O	1:J:297:LYS:HD3	2.06	0.56
1:E:393:ALA:HB2	1:E:425:TRP:CE2	2.41	0.56
1:H:162:THR:C	1:H:164:LEU:H	2.14	0.56
1:I:208:CYS:HA	1:I:211:ILE:HG12	1.88	0.56
1:L:83:THR:CG2	1:L:89:VAL:HB	2.35	0.56
1:E:35:VAL:CG1	1:E:70:LEU:HD21	2.36	0.55
1:F:55:SER:O	1:F:62:ARG:HG2	2.06	0.55
1:G:32:ILE:HD13	1:G:216:LEU:CD1	2.33	0.55
1:I:236:LEU:HB2	1:I:239:VAL:HG22	1.88	0.55
1:I:415:GLU:HG3	4:I:620:HOH:O	2.05	0.55
1:K:21:ILE:HD13	1:K:39:VAL:HA	1.87	0.55
1:K:50:VAL:O	1:K:69:TYR:HA	2.05	0.55
1:K:82:TRP:HZ3	1:K:221:ILE:HD11	1.71	0.55
1:D:102:THR:HB	1:D:103:PRO:HD2	1.87	0.55
1:I:23:LEU:HB2	1:I:35:VAL:CG1	2.36	0.55
1:B:138:PHE:HB3	1:B:147:THR:O	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ILE:HG22	1:C:351:LEU:HD12	1.89	0.55
1:C:261:GLU:HA	1:C:266:GLN:HG2	1.88	0.55
1:D:129:LEU:HD22	1:D:130:GLY:H	1.71	0.55
1:E:147:THR:C	1:E:149:GLU:H	2.15	0.55
1:E:402:ASN:OD1	1:E:403:GLU:N	2.39	0.55
1:F:260:ASP:O	1:F:266:GLN:HA	2.06	0.55
1:J:182:GLU:O	1:J:200:LYS:HD3	2.07	0.55
1:J:307:CYS:O	1:J:388:LEU:HG	2.06	0.55
1:C:33:LYS:O	1:C:34:ASN:HB3	2.06	0.55
1:E:266:GLN:HB2	1:E:326:ARG:HD2	1.88	0.55
1:F:223:ARG:C	1:F:225:HIS:H	2.14	0.55
1:G:72:PRO:HA	1:G:94:CYS:HA	1.88	0.55
1:G:306:PRO:HG2	1:G:335:ARG:HD3	1.88	0.55
1:L:355:LEU:C	1:L:357:GLY:H	2.15	0.55
1:A:67:ASP:O	1:A:68:MET:HG3	2.07	0.55
1:B:78:VAL:HG11	1:B:179:MET:HE2	1.89	0.55
1:E:288:VAL:O	1:E:291:PRO:HD3	2.06	0.55
1:F:160:ALA:HB3	1:F:169:ARG:NH2	2.22	0.55
1:G:223:ARG:C	1:G:225:HIS:H	2.15	0.55
1:G:370:ARG:HH22	1:G:383:ASN:HD22	1.52	0.55
1:H:34:ASN:ND2	1:H:34:ASN:C	2.64	0.55
1:K:127:PHE:CE2	1:K:351:LEU:HB2	2.42	0.55
1:L:285:PHE:C	1:L:285:PHE:CD1	2.84	0.55
1:A:314:GLN:HG2	1:B:64:GLU:OE1	2.07	0.55
1:B:138:PHE:CE2	1:B:150:LEU:HD23	2.41	0.55
1:C:25:PHE:CE1	1:C:33:LYS:HB2	2.42	0.55
1:D:249:SER:HA	1:D:258:PHE:CE1	2.42	0.55
1:I:182:GLU:O	1:I:200:LYS:HB2	2.07	0.55
1:J:83:THR:HB	1:J:89:VAL:HG23	1.88	0.55
1:L:74:LEU:H	1:L:74:LEU:CD2	2.20	0.55
1:D:26:THR:HG23	1:D:30:GLY:HA2	1.88	0.55
1:D:123:GLY:O	1:D:252:LYS:HG3	2.07	0.55
1:F:293:VAL:HG12	1:L:440:TYR:OH	2.07	0.55
1:G:58:GLU:HB2	1:G:62:ARG:HG2	1.89	0.55
1:H:421:LYS:HD3	1:H:424:GLU:OE2	2.07	0.55
1:K:98:ASN:HB2	1:K:102:THR:O	2.07	0.55
1:K:166:GLU:HB2	1:K:227:LEU:HD11	1.87	0.55
1:C:6:ARG:HG3	1:C:10:GLU:OE2	2.07	0.55
1:E:62:ARG:O	1:E:62:ARG:HD3	2.06	0.55
1:E:292:THR:HB	1:K:440:TYR:CE1	2.42	0.55
1:F:251:PHE:HD2	1:F:254:GLY:O	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:ALA:HA	1:G:50:VAL:HG23	1.88	0.55
1:G:368:ILE:HD13	1:G:372:ILE:CG1	2.37	0.55
1:G:380:ARG:HB3	1:G:385:ILE:O	2.06	0.55
1:H:118:GLU:O	1:H:122:LEU:HD13	2.07	0.55
1:I:291:PRO:O	1:I:392:LEU:HD13	2.06	0.55
1:J:321:ARG:O	1:J:323:PRO:HD3	2.07	0.55
1:K:402:ASN:O	1:K:406:VAL:HG23	2.07	0.55
1:B:124:PHE:HA	1:B:252:LYS:HA	1.89	0.55
1:F:127:PHE:CZ	1:F:248:LEU:HD22	2.42	0.55
1:H:243:GLY:C	1:H:339:PRO:HD3	2.32	0.55
1:I:248:LEU:HD11	1:I:334:VAL:CG2	2.30	0.55
1:J:114:ARG:HH12	1:J:115:ILE:HD11	1.71	0.55
1:J:281:HIS:CE1	1:J:404:VAL:HG11	2.41	0.55
1:K:33:LYS:CA	1:L:158:ASP:HA	2.29	0.55
1:A:310:ALA:HB3	1:A:372:ILE:CD1	2.33	0.55
1:C:33:LYS:NZ	1:C:56:SER:O	2.40	0.55
1:C:400:LYS:HG3	1:C:418:ILE:HD12	1.88	0.55
1:E:126:ASP:OD1	1:E:251:PHE:HB2	2.07	0.55
1:E:170:ARG:HG2	1:E:170:ARG:HH11	1.72	0.55
1:I:338:ASP:OD2	1:I:340:ALA:HB3	2.06	0.55
1:J:173:VAL:HG13	1:J:183:ILE:HD12	1.87	0.55
1:J:190:VAL:HG13	1:J:191:ALA:N	2.17	0.55
1:J:399:PHE:HZ	1:J:409:LEU:HD22	1.71	0.55
1:K:109:ARG:HG2	1:K:109:ARG:HH21	1.72	0.55
1:L:150:LEU:CD1	1:L:192:PRO:HG2	2.37	0.55
1:D:139:LYS:HE3	1:D:149:GLU:CB	2.38	0.54
1:F:319:LEU:HG	1:F:320:ILE:CD1	2.37	0.54
1:F:342:ASN:HB3	1:F:345:LEU:HD12	1.89	0.54
1:I:122:LEU:HD22	1:I:355:LEU:HD22	1.88	0.54
1:A:78:VAL:HB	1:A:91:ARG:NH1	2.22	0.54
1:A:137:LEU:HA	1:A:228:HIS:O	2.08	0.54
1:A:328:ILE:C	1:A:328:ILE:HD12	2.32	0.54
1:G:119:MET:SD	1:G:127:PHE:HB2	2.47	0.54
1:G:306:PRO:CG	1:G:335:ARG:HH21	2.20	0.54
1:I:13:VAL:HG13	1:I:18:VAL:HB	1.88	0.54
1:I:37:ILE:HG22	1:J:185:ALA:HB2	1.89	0.54
1:I:286:THR:O	1:I:290:ASN:N	2.40	0.54
1:I:355:LEU:C	1:I:357:GLY:H	2.15	0.54
1:J:49:LYS:HE3	1:J:49:LYS:HA	1.89	0.54
1:L:82:TRP:CH2	1:L:217:VAL:HG22	2.40	0.54
1:A:41:GLN:NE2	1:F:200:LYS:HE2	2.18	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:PHE:CZ	1:A:106:GLY:HA3	2.43	0.54
1:A:224:LYS:HB2	1:F:164:LEU:CD1	2.38	0.54
1:B:131:PRO:HG2	1:B:199:PHE:HD1	1.71	0.54
1:D:351:LEU:O	1:D:351:LEU:HD13	2.07	0.54
1:H:67:ASP:O	1:H:99:PRO:HG3	2.07	0.54
1:J:211:ILE:O	1:J:215:LYS:HG3	2.07	0.54
1:K:54:GLY:C	1:K:56:SER:N	2.63	0.54
1:A:64:GLU:HG2	1:F:316:ARG:CA	2.38	0.54
1:A:115:ILE:HG22	1:A:351:LEU:HD23	1.90	0.54
1:B:207:SER:O	1:B:211:ILE:HG13	2.08	0.54
1:B:295:SER:O	1:B:299:LEU:HD13	2.07	0.54
1:F:372:ILE:HA	1:F:375:MET:HG3	1.88	0.54
1:G:267:LEU:CD2	1:G:326:ARG:NH1	2.70	0.54
1:I:114:ARG:HH11	1:I:114:ARG:CB	2.20	0.54
1:J:383:ASN:HB2	1:J:385:ILE:HG12	1.90	0.54
1:K:236:LEU:HB2	1:K:239:VAL:HG21	1.88	0.54
1:K:338:ASP:OD2	1:K:338:ASP:C	2.50	0.54
1:A:252:LYS:HB2	1:A:252:LYS:HZ3	1.73	0.54
1:C:260:ASP:O	1:C:266:GLN:HA	2.08	0.54
1:C:282:ALA:C	1:C:284:SER:N	2.66	0.54
1:D:127:PHE:CZ	1:D:351:LEU:HD23	2.42	0.54
1:E:271:ALA:O	1:E:272:LYS:C	2.50	0.54
1:F:319:LEU:HD13	1:F:388:LEU:HD11	1.90	0.54
1:G:384:GLY:C	1:G:385:ILE:HD13	2.31	0.54
1:J:396:LEU:HD11	1:J:421:LYS:HB3	1.88	0.54
1:K:270:THR:CG2	1:K:358:ILE:HD12	2.37	0.54
1:L:114:ARG:HH21	1:L:115:ILE:HG13	1.73	0.54
1:A:170:ARG:NH1	1:B:84:ALA:HB1	2.23	0.54
1:F:85:GLU:C	1:F:87:GLY:H	2.15	0.54
1:G:77:PHE:HZ	1:G:79:ILE:HD11	1.72	0.54
1:G:402:ASN:C	1:G:402:ASN:OD1	2.51	0.54
1:H:49:LYS:HD3	1:H:69:TYR:HE2	1.72	0.54
1:J:33:LYS:HE2	1:K:158:ASP:OD1	2.07	0.54
1:K:18:VAL:HA	1:K:88:LYS:HB2	1.90	0.54
1:K:83:THR:HG22	1:K:89:VAL:HG23	1.90	0.54
1:K:310:ALA:CB	1:K:372:ILE:HD13	2.37	0.54
1:C:244:MET:HB2	1:C:339:PRO:HD3	1.88	0.54
1:D:115:ILE:CG2	1:D:351:LEU:HD12	2.38	0.54
1:E:170:ARG:O	1:E:174:LEU:HG	2.08	0.54
1:E:400:LYS:HA	1:E:414:PHE:HZ	1.72	0.54
1:G:160:ALA:CB	1:G:188:HIS:HD2	2.18	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:328:ILE:HG12	1:I:329:SER:N	2.20	0.54
1:K:27:ASP:C	1:K:27:ASP:OD2	2.51	0.54
1:A:272:LYS:NZ	1:A:311:TRP:CH2	2.76	0.54
1:B:2:ALA:O	1:B:3:LYS:HB2	2.08	0.54
1:B:95:ASP:O	1:B:97:TYR:HD1	1.90	0.54
1:C:145:GLU:HA	1:C:145:GLU:OE1	2.08	0.54
1:D:104:PHE:CE2	1:D:106:GLY:HA3	2.43	0.54
1:D:128:ASN:HD22	1:D:203:GLY:HA2	1.73	0.54
1:D:264:ASP:C	1:D:266:GLN:N	2.64	0.54
1:E:368:ILE:HG21	1:E:372:ILE:CG2	2.38	0.54
1:F:376:SER:O	1:F:380:ARG:HG3	2.07	0.54
1:G:169:ARG:NH2	1:G:195:HIS:ND1	2.56	0.54
1:G:204:ALA:HB1	1:G:347:LEU:HD23	1.90	0.54
1:G:325:SER:CB	1:G:331:ARG:NH2	2.70	0.54
1:H:236:LEU:HB2	1:H:239:VAL:HG22	1.89	0.54
1:H:236:LEU:HB2	1:H:239:VAL:HG21	1.89	0.54
1:H:384:GLY:O	1:H:386:VAL:HG23	2.08	0.54
1:J:85:GLU:C	1:J:87:GLY:H	2.16	0.54
1:J:281:HIS:HE1	1:J:356:ASP:OD1	1.90	0.54
1:B:129:LEU:HG	1:B:347:LEU:CD2	2.37	0.54
1:B:278:ILE:CG2	1:B:320:ILE:HD11	2.38	0.54
1:D:256:ASN:ND2	1:D:328:ILE:O	2.41	0.54
1:E:223:ARG:C	1:E:225:HIS:H	2.16	0.54
1:E:393:ALA:HB2	1:E:425:TRP:CD2	2.43	0.54
1:F:96:ILE:HD12	1:F:96:ILE:H	1.73	0.54
1:F:409:LEU:O	1:F:413:LEU:HB2	2.07	0.54
1:H:258:PHE:HA	1:H:271:ALA:HB2	1.89	0.54
1:I:68:MET:HE3	1:I:98:ASN:HA	1.90	0.54
1:J:169:ARG:HG3	1:J:195:HIS:HB3	1.90	0.54
1:A:281:HIS:O	1:A:284:SER:HB2	2.09	0.54
1:A:316:ARG:HD3	1:B:63:ILE:O	2.08	0.54
1:A:323:PRO:HD2	1:A:331:ARG:O	2.08	0.54
1:C:252:LYS:HB2	1:C:252:LYS:NZ	2.23	0.54
1:E:199:PHE:HZ	1:E:214:PHE:CG	2.26	0.54
1:F:393:ALA:HB2	1:F:425:TRP:CE2	2.43	0.54
1:G:127:PHE:N	4:G:608:HOH:O	2.36	0.54
1:H:27:ASP:HB2	1:H:57:ILE:O	2.07	0.54
1:H:323:PRO:HD2	1:H:331:ARG:O	2.08	0.54
1:J:172:ILE:O	1:J:176:LEU:HG	2.07	0.54
1:B:126:ASP:CB	1:B:251:PHE:HB2	2.25	0.53
1:B:211:ILE:CG2	1:B:215:LYS:HE3	2.37	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:GLU:CD	1:E:142:GLU:H	2.15	0.53
1:G:256:ASN:ND2	1:G:330:THR:HB	2.23	0.53
1:G:325:SER:HB2	1:G:331:ARG:HH21	1.71	0.53
1:H:91:ARG:HD2	1:H:91:ARG:C	2.33	0.53
1:A:27:ASP:CG	1:A:31:THR:HB	2.34	0.53
1:C:97:TYR:HD2	1:C:101:GLY:O	1.91	0.53
1:E:55:SER:HB2	1:E:62:ARG:HB2	1.89	0.53
1:E:201:TYR:O	1:E:202:ALA:HB2	2.08	0.53
1:H:49:LYS:HD3	1:H:69:TYR:CE2	2.43	0.53
1:I:206:ARG:O	1:I:206:ARG:HD3	2.09	0.53
1:I:328:ILE:HD13	1:I:328:ILE:N	2.12	0.53
1:L:310:ALA:HB1	1:L:368:ILE:HB	1.90	0.53
1:B:291:PRO:HB2	1:B:421:LYS:HE3	1.90	0.53
1:D:68:MET:HE2	1:D:98:ASN:HA	1.90	0.53
1:D:353:ALA:HB2	1:D:405:MET:HE1	1.90	0.53
1:E:345:LEU:HD22	1:E:409:LEU:HD22	1.88	0.53
1:F:281:HIS:CE1	1:F:404:VAL:HG11	2.43	0.53
1:H:28:ILE:HD11	1:H:417:PHE:CA	2.39	0.53
1:I:440:TYR:HD1	1:I:444:TYR:CE2	2.25	0.53
1:J:81:PRO:HG2	1:J:82:TRP:CE3	2.44	0.53
1:K:378:GLU:HA	1:K:381:MET:HG2	1.91	0.53
1:L:6:ARG:HD2	1:L:46:LEU:HD13	1.89	0.53
1:L:96:ILE:N	1:L:96:ILE:HD12	2.22	0.53
1:L:316:ARG:HH11	1:L:316:ARG:HG3	1.74	0.53
1:A:223:ARG:HG3	1:A:223:ARG:NH1	2.23	0.53
1:A:338:ASP:HB2	1:A:339:PRO:CD	2.38	0.53
1:A:360:ASN:O	1:A:361:LYS:C	2.50	0.53
1:B:201:TYR:N	1:B:201:TYR:CD1	2.77	0.53
1:D:275:ILE:O	1:D:279:VAL:HG23	2.08	0.53
1:E:51:MET:SD	1:E:67:ASP:HB3	2.48	0.53
1:E:319:LEU:CG	1:E:320:ILE:HD12	2.27	0.53
1:G:21:ILE:CD1	1:G:42:LEU:HD13	2.37	0.53
1:G:146:PRO:HG3	1:G:228:HIS:CD2	2.44	0.53
1:I:116:LEU:O	1:I:119:MET:HB3	2.09	0.53
1:J:112:LEU:O	1:J:116:LEU:HG	2.09	0.53
1:J:423:ILE:O	1:J:427:MET:HG3	2.07	0.53
1:L:231:PHE:HB3	1:L:339:PRO:CB	2.38	0.53
1:A:107:ASP:OD2	1:A:110:ASN:N	2.41	0.53
1:A:291:PRO:HG3	1:A:341:ALA:HA	1.90	0.53
1:B:278:ILE:HG22	1:B:320:ILE:HD11	1.88	0.53
1:C:24:GLN:HE21	1:C:91:ARG:HB2	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ARG:C	1:C:91:ARG:HD2	2.34	0.53
1:E:160:ALA:HB2	1:E:188:HIS:HD2	1.73	0.53
1:E:231:PHE:HB3	1:E:339:PRO:HB2	1.90	0.53
1:E:263:ALA:O	1:E:266:GLN:HA	2.09	0.53
1:F:182:GLU:HB3	1:F:200:LYS:CD	2.34	0.53
1:G:231:PHE:O	1:G:339:PRO:HG2	2.08	0.53
1:H:371:ASN:OD1	1:H:373:TYR:HD1	1.91	0.53
1:I:418:ILE:HG22	1:I:422:GLU:HG3	1.89	0.53
1:J:247:ASN:ND2	1:J:331:ARG:HD2	2.22	0.53
1:K:348:SER:O	1:K:352:ALA:HB2	2.09	0.53
1:L:215:LYS:O	1:L:219:LYS:HG2	2.09	0.53
1:L:368:ILE:HG12	1:L:385:ILE:HG23	1.90	0.53
1:C:402:ASN:OD1	1:C:402:ASN:C	2.51	0.53
1:I:28:ILE:O	1:I:28:ILE:HD13	2.08	0.53
1:K:399:PHE:CE1	1:K:405:MET:HB3	2.44	0.53
1:A:399:PHE:HZ	1:A:409:LEU:HD12	1.73	0.53
1:D:19:LYS:HD2	1:D:86:LYS:O	2.08	0.53
1:D:375:MET:SD	1:D:379:GLU:HB3	2.48	0.53
1:G:151:ASN:HD22	1:G:166:GLU:CD	2.17	0.53
1:I:96:ILE:HD12	1:I:96:ILE:N	2.23	0.53
1:I:123:GLY:O	1:I:252:LYS:HG3	2.08	0.53
1:I:328:ILE:C	1:I:330:THR:H	2.16	0.53
1:A:35:VAL:HG11	1:A:70:LEU:CD2	2.39	0.53
1:A:146:PRO:HB3	1:A:228:HIS:ND1	2.23	0.53
1:C:197:ILE:HD12	1:C:214:PHE:CZ	2.43	0.53
1:D:349:VAL:HB	1:D:405:MET:SD	2.49	0.53
1:F:9:ILE:HG13	1:F:74:LEU:HD12	1.91	0.53
1:F:175:GLU:HG3	1:F:221:ILE:HD11	1.91	0.53
1:F:234:LYS:HB3	1:F:294:ASN:HD21	1.73	0.53
1:G:182:GLU:O	1:G:200:LYS:HG3	2.09	0.53
1:H:20:TYR:CZ	1:H:36:GLU:HB3	2.44	0.53
1:H:282:ALA:C	1:H:284:SER:H	2.17	0.53
1:I:423:ILE:O	1:I:427:MET:HG3	2.08	0.53
1:J:125:SER:HB3	1:J:126:ASP:OD1	2.09	0.53
1:J:160:ALA:O	1:J:161:PRO:C	2.51	0.53
1:L:380:ARG:CB	1:L:380:ARG:HH11	2.22	0.53
1:C:332:VAL:HG13	1:C:332:VAL:O	2.08	0.53
1:C:368:ILE:HD13	1:C:384:GLY:O	2.09	0.53
1:D:249:SER:HB3	1:D:331:ARG:CB	2.39	0.53
1:E:326:ARG:HG2	1:E:326:ARG:HH11	1.74	0.53
1:F:128:ASN:OD1	1:F:201:TYR:CE1	2.62	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:169:ARG:O	1:F:172:ILE:HB	2.09	0.53
1:F:297:LYS:HE3	1:L:436:GLU:CD	2.34	0.53
1:F:419:GLU:O	1:F:423:ILE:HG23	2.09	0.53
1:H:282:ALA:HA	1:H:285:PHE:CE2	2.44	0.53
1:H:316:ARG:HB2	1:H:371:ASN:HD21	1.73	0.53
1:J:288:VAL:O	1:J:291:PRO:HD3	2.09	0.53
1:L:261:GLU:HA	1:L:266:GLN:HE21	1.73	0.53
1:D:281:HIS:NE2	1:D:404:VAL:HG21	2.24	0.53
1:G:175:GLU:O	1:G:178:GLU:HB3	2.09	0.53
1:I:35:VAL:HG13	1:I:35:VAL:O	2.08	0.53
1:I:35:VAL:HG11	1:I:70:LEU:HD23	1.90	0.53
1:K:82:TRP:CZ3	1:K:221:ILE:HD11	2.43	0.53
1:K:282:ALA:C	1:K:284:SER:H	2.16	0.53
1:L:147:THR:C	1:L:149:GLU:H	2.16	0.53
1:L:278:ILE:O	1:L:282:ALA:HB2	2.08	0.53
1:A:281:HIS:HD2	1:A:402:ASN:ND2	2.07	0.52
1:B:159:LEU:CD1	1:C:22:ARG:NH1	2.72	0.52
1:B:243:GLY:CA	1:B:298:ARG:NH1	2.72	0.52
1:C:3:LYS:HG2	1:C:4:TYR:HD1	1.73	0.52
1:D:371:ASN:OD1	1:D:375:MET:HB2	2.09	0.52
1:E:259:PHE:O	1:E:268:SER:HB3	2.09	0.52
1:E:297:LYS:HE3	1:K:436:GLU:CD	2.34	0.52
1:F:24:GLN:NE2	1:F:91:ARG:NH1	2.57	0.52
1:H:5:THR:C	1:H:7:GLU:N	2.65	0.52
1:H:244:MET:N	1:H:338:ASP:HA	2.25	0.52
1:I:168:CYS:O	1:I:172:ILE:HG13	2.09	0.52
1:I:371:ASN:ND2	1:I:375:MET:HG2	2.23	0.52
1:J:160:ALA:HB2	1:J:188:HIS:CD2	2.43	0.52
1:J:377:LYS:H	1:J:377:LYS:CD	2.13	0.52
1:K:95:ASP:OD1	1:K:109:ARG:HG2	2.09	0.52
1:L:52:PHE:HE2	1:L:56:SER:OG	1.93	0.52
1:A:35:VAL:HG13	1:A:35:VAL:O	2.08	0.52
1:B:265:LEU:O	1:B:266:GLN:HB2	2.09	0.52
1:B:285:PHE:HB2	1:B:349:VAL:CG1	2.39	0.52
1:D:399:PHE:CE1	1:D:405:MET:HB3	2.44	0.52
1:E:160:ALA:HB1	1:E:161:PRO:CD	2.38	0.52
1:E:319:LEU:C	1:E:320:ILE:HD12	2.34	0.52
1:E:361:LYS:O	1:E:362:LEU:HD23	2.09	0.52
1:F:183:ILE:HD12	1:F:197:ILE:CG2	2.39	0.52
1:F:297:LYS:HE3	1:L:436:GLU:OE2	2.09	0.52
1:I:114:ARG:NH2	1:I:407:LYS:O	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:355:LEU:C	1:I:357:GLY:N	2.66	0.52
1:K:98:ASN:C	1:K:100:ASP:H	2.16	0.52
1:K:152:ASP:CB	1:K:161:PRO:HG3	2.37	0.52
1:K:326:ARG:HG3	1:K:327:GLY:N	2.23	0.52
1:A:380:ARG:HA	1:A:383:ASN:HD22	1.73	0.52
1:C:115:ILE:HD11	1:C:408:ALA:O	2.09	0.52
1:D:83:THR:HB	1:D:87:GLY:O	2.09	0.52
1:F:133:PRO:HG2	1:F:199:PHE:HE1	1.75	0.52
1:G:33:LYS:HD3	1:H:158:ASP:OD1	2.10	0.52
1:G:360:ASN:O	1:G:361:LYS:C	2.53	0.52
1:G:368:ILE:O	1:G:369:ASP:HB2	2.09	0.52
1:J:121:ASP:C	1:J:122:LEU:HD22	2.34	0.52
1:J:162:THR:O	1:J:164:LEU:N	2.43	0.52
1:J:402:ASN:CG	1:J:405:MET:HG2	2.34	0.52
1:K:170:ARG:HG2	1:K:174:LEU:CD2	2.40	0.52
1:K:232:MET:HB3	1:K:235:PRO:HG3	1.91	0.52
1:L:34:ASN:C	1:L:34:ASN:HD22	2.18	0.52
1:A:337:VAL:HG12	1:A:338:ASP:H	1.73	0.52
1:B:231:PHE:HB3	1:B:339:PRO:HB2	1.90	0.52
1:C:435:TRP:CZ2	1:C:439:GLN:HG3	2.44	0.52
1:D:34:ASN:C	1:D:34:ASN:HD22	2.17	0.52
1:E:234:LYS:HB3	1:E:294:ASN:HD21	1.74	0.52
1:G:33:LYS:HE3	1:H:156:TYR:O	2.10	0.52
1:H:168:CYS:O	1:H:169:ARG:C	2.53	0.52
1:H:276:ALA:HA	1:H:364:ALA:HB2	1.91	0.52
1:H:286:THR:HG23	1:H:290:ASN:ND2	2.25	0.52
1:I:166:GLU:O	1:I:168:CYS:N	2.42	0.52
1:I:261:GLU:CA	1:I:266:GLN:HG2	2.27	0.52
1:J:207:SER:O	1:J:208:CYS:C	2.51	0.52
1:J:272:LYS:CA	1:J:275:ILE:HD12	2.29	0.52
1:K:259:PHE:CD1	1:K:326:ARG:HD2	2.42	0.52
1:A:53:ASP:OD2	1:A:55:SER:HB3	2.09	0.52
1:B:68:MET:SD	1:B:96:ILE:CG2	2.98	0.52
1:B:120:GLU:C	1:B:122:LEU:N	2.68	0.52
1:B:236:LEU:HB2	1:B:239:VAL:HG21	1.92	0.52
1:B:248:LEU:O	1:B:331:ARG:HB2	2.09	0.52
1:D:318:PRO:O	1:D:335:ARG:HD2	2.10	0.52
1:E:164:LEU:HG	1:F:82:TRP:HB3	1.92	0.52
1:F:136:PHE:HB3	1:F:138:PHE:HE1	1.75	0.52
1:F:261:GLU:HA	1:F:266:GLN:HE21	1.74	0.52
1:F:323:PRO:HD2	1:F:331:ARG:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:315:ASN:HB3	1:G:318:PRO:HD3	1.92	0.52
1:K:135:PHE:HB3	1:K:231:PHE:CD1	2.45	0.52
1:L:5:THR:HG23	1:L:8:ASP:OD2	2.09	0.52
1:L:274:PHE:HD1	1:L:358:ILE:HD11	1.75	0.52
1:A:150:LEU:CD1	1:A:192:PRO:HB2	2.39	0.52
1:B:243:GLY:HA3	1:B:298:ARG:NH1	2.23	0.52
1:C:297:LYS:HE2	1:I:429:ARG:O	2.09	0.52
1:D:168:CYS:O	1:D:169:ARG:C	2.52	0.52
1:F:91:ARG:HD2	1:F:91:ARG:C	2.34	0.52
1:F:319:LEU:C	1:F:320:ILE:HD12	2.34	0.52
1:G:333:GLU:HG2	1:G:335:ARG:HG2	1.90	0.52
1:H:79:ILE:O	1:H:79:ILE:HG22	2.08	0.52
1:H:131:PRO:C	1:H:133:PRO:HD3	2.34	0.52
1:J:39:VAL:HG13	1:J:40:SER:N	2.23	0.52
1:K:322:ILE:O	1:K:322:ILE:HG22	2.10	0.52
1:L:73:ASP:HB3	1:L:76:THR:OG1	2.09	0.52
1:L:237:PHE:CD1	1:L:238:GLY:N	2.78	0.52
1:A:86:LYS:HD2	1:F:178:GLU:OE1	2.10	0.52
1:A:105:GLU:H	1:A:105:GLU:CD	2.18	0.52
1:A:274:PHE:HE2	1:A:332:VAL:HG21	1.74	0.52
1:B:291:PRO:O	1:B:392:LEU:HD13	2.09	0.52
1:B:375:MET:HB3	1:B:379:GLU:HB2	1.92	0.52
1:E:27:ASP:HA	1:E:57:ILE:HG23	1.91	0.52
1:F:206:ARG:HB2	4:F:621:HOH:O	2.10	0.52
1:G:33:LYS:HD3	1:H:158:ASP:HA	1.92	0.52
1:G:157:PHE:CE1	1:L:35:VAL:HG12	2.45	0.52
1:H:309:VAL:HG13	1:H:319:LEU:HD23	1.92	0.52
1:H:347:LEU:O	1:H:348:SER:C	2.52	0.52
1:J:404:VAL:HG13	1:J:405:MET:CE	2.38	0.52
1:A:37:ILE:H	1:A:37:ILE:HD13	1.74	0.52
1:B:397:GLU:HA	1:B:400:LYS:HE2	1.91	0.52
1:C:203:GLY:O	1:C:204:ALA:C	2.53	0.52
1:D:23:LEU:HD13	1:D:70:LEU:HD23	1.92	0.52
1:E:91:ARG:C	1:E:91:ARG:CD	2.82	0.52
1:E:278:ILE:HG23	1:E:285:PHE:CZ	2.45	0.52
1:E:285:PHE:HB3	1:E:405:MET:SD	2.50	0.52
1:G:286:THR:HA	1:G:289:THR:OG1	2.10	0.52
1:H:360:ASN:O	1:H:361:LYS:C	2.51	0.52
1:I:224:LYS:HD3	1:J:164:LEU:HD11	1.90	0.52
1:I:406:VAL:HG22	1:I:414:PHE:CZ	2.44	0.52
1:J:150:LEU:HD13	1:J:192:PRO:HG2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:184:GLU:OE1	1:L:200:LYS:HG2	2.10	0.52
1:L:203:GLY:O	1:L:204:ALA:C	2.52	0.52
1:A:379:GLU:HG2	1:A:379:GLU:O	2.08	0.52
1:C:58:GLU:HG2	1:C:416:HIS:CD2	2.44	0.52
1:C:143:LYS:HE2	1:C:143:LYS:HA	1.90	0.52
1:D:84:ALA:C	1:D:86:LYS:H	2.18	0.52
1:D:297:LYS:HE3	1:J:436:GLU:OE1	2.08	0.52
1:D:306:PRO:O	1:D:388:LEU:HD12	2.09	0.52
1:F:160:ALA:HB3	1:F:169:ARG:HH21	1.74	0.52
1:F:380:ARG:NH1	1:F:385:ILE:HG21	2.25	0.52
1:F:397:GLU:HA	1:F:400:LYS:HD3	1.91	0.52
1:G:259:PHE:HB2	1:G:330:THR:HG21	1.91	0.52
1:H:372:ILE:HG13	1:H:385:ILE:HD12	1.90	0.52
1:I:127:PHE:HZ	1:I:248:LEU:HD23	1.75	0.52
1:L:82:TRP:HE1	1:L:221:ILE:HD11	1.74	0.52
1:C:22:ARG:NH1	1:C:36:GLU:OE2	2.43	0.52
1:D:127:PHE:CD2	1:D:351:LEU:HD23	2.45	0.52
1:E:281:HIS:HD2	1:E:402:ASN:ND2	2.00	0.52
1:E:345:LEU:HD22	1:E:409:LEU:CD2	2.40	0.52
1:F:13:VAL:HG21	1:F:42:LEU:HD21	1.92	0.52
1:F:52:PHE:CZ	1:F:54:GLY:HA2	2.46	0.52
1:F:375:MET:O	1:F:380:ARG:NH2	2.43	0.52
1:F:427:MET:HE2	1:L:435:TRP:HZ2	1.75	0.52
1:G:167:ASN:HD22	1:G:170:ARG:CZ	2.23	0.52
1:H:8:ASP:O	1:H:12:LEU:HG	2.10	0.52
1:H:78:VAL:HB	1:H:91:ARG:HG3	1.92	0.52
1:H:370:ARG:O	1:H:372:ILE:HG23	2.10	0.52
1:H:378:GLU:O	1:H:381:MET:HG3	2.09	0.52
1:J:151:ASN:HD22	1:J:166:GLU:CD	2.17	0.52
1:L:355:LEU:C	1:L:357:GLY:N	2.67	0.52
1:B:159:LEU:HD13	1:C:34:ASN:CG	2.34	0.51
1:D:135:PHE:HB3	1:D:231:PHE:CE1	2.45	0.51
1:E:128:ASN:HA	1:E:202:ALA:O	2.09	0.51
1:E:404:VAL:HG13	1:E:405:MET:HE2	1.92	0.51
1:G:76:THR:HG21	1:G:93:ILE:HB	1.92	0.51
1:G:120:GLU:HA	1:G:124:PHE:O	2.10	0.51
1:G:211:ILE:HD13	1:G:244:MET:HE1	1.92	0.51
1:J:97:TYR:CE2	1:J:103:PRO:HG3	2.45	0.51
1:L:34:ASN:ND2	1:L:34:ASN:O	2.43	0.51
1:L:131:PRO:HG2	1:L:199:PHE:HD2	1.75	0.51
1:A:250:LEU:HD12	1:A:258:PHE:CE2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:GLY:HA2	1:D:362:LEU:HD22	1.92	0.51
1:F:244:MET:N	1:F:338:ASP:HA	2.25	0.51
1:G:63:ILE:HG13	1:G:64:GLU:H	1.75	0.51
1:G:311:TRP:HB3	1:G:320:ILE:HB	1.92	0.51
1:H:364:ALA:HB1	1:H:365:PRO:HD2	1.92	0.51
1:I:131:PRO:HD2	1:I:199:PHE:HB2	1.93	0.51
1:I:402:ASN:OD1	1:I:404:VAL:HG12	2.10	0.51
1:J:11:LYS:O	1:J:15:GLU:HG3	2.10	0.51
1:A:35:VAL:HG11	1:A:70:LEU:HD23	1.93	0.51
1:A:343:PRO:O	1:A:347:LEU:HB2	2.10	0.51
1:C:369:ASP:CG	1:C:370:ARG:H	2.18	0.51
1:E:285:PHE:CB	1:E:349:VAL:HG13	2.41	0.51
1:F:325:SER:O	1:F:326:ARG:HD3	2.10	0.51
1:H:68:MET:HE1	1:H:104:PHE:CZ	2.45	0.51
1:H:349:VAL:CG2	1:H:405:MET:SD	2.99	0.51
1:I:155:GLY:O	1:I:158:ASP:HB2	2.11	0.51
1:I:319:LEU:HB3	1:I:320:ILE:HD12	1.93	0.51
1:J:356:ASP:HA	1:J:359:LYS:HE2	1.92	0.51
1:J:434:PRO:O	1:J:438:GLU:HG3	2.11	0.51
1:K:3:LYS:HE2	1:K:4:TYR:OH	2.10	0.51
1:L:344:TYR:O	1:L:348:SER:HB2	2.09	0.51
1:L:372:ILE:HG22	1:L:385:ILE:HD13	1.92	0.51
1:A:110:ASN:O	1:A:113:LYS:HB2	2.11	0.51
1:A:386:VAL:HG12	1:A:387:ASP:N	2.24	0.51
1:B:135:PHE:HB3	1:B:231:PHE:CD1	2.45	0.51
1:B:286:THR:HG21	1:B:388:LEU:HD22	1.92	0.51
1:C:159:LEU:HD12	1:D:34:ASN:CG	2.35	0.51
1:D:236:LEU:HB2	1:D:239:VAL:HG21	1.90	0.51
1:E:91:ARG:NH1	1:E:93:ILE:HD11	2.25	0.51
1:F:48:ASN:HB3	1:F:71:TYR:CE1	2.46	0.51
1:F:203:GLY:O	1:F:204:ALA:C	2.52	0.51
1:F:379:GLU:HG3	1:F:385:ILE:CD1	2.41	0.51
1:J:349:VAL:HG23	1:J:409:LEU:CD1	2.40	0.51
1:L:375:MET:HG3	1:L:379:GLU:CG	2.38	0.51
1:A:288:VAL:O	1:A:291:PRO:HD3	2.10	0.51
1:A:421:LYS:HD3	1:A:424:GLU:OE2	2.10	0.51
1:C:323:PRO:HD2	1:C:331:ARG:O	2.10	0.51
1:D:52:PHE:CE2	1:D:54:GLY:HA2	2.45	0.51
1:D:211:ILE:HG22	1:D:215:LYS:HE3	1.91	0.51
1:E:417:PHE:HD2	1:E:418:ILE:HD12	1.75	0.51
1:F:267:LEU:HD21	1:F:326:ARG:NH1	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:271:ALA:O	1:F:275:ILE:HG12	2.11	0.51
1:H:96:ILE:HD13	1:H:107:ASP:CG	2.36	0.51
1:J:191:ALA:HB2	1:J:240:ASN:HB2	1.93	0.51
1:J:207:SER:O	1:J:210:ASP:N	2.43	0.51
1:K:21:ILE:HD12	1:K:21:ILE:N	2.24	0.51
1:K:377:LYS:HA	1:K:380:ARG:NH2	2.25	0.51
1:A:36:GLU:CD	1:F:169:ARG:HH12	2.18	0.51
1:A:166:GLU:CD	1:A:167:ASN:H	2.19	0.51
1:B:300:VAL:HA	1:H:429:ARG:HH22	1.75	0.51
1:D:22:ARG:NH1	1:D:36:GLU:OE2	2.43	0.51
1:D:406:VAL:HG22	1:D:414:PHE:CZ	2.45	0.51
1:E:402:ASN:CG	1:E:405:MET:HG2	2.35	0.51
1:F:114:ARG:NH2	1:F:407:LYS:O	2.44	0.51
1:H:345:LEU:O	1:H:349:VAL:HG12	2.11	0.51
1:I:150:LEU:HD13	1:I:192:PRO:HB2	1.93	0.51
1:J:140:LEU:HD12	1:J:226:GLY:C	2.36	0.51
1:J:328:ILE:HD12	1:J:328:ILE:C	2.35	0.51
1:K:380:ARG:NH1	1:K:380:ARG:HB2	2.26	0.51
1:L:23:LEU:HB2	1:L:35:VAL:HG22	1.92	0.51
1:L:383:ASN:HB2	1:L:385:ILE:CG1	2.40	0.51
1:A:237:PHE:CD1	1:A:238:GLY:N	2.79	0.51
1:B:393:ALA:HB2	1:B:425:TRP:CE2	2.45	0.51
1:C:380:ARG:HH11	1:C:380:ARG:CB	2.23	0.51
1:D:20:TYR:CZ	1:D:36:GLU:HB3	2.45	0.51
1:D:406:VAL:HG22	1:D:414:PHE:CE1	2.45	0.51
1:G:281:HIS:CD2	1:G:402:ASN:HD21	2.28	0.51
1:I:37:ILE:HG22	1:J:185:ALA:CB	2.41	0.51
1:I:201:TYR:CD1	1:I:201:TYR:C	2.88	0.51
1:I:203:GLY:O	1:I:207:SER:N	2.38	0.51
1:I:285:PHE:HB2	1:I:349:VAL:HG11	1.93	0.51
1:K:83:THR:CG2	1:K:89:VAL:H	2.04	0.51
1:L:30:GLY:HA2	1:L:342:ASN:ND2	2.25	0.51
1:L:242:SER:O	1:L:298:ARG:NE	2.44	0.51
1:L:311:TRP:NE1	1:L:367:PRO:HA	2.25	0.51
1:A:38:PRO:HD2	1:A:41:GLN:HG3	1.93	0.51
1:A:191:ALA:HB3	1:A:194:GLN:NE2	2.25	0.51
1:A:300:VAL:HG22	1:G:429:ARG:NH2	2.26	0.51
1:D:57:ILE:HD11	1:D:96:ILE:HG21	1.91	0.51
1:E:85:GLU:H	1:E:85:GLU:CD	2.16	0.51
1:G:37:ILE:HG22	1:H:185:ALA:CB	2.41	0.51
1:G:98:ASN:ND2	1:G:104:PHE:HA	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:429:ARG:HD3	4:J:610:HOH:O	2.10	0.51
1:K:19:LYS:HA	1:K:39:VAL:HB	1.91	0.51
1:L:9:ILE:O	1:L:13:VAL:HG23	2.11	0.51
1:L:316:ARG:HB2	1:L:370:ARG:NH1	2.26	0.51
1:A:158:ASP:OD2	1:B:33:LYS:HE2	2.11	0.51
1:D:128:ASN:ND2	1:D:203:GLY:HA2	2.26	0.51
1:D:315:ASN:ND2	1:D:370:ARG:HA	2.26	0.51
1:F:281:HIS:O	1:F:284:SER:N	2.42	0.51
1:G:370:ARG:NH2	1:G:383:ASN:HD22	2.08	0.51
1:J:91:ARG:C	1:J:91:ARG:CD	2.82	0.51
1:J:282:ALA:C	1:J:284:SER:H	2.18	0.51
1:L:109:ARG:HG2	1:L:109:ARG:HH21	1.76	0.51
1:L:306:PRO:O	1:L:388:LEU:HD12	2.11	0.51
1:B:370:ARG:NH2	1:B:375:MET:CG	2.71	0.51
1:C:124:PHE:CE2	1:C:250:LEU:HD13	2.46	0.51
1:D:159:LEU:CD1	1:E:22:ARG:HH11	2.23	0.51
1:E:145:GLU:OE1	1:E:145:GLU:HA	2.11	0.51
1:E:206:ARG:O	1:E:209:ASP:HB2	2.11	0.51
1:F:146:PRO:O	1:F:147:THR:HG23	2.10	0.51
1:F:205:VAL:CG1	1:F:206:ARG:N	2.74	0.51
1:F:386:VAL:HG23	1:F:386:VAL:O	2.11	0.51
1:G:260:ASP:HB3	1:G:263:ALA:HB3	1.93	0.51
1:H:223:ARG:O	1:H:226:GLY:N	2.41	0.51
1:I:27:ASP:C	1:I:27:ASP:OD2	2.53	0.51
1:I:116:LEU:HD23	1:I:351:LEU:HD11	1.93	0.51
1:K:107:ASP:OD2	1:K:110:ASN:OD1	2.29	0.51
1:K:129:LEU:HD23	1:K:207:SER:OG	2.10	0.51
1:D:34:ASN:ND2	1:D:34:ASN:O	2.44	0.50
1:D:253:ASN:O	1:D:255:VAL:HG13	2.11	0.50
1:D:311:TRP:CD1	1:D:365:PRO:HG2	2.46	0.50
1:E:356:ASP:O	1:E:360:ASN:HB2	2.11	0.50
1:E:374:VAL:HG23	1:E:375:MET:N	2.26	0.50
1:F:437:ARG:HD3	1:L:148:LEU:CD2	2.41	0.50
1:G:402:ASN:CG	1:G:405:MET:HG2	2.36	0.50
1:G:406:VAL:HA	1:G:414:PHE:CD1	2.46	0.50
1:K:35:VAL:HG13	1:K:35:VAL:O	2.12	0.50
1:L:13:VAL:HG13	1:L:18:VAL:HB	1.93	0.50
1:L:23:LEU:HB3	1:L:70:LEU:HD23	1.93	0.50
1:L:82:TRP:HE1	1:L:221:ILE:HD13	1.76	0.50
1:L:371:ASN:HD21	1:L:374:VAL:HB	1.75	0.50
1:A:36:GLU:OE2	1:F:169:ARG:NH1	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:PRO:HA	1:A:394:GLU:OE1	2.11	0.50
1:C:160:ALA:O	1:C:161:PRO:C	2.54	0.50
1:D:167:ASN:HD22	1:D:170:ARG:HB3	1.76	0.50
1:F:3:LYS:HE2	1:F:4:TYR:CE2	2.46	0.50
1:F:53:ASP:OD1	1:F:62:ARG:NH2	2.43	0.50
1:F:172:ILE:HD12	1:F:218:VAL:HA	1.92	0.50
1:G:315:ASN:HB3	1:G:318:PRO:HG3	1.93	0.50
1:H:5:THR:O	1:H:7:GLU:N	2.44	0.50
1:H:351:LEU:CD2	1:H:355:LEU:HG	2.42	0.50
1:I:293:VAL:HG11	1:I:428:PHE:CD1	2.46	0.50
1:A:170:ARG:NH1	1:A:171:ASP:OD2	2.44	0.50
1:A:437:ARG:O	1:A:441:MET:HB2	2.11	0.50
1:C:142:GLU:CD	1:C:142:GLU:H	2.20	0.50
1:D:160:ALA:HB3	1:D:169:ARG:HH22	1.76	0.50
1:E:378:GLU:O	1:E:382:GLU:HG3	2.11	0.50
1:F:140:LEU:HD12	1:F:226:GLY:C	2.37	0.50
1:G:237:PHE:CD2	1:G:238:GLY:N	2.79	0.50
1:G:267:LEU:CD2	1:G:326:ARG:HH12	2.24	0.50
1:H:372:ILE:HA	1:H:375:MET:SD	2.51	0.50
1:I:35:VAL:HG11	1:I:70:LEU:HD21	1.92	0.50
1:J:160:ALA:O	1:J:161:PRO:O	2.30	0.50
1:L:135:PHE:HB3	1:L:231:PHE:CD1	2.46	0.50
1:B:35:VAL:HG13	1:B:35:VAL:O	2.11	0.50
1:B:371:ASN:HD22	1:B:372:ILE:N	2.10	0.50
1:E:119:MET:HE1	1:E:126:ASP:HA	1.94	0.50
1:E:437:ARG:O	1:E:441:MET:HB3	2.12	0.50
1:F:60:PHE:CZ	1:F:423:ILE:HD11	2.46	0.50
1:G:164:LEU:CD1	1:L:224:LYS:HD3	2.41	0.50
1:G:375:MET:SD	1:G:380:ARG:HA	2.51	0.50
1:G:399:PHE:HZ	1:G:409:LEU:CD2	2.21	0.50
1:G:423:ILE:O	1:G:424:GLU:C	2.54	0.50
1:H:52:PHE:HE2	1:H:56:SER:OG	1.95	0.50
1:H:166:GLU:O	1:H:166:GLU:CD	2.54	0.50
1:H:203:GLY:O	1:H:206:ARG:N	2.42	0.50
1:H:399:PHE:HZ	1:H:409:LEU:HD12	1.76	0.50
1:J:169:ARG:HG3	1:J:169:ARG:HH21	1.76	0.50
1:J:224:LYS:HB2	1:K:164:LEU:HD12	1.93	0.50
1:K:20:TYR:OH	1:K:36:GLU:HG3	2.11	0.50
1:K:81:PRO:HG2	1:K:82:TRP:CE3	2.47	0.50
1:L:306:PRO:HB3	1:L:319:LEU:HA	1.93	0.50
1:L:376:SER:H	1:L:379:GLU:CG	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASN:O	1:A:255:VAL:HG23	2.12	0.50
1:B:165:GLY:HA3	1:C:223:ARG:HH21	1.77	0.50
1:F:133:PRO:HD2	1:F:197:ILE:O	2.11	0.50
1:G:429:ARG:NH1	1:G:430:THR:HG22	2.26	0.50
1:H:116:LEU:HD22	1:H:119:MET:CE	2.40	0.50
1:I:199:PHE:N	1:I:199:PHE:CD1	2.79	0.50
1:I:267:LEU:HG	1:I:326:ARG:HH12	1.75	0.50
1:J:52:PHE:CZ	1:J:54:GLY:HA2	2.47	0.50
1:J:234:LYS:HB3	1:J:294:ASN:ND2	2.27	0.50
1:J:351:LEU:CD2	1:J:355:LEU:HG	2.40	0.50
1:L:287:ALA:HB2	1:L:395:ALA:C	2.36	0.50
1:A:91:ARG:NH2	1:A:213:THR:OG1	2.43	0.50
1:A:133:PRO:O	1:A:196:GLU:HG3	2.12	0.50
1:A:267:LEU:HD21	1:A:326:ARG:HH12	1.77	0.50
1:B:405:MET:HE2	1:B:405:MET:HA	1.92	0.50
1:C:127:PHE:CE2	1:C:351:LEU:HB2	2.47	0.50
1:D:68:MET:CE	1:D:104:PHE:HB2	2.40	0.50
1:D:121:ASP:O	1:D:122:LEU:HD23	2.12	0.50
1:F:16:GLU:HG3	1:F:88:LYS:HE3	1.94	0.50
1:G:147:THR:C	1:G:149:GLU:H	2.20	0.50
1:H:79:ILE:O	1:H:80:PHE:C	2.55	0.50
1:I:169:ARG:HG3	1:I:195:HIS:CG	2.47	0.50
1:I:199:PHE:N	1:I:199:PHE:HD1	2.10	0.50
1:I:216:LEU:HD11	1:J:159:LEU:HD13	1.93	0.50
1:I:282:ALA:C	1:I:284:SER:N	2.70	0.50
1:J:46:LEU:CD2	1:J:74:LEU:HD11	2.41	0.50
1:J:176:LEU:CB	1:J:183:ILE:HD11	2.40	0.50
1:L:81:PRO:HG2	1:L:82:TRP:H	1.76	0.50
1:A:281:HIS:HD2	1:A:402:ASN:HD21	1.59	0.50
1:A:321:ARG:HG2	1:A:322:ILE:N	2.25	0.50
1:B:97:TYR:CE2	1:B:103:PRO:HG3	2.47	0.50
1:C:326:ARG:HA	1:C:330:THR:OG1	2.11	0.50
1:C:402:ASN:CG	1:C:404:VAL:HG12	2.36	0.50
1:G:100:ASP:OD2	1:G:101:GLY:N	2.41	0.50
1:G:434:PRO:O	1:G:438:GLU:HG3	2.12	0.50
1:I:84:ALA:HB3	1:I:87:GLY:O	2.12	0.50
1:I:142:GLU:OE2	1:I:142:GLU:N	2.38	0.50
1:I:396:LEU:HD11	1:I:421:LYS:HB3	1.94	0.50
1:J:64:GLU:HG2	1:K:315:ASN:O	2.12	0.50
1:J:162:THR:HG22	1:J:163:ASP:N	2.26	0.50
1:J:196:GLU:O	1:J:197:ILE:HD13	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:236:LEU:HD12	1:J:239:VAL:HG21	1.93	0.50
1:J:257:ALA:O	1:J:270:THR:HG23	2.12	0.50
1:J:399:PHE:HE1	1:J:405:MET:HB3	1.76	0.50
1:L:286:THR:HG23	1:L:290:ASN:HD22	1.77	0.50
1:A:164:LEU:HD11	1:B:224:LYS:HD3	1.93	0.50
1:A:275:ILE:O	1:A:279:VAL:HG23	2.12	0.50
1:C:338:ASP:HB2	1:C:339:PRO:HD2	1.94	0.50
1:E:375:MET:HB3	1:E:379:GLU:HG2	1.94	0.50
1:F:22:ARG:HG2	1:F:22:ARG:HH11	1.76	0.50
1:F:45:ALA:HA	1:F:50:VAL:CG2	2.35	0.50
1:G:132:GLU:OE2	4:G:615:HOH:O	2.19	0.50
1:G:440:TYR:O	1:G:441:MET:C	2.55	0.50
1:H:95:ASP:OD1	1:H:109:ARG:HD3	2.12	0.50
1:H:160:ALA:HB3	1:H:169:ARG:HH12	1.77	0.50
1:I:34:ASN:C	1:I:34:ASN:HD22	2.20	0.50
1:K:372:ILE:O	1:K:373:TYR:HD2	1.94	0.50
1:A:435:TRP:O	1:A:439:GLN:HG2	2.12	0.50
1:B:381:MET:C	1:B:382:GLU:HG3	2.37	0.50
1:D:140:LEU:CD2	1:D:228:HIS:HB2	2.42	0.50
1:D:200:LYS:CE	1:E:41:GLN:HE22	2.25	0.50
1:E:148:LEU:HD13	1:E:148:LEU:N	2.26	0.50
1:F:402:ASN:OD1	1:F:404:VAL:HG12	2.12	0.50
1:G:245:HIS:CD2	1:G:335:ARG:HB3	2.47	0.50
1:I:236:LEU:HD12	1:I:239:VAL:HG21	1.94	0.50
1:K:5:THR:HG23	1:K:8:ASP:H	1.77	0.50
1:L:156:TYR:CE1	1:L:189:GLU:OE1	2.64	0.50
1:L:281:HIS:CE1	1:L:404:VAL:HG11	2.47	0.50
1:C:3:LYS:HB3	1:C:75:ASN:OD1	2.12	0.49
1:C:182:GLU:HG2	1:C:200:LYS:HD2	1.94	0.49
1:D:282:ALA:HA	1:D:285:PHE:CZ	2.46	0.49
1:G:112:LEU:HD12	1:G:344:TYR:HD2	1.77	0.49
1:H:20:TYR:O	1:H:89:VAL:HG13	2.11	0.49
1:H:111:ASN:O	1:H:115:ILE:HG12	2.11	0.49
1:H:184:GLU:HB2	1:H:199:PHE:O	2.12	0.49
1:H:311:TRP:HB3	1:H:320:ILE:HB	1.93	0.49
1:I:80:PHE:CE1	1:I:91:ARG:HG2	2.42	0.49
1:I:156:TYR:O	1:I:158:ASP:N	2.44	0.49
1:K:115:ILE:HG22	1:K:351:LEU:CD1	2.38	0.49
1:L:83:THR:C	1:L:85:GLU:OE2	2.55	0.49
1:L:261:GLU:O	1:L:266:GLN:HG2	2.12	0.49
1:L:353:ALA:HB2	1:L:405:MET:HE1	1.92	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ALA:HB2	1:B:425:TRP:CD2	2.46	0.49
1:D:161:PRO:HB2	1:D:167:ASN:OD1	2.12	0.49
1:D:174:LEU:HD13	1:E:86:LYS:HB2	1.94	0.49
1:E:169:ARG:HH21	1:F:36:GLU:CD	2.19	0.49
1:G:27:ASP:HB2	1:G:57:ILE:HA	1.93	0.49
1:H:74:LEU:HD22	1:H:74:LEU:N	2.17	0.49
1:H:82:TRP:HE1	1:H:221:ILE:HD11	1.75	0.49
1:H:189:GLU:OE2	1:H:190:VAL:HG23	2.12	0.49
1:H:224:LYS:HB2	1:I:164:LEU:HD13	1.93	0.49
1:I:368:ILE:HG21	1:I:372:ILE:CG2	2.42	0.49
1:J:162:THR:CG2	1:J:163:ASP:N	2.75	0.49
1:J:208:CYS:HA	1:J:343:PRO:HB2	1.94	0.49
1:J:309:VAL:CG2	1:J:386:VAL:HB	2.42	0.49
1:K:48:ASN:HB3	1:K:71:TYR:CD1	2.47	0.49
1:K:391:THR:OG1	1:K:394:GLU:HB2	2.12	0.49
1:B:399:PHE:HZ	1:B:409:LEU:HD12	1.77	0.49
1:C:156:TYR:CE2	1:D:62:ARG:NH1	2.80	0.49
1:C:179:MET:HE3	1:C:217:VAL:HG21	1.93	0.49
1:C:203:GLY:O	1:C:205:VAL:N	2.45	0.49
1:D:346:ALA:O	1:D:347:LEU:C	2.56	0.49
1:E:201:TYR:C	1:E:201:TYR:CD2	2.88	0.49
1:E:293:VAL:HG11	1:E:428:PHE:CE2	2.47	0.49
1:E:429:ARG:NH2	1:K:300:VAL:HG12	2.26	0.49
1:F:24:GLN:HE21	1:F:91:ARG:HH11	1.59	0.49
1:F:309:VAL:O	1:F:310:ALA:HB2	2.12	0.49
1:H:76:THR:O	1:H:78:VAL:HG23	2.12	0.49
1:H:100:ASP:CG	1:H:101:GLY:H	2.21	0.49
1:I:402:ASN:CG	1:I:405:MET:HG2	2.37	0.49
1:K:115:ILE:HD11	1:K:408:ALA:O	2.12	0.49
1:K:183:ILE:HD12	1:K:183:ILE:N	2.27	0.49
1:L:58:GLU:O	1:L:61:VAL:HG22	2.12	0.49
1:A:52:PHE:CE1	1:A:70:LEU:CD1	2.95	0.49
1:B:107:ASP:HB3	1:B:110:ASN:HB2	1.95	0.49
1:B:109:ARG:HG3	1:B:344:TYR:CE2	2.48	0.49
1:B:409:LEU:O	1:B:413:LEU:HB2	2.12	0.49
1:C:402:ASN:ND2	1:C:404:VAL:HG12	2.28	0.49
1:D:311:TRP:HA	1:D:320:ILE:HB	1.94	0.49
1:E:45:ALA:HA	1:E:50:VAL:HG23	1.95	0.49
1:E:48:ASN:OD1	1:E:72:PRO:HD2	2.13	0.49
1:E:74:LEU:H	1:E:74:LEU:CD2	2.26	0.49
1:F:129:LEU:HD22	1:F:131:PRO:CD	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:LEU:HB3	1:G:70:LEU:HD23	1.94	0.49
1:G:239:VAL:HG23	1:G:239:VAL:O	2.11	0.49
1:H:328:ILE:HD13	1:H:329:SER:H	1.76	0.49
1:I:256:ASN:ND2	1:I:328:ILE:O	2.46	0.49
1:I:273:HIS:O	1:I:276:ALA:HB3	2.12	0.49
1:I:399:PHE:HZ	1:I:409:LEU:HD11	1.76	0.49
1:I:410:GLY:O	1:I:411:GLU:C	2.55	0.49
1:J:129:LEU:O	1:J:201:TYR:HA	2.12	0.49
1:A:166:GLU:CD	1:A:167:ASN:N	2.71	0.49
1:B:380:ARG:HA	1:B:383:ASN:HD22	1.77	0.49
1:C:212:GLN:OE1	1:C:212:GLN:HA	2.11	0.49
1:C:297:LYS:HD2	1:C:297:LYS:N	2.28	0.49
1:D:293:VAL:HG23	1:J:440:TYR:OH	2.12	0.49
1:E:326:ARG:HH11	1:E:326:ARG:CG	2.25	0.49
1:G:145:GLU:OE1	1:G:145:GLU:HA	2.13	0.49
1:H:161:PRO:O	1:H:167:ASN:ND2	2.45	0.49
1:I:52:PHE:CD1	1:I:70:LEU:HD22	2.48	0.49
1:I:133:PRO:CA	1:I:244:MET:HG3	2.43	0.49
1:I:308:TYR:OH	1:I:380:ARG:HD2	2.12	0.49
1:I:312:SER:OG	1:I:369:ASP:HA	2.13	0.49
1:I:320:ILE:HG22	1:I:321:ARG:N	2.26	0.49
1:F:119:MET:O	1:F:124:PHE:HB2	2.12	0.49
1:F:197:ILE:HD12	1:F:214:PHE:CE1	2.48	0.49
1:F:280:LYS:HG3	1:F:281:HIS:CD2	2.46	0.49
1:G:309:VAL:HA	1:G:319:LEU:HD22	1.95	0.49
1:G:310:ALA:HB3	1:G:372:ILE:HD11	1.93	0.49
1:H:6:ARG:HG3	1:H:6:ARG:O	2.13	0.49
1:H:235:PRO:O	1:H:236:LEU:HD23	2.12	0.49
1:H:286:THR:HG23	1:H:290:ASN:HD22	1.77	0.49
1:J:22:ARG:HG2	1:J:22:ARG:HH11	1.77	0.49
1:K:91:ARG:HD2	1:K:91:ARG:C	2.37	0.49
1:K:271:ALA:O	1:K:275:ILE:HG13	2.13	0.49
1:A:138:PHE:CE2	1:A:236:LEU:HD11	2.47	0.49
1:D:11:LYS:HG3	1:D:15:GLU:OE2	2.13	0.49
1:D:13:VAL:HG21	1:D:42:LEU:CD2	2.42	0.49
1:D:443:GLN:CA	1:D:443:GLN:HE21	2.25	0.49
1:F:127:PHE:CD2	1:F:351:LEU:HG	2.47	0.49
1:J:120:GLU:C	1:J:122:LEU:H	2.21	0.49
1:K:25:PHE:HB2	1:K:96:ILE:HD11	1.94	0.49
1:A:52:PHE:HE1	1:A:70:LEU:HD13	1.77	0.49
1:A:319:LEU:HD23	1:A:319:LEU:C	2.38	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:GLU:O	1:B:423:ILE:HG12	2.12	0.49
1:C:18:VAL:CG2	1:C:79:ILE:HD12	2.42	0.49
1:C:54:GLY:O	1:C:57:ILE:HG12	2.12	0.49
1:C:79:ILE:HD13	1:C:90:ALA:HB2	1.95	0.49
1:D:78:VAL:HG21	1:D:91:ARG:HH21	1.76	0.49
1:D:80:PHE:N	1:D:80:PHE:CD2	2.81	0.49
1:D:243:GLY:N	1:D:298:ARG:NH1	2.61	0.49
1:F:146:PRO:CG	1:F:228:HIS:CD2	2.87	0.49
1:F:187:HIS:CE1	1:F:196:GLU:OE1	2.62	0.49
1:F:322:ILE:HD12	1:F:322:ILE:N	2.28	0.49
1:F:433:HIS:O	1:F:436:GLU:HB2	2.13	0.49
1:G:371:ASN:O	1:G:372:ILE:HB	2.13	0.49
1:I:58:GLU:O	1:I:61:VAL:HG22	2.13	0.49
1:I:67:ASP:O	1:I:99:PRO:HG3	2.12	0.49
1:K:51:MET:HE3	1:K:69:TYR:CZ	2.48	0.49
1:B:129:LEU:CD1	1:B:207:SER:HB3	2.42	0.49
1:D:200:LYS:HE2	1:E:41:GLN:HE22	1.78	0.49
1:G:73:ASP:HA	4:G:612:HOH:O	2.11	0.49
1:H:166:GLU:O	1:H:166:GLU:OE1	2.31	0.49
1:I:63:ILE:H	1:I:63:ILE:HD12	1.77	0.49
1:I:169:ARG:NH2	1:I:195:HIS:HD1	2.10	0.49
1:J:24:GLN:NE2	1:J:32:ILE:HD11	2.27	0.49
1:J:129:LEU:HD22	1:J:131:PRO:CD	2.43	0.49
1:J:258:PHE:HA	1:J:271:ALA:HB2	1.93	0.49
1:A:27:ASP:OD1	1:A:31:THR:HB	2.12	0.49
1:C:18:VAL:HG21	1:C:79:ILE:CD1	2.42	0.49
1:D:286:THR:HA	1:D:289:THR:OG1	2.12	0.49
1:D:351:LEU:O	1:D:355:LEU:HG	2.13	0.49
1:E:380:ARG:O	1:E:385:ILE:O	2.31	0.49
1:F:52:PHE:CD1	1:F:70:LEU:HD13	2.48	0.49
1:F:283:THR:HG23	1:F:309:VAL:HG21	1.95	0.49
1:G:174:LEU:HD23	1:L:86:LYS:HB3	1.95	0.49
1:G:328:ILE:C	1:G:330:THR:H	2.20	0.49
1:I:5:THR:HG22	1:I:8:ASP:CG	2.38	0.49
1:J:78:VAL:HB	1:J:91:ARG:HG3	1.94	0.49
1:K:317:SER:N	1:K:318:PRO:HD3	2.28	0.49
1:L:124:PHE:CZ	1:L:358:ILE:HG21	2.48	0.49
1:A:23:LEU:HB2	1:A:35:VAL:CG1	2.43	0.48
1:A:281:HIS:CD2	1:A:402:ASN:HD21	2.30	0.48
1:B:45:ALA:HA	1:B:50:VAL:HG23	1.95	0.48
1:B:308:TYR:HE1	1:B:373:TYR:CE1	2.31	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:ASN:HD22	1:B:318:PRO:HD3	1.78	0.48
1:B:370:ARG:HH12	1:B:375:MET:HG3	1.78	0.48
1:D:177:GLU:HA	1:D:177:GLU:OE2	2.13	0.48
1:D:199:PHE:HZ	1:D:214:PHE:HB2	1.78	0.48
1:F:54:GLY:HA3	1:F:68:MET:HE3	1.95	0.48
1:F:66:SER:O	1:F:68:MET:N	2.47	0.48
1:F:308:TYR:CD1	1:F:372:ILE:HG21	2.48	0.48
1:G:140:LEU:HD12	1:G:226:GLY:C	2.37	0.48
1:L:140:LEU:HD12	1:L:226:GLY:HA2	1.94	0.48
1:A:206:ARG:CG	1:A:206:ARG:NH1	2.74	0.48
1:A:300:VAL:HG13	1:A:301:PRO:HD2	1.94	0.48
1:A:324:ALA:O	1:A:325:SER:O	2.31	0.48
1:C:129:LEU:HD22	1:C:131:PRO:CD	2.41	0.48
1:C:160:ALA:HB1	1:C:161:PRO:CD	2.43	0.48
1:F:48:ASN:OD1	1:F:72:PRO:HD2	2.12	0.48
1:G:203:GLY:O	1:G:206:ARG:N	2.46	0.48
1:G:258:PHE:HB3	1:G:271:ALA:N	2.29	0.48
1:G:281:HIS:CD2	1:G:404:VAL:HG11	2.47	0.48
1:G:404:VAL:HG22	1:G:405:MET:HE2	1.95	0.48
1:H:371:ASN:OD1	1:H:374:VAL:HG22	2.12	0.48
1:I:208:CYS:HA	1:I:211:ILE:CG1	2.43	0.48
1:J:76:THR:O	1:J:78:VAL:HG23	2.13	0.48
1:J:160:ALA:HB2	1:J:188:HIS:HD2	1.79	0.48
1:J:268:SER:OG	1:J:270:THR:HG23	2.13	0.48
1:C:286:THR:HG22	1:C:290:ASN:ND2	2.28	0.48
1:D:273:HIS:CE1	1:D:361:LYS:CA	2.96	0.48
1:E:260:ASP:HB2	1:E:268:SER:HA	1.95	0.48
1:F:129:LEU:HD23	1:F:130:GLY:H	1.78	0.48
1:J:30:GLY:CA	1:J:342:ASN:ND2	2.74	0.48
1:J:199:PHE:HZ	1:J:214:PHE:CG	2.31	0.48
1:J:306:PRO:CG	1:J:335:ARG:HB2	2.37	0.48
1:K:37:ILE:HG22	1:L:185:ALA:HA	1.94	0.48
1:K:104:PHE:CZ	1:K:106:GLY:HA3	2.48	0.48
1:K:138:PHE:HB3	1:K:147:THR:O	2.13	0.48
1:K:234:LYS:HB3	1:K:294:ASN:HD21	1.78	0.48
1:L:380:ARG:HH11	1:L:380:ARG:HB3	1.77	0.48
1:C:291:PRO:HG2	1:C:292:THR:H	1.78	0.48
1:D:173:VAL:HG13	1:D:183:ILE:HG13	1.96	0.48
1:E:78:VAL:HB	1:E:91:ARG:HG3	1.95	0.48
1:G:178:GLU:HG2	1:L:86:LYS:HE2	1.94	0.48
4:G:604:HOH:O	1:H:157:PHE:HZ	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:21:ILE:O	1:H:21:ILE:HG12	2.13	0.48
1:J:259:PHE:CE1	1:J:326:ARG:HB3	2.48	0.48
1:L:310:ALA:HB1	1:L:368:ILE:CB	2.43	0.48
1:C:321:ARG:O	1:C:323:PRO:HD3	2.13	0.48
1:E:331:ARG:HG2	1:E:331:ARG:NH2	2.28	0.48
1:E:375:MET:HA	1:E:379:GLU:OE1	2.13	0.48
1:F:160:ALA:HB1	1:F:161:PRO:CD	2.39	0.48
1:F:232:MET:HE1	1:L:437:ARG:CA	2.42	0.48
1:I:63:ILE:HD12	1:I:63:ILE:N	2.28	0.48
1:K:116:LEU:O	1:K:119:MET:HB3	2.13	0.48
1:L:440:TYR:HD1	1:L:444:TYR:CE2	2.32	0.48
1:D:325:SER:OG	1:D:329:SER:HB2	2.14	0.48
1:E:19:LYS:HA	1:E:39:VAL:HB	1.94	0.48
1:H:272:LYS:NZ	1:H:364:ALA:H	2.09	0.48
1:H:291:PRO:HG3	1:H:341:ALA:HA	1.94	0.48
1:I:282:ALA:HB1	1:I:319:LEU:HD21	1.96	0.48
1:I:311:TRP:HB3	1:I:320:ILE:HB	1.96	0.48
1:J:232:MET:HE2	1:J:294:ASN:OD1	2.13	0.48
1:J:285:PHE:CD1	1:J:285:PHE:C	2.92	0.48
1:K:129:LEU:HD11	1:K:246:CYS:HB3	1.95	0.48
1:K:426:ASP:HA	1:K:429:ARG:HG2	1.95	0.48
1:L:176:LEU:O	1:L:181:PHE:HB2	2.13	0.48
1:L:310:ALA:HB2	1:L:385:ILE:HG22	1.96	0.48
1:L:396:LEU:O	1:L:400:LYS:HG3	2.12	0.48
1:A:111:ASN:O	1:A:115:ILE:HG12	2.14	0.48
1:A:243:GLY:HA3	1:A:298:ARG:NH1	2.29	0.48
1:A:402:ASN:OD1	1:A:404:VAL:HG12	2.13	0.48
1:B:252:LYS:O	1:B:253:ASN:HB2	2.12	0.48
1:B:380:ARG:HA	1:B:383:ASN:ND2	2.29	0.48
1:C:100:ASP:O	1:C:102:THR:HG22	2.14	0.48
1:C:164:LEU:CD1	1:D:224:LYS:HD3	2.38	0.48
1:D:208:CYS:SG	1:D:347:LEU:HD12	2.53	0.48
1:D:242:SER:O	1:D:339:PRO:HD2	2.13	0.48
1:D:280:LYS:HD3	1:D:281:HIS:CE1	2.49	0.48
1:F:35:VAL:HG13	1:F:35:VAL:O	2.13	0.48
1:F:97:TYR:CD1	1:F:103:PRO:HA	2.48	0.48
1:F:189:GLU:HB3	1:F:194:GLN:NE2	2.29	0.48
1:F:359:LYS:C	1:F:360:ASN:HD22	2.21	0.48
1:G:23:LEU:HB2	1:G:35:VAL:CG1	2.41	0.48
1:G:119:MET:HG2	1:G:124:PHE:HB2	1.95	0.48
1:G:271:ALA:O	1:G:275:ILE:HD12	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:167:ASN:O	1:J:171:ASP:OD1	2.31	0.48
1:J:173:VAL:HG13	1:J:183:ILE:CD1	2.44	0.48
1:K:22:ARG:NH1	1:K:36:GLU:OE2	2.45	0.48
1:K:236:LEU:HB2	1:K:239:VAL:HG23	1.96	0.48
1:K:236:LEU:O	1:K:239:VAL:HG23	2.13	0.48
1:L:24:GLN:HE22	1:L:91:ARG:HH11	1.60	0.48
1:A:131:PRO:HG2	1:A:211:ILE:HD11	1.96	0.48
1:A:156:TYR:O	1:A:158:ASP:N	2.46	0.48
1:A:402:ASN:OD1	1:A:402:ASN:C	2.56	0.48
1:C:239:VAL:O	1:C:240:ASN:C	2.57	0.48
1:D:205:VAL:HG23	1:D:206:ARG:N	2.26	0.48
1:D:360:ASN:O	1:D:361:LYS:C	2.56	0.48
1:E:328:ILE:C	1:E:330:THR:H	2.21	0.48
1:G:13:VAL:CG1	1:G:18:VAL:HB	2.41	0.48
1:G:20:TYR:OH	1:G:36:GLU:HB3	2.13	0.48
1:I:6:ARG:NH2	1:I:47:ASP:OD1	2.46	0.48
1:I:150:LEU:HD12	1:I:192:PRO:HB2	1.96	0.48
1:I:212:GLN:O	1:I:213:THR:C	2.57	0.48
1:K:234:LYS:N	1:K:235:PRO:HD3	2.29	0.48
1:L:205:VAL:O	1:L:206:ARG:C	2.57	0.48
1:C:109:ARG:HD2	1:C:344:TYR:CE2	2.49	0.48
1:C:252:LYS:C	1:C:254:GLY:H	2.20	0.48
1:D:251:PHE:CD1	1:D:251:PHE:N	2.82	0.48
1:D:292:THR:OG1	1:D:295:SER:HB2	2.13	0.48
1:F:429:ARG:HH21	1:L:300:VAL:CG2	2.15	0.48
1:G:261:GLU:O	1:G:266:GLN:HG2	2.13	0.48
1:H:41:GLN:NE2	1:I:200:LYS:NZ	2.56	0.48
1:J:51:MET:SD	1:J:67:ASP:HB3	2.54	0.48
1:J:260:ASP:CG	1:J:263:ALA:HB2	2.38	0.48
1:K:22:ARG:NH1	1:L:159:LEU:HD13	2.28	0.48
1:L:404:VAL:HG13	1:L:405:MET:CE	2.40	0.48
1:A:156:TYR:C	1:A:158:ASP:H	2.22	0.48
1:B:55:SER:OG	1:B:62:ARG:NE	2.46	0.48
1:B:203:GLY:O	1:B:204:ALA:C	2.57	0.48
1:C:393:ALA:HB2	1:C:425:TRP:CE2	2.48	0.48
1:D:77:PHE:CE1	1:D:90:ALA:HB1	2.49	0.48
1:D:160:ALA:O	1:D:161:PRO:C	2.57	0.48
1:D:218:VAL:O	1:D:222:ALA:HB2	2.14	0.48
1:E:32:ILE:CD1	1:E:216:LEU:HD13	2.44	0.48
1:E:53:ASP:CG	1:E:65:GLU:HG3	2.39	0.48
1:E:272:LYS:O	1:E:275:ILE:HB	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:97:TYR:C	1:F:98:ASN:HD22	2.22	0.48
1:G:158:ASP:N	1:G:158:ASP:OD1	2.47	0.48
1:H:137:LEU:HD12	1:H:195:HIS:HE2	1.79	0.48
1:H:250:LEU:HB2	1:H:258:PHE:CZ	2.48	0.48
1:H:423:ILE:O	1:H:427:MET:HG3	2.14	0.48
1:J:135:PHE:HB3	1:J:231:PHE:CE1	2.49	0.48
1:J:212:GLN:OE1	1:J:212:GLN:CA	2.58	0.48
1:J:299:LEU:N	1:J:299:LEU:CD1	2.77	0.48
1:L:189:GLU:HB3	1:L:194:GLN:NE2	2.29	0.48
1:L:418:ILE:O	1:L:422:GLU:HG3	2.13	0.48
1:A:78:VAL:HG12	1:A:91:ARG:CG	2.44	0.47
1:A:311:TRP:HA	1:A:320:ILE:O	2.14	0.47
1:A:315:ASN:OD1	1:A:371:ASN:HA	2.14	0.47
1:A:436:GLU:CD	1:G:297:LYS:HZ2	2.21	0.47
1:B:279:VAL:HG13	1:B:309:VAL:HG12	1.95	0.47
1:C:20:TYR:HB3	1:C:89:VAL:HG22	1.96	0.47
1:D:413:LEU:HD23	1:D:413:LEU:HA	1.73	0.47
1:E:278:ILE:HG23	1:E:285:PHE:CE2	2.49	0.47
1:E:294:ASN:HD22	1:E:297:LYS:HG3	1.79	0.47
1:F:264:ASP:O	1:F:265:LEU:HB2	2.14	0.47
1:F:286:THR:O	1:F:290:ASN:N	2.45	0.47
1:H:28:ILE:HD11	1:H:417:PHE:HA	1.96	0.47
1:H:272:LYS:HZ1	1:H:276:ALA:HB2	1.79	0.47
1:I:319:LEU:CB	1:I:320:ILE:HD12	2.44	0.47
1:J:138:PHE:CD2	1:J:148:LEU:HA	2.48	0.47
1:K:270:THR:HG22	1:K:358:ILE:CD1	2.40	0.47
1:K:311:TRP:HA	1:K:320:ILE:HB	1.96	0.47
1:K:326:ARG:HD3	1:K:330:THR:OG1	2.14	0.47
1:L:156:TYR:HB2	1:L:190:VAL:HA	1.96	0.47
1:C:295:SER:O	1:C:299:LEU:HD13	2.15	0.47
1:C:316:ARG:HG2	1:C:373:TYR:CG	2.49	0.47
1:D:134:GLU:HG3	1:D:243:GLY:O	2.13	0.47
1:F:201:TYR:CD1	1:F:201:TYR:C	2.93	0.47
1:F:342:ASN:HD21	1:F:344:TYR:HD1	1.62	0.47
1:F:347:LEU:HD22	1:F:347:LEU:N	2.29	0.47
1:G:79:ILE:HD13	1:G:90:ALA:HB2	1.96	0.47
1:G:160:ALA:HB3	1:G:169:ARG:HH12	1.79	0.47
1:G:309:VAL:HB	1:G:386:VAL:HG23	1.95	0.47
1:G:370:ARG:HG3	1:G:370:ARG:HH11	1.79	0.47
1:H:140:LEU:HD12	1:H:226:GLY:HA2	1.96	0.47
1:H:349:VAL:HG23	1:H:405:MET:SD	2.53	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:116:LEU:HD23	1:I:351:LEU:CD1	2.44	0.47
1:I:200:LYS:O	1:I:201:TYR:C	2.56	0.47
1:I:317:SER:C	1:I:373:TYR:OH	2.57	0.47
1:L:291:PRO:HG2	1:L:292:THR:HG23	1.96	0.47
1:A:27:ASP:C	1:A:27:ASP:OD2	2.55	0.47
1:A:200:LYS:NZ	1:B:41:GLN:NE2	2.59	0.47
1:B:231:PHE:O	1:B:339:PRO:HG2	2.14	0.47
1:B:262:ASN:HD22	1:B:262:ASN:N	2.08	0.47
1:B:300:VAL:HG11	1:H:430:THR:CG2	2.44	0.47
1:B:315:ASN:HD22	1:B:318:PRO:CD	2.27	0.47
1:C:114:ARG:HH21	1:C:115:ILE:HD11	1.78	0.47
1:C:228:HIS:HE1	1:I:441:MET:O	1.96	0.47
1:D:55:SER:HB2	1:D:62:ARG:HB2	1.95	0.47
1:D:167:ASN:ND2	1:D:170:ARG:HB2	2.29	0.47
1:D:176:LEU:HD11	1:D:214:PHE:CD1	2.49	0.47
1:D:297:LYS:HE3	1:J:436:GLU:CD	2.39	0.47
1:E:80:PHE:CE1	1:E:91:ARG:HB3	2.49	0.47
1:G:148:LEU:HD22	1:G:148:LEU:N	2.29	0.47
1:G:306:PRO:HA	1:G:317:SER:HB2	1.96	0.47
1:G:368:ILE:HD13	1:G:372:ILE:HG13	1.96	0.47
1:I:126:ASP:HB2	1:I:251:PHE:HB2	1.96	0.47
1:J:36:GLU:HG2	1:K:186:SER:O	2.14	0.47
1:J:48:ASN:HB3	1:J:71:TYR:CD1	2.49	0.47
1:J:370:ARG:HB3	1:J:375:MET:HE2	1.96	0.47
1:K:129:LEU:HB3	1:K:207:SER:OG	2.15	0.47
1:L:325:SER:HB2	1:L:329:SER:HB3	1.96	0.47
1:B:147:THR:HG22	1:B:149:GLU:HG3	1.94	0.47
1:B:203:GLY:O	1:B:206:ARG:N	2.47	0.47
1:B:261:GLU:HA	1:B:266:GLN:HE22	1.80	0.47
1:B:308:TYR:HE1	1:B:373:TYR:CD1	2.32	0.47
1:C:127:PHE:CE2	1:C:347:LEU:HD22	2.49	0.47
1:C:244:MET:O	1:C:337:VAL:HB	2.13	0.47
1:D:156:TYR:HB2	1:D:190:VAL:HA	1.96	0.47
1:D:160:ALA:HB2	1:D:188:HIS:CD2	2.49	0.47
1:E:140:LEU:HD12	1:E:227:LEU:N	2.29	0.47
1:F:172:ILE:O	1:F:176:LEU:HG	2.14	0.47
1:G:52:PHE:CD1	1:G:70:LEU:HD13	2.48	0.47
1:G:245:HIS:NE2	1:G:335:ARG:HB3	2.29	0.47
1:I:114:ARG:HH12	1:I:115:ILE:CD1	2.26	0.47
1:J:17:ASN:O	1:J:17:ASN:CG	2.57	0.47
1:K:34:ASN:ND2	1:K:34:ASN:C	2.69	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LYS:HD2	1:A:15:GLU:OE1	2.14	0.47
1:A:48:ASN:OD1	1:A:71:TYR:HA	2.14	0.47
1:A:402:ASN:CG	1:A:405:MET:HG2	2.40	0.47
1:B:25:PHE:CE1	1:B:33:LYS:HB2	2.49	0.47
1:C:375:MET:HA	1:C:379:GLU:OE1	2.14	0.47
1:D:345:LEU:HD22	1:D:409:LEU:CD2	2.44	0.47
1:E:74:LEU:HD22	1:E:74:LEU:N	2.29	0.47
1:E:399:PHE:CE2	1:E:418:ILE:HD11	2.49	0.47
1:F:309:VAL:HG23	1:F:386:VAL:O	2.14	0.47
1:H:271:ALA:O	1:H:275:ILE:HG12	2.14	0.47
1:I:63:ILE:O	1:J:316:ARG:NH1	2.47	0.47
1:J:129:LEU:CD2	1:J:130:GLY:N	2.74	0.47
1:J:402:ASN:C	1:J:402:ASN:OD1	2.58	0.47
1:K:5:THR:H	1:K:8:ASP:HB2	1.80	0.47
1:K:84:ALA:O	1:K:85:GLU:C	2.58	0.47
1:L:58:GLU:HG3	1:L:416:HIS:ND1	2.29	0.47
1:C:274:PHE:CE2	1:C:332:VAL:HG11	2.49	0.47
1:C:435:TRP:CE2	1:C:439:GLN:HG3	2.49	0.47
1:F:23:LEU:HB3	1:F:70:LEU:HD23	1.95	0.47
1:G:208:CYS:O	1:G:212:GLN:HG2	2.15	0.47
1:I:5:THR:H	1:I:8:ASP:HB2	1.80	0.47
1:J:328:ILE:C	1:J:330:THR:H	2.22	0.47
1:K:168:CYS:SG	1:K:227:LEU:HD12	2.54	0.47
1:K:291:PRO:CG	1:K:341:ALA:HA	2.40	0.47
1:A:5:THR:O	1:A:9:ILE:HG12	2.15	0.47
1:A:11:LYS:HZ2	1:A:15:GLU:HG3	1.80	0.47
1:A:232:MET:CE	1:A:235:PRO:HA	2.42	0.47
1:A:337:VAL:HG12	1:A:338:ASP:N	2.30	0.47
1:B:147:THR:C	1:B:149:GLU:H	2.21	0.47
1:B:243:GLY:HA3	1:B:298:ARG:HH12	1.79	0.47
1:B:380:ARG:NH1	1:B:387:ASP:OD1	2.47	0.47
1:B:440:TYR:O	1:B:444:TYR:HB2	2.14	0.47
1:C:124:PHE:CZ	1:C:358:ILE:HD13	2.50	0.47
1:C:185:ALA:CB	1:D:37:ILE:HG22	2.45	0.47
1:C:321:ARG:O	1:C:333:GLU:HB3	2.14	0.47
1:C:402:ASN:HD21	1:C:404:VAL:HG12	1.78	0.47
1:C:404:VAL:HG13	1:C:405:MET:CE	2.36	0.47
1:D:4:TYR:CE2	1:D:12:LEU:HD11	2.50	0.47
1:D:167:ASN:HD22	1:D:170:ARG:CB	2.28	0.47
1:D:375:MET:HG2	1:D:376:SER:N	2.29	0.47
1:D:412:HIS:O	1:D:413:LEU:C	2.58	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:THR:O	1:E:8:ASP:HB2	2.15	0.47
1:E:170:ARG:NH1	1:E:170:ARG:HG2	2.29	0.47
1:E:247:ASN:HD22	1:E:331:ARG:NE	2.12	0.47
1:F:215:LYS:O	1:F:219:LYS:HB2	2.14	0.47
1:F:223:ARG:C	1:F:225:HIS:N	2.71	0.47
1:F:281:HIS:O	1:F:282:ALA:C	2.58	0.47
1:F:285:PHE:CD1	1:F:285:PHE:C	2.93	0.47
1:F:326:ARG:HD2	1:F:330:THR:HG23	1.96	0.47
1:F:410:GLY:O	1:F:411:GLU:C	2.57	0.47
1:F:436:GLU:CD	1:L:297:LYS:HE3	2.40	0.47
1:G:3:LYS:HB3	1:G:75:ASN:ND2	2.29	0.47
1:G:211:ILE:HD13	1:G:244:MET:CE	2.45	0.47
1:H:5:THR:H	1:H:8:ASP:CB	2.17	0.47
1:H:125:SER:OG	1:H:253:ASN:N	2.48	0.47
1:H:135:PHE:HB3	1:H:231:PHE:CD1	2.50	0.47
1:H:139:LYS:HA	1:H:227:LEU:HD23	1.96	0.47
1:H:175:GLU:O	1:H:179:MET:HG3	2.15	0.47
1:H:183:ILE:HG23	1:H:198:ASP:O	2.14	0.47
1:I:370:ARG:HD3	1:I:370:ARG:N	2.29	0.47
1:J:17:ASN:ND2	1:J:87:GLY:HA2	2.30	0.47
1:J:176:LEU:HD12	1:J:183:ILE:HD11	1.95	0.47
1:J:289:THR:HB	1:J:337:VAL:HG22	1.96	0.47
1:K:351:LEU:O	1:K:351:LEU:HD13	2.14	0.47
1:L:85:GLU:CD	1:L:85:GLU:N	2.73	0.47
1:L:309:VAL:HG21	1:L:386:VAL:HB	1.96	0.47
1:L:396:LEU:HD22	1:L:418:ILE:HD13	1.97	0.47
1:A:150:LEU:HD12	1:A:192:PRO:HB2	1.96	0.47
1:A:306:PRO:HB3	1:A:319:LEU:CA	2.37	0.47
1:B:277:GLY:HA3	1:B:353:ALA:O	2.14	0.47
1:C:232:MET:HE2	1:I:441:MET:HA	1.97	0.47
1:C:405:MET:HA	1:C:405:MET:HE2	1.96	0.47
1:D:159:LEU:HD13	1:E:22:ARG:HH11	1.80	0.47
1:E:421:LYS:HD3	1:E:424:GLU:OE1	2.15	0.47
1:F:221:ILE:O	1:F:225:HIS:HD2	1.98	0.47
1:J:24:GLN:HE21	1:J:32:ILE:HD11	1.80	0.47
1:J:141:ASP:OD2	1:J:141:ASP:C	2.57	0.47
1:A:160:ALA:HB2	1:A:188:HIS:CD2	2.50	0.47
1:A:264:ASP:C	1:A:265:LEU:HD12	2.40	0.47
1:B:119:MET:SD	1:B:127:PHE:HB2	2.54	0.47
1:B:142:GLU:HG3	1:B:143:LYS:H	1.80	0.47
1:B:167:ASN:HD22	1:B:170:ARG:CZ	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:THR:HB	1:B:398:GLU:OE1	2.15	0.47
1:D:375:MET:HE2	1:D:379:GLU:HB3	1.97	0.47
1:E:32:ILE:HD13	1:E:216:LEU:HB2	1.96	0.47
1:E:68:MET:HE1	1:E:104:PHE:CG	2.49	0.47
1:E:142:GLU:CD	1:E:142:GLU:N	2.73	0.47
1:E:208:CYS:SG	1:E:347:LEU:HD12	2.55	0.47
1:E:322:ILE:N	1:E:322:ILE:CD1	2.77	0.47
1:F:109:ARG:HG2	1:F:109:ARG:NH2	2.29	0.47
1:G:17:ASN:ND2	1:G:87:GLY:HA2	2.30	0.47
1:G:57:ILE:O	1:G:59:GLY:N	2.47	0.47
1:G:156:TYR:CE2	1:L:62:ARG:NH1	2.83	0.47
1:G:291:PRO:HG3	1:G:341:ALA:HA	1.96	0.47
1:I:216:LEU:HD21	1:J:162:THR:OG1	2.15	0.47
1:J:285:PHE:HB2	1:J:349:VAL:CG1	2.45	0.47
1:L:383:ASN:HB2	1:L:385:ILE:HD11	1.96	0.47
1:A:160:ALA:CB	1:A:188:HIS:CD2	2.98	0.47
1:B:258:PHE:HZ	1:B:274:PHE:CG	2.33	0.47
1:C:9:ILE:O	1:C:12:LEU:N	2.47	0.47
1:C:27:ASP:OD1	1:C:33:LYS:HE3	2.15	0.47
1:C:153:LYS:NZ	1:D:145:GLU:OE1	2.45	0.47
1:C:174:LEU:O	1:C:178:GLU:HG2	2.14	0.47
1:D:21:ILE:CD1	1:D:39:VAL:HA	2.45	0.47
1:D:23:LEU:HB3	1:D:94:CYS:SG	2.55	0.47
1:E:48:ASN:O	1:E:69:TYR:HD2	1.97	0.47
1:E:131:PRO:HG2	1:E:199:PHE:CD1	2.49	0.47
1:G:417:PHE:O	1:G:418:ILE:C	2.58	0.47
1:H:58:GLU:HG2	1:H:416:HIS:CD2	2.50	0.47
1:H:325:SER:HB2	1:H:331:ARG:HH22	1.80	0.47
1:I:156:TYR:C	1:I:158:ASP:N	2.72	0.47
1:I:381:MET:HE2	1:I:381:MET:N	2.29	0.47
1:J:325:SER:HB3	1:J:329:SER:CB	2.45	0.47
1:K:319:LEU:HG	1:K:320:ILE:CD1	2.45	0.47
1:L:226:GLY:O	1:L:227:LEU:HD23	2.15	0.47
1:B:41:GLN:NE2	1:B:44:LYS:HD2	2.29	0.46
1:B:49:LYS:HE2	1:B:49:LYS:HA	1.98	0.46
1:C:23:LEU:HB3	1:C:94:CYS:SG	2.55	0.46
1:C:45:ALA:O	1:C:72:PRO:HG3	2.15	0.46
1:C:429:ARG:HH11	1:C:429:ARG:HG3	1.80	0.46
1:E:200:LYS:HG2	1:E:201:TYR:H	1.80	0.46
1:E:236:LEU:HB2	1:E:239:VAL:HG21	1.97	0.46
1:F:4:TYR:HB3	1:F:9:ILE:CD1	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:143:LYS:HD3	1:G:143:LYS:N	2.29	0.46
1:H:37:ILE:HG22	1:I:185:ALA:CB	2.45	0.46
1:H:281:HIS:CE1	1:H:404:VAL:HG11	2.51	0.46
1:H:409:LEU:O	1:H:413:LEU:HB2	2.15	0.46
1:J:127:PHE:CE2	1:J:351:LEU:HG	2.50	0.46
1:J:322:ILE:CD1	1:J:332:VAL:HG13	2.45	0.46
1:K:215:LYS:HG2	1:K:231:PHE:CE2	2.50	0.46
1:K:351:LEU:O	1:K:351:LEU:HD22	2.14	0.46
1:K:405:MET:HA	1:K:405:MET:HE2	1.96	0.46
1:L:311:TRP:HA	1:L:320:ILE:HB	1.97	0.46
1:A:57:ILE:HD13	1:A:96:ILE:HG13	1.96	0.46
1:A:310:ALA:CB	1:A:372:ILE:HD13	2.40	0.46
1:A:368:ILE:HD12	1:A:385:ILE:HD11	1.96	0.46
1:A:383:ASN:C	1:A:385:ILE:H	2.22	0.46
1:B:141:ASP:OD2	1:B:141:ASP:C	2.59	0.46
1:B:146:PRO:HG3	1:B:228:HIS:CD2	2.50	0.46
1:C:270:THR:O	1:C:274:PHE:HB2	2.15	0.46
1:C:371:ASN:OD1	1:C:374:VAL:HG22	2.15	0.46
1:D:4:TYR:HB3	1:D:9:ILE:HD11	1.97	0.46
1:E:67:ASP:C	1:E:68:MET:HG2	2.40	0.46
1:E:315:ASN:OD1	1:E:372:ILE:HG12	2.16	0.46
1:F:170:ARG:NH1	1:F:171:ASP:OD2	2.48	0.46
1:F:368:ILE:HG21	1:F:372:ILE:HD11	1.94	0.46
1:G:48:ASN:OD1	1:G:72:PRO:HD2	2.14	0.46
1:H:4:TYR:CB	1:H:9:ILE:HG13	2.45	0.46
1:H:236:LEU:O	1:H:239:VAL:HG22	2.15	0.46
1:H:272:LYS:NZ	1:H:276:ALA:HB2	2.31	0.46
1:I:160:ALA:CB	1:I:169:ARG:HH12	2.26	0.46
1:I:207:SER:O	1:I:211:ILE:HG12	2.16	0.46
1:J:100:ASP:OD1	1:J:101:GLY:N	2.48	0.46
1:J:163:ASP:HA	1:J:170:ARG:NH1	2.31	0.46
1:J:310:ALA:CA	1:J:368:ILE:HG13	2.43	0.46
1:K:48:ASN:HB3	1:K:71:TYR:CE1	2.50	0.46
1:K:49:LYS:HD3	1:K:69:TYR:HE2	1.78	0.46
1:K:54:GLY:O	1:K:56:SER:N	2.48	0.46
1:K:264:ASP:C	1:K:266:GLN:N	2.74	0.46
1:K:296:TYR:N	1:K:296:TYR:CD1	2.84	0.46
1:L:183:ILE:HD12	1:L:183:ILE:H	1.81	0.46
1:A:271:ALA:O	1:A:275:ILE:HG13	2.15	0.46
1:B:155:GLY:H	1:B:158:ASP:CG	2.23	0.46
1:B:162:THR:HG21	1:C:220:THR:OG1	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:ASN:OD1	1:B:405:MET:HG2	2.15	0.46
1:C:39:VAL:C	1:C:41:GLN:H	2.23	0.46
1:C:85:GLU:OE2	1:C:86:LYS:N	2.48	0.46
1:C:114:ARG:HH21	1:C:115:ILE:CD1	2.28	0.46
1:C:114:ARG:NH2	1:C:115:ILE:HD11	2.30	0.46
1:D:176:LEU:HD11	1:D:214:PHE:HD1	1.78	0.46
1:E:139:LYS:HB2	1:E:149:GLU:HB3	1.97	0.46
1:F:310:ALA:HB1	1:F:368:ILE:HG12	1.98	0.46
1:G:46:LEU:HD22	1:G:74:LEU:HD11	1.97	0.46
1:H:160:ALA:CB	1:H:169:ARG:HH12	2.28	0.46
1:H:172:ILE:HD13	1:H:221:ILE:HB	1.97	0.46
1:H:318:PRO:HB2	1:H:320:ILE:O	2.15	0.46
1:I:232:MET:HE2	1:I:234:LYS:C	2.40	0.46
1:I:392:LEU:HD21	1:I:421:LYS:HB3	1.97	0.46
1:J:17:ASN:HD21	1:J:87:GLY:HA2	1.81	0.46
1:K:360:ASN:HB2	1:K:362:LEU:CD1	2.45	0.46
1:A:167:ASN:C	1:A:167:ASN:HD22	2.22	0.46
1:C:444:TYR:OH	1:I:29:LEU:HD22	2.16	0.46
1:D:5:THR:O	1:D:8:ASP:N	2.48	0.46
1:D:164:LEU:HD23	1:E:220:THR:CG2	2.46	0.46
1:D:168:CYS:SG	1:D:227:LEU:HD12	2.55	0.46
1:D:294:ASN:HB2	1:J:436:GLU:HB3	1.97	0.46
1:E:115:ILE:O	1:E:118:GLU:HB3	2.15	0.46
1:F:131:PRO:HG2	1:F:199:PHE:CD1	2.50	0.46
1:F:188:HIS:HE1	1:F:191:ALA:O	1.97	0.46
1:F:420:ALA:O	1:F:423:ILE:HG13	2.15	0.46
1:H:116:LEU:O	1:H:119:MET:HB3	2.15	0.46
1:J:72:PRO:N	1:J:94:CYS:HB3	2.31	0.46
1:J:82:TRP:HE1	1:K:163:ASP:HB2	1.81	0.46
1:J:208:CYS:N	1:J:211:ILE:HD12	2.30	0.46
1:K:83:THR:OG1	1:K:88:LYS:HD3	2.15	0.46
1:K:115:ILE:CG2	1:K:351:LEU:HD12	2.39	0.46
1:K:311:TRP:O	1:K:312:SER:HB3	2.14	0.46
1:L:124:PHE:HZ	1:L:358:ILE:HG21	1.80	0.46
1:L:386:VAL:CG1	1:L:387:ASP:H	2.12	0.46
1:A:117:LYS:C	1:A:119:MET:N	2.74	0.46
1:B:239:VAL:O	1:B:239:VAL:HG23	2.14	0.46
1:B:405:MET:O	1:B:406:VAL:C	2.58	0.46
1:C:116:LEU:HD11	1:C:204:ALA:HB3	1.97	0.46
1:D:310:ALA:CB	1:D:368:ILE:HG21	2.42	0.46
1:E:119:MET:HG2	1:E:124:PHE:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:200:LYS:O	1:F:201:TYR:C	2.58	0.46
1:F:370:ARG:HH21	1:F:372:ILE:CD1	2.29	0.46
1:F:430:THR:HG22	1:L:300:VAL:HG21	1.97	0.46
1:H:63:ILE:HG22	1:H:64:GLU:HG3	1.97	0.46
1:H:278:ILE:O	1:H:282:ALA:HB2	2.15	0.46
1:H:315:ASN:ND2	1:H:371:ASN:HA	2.31	0.46
1:I:285:PHE:HB2	1:I:349:VAL:HG13	1.96	0.46
1:I:371:ASN:HB2	1:I:374:VAL:HG22	1.97	0.46
1:J:82:TRP:HE1	1:K:163:ASP:CB	2.29	0.46
1:K:60:PHE:CD1	1:K:60:PHE:C	2.93	0.46
1:L:91:ARG:HD2	1:L:92:PHE:N	2.29	0.46
1:A:80:PHE:HA	1:A:81:PRO:HD3	1.78	0.46
1:A:108:PRO:O	1:A:344:TYR:HB3	2.16	0.46
1:A:259:PHE:HE2	1:A:261:GLU:OE2	1.99	0.46
1:B:436:GLU:CD	1:H:297:LYS:HE3	2.40	0.46
1:C:164:LEU:HD23	1:C:164:LEU:C	2.40	0.46
1:C:267:LEU:CD2	1:C:326:ARG:NH1	2.78	0.46
1:D:289:THR:C	1:D:290:ASN:ND2	2.73	0.46
1:D:443:GLN:HE21	1:D:443:GLN:HA	1.81	0.46
1:E:234:LYS:HB3	1:E:294:ASN:ND2	2.30	0.46
1:H:182:GLU:HB3	1:H:200:LYS:CD	2.31	0.46
1:I:151:ASN:HD22	1:I:166:GLU:CD	2.23	0.46
1:I:160:ALA:HB3	1:I:169:ARG:HH12	1.79	0.46
1:J:54:GLY:HA3	1:J:68:MET:HE3	1.96	0.46
1:K:289:THR:C	1:K:290:ASN:ND2	2.74	0.46
1:K:312:SER:HB2	1:K:369:ASP:OD1	2.16	0.46
1:B:287:ALA:HB2	1:B:395:ALA:HB1	1.98	0.46
1:C:111:ASN:OD1	1:C:409:LEU:HA	2.15	0.46
1:C:274:PHE:HE2	1:C:332:VAL:HG11	1.80	0.46
1:C:431:GLN:O	1:I:297:LYS:HD2	2.16	0.46
1:D:71:TYR:C	1:D:94:CYS:HB3	2.41	0.46
1:D:342:ASN:HB3	1:D:345:LEU:HB2	1.96	0.46
1:E:151:ASN:HD22	1:E:166:GLU:CD	2.24	0.46
1:E:376:SER:O	1:E:380:ARG:HG3	2.16	0.46
1:F:129:LEU:CD2	1:F:130:GLY:N	2.78	0.46
1:F:345:LEU:CD2	1:F:409:LEU:HD22	2.45	0.46
1:G:34:ASN:CG	1:H:159:LEU:HG	2.41	0.46
1:I:267:LEU:HG	1:I:326:ARG:NH1	2.31	0.46
1:J:273:HIS:CE1	1:J:361:LYS:CA	2.99	0.46
1:K:143:LYS:O	1:K:144:GLY:C	2.57	0.46
1:L:232:MET:SD	1:L:235:PRO:HA	2.56	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:VAL:CG2	1:G:429:ARG:HH12	2.28	0.46
1:A:327:GLY:C	1:A:329:SER:H	2.23	0.46
1:B:138:PHE:CE2	1:B:150:LEU:CD2	2.99	0.46
1:C:21:ILE:HD13	1:C:39:VAL:HA	1.97	0.46
1:C:360:ASN:O	1:C:361:LYS:C	2.57	0.46
1:C:380:ARG:HA	1:C:385:ILE:HD12	1.97	0.46
1:C:433:HIS:N	1:C:436:GLU:OE1	2.48	0.46
1:D:288:VAL:O	1:D:291:PRO:HD3	2.15	0.46
1:E:189:GLU:HB3	1:E:194:GLN:OE1	2.15	0.46
1:E:211:ILE:HG22	1:E:215:LYS:HE2	1.98	0.46
1:H:282:ALA:HB1	1:H:319:LEU:HD21	1.97	0.46
1:H:332:VAL:HG13	1:H:332:VAL:O	2.16	0.46
1:I:27:ASP:OD2	1:I:29:LEU:N	2.48	0.46
1:I:124:PHE:CE1	1:I:358:ILE:HD13	2.51	0.46
1:I:357:GLY:HA2	1:I:362:LEU:HD13	1.98	0.46
1:I:418:ILE:HG22	1:I:422:GLU:CG	2.45	0.46
1:J:33:LYS:HB3	1:K:157:PHE:O	2.16	0.46
1:K:98:ASN:O	1:K:100:ASP:N	2.49	0.46
1:A:58:GLU:O	1:A:61:VAL:HG22	2.16	0.46
1:A:372:ILE:O	1:A:380:ARG:NH2	2.48	0.46
1:B:159:LEU:HD12	1:C:22:ARG:NH1	2.27	0.46
1:B:159:LEU:HB2	1:C:32:ILE:O	2.15	0.46
1:C:62:ARG:HH21	1:C:65:GLU:HB3	1.81	0.46
1:C:127:PHE:HE2	1:C:347:LEU:HD22	1.80	0.46
1:F:231:PHE:HB3	1:F:339:PRO:HB2	1.97	0.46
1:F:309:VAL:HB	1:F:386:VAL:CG2	2.41	0.46
1:F:355:LEU:HD23	1:F:355:LEU:HA	1.67	0.46
1:G:315:ASN:HB3	1:G:318:PRO:CG	2.46	0.46
1:I:25:PHE:CE1	1:I:33:LYS:HB2	2.50	0.46
1:I:282:ALA:O	1:I:284:SER:N	2.49	0.46
1:J:23:LEU:HB3	1:J:70:LEU:HD23	1.97	0.46
1:J:206:ARG:HG3	1:J:206:ARG:NH1	2.31	0.46
1:K:46:LEU:C	1:K:48:ASN:H	2.24	0.46
1:L:33:LYS:O	1:L:34:ASN:HB3	2.16	0.46
1:L:73:ASP:O	1:L:75:ASN:N	2.49	0.46
1:A:252:LYS:CE	1:A:253:ASN:ND2	2.78	0.46
1:A:306:PRO:O	1:A:388:LEU:HD12	2.16	0.46
1:A:309:VAL:HG23	1:A:386:VAL:O	2.16	0.46
1:B:300:VAL:HG11	1:H:430:THR:HG22	1.98	0.46
1:C:296:TYR:CE1	1:C:392:LEU:HA	2.51	0.46
1:C:399:PHE:HZ	1:C:409:LEU:HD11	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:TYR:H	1:E:201:TYR:HD2	1.63	0.46
1:E:436:GLU:HG2	1:K:294:ASN:HB2	1.98	0.46
1:G:406:VAL:HG22	1:G:414:PHE:CZ	2.50	0.46
1:I:127:PHE:CZ	1:I:248:LEU:HD23	2.50	0.46
1:I:272:LYS:HA	1:I:275:ILE:HD12	1.97	0.46
1:J:58:GLU:O	1:J:59:GLY:C	2.58	0.46
1:J:167:ASN:HD22	1:J:167:ASN:HA	1.51	0.46
1:J:320:ILE:HG22	1:J:321:ARG:H	1.81	0.46
1:J:368:ILE:CD1	1:J:385:ILE:HG23	2.46	0.46
1:K:151:ASN:HB2	1:K:166:GLU:OE2	2.16	0.46
1:A:259:PHE:CE2	1:A:261:GLU:OE2	2.69	0.45
1:A:306:PRO:CB	1:A:319:LEU:HA	2.37	0.45
1:B:261:GLU:HA	1:B:266:GLN:NE2	2.31	0.45
1:B:264:ASP:C	1:B:266:GLN:N	2.73	0.45
1:C:429:ARG:O	1:I:297:LYS:HD3	2.16	0.45
1:D:9:ILE:O	1:D:13:VAL:HG23	2.16	0.45
1:D:169:ARG:O	1:D:170:ARG:C	2.58	0.45
1:D:436:GLU:OE2	1:J:297:LYS:HG3	2.15	0.45
1:E:100:ASP:OD2	1:E:102:THR:HG23	2.16	0.45
1:G:13:VAL:HG21	1:G:42:LEU:HD21	1.97	0.45
1:G:86:LYS:HG3	1:H:174:LEU:CB	2.43	0.45
1:G:166:GLU:HG2	1:G:168:CYS:H	1.81	0.45
1:H:242:SER:O	1:H:339:PRO:CD	2.61	0.45
1:J:19:LYS:HG3	1:J:87:GLY:HA3	1.97	0.45
1:J:27:ASP:OD2	1:J:27:ASP:C	2.59	0.45
1:J:140:LEU:HD11	1:J:227:LEU:O	2.16	0.45
1:J:371:ASN:HD21	1:J:373:TYR:HB2	1.79	0.45
1:K:35:VAL:CG1	1:K:70:LEU:HD11	2.46	0.45
1:K:51:MET:HA	1:K:68:MET:O	2.16	0.45
1:K:309:VAL:HG13	1:K:319:LEU:CD2	2.43	0.45
1:L:91:ARG:C	1:L:91:ARG:CD	2.83	0.45
1:L:114:ARG:NH2	1:L:115:ILE:CD1	2.78	0.45
1:L:275:ILE:O	1:L:279:VAL:HG23	2.16	0.45
1:A:33:LYS:HE2	1:F:158:ASP:OD2	2.16	0.45
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.75	0.45
1:A:356:ASP:O	1:A:360:ASN:HB2	2.16	0.45
1:A:407:LYS:O	1:A:408:ALA:C	2.59	0.45
1:C:159:LEU:O	1:C:160:ALA:O	2.33	0.45
1:D:26:THR:OG1	1:D:212:GLN:NE2	2.47	0.45
1:D:138:PHE:HA	1:D:149:GLU:O	2.16	0.45
1:D:308:TYR:HA	1:D:387:ASP:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:85:GLU:C	1:F:87:GLY:N	2.74	0.45
1:I:78:VAL:HG11	1:I:179:MET:HE3	1.98	0.45
1:I:80:PHE:HB2	1:I:89:VAL:O	2.15	0.45
1:I:418:ILE:O	1:I:419:GLU:C	2.59	0.45
1:J:64:GLU:HG2	1:K:315:ASN:C	2.42	0.45
1:J:112:LEU:HD11	1:J:208:CYS:SG	2.56	0.45
1:K:20:TYR:C	1:K:21:ILE:HD12	2.40	0.45
1:A:9:ILE:HG21	1:A:92:PHE:HZ	1.81	0.45
1:A:326:ARG:HD3	1:A:326:ARG:HA	1.82	0.45
1:D:4:TYR:HB3	1:D:9:ILE:CD1	2.47	0.45
1:D:184:GLU:HG3	1:E:44:LYS:NZ	2.31	0.45
1:E:68:MET:HE1	1:E:104:PHE:HB2	1.97	0.45
1:E:252:LYS:O	1:E:255:VAL:HG22	2.16	0.45
1:F:345:LEU:HD22	1:F:409:LEU:HD22	1.98	0.45
1:G:410:GLY:O	1:G:411:GLU:C	2.59	0.45
1:H:20:TYR:OH	1:H:36:GLU:HB3	2.16	0.45
1:H:273:HIS:NE2	1:H:361:LYS:HA	2.32	0.45
1:I:236:LEU:HB2	1:I:239:VAL:CG2	2.46	0.45
1:J:37:ILE:HG13	1:J:41:GLN:HB2	1.97	0.45
1:K:234:LYS:HB3	1:K:294:ASN:ND2	2.32	0.45
1:K:264:ASP:C	1:K:266:GLN:H	2.25	0.45
1:L:130:GLY:O	1:L:247:ASN:ND2	2.49	0.45
1:L:214:PHE:O	1:L:215:LYS:C	2.57	0.45
1:A:211:ILE:O	1:A:214:PHE:HB3	2.16	0.45
1:A:376:SER:HB3	1:A:378:GLU:OE1	2.17	0.45
1:B:110:ASN:O	1:B:113:LYS:HB2	2.17	0.45
1:C:18:VAL:HG21	1:C:79:ILE:HD12	1.98	0.45
1:C:127:PHE:CZ	1:C:248:LEU:HD22	2.51	0.45
1:C:232:MET:HE3	1:C:235:PRO:CB	2.44	0.45
1:C:347:LEU:HD23	1:C:347:LEU:HA	1.80	0.45
1:D:184:GLU:OE1	1:D:200:LYS:HG2	2.16	0.45
1:E:134:GLU:HG2	1:E:196:GLU:HG3	1.99	0.45
1:E:169:ARG:NH2	1:F:36:GLU:OE2	2.45	0.45
1:F:56:SER:HA	1:F:62:ARG:HD2	1.98	0.45
1:F:175:GLU:HG3	1:F:221:ILE:CD1	2.46	0.45
1:G:172:ILE:O	1:G:176:LEU:HG	2.16	0.45
1:I:53:ASP:OD2	1:I:53:ASP:C	2.60	0.45
1:J:308:TYR:CD1	1:J:372:ILE:HG21	2.51	0.45
1:K:85:GLU:HG2	1:L:170:ARG:NH1	2.27	0.45
1:K:290:ASN:HB3	1:K:295:SER:HB3	1.99	0.45
1:K:309:VAL:HG22	1:K:319:LEU:HD22	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:132:GLU:HB3	1:L:196:GLU:OE1	2.16	0.45
1:L:345:LEU:HD22	1:L:409:LEU:CD1	2.47	0.45
1:A:20:TYR:OH	1:A:36:GLU:HG3	2.17	0.45
1:B:176:LEU:HD11	1:B:214:PHE:CE1	2.51	0.45
1:C:416:HIS:O	1:C:417:PHE:C	2.60	0.45
1:D:166:GLU:HA	1:D:225:HIS:CD2	2.52	0.45
1:E:247:ASN:ND2	1:E:331:ARG:HE	2.14	0.45
1:E:429:ARG:NH1	1:K:300:VAL:HG12	2.32	0.45
1:F:84:ALA:HB3	1:F:87:GLY:O	2.16	0.45
1:F:119:MET:HA	1:F:355:LEU:CD1	2.46	0.45
1:G:45:ALA:HA	1:G:50:VAL:CG2	2.46	0.45
1:G:237:PHE:O	1:G:239:VAL:N	2.49	0.45
1:I:106:GLY:HA2	1:I:413:LEU:HG	1.98	0.45
1:J:322:ILE:HD11	1:J:332:VAL:HG13	1.98	0.45
1:K:244:MET:H	1:K:338:ASP:HA	1.80	0.45
1:A:169:ARG:NH2	1:A:195:HIS:ND1	2.64	0.45
1:A:280:LYS:HD2	1:A:362:LEU:HD21	1.98	0.45
1:C:255:VAL:HG12	1:C:256:ASN:H	1.81	0.45
1:C:315:ASN:HD21	1:C:369:ASP:CB	2.29	0.45
1:C:321:ARG:HD3	1:C:333:GLU:OE1	2.17	0.45
1:D:179:MET:HE2	1:D:179:MET:HB3	1.84	0.45
1:G:95:ASP:OD1	1:G:109:ARG:NH2	2.49	0.45
1:G:204:ALA:HB1	1:G:347:LEU:CD2	2.47	0.45
1:G:285:PHE:CD1	1:G:285:PHE:C	2.95	0.45
1:I:203:GLY:O	1:I:204:ALA:C	2.60	0.45
1:J:274:PHE:C	1:J:274:PHE:CD2	2.95	0.45
1:K:127:PHE:HZ	1:K:248:LEU:HD22	1.73	0.45
1:K:258:PHE:CA	1:K:271:ALA:HB2	2.47	0.45
1:L:156:TYR:C	1:L:158:ASP:H	2.24	0.45
1:A:276:ALA:HB2	1:A:364:ALA:HB2	1.97	0.45
1:A:320:ILE:HD12	1:A:320:ILE:N	2.32	0.45
1:A:380:ARG:HD3	1:A:387:ASP:OD1	2.17	0.45
1:B:30:GLY:N	1:B:342:ASN:HD22	2.15	0.45
1:B:364:ALA:HB1	1:B:365:PRO:HD2	1.99	0.45
1:E:96:ILE:H	1:E:96:ILE:CD1	2.22	0.45
1:E:170:ARG:NH1	1:F:84:ALA:HB1	2.31	0.45
1:E:260:ASP:O	1:E:266:GLN:HA	2.17	0.45
1:E:406:VAL:HG22	1:E:414:PHE:CZ	2.51	0.45
1:F:230:THR:HG23	1:F:230:THR:O	2.17	0.45
1:H:78:VAL:HG12	1:H:79:ILE:N	2.32	0.45
1:I:360:ASN:O	1:I:361:LYS:C	2.60	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:426:ASP:HA	1:I:429:ARG:HG2	1.98	0.45
1:J:163:ASP:O	1:J:164:LEU:HB2	2.17	0.45
1:K:396:LEU:HD22	1:K:418:ILE:HD13	1.98	0.45
1:A:203:GLY:O	1:A:204:ALA:C	2.60	0.45
1:A:264:ASP:C	1:A:266:GLN:N	2.73	0.45
1:B:297:LYS:HD3	1:H:429:ARG:O	2.17	0.45
1:C:35:VAL:HG13	1:C:35:VAL:O	2.17	0.45
1:C:383:ASN:N	1:C:383:ASN:ND2	2.64	0.45
1:C:383:ASN:N	1:C:383:ASN:HD22	2.14	0.45
1:D:96:ILE:HD13	1:D:96:ILE:N	2.32	0.45
1:D:145:GLU:OE2	1:D:146:PRO:HD2	2.17	0.45
1:D:259:PHE:HZ	1:D:261:GLU:HG3	1.82	0.45
1:E:324:ALA:O	1:E:325:SER:C	2.60	0.45
1:F:298:ARG:O	1:F:298:ARG:HD2	2.17	0.45
1:F:399:PHE:HE1	1:F:405:MET:HB3	1.80	0.45
1:H:86:LYS:HB2	1:I:174:LEU:HD23	1.99	0.45
1:H:368:ILE:HG21	1:H:372:ILE:HD12	1.98	0.45
1:K:282:ALA:HA	1:K:285:PHE:CE1	2.51	0.45
1:K:419:GLU:O	1:K:423:ILE:HG12	2.16	0.45
1:A:129:LEU:HD13	1:A:131:PRO:HG3	1.99	0.45
1:A:142:GLU:CD	1:A:142:GLU:N	2.74	0.45
1:B:148:LEU:CD2	1:H:437:ARG:HD3	2.44	0.45
1:B:213:THR:O	1:B:217:VAL:HG23	2.17	0.45
1:B:260:ASP:HB2	1:B:268:SER:CA	2.47	0.45
1:B:430:THR:CG2	1:H:300:VAL:HG21	2.47	0.45
1:C:316:ARG:HG2	1:C:373:TYR:CD2	2.52	0.45
1:D:158:ASP:OD2	1:E:33:LYS:HE2	2.17	0.45
1:D:183:ILE:HD13	1:D:183:ILE:N	2.31	0.45
1:E:282:ALA:C	1:E:284:SER:N	2.73	0.45
1:G:35:VAL:HG13	1:G:35:VAL:O	2.17	0.45
1:H:248:LEU:O	1:H:331:ARG:HB2	2.16	0.45
1:I:68:MET:CE	1:I:98:ASN:HA	2.46	0.45
1:I:368:ILE:O	1:I:368:ILE:HG22	2.17	0.45
1:J:6:ARG:HG3	1:J:46:LEU:HD13	1.99	0.45
1:J:296:TYR:HE2	1:J:389:PRO:HG2	1.82	0.45
1:J:406:VAL:HG22	1:J:414:PHE:CE1	2.51	0.45
1:K:129:LEU:CD1	1:K:246:CYS:HB3	2.46	0.45
1:L:282:ALA:C	1:L:284:SER:H	2.25	0.45
1:A:11:LYS:HZ2	1:A:15:GLU:CG	2.30	0.45
1:B:48:ASN:HB3	1:B:71:TYR:CD1	2.51	0.45
1:B:212:GLN:O	1:B:213:THR:C	2.60	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:SER:HB3	1:B:315:ASN:HB2	1.99	0.45
1:C:9:ILE:CD1	1:C:74:LEU:HB3	2.46	0.45
1:D:6:ARG:NE	1:D:46:LEU:HD13	2.32	0.45
1:D:58:GLU:O	1:D:61:VAL:HG22	2.17	0.45
1:D:322:ILE:HD12	1:D:322:ILE:N	2.32	0.45
1:E:70:LEU:O	1:E:72:PRO:HD3	2.17	0.45
1:E:175:GLU:O	1:E:179:MET:HB2	2.17	0.45
1:H:309:VAL:HG13	1:H:319:LEU:CD2	2.47	0.45
1:I:280:LYS:HG2	1:I:281:HIS:CD2	2.51	0.45
1:J:28:ILE:C	1:J:30:GLY:H	2.24	0.45
1:K:48:ASN:OD1	1:K:71:TYR:HA	2.17	0.45
1:K:57:ILE:C	1:K:59:GLY:H	2.24	0.45
1:K:285:PHE:C	1:K:285:PHE:CD1	2.95	0.45
1:K:316:ARG:HE	1:K:370:ARG:NH1	2.14	0.45
1:L:18:VAL:HG21	1:L:79:ILE:HD12	1.98	0.45
1:L:129:LEU:CG	1:L:347:LEU:HD21	2.46	0.45
1:L:325:SER:HB2	1:L:329:SER:CB	2.48	0.45
1:B:309:VAL:HB	1:B:386:VAL:HG13	1.99	0.44
1:C:74:LEU:N	1:C:74:LEU:HD23	2.32	0.44
1:C:100:ASP:O	1:C:102:THR:N	2.50	0.44
1:C:114:ARG:O	1:C:117:LYS:HB2	2.17	0.44
1:C:217:VAL:HG12	1:C:221:ILE:HD12	1.99	0.44
1:D:150:LEU:CD1	1:D:192:PRO:HB2	2.37	0.44
1:D:211:ILE:O	1:D:215:LYS:HG3	2.17	0.44
1:D:390:ALA:HB1	1:J:429:ARG:NE	2.29	0.44
1:D:437:ARG:NH1	1:J:235:PRO:O	2.45	0.44
1:E:429:ARG:HH12	1:K:300:VAL:CG1	2.30	0.44
1:F:321:ARG:HD3	1:F:335:ARG:HD2	1.98	0.44
1:F:402:ASN:OD1	1:F:404:VAL:CG1	2.65	0.44
1:G:223:ARG:O	1:G:226:GLY:N	2.50	0.44
1:I:286:THR:HG23	1:I:290:ASN:ND2	2.31	0.44
1:I:380:ARG:CB	1:I:381:MET:HE2	2.47	0.44
1:K:416:HIS:O	1:K:417:PHE:C	2.60	0.44
1:L:51:MET:HE1	1:L:67:ASP:HB3	1.99	0.44
1:A:160:ALA:O	1:A:161:PRO:O	2.35	0.44
1:A:384:GLY:C	1:A:385:ILE:HG13	2.40	0.44
1:A:410:GLY:O	1:A:411:GLU:C	2.59	0.44
1:B:134:GLU:HG3	1:B:243:GLY:O	2.16	0.44
1:B:150:LEU:HD13	1:B:192:PRO:HB2	1.98	0.44
1:C:97:TYR:CD2	1:C:101:GLY:O	2.70	0.44
1:D:440:TYR:CE1	1:J:292:THR:HB	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:ARG:HH11	1:E:195:HIS:CD2	2.32	0.44
1:F:35:VAL:HG11	1:F:70:LEU:HD22	1.99	0.44
1:F:189:GLU:HB3	1:F:194:GLN:HE21	1.82	0.44
1:G:223:ARG:CB	1:G:223:ARG:HH11	2.31	0.44
1:H:162:THR:C	1:H:164:LEU:N	2.74	0.44
1:H:311:TRP:HA	1:H:320:ILE:O	2.17	0.44
1:L:73:ASP:O	1:L:76:THR:N	2.37	0.44
1:L:375:MET:HG2	1:L:380:ARG:CG	2.46	0.44
1:A:55:SER:CB	1:A:62:ARG:HE	2.31	0.44
1:A:163:ASP:O	1:A:165:GLY:N	2.50	0.44
1:A:319:LEU:HD22	1:A:320:ILE:HD11	1.99	0.44
1:C:286:THR:O	1:C:290:ASN:N	2.50	0.44
1:C:418:ILE:O	1:C:422:GLU:HG3	2.17	0.44
1:D:167:ASN:ND2	1:D:170:ARG:CB	2.79	0.44
1:D:293:VAL:HG11	1:D:428:PHE:CG	2.52	0.44
1:D:435:TRP:CE2	1:D:439:GLN:HG3	2.52	0.44
1:E:5:THR:O	1:E:9:ILE:HG12	2.17	0.44
1:E:400:LYS:HA	1:E:414:PHE:CZ	2.52	0.44
1:H:68:MET:HE1	1:H:104:PHE:CE2	2.51	0.44
1:H:308:TYR:HA	1:H:387:ASP:HA	1.99	0.44
1:I:98:ASN:O	1:I:99:PRO:C	2.60	0.44
1:J:383:ASN:HB2	1:J:385:ILE:CG1	2.48	0.44
1:K:281:HIS:CE1	1:K:404:VAL:HG21	2.52	0.44
1:L:166:GLU:O	1:L:166:GLU:OE2	2.35	0.44
1:L:253:ASN:O	1:L:255:VAL:HG23	2.18	0.44
1:L:423:ILE:O	1:L:427:MET:HG3	2.17	0.44
1:A:2:ALA:O	1:A:3:LYS:HB2	2.17	0.44
1:A:39:VAL:C	1:A:41:GLN:H	2.25	0.44
1:C:25:PHE:CE1	1:C:33:LYS:CB	3.00	0.44
1:C:96:ILE:N	1:C:96:ILE:CD1	2.81	0.44
1:C:248:LEU:HB2	1:C:332:VAL:HG13	1.99	0.44
1:D:372:ILE:HG13	1:D:373:TYR:N	2.33	0.44
1:E:138:PHE:HD2	1:E:148:LEU:HA	1.81	0.44
1:F:151:ASN:ND2	1:F:166:GLU:OE2	2.50	0.44
1:F:326:ARG:HD3	1:F:326:ARG:HA	1.79	0.44
1:G:32:ILE:HG22	1:H:159:LEU:HD12	1.98	0.44
1:G:311:TRP:O	1:G:368:ILE:HG13	2.17	0.44
1:H:140:LEU:HD12	1:H:226:GLY:C	2.42	0.44
1:I:78:VAL:CG1	1:I:179:MET:HE3	2.48	0.44
1:I:86:LYS:CB	1:J:174:LEU:HD13	2.38	0.44
1:J:48:ASN:O	1:J:69:TYR:HD2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:73:ASP:O	1:K:74:LEU:C	2.58	0.44
1:K:202:ALA:O	1:K:203:GLY:C	2.59	0.44
1:L:256:ASN:OD1	1:L:258:PHE:N	2.50	0.44
1:L:282:ALA:C	1:L:284:SER:N	2.76	0.44
1:L:355:LEU:O	1:L:357:GLY:N	2.51	0.44
1:A:138:PHE:HZ	1:A:236:LEU:HD11	1.82	0.44
1:B:232:MET:HE1	1:H:437:ARG:CA	2.45	0.44
1:B:360:ASN:HB2	1:B:362:LEU:HD13	1.99	0.44
1:C:141:ASP:O	1:C:142:GLU:C	2.60	0.44
1:C:292:THR:O	1:C:293:VAL:C	2.61	0.44
1:C:315:ASN:HD21	1:C:369:ASP:HA	1.82	0.44
1:D:115:ILE:HG23	1:D:351:LEU:HD12	2.00	0.44
1:D:201:TYR:CD1	1:D:201:TYR:C	2.96	0.44
1:D:308:TYR:CD1	1:D:372:ILE:HB	2.53	0.44
1:E:41:GLN:O	1:E:42:LEU:C	2.60	0.44
1:E:374:VAL:HG23	1:E:375:MET:H	1.82	0.44
1:F:237:PHE:CD2	1:F:238:GLY:N	2.85	0.44
1:F:418:ILE:HG22	1:F:422:GLU:OE1	2.17	0.44
1:H:252:LYS:O	1:H:253:ASN:HB2	2.17	0.44
1:H:294:ASN:HA	1:H:297:LYS:HD3	1.99	0.44
1:H:370:ARG:HH11	1:H:370:ARG:CG	2.28	0.44
1:J:125:SER:C	1:J:126:ASP:CG	2.86	0.44
1:J:189:GLU:O	1:J:190:VAL:C	2.60	0.44
1:J:349:VAL:HG22	1:J:405:MET:SD	2.58	0.44
1:K:83:THR:O	1:K:84:ALA:HB3	2.16	0.44
1:K:282:ALA:C	1:K:284:SER:N	2.75	0.44
1:L:140:LEU:HD12	1:L:226:GLY:C	2.42	0.44
1:A:397:GLU:O	1:A:401:SER:HB3	2.17	0.44
1:C:45:ALA:HA	1:C:50:VAL:HG23	2.00	0.44
1:C:435:TRP:CD1	1:I:431:GLN:HE22	2.35	0.44
1:D:28:ILE:HG22	1:D:29:LEU:HG	1.99	0.44
1:D:351:LEU:HD13	1:D:351:LEU:C	2.43	0.44
1:E:298:ARG:O	1:E:298:ARG:HG2	2.18	0.44
1:E:370:ARG:NH1	1:E:370:ARG:HG3	2.32	0.44
1:E:443:GLN:HG2	1:E:443:GLN:O	2.16	0.44
1:F:440:TYR:HD1	1:F:444:TYR:HE2	1.65	0.44
1:G:162:THR:HG21	1:L:220:THR:OG1	2.17	0.44
1:G:323:PRO:HD2	1:G:331:ARG:O	2.18	0.44
1:H:383:ASN:C	1:H:385:ILE:H	2.25	0.44
1:I:250:LEU:HB2	1:I:258:PHE:CE2	2.53	0.44
1:I:279:VAL:HG13	1:I:309:VAL:CG1	2.45	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:53:ASP:OD2	1:J:53:ASP:C	2.61	0.44
1:J:138:PHE:HB3	1:J:147:THR:O	2.18	0.44
1:A:300:VAL:CG1	1:A:301:PRO:HD2	2.48	0.44
1:B:140:LEU:HD12	1:B:226:GLY:C	2.43	0.44
1:B:224:LYS:HE2	1:B:225:HIS:CE1	2.53	0.44
1:B:297:LYS:HE3	1:H:436:GLU:OE1	2.17	0.44
1:B:371:ASN:HD22	1:B:372:ILE:H	1.64	0.44
1:B:406:VAL:HG22	1:B:414:PHE:CE1	2.52	0.44
1:C:51:MET:CE	1:C:67:ASP:HB3	2.37	0.44
1:D:137:LEU:HD13	1:D:227:LEU:HD13	2.00	0.44
1:D:300:VAL:HG21	1:J:430:THR:HG22	1.99	0.44
1:E:70:LEU:HG	1:E:94:CYS:HB2	1.99	0.44
1:F:38:PRO:C	1:F:40:SER:N	2.74	0.44
1:F:280:LYS:HE2	1:F:281:HIS:NE2	2.33	0.44
1:F:282:ALA:HA	1:F:285:PHE:CE2	2.52	0.44
1:F:440:TYR:HD1	1:F:444:TYR:CE2	2.35	0.44
1:G:9:ILE:O	1:G:13:VAL:HG23	2.17	0.44
1:I:179:MET:HE2	1:I:179:MET:HB3	1.81	0.44
1:I:251:PHE:CD1	1:I:256:ASN:HA	2.53	0.44
1:J:5:THR:O	1:J:6:ARG:C	2.61	0.44
1:K:360:ASN:HB2	1:K:362:LEU:HD11	2.00	0.44
1:K:404:VAL:CG2	1:K:405:MET:HE3	2.42	0.44
1:L:316:ARG:HG3	1:L:316:ARG:NH1	2.33	0.44
1:B:54:GLY:C	1:B:56:SER:N	2.74	0.44
1:B:285:PHE:HB2	1:B:349:VAL:HG11	2.00	0.44
1:C:6:ARG:CD	1:C:46:LEU:HD13	2.48	0.44
1:D:23:LEU:HB2	1:D:35:VAL:HG13	2.00	0.44
1:D:54:GLY:C	1:D:56:SER:N	2.74	0.44
1:D:91:ARG:C	1:D:91:ARG:CD	2.80	0.44
1:D:324:ALA:O	1:D:325:SER:C	2.60	0.44
1:E:309:VAL:CG2	1:E:386:VAL:HG23	2.46	0.44
1:E:314:GLN:NE2	1:E:321:ARG:NH2	2.55	0.44
1:E:392:LEU:O	1:E:392:LEU:HG	2.18	0.44
1:E:418:ILE:HD12	1:E:418:ILE:N	2.33	0.44
1:F:286:THR:HA	1:F:289:THR:OG1	2.18	0.44
1:G:57:ILE:C	1:G:59:GLY:N	2.72	0.44
1:G:250:LEU:O	1:G:257:ALA:HB3	2.18	0.44
1:G:286:THR:HG23	1:G:290:ASN:OD1	2.18	0.44
1:G:370:ARG:NH2	1:G:383:ASN:ND2	2.66	0.44
1:H:16:GLU:O	1:H:88:LYS:HG3	2.18	0.44
1:H:380:ARG:HH11	1:H:380:ARG:CB	2.28	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:22:ARG:NH1	1:J:159:LEU:CD2	2.81	0.44
1:I:282:ALA:CB	1:I:319:LEU:HD21	2.47	0.44
1:I:285:PHE:CD1	1:I:285:PHE:C	2.96	0.44
1:J:54:GLY:O	1:J:56:SER:N	2.51	0.44
1:J:129:LEU:HD22	1:J:131:PRO:CG	2.48	0.44
1:J:399:PHE:CD1	1:J:405:MET:HB3	2.52	0.44
1:L:296:TYR:C	1:L:298:ARG:H	2.26	0.44
1:A:31:THR:HG22	1:A:33:LYS:HG3	1.98	0.44
1:A:36:GLU:H	1:A:36:GLU:HG2	1.67	0.44
1:A:39:VAL:O	1:A:39:VAL:HG22	2.17	0.44
1:B:27:ASP:OD2	1:B:27:ASP:C	2.61	0.44
1:D:166:GLU:O	1:D:167:ASN:C	2.60	0.44
1:E:80:PHE:HE1	1:E:91:ARG:HB3	1.82	0.44
1:E:185:ALA:HB2	1:F:37:ILE:HG22	1.99	0.44
1:F:437:ARG:CA	1:L:232:MET:HE1	2.46	0.44
1:G:115:ILE:N	1:G:115:ILE:HD12	2.32	0.44
1:G:131:PRO:HB3	1:G:244:MET:HE3	1.99	0.44
1:H:365:PRO:O	1:H:366:ALA:C	2.61	0.44
1:A:37:ILE:HG22	1:F:185:ALA:HB2	1.97	0.43
1:A:69:TYR:O	1:A:70:LEU:HD13	2.18	0.43
1:A:102:THR:HG22	1:A:103:PRO:HD2	2.00	0.43
1:A:324:ALA:O	1:A:325:SER:C	2.60	0.43
1:B:18:VAL:HG11	1:B:90:ALA:HB2	1.99	0.43
1:B:55:SER:HB2	1:B:62:ARG:HB2	2.00	0.43
1:B:124:PHE:CZ	1:B:358:ILE:HD13	2.53	0.43
1:B:158:ASP:HA	1:C:33:LYS:HA	1.98	0.43
1:B:232:MET:HE3	1:H:440:TYR:CB	2.25	0.43
1:C:32:ILE:N	1:C:32:ILE:CD1	2.79	0.43
1:C:117:LYS:O	1:C:120:GLU:N	2.51	0.43
1:D:76:THR:O	1:D:78:VAL:HG23	2.17	0.43
1:D:376:SER:O	1:D:380:ARG:HG3	2.18	0.43
1:E:117:LYS:HD3	1:E:117:LYS:C	2.42	0.43
1:F:372:ILE:HG23	1:F:375:MET:SD	2.58	0.43
1:G:274:PHE:CD2	1:G:274:PHE:C	2.96	0.43
1:G:312:SER:CB	1:G:315:ASN:HB2	2.47	0.43
1:J:142:GLU:CD	1:J:142:GLU:N	2.71	0.43
1:J:211:ILE:HG22	1:J:215:LYS:HE3	2.00	0.43
1:J:386:VAL:CG1	1:J:387:ASP:H	2.14	0.43
1:J:396:LEU:HD11	1:J:421:LYS:CB	2.48	0.43
1:K:156:TYR:C	1:K:158:ASP:H	2.26	0.43
1:K:167:ASN:O	1:K:168:CYS:C	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:252:LYS:HD2	1:K:252:LYS:C	2.42	0.43
1:L:259:PHE:CE1	1:L:326:ARG:HB3	2.53	0.43
1:L:359:LYS:C	1:L:361:LYS:H	2.26	0.43
1:A:44:LYS:HE2	1:A:49:LYS:O	2.18	0.43
1:B:273:HIS:O	1:B:276:ALA:HB3	2.18	0.43
1:B:368:ILE:CG2	1:B:370:ARG:HG3	2.48	0.43
1:C:213:THR:O	1:C:217:VAL:HG23	2.18	0.43
1:D:45:ALA:CA	1:D:50:VAL:HG23	2.46	0.43
1:D:46:LEU:HD22	1:D:74:LEU:HD21	2.00	0.43
1:D:359:LYS:C	1:D:361:LYS:H	2.26	0.43
1:E:285:PHE:CD1	1:E:285:PHE:C	2.96	0.43
1:F:153:LYS:O	1:F:153:LYS:HG2	2.18	0.43
1:F:380:ARG:NH1	1:F:385:ILE:CG2	2.80	0.43
1:I:51:MET:SD	1:I:67:ASP:HB3	2.57	0.43
1:I:271:ALA:O	1:I:275:ILE:HD12	2.17	0.43
1:J:285:PHE:HB2	1:J:349:VAL:HG13	2.00	0.43
1:K:28:ILE:HD11	1:K:417:PHE:HA	1.99	0.43
1:K:189:GLU:HB3	1:K:194:GLN:NE2	2.33	0.43
1:K:261:GLU:C	1:K:262:ASN:HD22	2.26	0.43
1:K:406:VAL:HG13	1:K:414:PHE:CD2	2.54	0.43
1:L:316:ARG:HG2	1:L:373:TYR:HB2	2.00	0.43
1:L:383:ASN:HB2	1:L:385:ILE:HG12	1.99	0.43
1:A:80:PHE:HB3	1:A:82:TRP:CE3	2.53	0.43
1:A:252:LYS:NZ	1:A:253:ASN:ND2	2.65	0.43
1:B:4:TYR:HB3	1:B:9:ILE:HD11	1.98	0.43
1:B:129:LEU:HD22	1:B:130:GLY:H	1.80	0.43
1:C:48:ASN:O	1:C:69:TYR:HD2	2.01	0.43
1:C:55:SER:CB	1:C:62:ARG:HG2	2.46	0.43
1:C:156:TYR:C	1:C:158:ASP:N	2.76	0.43
1:C:402:ASN:OD1	1:C:404:VAL:CG1	2.65	0.43
1:D:5:THR:HG23	1:D:8:ASP:CG	2.43	0.43
1:D:6:ARG:HE	1:D:46:LEU:HD13	1.83	0.43
1:D:23:LEU:HB3	1:D:70:LEU:HD23	2.00	0.43
1:D:72:PRO:HA	1:D:94:CYS:HA	2.01	0.43
1:D:78:VAL:O	1:D:90:ALA:HA	2.18	0.43
1:D:388:LEU:HB3	1:D:389:PRO:HD2	2.00	0.43
1:E:184:GLU:OE2	1:F:44:LYS:HE3	2.18	0.43
1:E:407:LYS:HE2	1:E:407:LYS:HA	2.01	0.43
1:G:308:TYR:CD2	1:G:380:ARG:HD3	2.52	0.43
1:H:171:ASP:O	1:H:172:ILE:C	2.60	0.43
1:H:206:ARG:O	1:H:206:ARG:HD3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:223:ARG:O	1:H:225:HIS:N	2.52	0.43
1:I:133:PRO:HA	1:I:244:MET:HG3	2.00	0.43
1:I:287:ALA:HB2	1:I:395:ALA:CB	2.46	0.43
1:J:54:GLY:C	1:J:56:SER:H	2.26	0.43
1:J:82:TRP:HH2	1:J:217:VAL:HG22	1.83	0.43
1:J:183:ILE:HG22	1:J:184:GLU:N	2.32	0.43
1:J:256:ASN:ND2	1:J:330:THR:HB	2.33	0.43
1:J:272:LYS:O	1:J:273:HIS:C	2.61	0.43
1:J:285:PHE:C	1:J:285:PHE:HD1	2.26	0.43
1:K:262:ASN:O	1:K:263:ALA:HB2	2.18	0.43
1:K:351:LEU:O	1:K:355:LEU:HG	2.19	0.43
1:A:245:HIS:CD2	1:A:335:ARG:HA	2.54	0.43
1:B:115:ILE:O	1:B:118:GLU:HB2	2.17	0.43
1:B:139:LYS:HA	1:B:227:LEU:HD23	2.00	0.43
1:B:290:ASN:OD1	1:B:338:ASP:OD1	2.37	0.43
1:C:162:THR:O	1:C:164:LEU:N	2.51	0.43
1:C:294:ASN:O	1:C:295:SER:C	2.61	0.43
1:D:8:ASP:O	1:D:11:LYS:HB3	2.19	0.43
1:D:45:ALA:HB2	1:D:50:VAL:HG21	2.01	0.43
1:D:321:ARG:O	1:D:333:GLU:HB3	2.18	0.43
1:G:112:LEU:HD11	1:G:208:CYS:SG	2.59	0.43
1:G:162:THR:HG22	1:G:163:ASP:N	2.34	0.43
1:H:240:ASN:HD22	1:H:240:ASN:HA	1.58	0.43
1:H:307:CYS:O	1:H:387:ASP:HA	2.18	0.43
1:J:338:ASP:C	1:J:338:ASP:OD2	2.62	0.43
1:J:406:VAL:HG22	1:J:414:PHE:CZ	2.54	0.43
1:K:412:HIS:O	1:K:413:LEU:C	2.61	0.43
1:L:137:LEU:HD23	1:L:229:ALA:HA	2.01	0.43
1:L:311:TRP:H	1:L:368:ILE:HD13	1.84	0.43
1:L:333:GLU:HG2	1:L:335:ARG:HG2	2.01	0.43
1:A:319:LEU:HD22	1:A:320:ILE:HD12	1.98	0.43
1:A:376:SER:O	1:A:380:ARG:HB2	2.19	0.43
1:B:28:ILE:O	1:B:28:ILE:HG12	2.18	0.43
1:B:201:TYR:OH	1:B:331:ARG:NE	2.49	0.43
1:C:74:LEU:HA	1:C:92:PHE:HE2	1.82	0.43
1:C:414:PHE:CE2	1:C:418:ILE:HG13	2.53	0.43
1:D:161:PRO:HD3	4:D:620:HOH:O	2.18	0.43
1:D:233:PRO:HG3	1:D:338:ASP:OD2	2.19	0.43
1:F:163:ASP:HA	1:F:167:ASN:HD22	1.83	0.43
1:G:132:GLU:HB3	1:G:196:GLU:OE1	2.19	0.43
1:G:152:ASP:OD1	1:G:193:GLY:HA2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:426:ASP:HA	1:G:429:ARG:HG2	2.00	0.43
1:G:429:ARG:HG3	1:G:430:THR:N	2.33	0.43
1:I:5:THR:HG22	1:I:8:ASP:OD1	2.18	0.43
1:I:9:ILE:HG13	1:I:74:LEU:CD1	2.48	0.43
1:I:321:ARG:O	1:I:333:GLU:HB3	2.18	0.43
1:J:28:ILE:HG12	1:J:57:ILE:O	2.19	0.43
1:J:389:PRO:CB	1:J:394:GLU:HB3	2.41	0.43
1:K:58:GLU:OE1	1:K:416:HIS:CD2	2.72	0.43
1:K:100:ASP:CG	1:K:102:THR:HG22	2.43	0.43
1:L:115:ILE:HD11	1:L:408:ALA:O	2.19	0.43
1:L:258:PHE:O	1:L:330:THR:HG21	2.18	0.43
1:L:272:LYS:HZ3	1:L:311:TRP:HH2	1.58	0.43
1:A:116:LEU:O	1:A:120:GLU:HG3	2.19	0.43
1:A:259:PHE:CE1	1:A:266:GLN:HB3	2.54	0.43
1:A:297:LYS:HD3	1:G:429:ARG:O	2.18	0.43
1:A:313:ALA:HA	1:A:321:ARG:HG3	2.00	0.43
1:B:127:PHE:CD2	1:B:351:LEU:HG	2.54	0.43
1:B:299:LEU:C	1:B:307:CYS:SG	3.02	0.43
1:B:300:VAL:HG22	1:H:429:ARG:NH2	2.33	0.43
1:C:39:VAL:C	1:C:41:GLN:N	2.76	0.43
1:C:271:ALA:O	1:C:275:ILE:HG13	2.18	0.43
1:C:300:VAL:O	1:C:300:VAL:HG13	2.19	0.43
1:C:325:SER:HB2	1:C:331:ARG:HH22	1.83	0.43
1:D:250:LEU:O	1:D:257:ALA:HB3	2.19	0.43
1:E:37:ILE:O	1:E:37:ILE:HG13	2.18	0.43
1:E:67:ASP:O	1:E:68:MET:HG2	2.19	0.43
1:E:278:ILE:O	1:E:282:ALA:N	2.52	0.43
1:E:329:SER:O	1:E:331:ARG:NH2	2.51	0.43
1:E:423:ILE:O	1:E:424:GLU:C	2.61	0.43
1:F:37:ILE:O	1:F:37:ILE:HG13	2.17	0.43
1:F:120:GLU:C	1:F:122:LEU:N	2.76	0.43
1:F:402:ASN:OD1	1:F:402:ASN:C	2.61	0.43
1:F:430:THR:HG22	1:L:300:VAL:HG11	2.00	0.43
1:F:440:TYR:CD1	1:F:444:TYR:HE2	2.35	0.43
1:G:178:GLU:OE1	1:L:86:LYS:HE3	2.19	0.43
1:G:219:LYS:NZ	1:G:229:ALA:O	2.47	0.43
1:G:322:ILE:HA	1:G:323:PRO:HD2	1.84	0.43
1:G:346:ALA:O	1:G:350:LEU:HB2	2.19	0.43
1:I:68:MET:HB3	1:I:97:TYR:O	2.19	0.43
1:I:175:GLU:HG3	1:I:221:ILE:CD1	2.48	0.43
1:I:249:SER:HB3	1:I:331:ARG:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:264:ASP:C	1:J:266:GLN:H	2.26	0.43
1:K:74:LEU:H	1:K:74:LEU:CD2	2.32	0.43
1:K:261:GLU:HG3	1:K:262:ASN:ND2	2.34	0.43
1:L:166:GLU:C	1:L:168:CYS:N	2.77	0.43
1:L:316:ARG:HG2	1:L:373:TYR:CB	2.48	0.43
1:A:402:ASN:OD1	1:A:405:MET:HG2	2.19	0.43
1:B:160:ALA:HB3	1:B:169:ARG:NH1	2.34	0.43
1:B:351:LEU:CD2	1:B:355:LEU:HG	2.49	0.43
1:C:117:LYS:O	1:C:118:GLU:C	2.60	0.43
1:D:203:GLY:O	1:D:204:ALA:C	2.61	0.43
1:D:306:PRO:HB3	1:D:319:LEU:HA	2.01	0.43
1:D:430:THR:HG22	1:J:300:VAL:HG22	2.01	0.43
1:F:181:PHE:CE2	1:F:210:ASP:HB3	2.53	0.43
1:G:2:ALA:HB1	1:G:75:ASN:OD1	2.19	0.43
1:G:51:MET:HE1	1:H:324:ALA:HB3	2.00	0.43
1:G:66:SER:HA	1:H:314:GLN:OE1	2.19	0.43
1:I:100:ASP:HB2	1:I:101:GLY:H	1.32	0.43
1:I:259:PHE:HA	1:I:330:THR:HG21	2.00	0.43
1:L:360:ASN:HB2	1:L:362:LEU:HD13	2.01	0.43
1:A:436:GLU:OE1	1:G:297:LYS:NZ	2.52	0.43
1:B:378:GLU:H	1:B:378:GLU:CD	2.27	0.43
1:D:244:MET:H	1:D:338:ASP:HA	1.83	0.43
1:D:355:LEU:O	1:D:356:ASP:C	2.60	0.43
1:E:183:ILE:HG22	1:E:198:ASP:O	2.19	0.43
1:F:20:TYR:CZ	1:F:36:GLU:HB2	2.54	0.43
1:F:432:VAL:HB	1:L:237:PHE:HB2	2.00	0.43
1:G:162:THR:O	1:G:164:LEU:O	2.36	0.43
1:H:23:LEU:HD11	1:H:37:ILE:HD13	2.01	0.43
1:H:113:LYS:O	1:H:116:LEU:HB2	2.19	0.43
1:H:143:LYS:HE2	1:H:143:LYS:HA	2.00	0.43
1:H:162:THR:O	1:H:164:LEU:N	2.51	0.43
1:H:282:ALA:HA	1:H:285:PHE:CZ	2.53	0.43
1:H:372:ILE:O	1:H:380:ARG:HD3	2.19	0.43
1:H:376:SER:HB3	1:H:379:GLU:HB2	2.00	0.43
1:I:28:ILE:HD11	1:I:417:PHE:HB2	2.01	0.43
1:I:128:ASN:HB2	1:I:249:SER:OG	2.18	0.43
1:I:418:ILE:O	1:I:420:ALA:N	2.52	0.43
1:J:196:GLU:HG2	1:J:198:ASP:OD2	2.19	0.43
1:J:319:LEU:HD23	1:J:320:ILE:HD11	1.99	0.43
1:J:354:GLY:O	1:J:358:ILE:HG12	2.18	0.43
1:K:28:ILE:O	1:K:28:ILE:HG12	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:78:VAL:HB	1:K:91:ARG:CG	2.45	0.43
1:K:224:LYS:HG3	1:L:164:LEU:HD11	2.00	0.43
1:K:326:ARG:NH1	1:K:326:ARG:HB2	2.33	0.43
1:K:375:MET:HB2	1:K:379:GLU:HB2	2.01	0.43
1:L:100:ASP:O	1:L:102:THR:N	2.51	0.43
1:A:58:GLU:HB3	1:A:61:VAL:HG23	2.00	0.43
1:A:145:GLU:OE1	1:A:146:PRO:HD2	2.19	0.43
1:B:160:ALA:HB1	1:B:161:PRO:CD	2.44	0.43
1:B:374:VAL:HG23	1:B:375:MET:N	2.34	0.43
1:B:384:GLY:C	1:B:385:ILE:HG13	2.44	0.43
1:B:418:ILE:HG22	1:B:419:GLU:N	2.33	0.43
1:D:26:THR:HG1	1:D:212:GLN:HE21	1.66	0.43
1:D:260:ASP:HB2	1:D:268:SER:HB3	2.00	0.43
1:E:360:ASN:O	1:E:361:LYS:O	2.37	0.43
1:F:369:ASP:OD1	1:F:369:ASP:N	2.52	0.43
1:F:376:SER:O	1:F:379:GLU:HG2	2.19	0.43
1:G:338:ASP:C	1:G:338:ASP:OD2	2.62	0.43
1:G:393:ALA:HB2	1:G:425:TRP:CE2	2.54	0.43
1:H:9:ILE:O	1:H:13:VAL:HG23	2.18	0.43
1:H:96:ILE:HD12	1:H:96:ILE:H	1.82	0.43
1:H:147:THR:C	1:H:149:GLU:H	2.27	0.43
1:H:183:ILE:HD12	1:H:183:ILE:H	1.83	0.43
1:I:200:LYS:O	1:I:201:TYR:O	2.37	0.43
1:J:91:ARG:HD2	1:J:92:PHE:N	2.34	0.43
1:J:371:ASN:O	1:J:375:MET:HG3	2.19	0.43
1:K:83:THR:HA	1:K:85:GLU:OE2	2.18	0.43
1:K:172:ILE:HG22	1:K:173:VAL:N	2.33	0.43
1:A:37:ILE:HD13	1:A:37:ILE:N	2.33	0.43
1:A:102:THR:HG21	4:A:610:HOH:O	2.18	0.43
1:B:256:ASN:C	1:B:258:PHE:H	2.26	0.43
1:B:285:PHE:HB2	1:B:349:VAL:HG13	2.00	0.43
1:B:306:PRO:HB3	1:B:319:LEU:HA	2.01	0.43
1:C:114:ARG:O	1:C:115:ILE:C	2.61	0.43
1:C:337:VAL:CG1	1:C:338:ASP:N	2.82	0.43
1:E:136:PHE:CE1	1:E:235:PRO:HG2	2.53	0.43
1:E:273:HIS:NE2	1:E:361:LYS:CA	2.82	0.43
1:G:32:ILE:O	1:H:159:LEU:HB2	2.19	0.43
1:G:131:PRO:HG2	1:G:199:PHE:HE1	1.84	0.43
1:G:151:ASN:ND2	1:G:166:GLU:OE1	2.52	0.43
1:G:160:ALA:CB	1:G:169:ARG:HH12	2.32	0.43
1:G:201:TYR:C	1:G:201:TYR:CD2	2.96	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:21:ILE:HD12	1:H:39:VAL:HA	2.01	0.43
1:J:52:PHE:CD1	1:J:70:LEU:HD13	2.53	0.43
1:J:54:GLY:C	1:J:56:SER:N	2.76	0.43
1:J:409:LEU:O	1:J:413:LEU:HB2	2.19	0.43
1:K:63:ILE:HG22	1:K:64:GLU:HG3	2.01	0.43
1:L:156:TYR:O	1:L:158:ASP:N	2.52	0.43
1:L:225:HIS:O	1:L:227:LEU:HG	2.19	0.43
1:L:434:PRO:O	1:L:435:TRP:C	2.62	0.43
1:A:212:GLN:O	1:A:213:THR:C	2.61	0.42
1:B:18:VAL:HG12	1:B:21:ILE:HD12	2.00	0.42
1:C:315:ASN:HD21	1:C:369:ASP:CA	2.32	0.42
1:C:388:LEU:HD23	1:C:388:LEU:HA	1.85	0.42
1:E:28:ILE:HD11	1:E:417:PHE:HB2	2.01	0.42
1:E:112:LEU:O	1:E:116:LEU:HG	2.19	0.42
1:E:274:PHE:CE1	1:E:354:GLY:HA3	2.54	0.42
1:F:28:ILE:HD11	1:F:417:PHE:HB2	2.00	0.42
1:F:39:VAL:C	1:F:41:GLN:H	2.27	0.42
1:F:104:PHE:HD2	1:F:107:ASP:HB2	1.84	0.42
1:F:172:ILE:CD1	1:F:221:ILE:HB	2.49	0.42
1:F:274:PHE:HD2	1:F:332:VAL:HG21	1.84	0.42
1:G:66:SER:HA	1:H:314:GLN:CD	2.43	0.42
1:G:314:GLN:HE22	1:L:66:SER:CA	2.31	0.42
1:G:338:ASP:CB	1:G:339:PRO:HD2	2.47	0.42
1:H:437:ARG:O	1:H:441:MET:CB	2.67	0.42
1:I:19:LYS:HA	1:I:39:VAL:HB	1.99	0.42
1:I:20:TYR:HB2	1:J:174:LEU:HD21	2.01	0.42
1:I:140:LEU:HA	1:I:145:GLU:O	2.18	0.42
1:I:371:ASN:O	1:I:372:ILE:HG23	2.18	0.42
1:J:45:ALA:HA	1:J:50:VAL:HG23	2.00	0.42
1:K:57:ILE:C	1:K:59:GLY:N	2.77	0.42
1:K:224:LYS:HG3	1:L:164:LEU:CD1	2.48	0.42
1:A:186:SER:HB2	1:A:196:GLU:O	2.19	0.42
1:A:191:ALA:H	1:A:194:GLN:NE2	2.17	0.42
1:B:6:ARG:HG2	1:B:10:GLU:OE1	2.18	0.42
1:C:133:PRO:HG3	1:C:199:PHE:HE1	1.83	0.42
1:C:169:ARG:HD3	1:C:186:SER:OG	2.19	0.42
1:C:244:MET:HE2	1:C:338:ASP:O	2.19	0.42
1:D:12:LEU:O	1:D:16:GLU:HB2	2.19	0.42
1:D:194:GLN:HE22	1:D:240:ASN:HB3	1.84	0.42
1:E:236:LEU:HB2	1:E:239:VAL:CG2	2.49	0.42
1:E:354:GLY:O	1:E:358:ILE:HG13	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:VAL:HG11	1:G:70:LEU:CD2	2.49	0.42
1:G:287:ALA:HB2	1:G:395:ALA:HB1	2.00	0.42
1:G:325:SER:HB3	1:G:329:SER:HB2	2.00	0.42
1:H:328:ILE:HG12	1:H:329:SER:N	2.35	0.42
1:H:370:ARG:O	1:H:372:ILE:N	2.52	0.42
1:I:116:LEU:O	1:I:120:GLU:HG2	2.19	0.42
1:I:129:LEU:CD2	1:I:131:PRO:HG3	2.35	0.42
1:J:349:VAL:HG23	1:J:409:LEU:HD13	2.00	0.42
1:L:282:ALA:HA	1:L:285:PHE:CZ	2.54	0.42
1:L:411:GLU:O	1:L:415:GLU:HB2	2.19	0.42
1:L:423:ILE:HD12	1:L:424:GLU:N	2.34	0.42
1:A:126:ASP:HB2	1:A:251:PHE:HB2	1.99	0.42
1:A:259:PHE:CE1	1:A:326:ARG:HB3	2.54	0.42
1:A:265:LEU:HD12	1:A:265:LEU:N	2.34	0.42
1:B:73:ASP:O	1:B:76:THR:OG1	2.30	0.42
1:B:276:ALA:HB2	1:B:364:ALA:HB2	2.01	0.42
1:B:375:MET:HE2	1:B:379:GLU:OE2	2.19	0.42
1:C:281:HIS:NE2	1:C:404:VAL:HG11	2.33	0.42
1:E:107:ASP:OD1	1:E:108:PRO:HD2	2.20	0.42
1:E:285:PHE:C	1:E:285:PHE:HD1	2.28	0.42
1:F:289:THR:O	1:F:341:ALA:HB2	2.19	0.42
1:G:409:LEU:O	1:G:413:LEU:HB2	2.19	0.42
1:H:316:ARG:HA	1:H:316:ARG:HD2	1.90	0.42
1:I:399:PHE:CZ	1:I:409:LEU:HD11	2.54	0.42
1:J:196:GLU:C	1:J:197:ILE:HD13	2.44	0.42
1:J:351:LEU:HD23	1:J:355:LEU:HG	2.01	0.42
1:K:45:ALA:C	1:K:46:LEU:O	2.61	0.42
1:K:216:LEU:HD12	1:K:216:LEU:HA	1.88	0.42
1:L:55:SER:HA	1:L:58:GLU:OE2	2.19	0.42
1:A:317:SER:N	1:A:318:PRO:CD	2.83	0.42
1:B:37:ILE:CD1	1:B:45:ALA:HB2	2.50	0.42
1:B:374:VAL:HG23	1:B:375:MET:HG3	2.02	0.42
1:C:114:ARG:HH12	1:C:410:GLY:CA	2.32	0.42
1:D:53:ASP:OD2	1:D:53:ASP:C	2.63	0.42
1:D:320:ILE:HG22	1:D:321:ARG:N	2.34	0.42
1:E:80:PHE:CD1	1:E:80:PHE:N	2.88	0.42
1:E:80:PHE:HA	1:E:81:PRO:HD3	1.85	0.42
1:E:124:PHE:HD2	1:E:252:LYS:HB2	1.84	0.42
1:E:131:PRO:HG3	1:E:211:ILE:HD11	2.01	0.42
1:E:163:ASP:OD1	1:F:89:VAL:HG21	2.19	0.42
1:E:297:LYS:HD2	1:K:431:GLN:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:ILE:HG13	1:F:74:LEU:CD1	2.50	0.42
1:F:430:THR:CG2	1:L:300:VAL:HG11	2.48	0.42
1:G:191:ALA:HB3	1:G:194:GLN:NE2	2.33	0.42
1:G:256:ASN:O	1:G:258:PHE:N	2.52	0.42
1:G:402:ASN:OD1	1:G:405:MET:HG2	2.19	0.42
1:H:57:ILE:C	1:H:59:GLY:H	2.27	0.42
1:H:267:LEU:HD21	1:H:326:ARG:HH12	1.82	0.42
1:I:208:CYS:CA	1:I:211:ILE:HG12	2.49	0.42
1:L:58:GLU:HB3	1:L:61:VAL:HG23	2.01	0.42
1:A:140:LEU:HD12	1:A:226:GLY:HA2	2.01	0.42
1:A:168:CYS:O	1:A:170:ARG:N	2.53	0.42
1:A:256:ASN:OD1	1:A:258:PHE:HB2	2.19	0.42
1:B:18:VAL:HG11	1:B:90:ALA:CB	2.49	0.42
1:B:76:THR:O	1:B:78:VAL:HG23	2.20	0.42
1:B:275:ILE:O	1:B:279:VAL:HG23	2.20	0.42
1:C:70:LEU:HD12	1:C:70:LEU:HA	1.88	0.42
1:C:281:HIS:ND1	1:C:353:ALA:HA	2.35	0.42
1:D:110:ASN:O	1:D:113:LYS:HB2	2.19	0.42
1:D:319:LEU:HD12	1:D:336:SER:CB	2.48	0.42
1:E:20:TYR:HB3	1:E:89:VAL:HG22	2.01	0.42
1:E:141:ASP:C	1:E:141:ASP:OD2	2.61	0.42
1:E:306:PRO:C	1:E:308:TYR:N	2.76	0.42
1:E:396:LEU:O	1:E:400:LYS:HG3	2.19	0.42
1:F:60:PHE:CD1	1:F:60:PHE:C	2.96	0.42
1:G:138:PHE:HB3	1:G:147:THR:O	2.18	0.42
1:G:148:LEU:HD22	1:G:148:LEU:H	1.84	0.42
1:G:223:ARG:C	1:G:225:HIS:N	2.75	0.42
1:G:267:LEU:O	1:G:268:SER:O	2.38	0.42
1:H:41:GLN:HE22	1:I:200:LYS:HZ3	1.66	0.42
1:I:68:MET:HE1	1:I:104:PHE:CB	2.49	0.42
1:J:16:GLU:O	1:J:17:ASN:HB3	2.18	0.42
1:J:37:ILE:HG13	1:J:41:GLN:CB	2.49	0.42
1:J:315:ASN:C	1:J:318:PRO:HD3	2.44	0.42
1:L:173:VAL:HG22	1:L:197:ILE:HD13	2.02	0.42
1:L:268:SER:C	1:L:270:THR:H	2.28	0.42
1:C:76:THR:O	1:C:78:VAL:HG23	2.19	0.42
1:C:402:ASN:CG	1:C:405:MET:HG2	2.45	0.42
1:D:260:ASP:OD1	1:D:263:ALA:HB2	2.20	0.42
1:E:162:THR:HG22	1:E:163:ASP:N	2.35	0.42
1:E:172:ILE:O	1:E:176:LEU:HG	2.19	0.42
1:E:296:TYR:HB3	1:E:390:ALA:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:280:LYS:HE2	1:F:281:HIS:HE2	1.84	0.42
1:F:426:ASP:O	1:F:430:THR:HG23	2.19	0.42
1:F:434:PRO:HD2	4:L:607:HOH:O	2.19	0.42
1:G:410:GLY:O	1:G:412:HIS:N	2.53	0.42
1:H:3:LYS:HG2	1:H:4:TYR:CE1	2.54	0.42
1:H:59:GLY:C	1:H:61:VAL:H	2.27	0.42
1:J:9:ILE:HG13	1:J:74:LEU:CD1	2.41	0.42
1:J:310:ALA:HB2	1:J:385:ILE:HG22	2.01	0.42
1:J:326:ARG:HB3	1:J:327:GLY:H	1.67	0.42
1:J:383:ASN:C	1:J:385:ILE:H	2.25	0.42
1:K:258:PHE:HA	1:K:271:ALA:HB2	2.01	0.42
1:L:126:ASP:HB2	1:L:251:PHE:HB2	2.00	0.42
1:L:399:PHE:CD2	1:L:418:ILE:HD11	2.50	0.42
1:A:156:TYR:C	1:A:158:ASP:N	2.77	0.42
1:B:18:VAL:HG12	1:B:21:ILE:CD1	2.49	0.42
1:B:168:CYS:O	1:B:172:ILE:HG13	2.19	0.42
1:B:282:ALA:O	1:B:283:THR:C	2.62	0.42
1:B:400:LYS:HE3	1:B:400:LYS:HB2	1.80	0.42
1:B:405:MET:HE2	1:B:405:MET:CA	2.49	0.42
1:C:53:ASP:OD2	1:C:55:SER:OG	2.36	0.42
1:E:306:PRO:HB3	1:E:319:LEU:CA	2.48	0.42
1:F:187:HIS:CE1	1:F:196:GLU:CD	2.98	0.42
1:G:164:LEU:C	1:G:164:LEU:HD23	2.43	0.42
1:H:264:ASP:OD2	1:H:264:ASP:N	2.52	0.42
1:I:68:MET:HE2	1:I:97:TYR:O	2.19	0.42
1:I:257:ALA:O	1:I:270:THR:HB	2.20	0.42
1:J:282:ALA:HA	1:J:285:PHE:CE1	2.54	0.42
1:J:291:PRO:HG2	1:J:292:THR:H	1.84	0.42
1:K:359:LYS:C	1:K:361:LYS:H	2.28	0.42
1:L:146:PRO:HB3	1:L:228:HIS:CD2	2.55	0.42
1:A:13:VAL:HG11	1:A:42:LEU:HD22	2.01	0.42
1:A:216:LEU:HA	1:A:216:LEU:HD12	1.75	0.42
1:A:273:HIS:NE2	1:A:361:LYS:HA	2.33	0.42
1:A:341:ALA:HB1	1:A:346:ALA:HB2	2.02	0.42
1:B:137:LEU:HD23	1:B:229:ALA:HA	2.02	0.42
1:B:274:PHE:O	1:B:278:ILE:HD13	2.20	0.42
1:C:430:THR:HG22	1:I:300:VAL:HG11	2.01	0.42
1:D:318:PRO:HG2	1:D:320:ILE:O	2.19	0.42
1:E:30:GLY:CA	1:E:342:ASN:ND2	2.83	0.42
1:E:136:PHE:HE2	1:E:194:GLN:HB2	1.81	0.42
1:E:375:MET:HE2	1:E:379:GLU:OE2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:LYS:HD2	1:F:225:HIS:CD2	2.55	0.42
1:G:20:TYR:HB3	1:G:89:VAL:HG22	2.01	0.42
1:G:32:ILE:HG21	1:G:216:LEU:HD13	2.01	0.42
1:G:421:LYS:CD	1:G:424:GLU:OE2	2.66	0.42
1:H:248:LEU:HD21	1:H:347:LEU:HD11	2.00	0.42
1:I:73:ASP:OD1	1:I:73:ASP:C	2.63	0.42
1:I:418:ILE:HG22	1:I:422:GLU:CD	2.45	0.42
1:I:426:ASP:OD1	1:I:429:ARG:NH1	2.52	0.42
1:J:258:PHE:HZ	1:J:274:PHE:CD1	2.37	0.42
1:J:400:LYS:HA	1:J:414:PHE:CZ	2.55	0.42
1:K:115:ILE:O	1:K:118:GLU:HB2	2.20	0.42
1:L:19:LYS:HA	1:L:39:VAL:CG1	2.49	0.42
1:L:355:LEU:HD23	1:L:355:LEU:HA	1.77	0.42
1:A:282:ALA:C	1:A:284:SER:H	2.28	0.42
1:A:285:PHE:CD1	1:A:285:PHE:C	2.98	0.42
1:B:28:ILE:HD11	1:B:417:PHE:HB2	2.02	0.42
1:B:62:ARG:O	1:B:62:ARG:HG3	2.20	0.42
1:B:150:LEU:CD1	1:B:192:PRO:HB2	2.50	0.42
1:B:253:ASN:O	1:B:255:VAL:HG23	2.20	0.42
1:B:282:ALA:HA	1:B:285:PHE:CE1	2.55	0.42
1:B:317:SER:HB2	1:B:335:ARG:HH22	1.84	0.42
1:C:206:ARG:HG3	4:C:604:HOH:O	2.19	0.42
1:C:209:ASP:O	1:C:212:GLN:HB2	2.20	0.42
1:C:372:ILE:O	1:C:380:ARG:HD3	2.20	0.42
1:E:9:ILE:HG13	1:E:74:LEU:CD1	2.29	0.42
1:E:12:LEU:HA	1:E:15:GLU:OE1	2.19	0.42
1:E:53:ASP:OD1	1:E:65:GLU:HG3	2.20	0.42
1:E:431:GLN:HG2	1:K:435:TRP:CD1	2.54	0.42
1:F:9:ILE:HD12	1:F:77:PHE:CG	2.55	0.42
1:F:22:ARG:HG2	1:F:22:ARG:NH1	2.34	0.42
1:H:258:PHE:CA	1:H:271:ALA:HB2	2.50	0.42
1:I:137:LEU:HD23	1:I:229:ALA:HA	2.02	0.42
1:J:208:CYS:HA	1:J:211:ILE:HD12	2.01	0.42
1:J:267:LEU:CD2	1:J:326:ARG:HH12	2.33	0.42
1:J:368:ILE:HD11	1:J:384:GLY:O	2.20	0.42
1:K:169:ARG:HG3	1:K:169:ARG:NH2	2.34	0.42
1:L:32:ILE:CD1	1:L:216:LEU:HD22	2.50	0.42
1:L:35:VAL:O	1:L:35:VAL:HG23	2.20	0.42
1:L:399:PHE:CE1	1:L:405:MET:HB3	2.55	0.42
1:A:52:PHE:HZ	1:A:57:ILE:HD11	1.85	0.42
1:A:129:LEU:HD22	1:A:130:GLY:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:ARG:O	1:A:438:GLU:C	2.61	0.42
1:B:52:PHE:CD1	1:B:70:LEU:HD13	2.55	0.42
1:C:52:PHE:CZ	1:C:54:GLY:HA2	2.54	0.42
1:C:300:VAL:HG21	1:I:430:THR:HG22	2.01	0.42
1:D:11:LYS:CG	1:D:15:GLU:OE2	2.67	0.42
1:E:259:PHE:CE2	1:E:326:ARG:HD3	2.55	0.42
1:E:306:PRO:C	1:E:308:TYR:H	2.27	0.42
1:E:441:MET:O	1:E:441:MET:HG3	2.19	0.42
1:F:108:PRO:O	1:F:111:ASN:N	2.53	0.42
1:G:137:LEU:O	1:G:151:ASN:HB3	2.19	0.42
1:H:116:LEU:O	1:H:117:LYS:C	2.63	0.42
1:H:380:ARG:HB2	1:H:380:ARG:CZ	2.50	0.42
1:I:223:ARG:O	1:I:226:GLY:N	2.53	0.42
1:J:191:ALA:HB3	1:J:194:GLN:NE2	2.34	0.42
1:J:260:ASP:OD1	1:J:263:ALA:HB2	2.20	0.42
1:K:37:ILE:HD12	1:K:38:PRO:O	2.20	0.42
1:K:112:LEU:HD12	1:K:205:VAL:HG22	2.02	0.42
1:K:315:ASN:HD22	1:K:315:ASN:HA	1.58	0.42
1:L:163:ASP:HA	1:L:167:ASN:HD22	1.85	0.42
1:L:437:ARG:HD2	4:L:622:HOH:O	2.18	0.42
1:A:58:GLU:HG2	1:A:58:GLU:H	1.66	0.41
1:A:83:THR:HG23	1:A:83:THR:O	2.20	0.41
1:A:184:GLU:CD	1:A:200:LYS:HZ2	2.28	0.41
1:A:354:GLY:O	1:A:358:ILE:HG12	2.20	0.41
1:A:403:GLU:C	1:A:405:MET:N	2.78	0.41
1:B:373:TYR:CD2	1:B:373:TYR:N	2.88	0.41
1:C:9:ILE:HD11	1:C:74:LEU:HB3	2.01	0.41
1:C:78:VAL:HB	1:C:91:ARG:HG3	2.02	0.41
1:C:137:LEU:HD12	1:C:195:HIS:HE2	1.85	0.41
1:C:283:THR:HG21	1:C:386:VAL:HG12	2.02	0.41
1:D:146:PRO:CG	1:D:228:HIS:CD2	3.03	0.41
1:E:34:ASN:OD1	1:E:35:VAL:N	2.53	0.41
1:E:141:ASP:OD2	1:E:144:GLY:N	2.53	0.41
1:E:272:LYS:O	1:E:273:HIS:C	2.61	0.41
1:E:380:ARG:HB3	1:E:380:ARG:HH11	1.85	0.41
1:F:4:TYR:CB	1:F:9:ILE:HD11	2.47	0.41
1:F:52:PHE:CE2	1:F:54:GLY:HA2	2.54	0.41
1:F:143:LYS:HE3	1:F:143:LYS:HB2	1.88	0.41
1:F:175:GLU:O	1:F:179:MET:HG3	2.20	0.41
1:F:282:ALA:HA	1:F:285:PHE:CZ	2.55	0.41
1:F:296:TYR:HB3	1:F:390:ALA:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:250:LEU:HB3	1:G:257:ALA:HB3	2.02	0.41
1:H:3:LYS:HB2	1:H:75:ASN:OD1	2.20	0.41
1:I:183:ILE:HD13	1:I:197:ILE:CG2	2.50	0.41
1:I:285:PHE:HB3	1:I:405:MET:SD	2.60	0.41
1:J:131:PRO:HG2	1:J:211:ILE:CG1	2.50	0.41
1:J:312:SER:HB3	1:J:315:ASN:HB2	2.02	0.41
1:K:98:ASN:HB3	1:K:100:ASP:OD2	2.19	0.41
1:K:360:ASN:N	1:K:360:ASN:ND2	2.68	0.41
1:K:380:ARG:CB	1:K:385:ILE:HD12	2.48	0.41
1:L:82:TRP:O	1:L:83:THR:C	2.63	0.41
1:L:175:GLU:HA	1:L:175:GLU:OE2	2.20	0.41
1:L:311:TRP:O	1:L:311:TRP:CG	2.73	0.41
1:A:3:LYS:HB3	1:A:3:LYS:HZ2	1.83	0.41
1:B:103:PRO:HB3	1:B:110:ASN:ND2	2.35	0.41
1:B:309:VAL:CG2	1:B:386:VAL:HG13	2.50	0.41
1:C:370:ARG:HB3	1:C:371:ASN:H	1.63	0.41
1:D:259:PHE:HB2	1:D:330:THR:OG1	2.20	0.41
1:F:133:PRO:HG2	1:F:199:PHE:CE1	2.55	0.41
1:F:342:ASN:CB	1:F:345:LEU:HD12	2.50	0.41
1:H:86:LYS:HG3	1:I:174:LEU:HB3	2.02	0.41
1:H:112:LEU:HD12	1:H:344:TYR:HA	2.02	0.41
1:H:328:ILE:N	1:H:328:ILE:CD1	2.81	0.41
1:I:116:LEU:HD23	1:I:116:LEU:HA	1.93	0.41
1:I:223:ARG:O	1:I:224:LYS:C	2.63	0.41
1:I:293:VAL:HG11	1:I:428:PHE:CG	2.54	0.41
1:J:9:ILE:O	1:J:13:VAL:HG23	2.19	0.41
1:J:139:LYS:HA	1:J:227:LEU:HD23	2.02	0.41
1:J:291:PRO:O	1:J:392:LEU:HD13	2.20	0.41
1:J:393:ALA:HB2	1:J:425:TRP:CE2	2.56	0.41
1:K:27:ASP:HA	1:K:57:ILE:HG23	2.02	0.41
1:K:141:ASP:C	1:K:141:ASP:OD2	2.63	0.41
1:L:276:ALA:O	1:L:279:VAL:HB	2.20	0.41
1:L:368:ILE:HG21	1:L:372:ILE:HG21	2.01	0.41
1:A:86:LYS:HG3	1:F:174:LEU:HB3	2.01	0.41
1:A:119:MET:CE	1:A:127:PHE:HB2	2.50	0.41
1:A:230:THR:OG1	1:A:232:MET:HB2	2.20	0.41
1:A:234:LYS:HE3	1:A:239:VAL:O	2.20	0.41
1:A:274:PHE:CE2	1:A:278:ILE:HD11	2.55	0.41
1:C:223:ARG:C	1:C:225:HIS:N	2.78	0.41
1:C:338:ASP:OD2	1:C:340:ALA:HB3	2.20	0.41
1:C:364:ALA:HB1	1:C:365:PRO:HD2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:LEU:HD11	1:D:350:LEU:HD13	2.02	0.41
1:E:80:PHE:HD2	1:E:82:TRP:CZ3	2.38	0.41
1:E:150:LEU:HD13	1:E:192:PRO:HG2	2.02	0.41
1:E:173:VAL:O	1:E:174:LEU:C	2.62	0.41
1:F:36:GLU:H	1:F:36:GLU:HG2	1.67	0.41
1:F:129:LEU:O	1:F:201:TYR:HA	2.21	0.41
1:F:133:PRO:CG	1:F:199:PHE:HE1	2.33	0.41
1:G:211:ILE:HG22	1:G:215:LYS:HE3	2.03	0.41
1:H:179:MET:HE2	1:H:179:MET:HB3	1.91	0.41
1:K:116:LEU:HD23	1:K:116:LEU:HA	1.90	0.41
1:L:172:ILE:O	1:L:176:LEU:HG	2.20	0.41
1:L:282:ALA:HA	1:L:285:PHE:CE1	2.56	0.41
1:L:314:GLN:HA	1:L:314:GLN:HE21	1.85	0.41
1:A:286:THR:HG21	1:A:389:PRO:HD2	2.03	0.41
1:A:300:VAL:HG22	1:G:429:ARG:NH1	2.33	0.41
1:A:440:TYR:OH	1:G:293:VAL:HG23	2.21	0.41
1:B:125:SER:O	1:B:126:ASP:CG	2.64	0.41
1:B:309:VAL:HG21	1:B:386:VAL:HG13	2.02	0.41
1:C:135:PHE:HB3	1:C:231:PHE:CE1	2.55	0.41
1:C:189:GLU:HA	1:C:189:GLU:OE2	2.18	0.41
1:D:5:THR:C	1:D:7:GLU:N	2.77	0.41
1:D:381:MET:HG2	4:D:605:HOH:O	2.20	0.41
1:E:12:LEU:HA	1:E:15:GLU:CD	2.45	0.41
1:E:23:LEU:HB3	1:E:70:LEU:HD23	2.02	0.41
1:E:73:ASP:OD2	1:E:76:THR:HG23	2.20	0.41
1:E:297:LYS:HD3	1:K:429:ARG:O	2.19	0.41
1:E:405:MET:O	1:E:408:ALA:N	2.47	0.41
1:F:80:PHE:HB3	1:F:82:TRP:CE3	2.55	0.41
1:F:156:TYR:C	1:F:158:ASP:H	2.29	0.41
1:F:319:LEU:CD1	1:F:336:SER:HB3	2.47	0.41
1:H:137:LEU:HD12	1:H:195:HIS:NE2	2.35	0.41
1:H:310:ALA:HB1	1:H:368:ILE:CG1	2.47	0.41
1:H:418:ILE:O	1:H:422:GLU:HG3	2.21	0.41
1:J:271:ALA:O	1:J:274:PHE:HB3	2.21	0.41
1:L:105:GLU:OE1	1:L:105:GLU:O	2.37	0.41
1:L:141:ASP:OD2	1:L:144:GLY:N	2.53	0.41
1:L:268:SER:C	1:L:270:THR:N	2.77	0.41
1:A:234:LYS:HB3	1:A:294:ASN:ND2	2.35	0.41
1:A:296:TYR:HB3	1:A:390:ALA:O	2.20	0.41
1:B:30:GLY:H	1:B:342:ASN:HD22	1.69	0.41
1:B:231:PHE:O	1:B:232:MET:C	2.62	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ASP:HB2	1:B:268:SER:HA	2.01	0.41
1:B:280:LYS:HD2	1:B:362:LEU:CD2	2.51	0.41
1:C:162:THR:O	1:C:163:ASP:C	2.63	0.41
1:C:232:MET:HA	1:C:233:PRO:HD3	1.86	0.41
1:C:291:PRO:O	1:C:392:LEU:HD13	2.20	0.41
1:C:321:ARG:HB2	1:C:335:ARG:HD2	2.03	0.41
1:C:345:LEU:CD2	1:C:413:LEU:HD13	2.50	0.41
1:D:6:ARG:HD3	1:D:6:ARG:O	2.21	0.41
1:D:163:ASP:OD1	1:E:89:VAL:HG21	2.20	0.41
1:D:164:LEU:HD11	1:E:224:LYS:NZ	2.35	0.41
1:E:360:ASN:O	1:E:361:LYS:C	2.62	0.41
1:E:439:GLN:HB2	1:E:440:TYR:H	1.72	0.41
1:F:279:VAL:HG13	1:F:309:VAL:HG12	2.02	0.41
1:F:281:HIS:HE1	1:F:356:ASP:OD2	2.04	0.41
1:G:23:LEU:O	1:G:35:VAL:HG12	2.20	0.41
1:G:91:ARG:C	1:G:91:ARG:CD	2.81	0.41
1:G:256:ASN:O	1:G:257:ALA:C	2.63	0.41
1:H:383:ASN:C	1:H:385:ILE:N	2.78	0.41
1:I:73:ASP:O	1:I:74:LEU:C	2.63	0.41
1:I:150:LEU:HD13	1:I:192:PRO:C	2.42	0.41
1:J:250:LEU:HB2	1:J:258:PHE:CZ	2.56	0.41
1:J:319:LEU:HD23	1:J:320:ILE:HG12	2.02	0.41
1:J:404:VAL:O	1:J:408:ALA:N	2.52	0.41
1:K:33:LYS:HA	1:L:158:ASP:CA	2.38	0.41
1:K:72:PRO:HA	1:K:94:CYS:HB3	2.03	0.41
1:K:163:ASP:O	1:K:164:LEU:HD23	2.20	0.41
1:K:247:ASN:HB3	1:K:331:ARG:CG	2.47	0.41
1:K:252:LYS:O	1:K:252:LYS:HD2	2.20	0.41
1:L:186:SER:O	1:L:187:HIS:HB3	2.20	0.41
1:A:119:MET:HG2	1:A:124:PHE:HB2	2.01	0.41
1:A:261:GLU:H	1:A:261:GLU:CD	2.27	0.41
1:B:351:LEU:HD22	1:B:355:LEU:HG	2.02	0.41
1:C:129:LEU:HD23	1:C:130:GLY:N	2.36	0.41
1:D:65:GLU:O	1:D:65:GLU:HG3	2.20	0.41
1:E:282:ALA:C	1:E:284:SER:H	2.28	0.41
1:F:41:GLN:HE21	1:F:41:GLN:HB3	1.59	0.41
1:F:57:ILE:C	1:F:59:GLY:N	2.79	0.41
1:F:82:TRP:HH2	1:F:217:VAL:HG22	1.85	0.41
1:F:146:PRO:HG3	1:F:228:HIS:HD2	1.75	0.41
1:F:150:LEU:HD22	1:F:192:PRO:O	2.21	0.41
1:F:170:ARG:HG2	1:F:170:ARG:HH11	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:221:ILE:O	1:F:225:HIS:CD2	2.73	0.41
1:G:32:ILE:HG21	1:G:216:LEU:CD1	2.51	0.41
1:G:131:PRO:HG2	1:G:199:PHE:CE1	2.55	0.41
1:H:223:ARG:O	1:H:224:LYS:C	2.62	0.41
1:I:9:ILE:CG1	1:I:74:LEU:HD12	2.50	0.41
1:I:212:GLN:OE1	1:I:212:GLN:HA	2.21	0.41
1:J:85:GLU:O	1:J:87:GLY:N	2.43	0.41
1:J:102:THR:HA	1:J:103:PRO:HD3	1.92	0.41
1:J:135:PHE:N	1:J:135:PHE:CD1	2.88	0.41
1:J:319:LEU:O	1:J:320:ILE:HD13	2.20	0.41
1:K:46:LEU:C	1:K:48:ASN:N	2.78	0.41
1:K:58:GLU:OE1	1:K:416:HIS:NE2	2.53	0.41
1:K:67:ASP:N	1:K:67:ASP:OD2	2.53	0.41
1:L:28:ILE:C	1:L:30:GLY:H	2.28	0.41
1:L:320:ILE:HG22	1:L:321:ARG:N	2.35	0.41
1:A:204:ALA:O	1:A:205:VAL:C	2.63	0.41
1:C:3:LYS:C	1:C:4:TYR:HD1	2.29	0.41
1:D:383:ASN:HD22	1:D:383:ASN:HA	1.60	0.41
1:E:91:ARG:CZ	1:E:93:ILE:HD11	2.51	0.41
1:E:96:ILE:HD13	1:E:107:ASP:OD1	2.21	0.41
1:G:306:PRO:HG2	1:G:335:ARG:HB2	2.02	0.41
1:H:60:PHE:CD1	1:H:60:PHE:C	2.98	0.41
1:I:248:LEU:HD13	1:I:332:VAL:HG23	2.02	0.41
1:I:436:GLU:O	1:I:437:ARG:C	2.63	0.41
1:I:442:SER:C	1:I:444:TYR:N	2.77	0.41
1:J:16:GLU:OE2	1:J:16:GLU:HA	2.20	0.41
1:J:114:ARG:NH1	1:J:115:ILE:HD11	2.35	0.41
1:K:423:ILE:O	1:K:427:MET:HG3	2.20	0.41
1:L:129:LEU:HD22	1:L:131:PRO:HD3	2.02	0.41
1:B:214:PHE:O	1:B:218:VAL:HG23	2.21	0.41
1:B:315:ASN:OD1	1:B:371:ASN:HA	2.21	0.41
1:C:24:GLN:HE22	1:C:91:ARG:HH11	1.64	0.41
1:C:232:MET:CG	1:C:294:ASN:HD22	2.34	0.41
1:C:378:GLU:OE1	1:C:378:GLU:N	2.48	0.41
1:C:427:MET:HB3	1:C:427:MET:HE2	1.71	0.41
1:E:100:ASP:OD2	1:E:100:ASP:C	2.64	0.41
1:E:169:ARG:O	1:E:171:ASP:N	2.54	0.41
1:E:176:LEU:HD11	1:E:214:PHE:CD1	2.56	0.41
1:F:205:VAL:HG13	1:F:206:ARG:H	1.85	0.41
1:G:44:LYS:HE3	1:G:49:LYS:O	2.21	0.41
1:G:55:SER:CB	1:G:62:ARG:HE	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:LEU:HD12	1:G:344:TYR:CD2	2.56	0.41
1:G:116:LEU:CD1	1:G:205:VAL:HG23	2.50	0.41
1:G:199:PHE:CD1	1:G:199:PHE:N	2.85	0.41
1:H:186:SER:HB2	1:H:197:ILE:HG12	2.02	0.41
1:H:223:ARG:C	1:H:225:HIS:N	2.78	0.41
1:H:346:ALA:O	1:H:350:LEU:HB2	2.20	0.41
1:I:140:LEU:HD12	1:I:227:LEU:N	2.36	0.41
1:I:223:ARG:O	1:I:225:HIS:N	2.54	0.41
1:I:321:ARG:HE	1:I:321:ARG:HB3	1.75	0.41
1:J:4:TYR:HB3	1:J:9:ILE:HD11	2.02	0.41
1:J:134:GLU:HG2	1:J:196:GLU:HB2	2.01	0.41
1:K:120:GLU:HA	1:K:124:PHE:O	2.19	0.41
1:A:375:MET:HE2	1:A:385:ILE:HD12	2.03	0.41
1:A:381:MET:HA	1:A:381:MET:CE	2.49	0.41
1:A:399:PHE:HZ	1:A:409:LEU:CD1	2.33	0.41
1:A:421:LYS:HD3	1:A:421:LYS:HA	1.89	0.41
1:A:429:ARG:HG3	1:A:429:ARG:HH11	1.86	0.41
1:B:32:ILE:HD13	1:B:216:LEU:HD12	2.02	0.41
1:B:68:MET:SD	1:B:96:ILE:HG22	2.60	0.41
1:B:109:ARG:O	1:B:112:LEU:HB3	2.21	0.41
1:B:112:LEU:O	1:B:116:LEU:HG	2.21	0.41
1:B:175:GLU:O	1:B:179:MET:HG3	2.21	0.41
1:B:399:PHE:C	1:B:401:SER:H	2.28	0.41
1:C:248:LEU:HB2	1:C:332:VAL:CG1	2.51	0.41
1:D:21:ILE:HD11	1:D:39:VAL:HA	2.03	0.41
1:D:39:VAL:C	1:D:41:GLN:H	2.28	0.41
1:D:170:ARG:O	1:D:174:LEU:HG	2.21	0.41
1:D:203:GLY:O	1:D:205:VAL:N	2.54	0.41
1:D:288:VAL:HG22	1:D:417:PHE:CE2	2.56	0.41
1:D:296:TYR:CD1	1:D:296:TYR:N	2.89	0.41
1:D:350:LEU:HD23	1:D:350:LEU:HA	1.87	0.41
1:E:182:GLU:HA	1:E:182:GLU:OE1	2.21	0.41
1:E:225:HIS:O	1:E:227:LEU:HG	2.21	0.41
1:E:306:PRO:CB	1:E:319:LEU:HA	2.47	0.41
1:E:371:ASN:HB3	1:E:375:MET:CG	2.51	0.41
1:E:399:PHE:CE1	1:E:405:MET:HB3	2.56	0.41
1:F:27:ASP:OD2	1:F:27:ASP:C	2.64	0.41
1:F:112:LEU:O	1:F:116:LEU:HG	2.21	0.41
1:F:241:GLY:HA3	1:F:298:ARG:CG	2.50	0.41
1:F:245:HIS:CD2	1:F:335:ARG:HA	2.56	0.41
1:F:275:ILE:O	1:F:279:VAL:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:343:PRO:O	1:F:347:LEU:HD23	2.21	0.41
1:F:369:ASP:CG	1:F:370:ARG:H	2.28	0.41
1:F:378:GLU:O	1:F:381:MET:HG2	2.21	0.41
1:G:13:VAL:HG21	1:G:42:LEU:CD2	2.51	0.41
1:G:20:TYR:OH	1:G:36:GLU:CB	2.69	0.41
1:G:41:GLN:NE2	1:G:44:LYS:HD3	2.36	0.41
1:G:281:HIS:O	1:G:282:ALA:C	2.64	0.41
1:H:3:LYS:HD3	1:H:4:TYR:HE1	1.86	0.41
1:H:124:PHE:CD2	1:H:250:LEU:HD13	2.56	0.41
1:H:135:PHE:HB3	1:H:231:PHE:CE1	2.54	0.41
1:H:393:ALA:HB2	1:H:425:TRP:CD2	2.55	0.41
1:H:397:GLU:HA	1:H:400:LYS:NZ	2.36	0.41
1:I:20:TYR:OH	1:I:36:GLU:HG3	2.20	0.41
1:I:152:ASP:OD2	1:I:188:HIS:NE2	2.39	0.41
1:I:232:MET:HE2	1:I:234:LYS:O	2.20	0.41
1:I:283:THR:HG22	1:I:388:LEU:HD23	2.02	0.41
1:I:393:ALA:HB2	1:I:425:TRP:CE2	2.56	0.41
1:I:396:LEU:HD11	1:I:421:LYS:CB	2.51	0.41
1:J:19:LYS:HD2	1:J:86:LYS:O	2.21	0.41
1:J:36:GLU:HG2	1:J:36:GLU:H	1.67	0.41
1:J:207:SER:O	1:J:209:ASP:N	2.53	0.41
1:J:343:PRO:O	1:J:347:LEU:HB2	2.21	0.41
1:K:28:ILE:HD11	1:K:417:PHE:N	2.36	0.41
1:K:141:ASP:HB3	1:K:147:THR:CG2	2.51	0.41
1:K:186:SER:HB2	1:K:196:GLU:O	2.21	0.41
1:L:20:TYR:CZ	1:L:36:GLU:HB3	2.56	0.41
1:L:100:ASP:C	1:L:102:THR:H	2.28	0.41
1:L:132:GLU:HG2	1:L:198:ASP:OD1	2.20	0.41
1:L:142:GLU:H	1:L:142:GLU:CD	2.29	0.41
1:L:152:ASP:OD2	1:L:188:HIS:NE2	2.40	0.41
1:L:185:ALA:O	1:L:186:SER:HB2	2.19	0.41
1:A:28:ILE:CG2	1:A:29:LEU:N	2.83	0.41
1:A:156:TYR:CE2	1:B:62:ARG:NH1	2.89	0.41
1:B:256:ASN:O	1:B:258:PHE:N	2.53	0.41
1:C:74:LEU:HA	1:C:92:PHE:CE2	2.56	0.41
1:C:129:LEU:HD23	1:C:130:GLY:H	1.86	0.41
1:C:169:ARG:O	1:C:172:ILE:HB	2.21	0.41
1:C:286:THR:O	1:C:290:ASN:HB2	2.21	0.41
1:C:301:PRO:HB3	1:C:308:TYR:OH	2.21	0.41
1:D:443:GLN:HA	1:D:443:GLN:NE2	2.36	0.41
1:E:172:ILE:HD11	1:E:221:ILE:HB	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:436:GLU:OE1	1:K:297:LYS:NZ	2.54	0.41
1:F:113:LYS:O	1:F:116:LEU:HB2	2.21	0.41
1:F:262:ASN:O	1:F:263:ALA:HB2	2.21	0.41
1:G:98:ASN:HD21	1:G:104:PHE:HA	1.86	0.41
1:H:125:SER:HB2	1:H:251:PHE:HB3	2.03	0.41
1:H:355:LEU:HD23	1:H:355:LEU:HA	1.86	0.41
1:I:58:GLU:CB	1:I:62:ARG:HB2	2.51	0.41
1:I:97:TYR:HE2	1:I:101:GLY:O	2.04	0.41
1:I:170:ARG:NH1	1:I:171:ASP:OD2	2.54	0.41
1:J:78:VAL:HG11	1:J:179:MET:CE	2.51	0.41
1:J:282:ALA:C	1:J:284:SER:N	2.79	0.41
1:J:306:PRO:HB3	1:J:319:LEU:HA	2.02	0.41
1:K:60:PHE:HZ	1:K:420:ALA:O	2.03	0.41
1:K:141:ASP:OD1	1:K:145:GLU:HB2	2.21	0.41
1:K:156:TYR:C	1:K:156:TYR:CD2	2.98	0.41
1:L:138:PHE:CZ	1:L:150:LEU:HD23	2.55	0.41
1:L:331:ARG:HG2	1:L:331:ARG:HH11	1.86	0.41
1:A:179:MET:HE2	1:A:179:MET:HB3	1.90	0.40
1:A:231:PHE:HB2	1:G:444:TYR:OXT	2.21	0.40
1:A:234:LYS:HB3	1:A:294:ASN:HD21	1.86	0.40
1:A:383:ASN:C	1:A:385:ILE:N	2.78	0.40
1:B:115:ILE:HD11	1:B:408:ALA:HA	2.04	0.40
1:B:281:HIS:CD2	1:B:404:VAL:HG21	2.56	0.40
1:B:371:ASN:O	1:B:374:VAL:HG22	2.21	0.40
1:B:441:MET:O	1:H:228:HIS:CE1	2.66	0.40
1:C:52:PHE:HE1	1:C:70:LEU:HD13	1.79	0.40
1:D:81:PRO:HA	4:D:619:HOH:O	2.21	0.40
1:D:139:LYS:O	1:D:147:THR:HG23	2.21	0.40
1:D:184:GLU:OE2	1:D:200:LYS:NZ	2.50	0.40
1:E:110:ASN:HD22	1:E:110:ASN:HA	1.71	0.40
1:E:262:ASN:HD22	1:E:262:ASN:HA	1.55	0.40
1:E:338:ASP:HB2	1:E:339:PRO:CD	2.50	0.40
1:F:5:THR:O	1:F:6:ARG:C	2.65	0.40
1:F:38:PRO:C	1:F:40:SER:H	2.30	0.40
1:G:150:LEU:HD13	1:G:192:PRO:O	2.21	0.40
1:G:156:TYR:O	1:G:158:ASP:N	2.54	0.40
1:H:34:ASN:C	1:H:34:ASN:HD22	2.28	0.40
1:H:370:ARG:CG	1:H:370:ARG:NH1	2.84	0.40
1:I:258:PHE:HA	1:I:271:ALA:HB2	2.03	0.40
1:J:37:ILE:HG22	1:K:185:ALA:HB2	2.03	0.40
1:J:116:LEU:HD23	1:J:351:LEU:CD1	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:277:GLY:C	1:J:279:VAL:N	2.79	0.40
1:K:33:LYS:HA	1:L:159:LEU:H	1.86	0.40
1:K:142:GLU:CD	1:K:142:GLU:H	2.27	0.40
1:K:258:PHE:CB	1:K:271:ALA:HB2	2.51	0.40
1:K:320:ILE:HG22	1:K:321:ARG:N	2.36	0.40
1:K:322:ILE:HA	1:K:323:PRO:HD2	1.95	0.40
1:L:53:ASP:CG	1:L:65:GLU:HG2	2.46	0.40
1:L:203:GLY:O	1:L:205:VAL:N	2.54	0.40
1:A:260:ASP:O	1:A:266:GLN:HA	2.20	0.40
1:B:274:PHE:CE1	1:B:354:GLY:HA3	2.56	0.40
1:B:377:LYS:HD3	1:B:387:ASP:OD2	2.20	0.40
1:C:9:ILE:O	1:C:10:GLU:C	2.64	0.40
1:C:106:GLY:O	1:C:413:LEU:HD21	2.21	0.40
1:C:112:LEU:HD12	1:C:344:TYR:CD2	2.51	0.40
1:D:45:ALA:HA	1:D:50:VAL:CG2	2.50	0.40
1:D:293:VAL:HG11	1:D:428:PHE:CD2	2.56	0.40
1:E:273:HIS:NE2	1:E:361:LYS:CB	2.85	0.40
1:E:409:LEU:HB3	1:E:413:LEU:HB2	2.03	0.40
1:E:440:TYR:HD1	1:E:444:TYR:CE2	2.38	0.40
1:G:78:VAL:HG11	1:G:91:ARG:NH2	2.36	0.40
1:G:167:ASN:HD22	1:G:170:ARG:NH1	2.18	0.40
1:G:183:ILE:HG21	1:G:197:ILE:HG22	2.03	0.40
1:G:250:LEU:CB	1:G:258:PHE:CZ	2.98	0.40
1:I:127:PHE:CE2	1:I:347:LEU:HD11	2.56	0.40
1:I:378:GLU:C	1:I:380:ARG:H	2.29	0.40
1:J:129:LEU:HD22	1:J:131:PRO:HD3	2.02	0.40
1:J:389:PRO:HG3	1:J:395:ALA:HB2	2.03	0.40
1:K:133:PRO:HD2	1:K:197:ILE:O	2.21	0.40
1:K:285:PHE:C	1:K:285:PHE:HD1	2.28	0.40
1:K:377:LYS:HA	1:K:380:ARG:CZ	2.52	0.40
1:L:110:ASN:HD22	1:L:110:ASN:HA	1.66	0.40
1:L:374:VAL:O	1:L:374:VAL:HG12	2.21	0.40
1:B:338:ASP:HB2	1:B:339:PRO:CD	2.47	0.40
1:C:159:LEU:HD12	1:C:159:LEU:HA	1.95	0.40
1:D:100:ASP:OD2	1:D:100:ASP:C	2.64	0.40
1:D:103:PRO:HB2	1:D:110:ASN:OD1	2.22	0.40
1:D:347:LEU:HD23	1:D:347:LEU:HA	1.90	0.40
1:D:378:GLU:OE1	1:D:382:GLU:HG3	2.21	0.40
1:E:274:PHE:CE2	1:E:278:ILE:HD11	2.56	0.40
1:E:411:GLU:O	1:E:412:HIS:C	2.64	0.40
1:F:122:LEU:HD12	1:F:355:LEU:HD13	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:351:LEU:CD2	1:F:355:LEU:HG	2.51	0.40
1:G:33:LYS:HD2	1:H:157:PHE:C	2.46	0.40
1:H:243:GLY:HA2	1:H:338:ASP:HA	2.03	0.40
1:I:129:LEU:HD23	1:I:130:GLY:N	2.36	0.40
1:J:115:ILE:O	1:J:115:ILE:HG22	2.19	0.40
1:K:355:LEU:O	1:K:356:ASP:C	2.65	0.40
1:L:296:TYR:CE1	1:L:392:LEU:HA	2.56	0.40
1:L:380:ARG:CB	1:L:380:ARG:NH1	2.85	0.40
1:A:402:ASN:HD21	1:A:404:VAL:HG12	1.87	0.40
1:B:18:VAL:HG22	1:B:88:LYS:HB2	2.04	0.40
1:C:155:GLY:O	1:C:158:ASP:HB2	2.21	0.40
1:C:232:MET:HG3	1:C:294:ASN:HD22	1.87	0.40
1:D:104:PHE:C	1:D:106:GLY:H	2.28	0.40
1:D:119:MET:HE1	1:D:126:ASP:HA	2.03	0.40
1:D:289:THR:HG22	1:D:337:VAL:HG13	2.03	0.40
1:F:82:TRP:CH2	1:F:217:VAL:HG22	2.56	0.40
1:F:109:ARG:HE	1:F:205:VAL:CG2	2.34	0.40
1:G:258:PHE:O	1:G:330:THR:HG21	2.22	0.40
1:G:351:LEU:CD2	1:G:355:LEU:HG	2.51	0.40
1:G:370:ARG:HH22	1:G:383:ASN:ND2	2.19	0.40
1:H:83:THR:HG23	1:H:83:THR:O	2.22	0.40
1:H:253:ASN:C	1:H:255:VAL:H	2.30	0.40
1:I:129:LEU:O	1:I:131:PRO:HD3	2.21	0.40
1:I:174:LEU:HD12	1:I:174:LEU:HA	1.90	0.40
1:I:259:PHE:CD1	1:I:260:ASP:N	2.89	0.40
1:J:273:HIS:CE1	1:J:361:LYS:HB3	2.57	0.40
1:K:124:PHE:CZ	1:K:358:ILE:HG21	2.56	0.40
1:K:207:SER:O	1:K:211:ILE:HG13	2.21	0.40
1:L:115:ILE:H	1:L:115:ILE:HD12	1.87	0.40
1:L:337:VAL:HG12	1:L:338:ASP:N	2.36	0.40
1:L:351:LEU:O	1:L:355:LEU:N	2.43	0.40
1:A:129:LEU:CD2	1:A:130:GLY:N	2.85	0.40
1:A:252:LYS:O	1:A:253:ASN:HB2	2.21	0.40
1:B:38:PRO:C	1:B:40:SER:N	2.80	0.40
1:B:116:LEU:HD23	1:B:351:LEU:HD11	2.03	0.40
1:B:159:LEU:HD11	1:C:22:ARG:NH1	2.34	0.40
1:B:343:PRO:O	1:B:347:LEU:HB2	2.21	0.40
1:C:22:ARG:HB3	1:C:34:ASN:HD22	1.86	0.40
1:C:282:ALA:HA	1:C:285:PHE:CZ	2.57	0.40
1:D:13:VAL:HG21	1:D:42:LEU:HD22	2.02	0.40
1:E:429:ARG:HG3	1:E:429:ARG:HH11	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:288:VAL:O	1:F:291:PRO:HD3	2.22	0.40
1:G:183:ILE:CG2	1:G:197:ILE:HG22	2.52	0.40
1:G:258:PHE:HA	1:G:268:SER:OG	2.22	0.40
1:G:342:ASN:C	1:G:342:ASN:ND2	2.79	0.40
1:H:20:TYR:OH	1:H:36:GLU:CB	2.69	0.40
1:H:318:PRO:O	1:H:319:LEU:C	2.63	0.40
1:I:355:LEU:O	1:I:357:GLY:N	2.54	0.40
1:J:19:LYS:HA	1:J:39:VAL:HB	2.02	0.40
1:K:345:LEU:O	1:K:349:VAL:HG22	2.21	0.40
1:K:406:VAL:HG22	1:K:414:PHE:CZ	2.56	0.40
1:L:10:GLU:O	1:L:11:LYS:C	2.63	0.40
1:L:308:TYR:OH	1:L:373:TYR:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/443 (98%)	358 (82%)	63 (14%)	14 (3%)	3	18
1	B	435/443 (98%)	367 (84%)	52 (12%)	16 (4%)	2	15
1	C	434/443 (98%)	341 (79%)	67 (15%)	26 (6%)	1	7
1	D	435/443 (98%)	347 (80%)	72 (17%)	16 (4%)	2	15
1	E	434/443 (98%)	344 (79%)	66 (15%)	24 (6%)	1	9
1	F	433/443 (98%)	345 (80%)	69 (16%)	19 (4%)	2	12
1	G	434/443 (98%)	353 (81%)	58 (13%)	23 (5%)	1	10
1	H	433/443 (98%)	356 (82%)	58 (13%)	19 (4%)	2	12
1	I	432/443 (98%)	364 (84%)	45 (10%)	23 (5%)	1	10
1	J	434/443 (98%)	342 (79%)	69 (16%)	23 (5%)	1	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	434/443 (98%)	356 (82%)	56 (13%)	22 (5%)	1	10
1	L	436/443 (98%)	346 (79%)	66 (15%)	24 (6%)	1	9
All	All	5209/5316 (98%)	4219 (81%)	741 (14%)	249 (5%)	2	11

All (249) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	161	PRO
1	A	166	GLU
1	A	325	SER
1	A	411	GLU
1	B	3	LYS
1	B	166	GLU
1	B	325	SER
1	C	101	GLY
1	C	166	GLU
1	C	314	GLN
1	C	369	ASP
1	D	161	PRO
1	D	163	ASP
1	D	371	ASN
1	E	166	GLU
1	E	361	LYS
1	E	369	ASP
1	E	411	GLU
1	F	84	ALA
1	F	101	GLY
1	F	161	PRO
1	F	166	GLU
1	F	190	VAL
1	F	316	ARG
1	G	3	LYS
1	G	63	ILE
1	G	78	VAL
1	G	156	TYR
1	G	166	GLU
1	G	325	SER
1	G	369	ASP
1	G	411	GLU
1	G	441	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	125	SER
1	H	167	ASN
1	H	190	VAL
1	I	100	ASP
1	I	158	ASP
1	I	201	TYR
1	I	325	SER
1	J	3	LYS
1	J	161	PRO
1	J	163	ASP
1	J	325	SER
1	J	368	ILE
1	K	156	TYR
1	K	161	PRO
1	K	162	THR
1	K	166	GLU
1	K	312	SER
1	L	82	TRP
1	L	167	ASN
1	L	386	VAL
1	A	101	GLY
1	A	157	PHE
1	A	164	LEU
1	A	201	TYR
1	A	204	ALA
1	A	314	GLN
1	A	410	GLY
1	B	256	ASN
1	B	292	THR
1	C	161	PRO
1	C	163	ASP
1	C	283	THR
1	C	365	PRO
1	D	85	GLU
1	D	204	ALA
1	D	412	HIS
1	E	161	PRO
1	E	163	ASP
1	E	170	ARG
1	E	325	SER
1	E	329	SER
1	F	67	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	157	PHE
1	F	260	ASP
1	G	58	GLU
1	G	157	PHE
1	G	161	PRO
1	G	256	ASN
1	G	257	ALA
1	G	268	SER
1	G	361	LYS
1	H	163	ASP
1	H	260	ASP
1	H	325	SER
1	H	371	ASN
1	I	3	LYS
1	I	157	PHE
1	I	161	PRO
1	I	166	GLU
1	I	167	ASN
1	I	260	ASP
1	I	283	THR
1	I	361	LYS
1	I	372	ILE
1	I	376	SER
1	I	441	MET
1	J	81	PRO
1	J	190	VAL
1	J	268	SER
1	J	291	PRO
1	J	292	THR
1	K	85	GLU
1	K	368	ILE
1	L	74	LEU
1	L	83	THR
1	L	101	GLY
1	L	157	PHE
1	L	166	GLU
1	L	204	ALA
1	L	325	SER
1	L	368	ILE
1	B	121	ASP
1	B	124	PHE
1	B	161	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	204	ALA
1	B	257	ALA
1	B	291	PRO
1	C	3	LYS
1	C	86	LYS
1	C	204	ALA
1	C	312	SER
1	C	348	SER
1	D	158	ASP
1	D	360	ASN
1	D	361	LYS
1	E	143	LYS
1	E	148	LEU
1	E	224	LYS
1	F	310	ALA
1	F	361	LYS
1	G	329	SER
1	H	3	LYS
1	H	6	ARG
1	H	101	GLY
1	H	161	PRO
1	H	261	GLU
1	J	55	SER
1	J	164	LEU
1	J	207	SER
1	J	283	THR
1	J	376	SER
1	K	148	LEU
1	K	169	ARG
1	K	313	ALA
1	L	13	VAL
1	L	159	LEU
1	L	163	ASP
1	L	220	THR
1	L	371	ASN
1	B	39	VAL
1	C	6	ARG
1	C	139	LYS
1	C	160	ALA
1	C	261	GLU
1	C	325	SER
1	C	368	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	74	LEU
1	D	166	GLU
1	D	315	ASN
1	D	370	ARG
1	D	411	GLU
1	E	57	ILE
1	E	157	PHE
1	E	200	LYS
1	E	202	ALA
1	E	262	ASN
1	E	268	SER
1	E	291	PRO
1	E	412	HIS
1	F	58	GLU
1	F	348	SER
1	F	412	HIS
1	G	85	GLU
1	G	163	ASP
1	G	224	LYS
1	G	238	GLY
1	H	100	ASP
1	H	160	ALA
1	H	224	LYS
1	H	372	ILE
1	H	375	MET
1	I	17	ASN
1	I	268	SER
1	I	329	SER
1	I	419	GLU
1	J	181	PHE
1	J	208	CYS
1	J	361	LYS
1	K	74	LEU
1	K	99	PRO
1	L	148	LEU
1	L	291	PRO
1	L	412	HIS
1	A	169	ARG
1	B	282	ALA
1	C	220	THR
1	D	169	ARG
1	E	144	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	376	SER
1	F	3	LYS
1	F	201	TYR
1	G	101	GLY
1	G	204	ALA
1	H	58	GLU
1	H	283	THR
1	I	162	THR
1	I	204	ALA
1	J	85	GLU
1	J	261	GLU
1	J	329	SER
1	K	75	ASN
1	K	83	THR
1	K	373	TYR
1	K	376	SER
1	K	411	GLU
1	L	29	LEU
1	L	190	VAL
1	L	276	ALA
1	L	369	ASP
1	A	17	ASN
1	B	283	THR
1	B	368	ILE
1	C	157	PHE
1	C	291	PRO
1	C	349	VAL
1	C	370	ARG
1	F	220	THR
1	J	58	GLU
1	L	324	ALA
1	B	101	GLY
1	F	386	VAL
1	C	337	VAL
1	E	101	GLY
1	I	368	ILE
1	K	367	PRO
1	K	374	VAL
1	C	190	VAL
1	F	160	ALA
1	K	160	ALA
1	K	337	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	101	GLY
1	D	385	ILE
1	E	372	ILE
1	I	160	ALA
1	K	190	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	380/382 (100%)	336 (88%)	44 (12%)	5	22
1	B	380/382 (100%)	353 (93%)	27 (7%)	13	41
1	C	379/382 (99%)	341 (90%)	38 (10%)	7	29
1	D	380/382 (100%)	340 (90%)	40 (10%)	6	26
1	E	379/382 (99%)	334 (88%)	45 (12%)	5	21
1	F	378/382 (99%)	337 (89%)	41 (11%)	6	25
1	G	379/382 (99%)	334 (88%)	45 (12%)	5	21
1	H	378/382 (99%)	342 (90%)	36 (10%)	8	30
1	I	377/382 (99%)	336 (89%)	41 (11%)	6	24
1	J	379/382 (99%)	334 (88%)	45 (12%)	5	21
1	K	379/382 (99%)	341 (90%)	38 (10%)	7	29
1	L	380/382 (100%)	341 (90%)	39 (10%)	7	27
All	All	4548/4584 (99%)	4069 (90%)	479 (10%)	6	26

All (479) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	29	LEU
1	A	31	THR
1	A	34	ASN
1	A	36	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	37	ILE
1	A	70	LEU
1	A	78	VAL
1	A	85	GLU
1	A	91	ARG
1	A	94	CYS
1	A	102	THR
1	A	105	GLU
1	A	112	LEU
1	A	129	LEU
1	A	151	ASN
1	A	159	LEU
1	A	161	PRO
1	A	164	LEU
1	A	169	ARG
1	A	174	LEU
1	A	186	SER
1	A	190	VAL
1	A	206	ARG
1	A	215	LYS
1	A	252	LYS
1	A	262	ASN
1	A	273	HIS
1	A	294	ASN
1	A	308	TYR
1	A	314	GLN
1	A	332	VAL
1	A	347	LEU
1	A	359	LYS
1	A	363	GLU
1	A	371	ASN
1	A	373	TYR
1	A	375	MET
1	A	380	ARG
1	A	401	SER
1	A	427	MET
1	A	429	ARG
1	A	431	GLN
1	A	441	MET
1	B	7	GLU
1	B	12	LEU
1	B	32	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	49	LYS
1	B	70	LEU
1	B	82	TRP
1	B	89	VAL
1	B	122	LEU
1	B	124	PHE
1	B	129	LEU
1	B	153	LYS
1	B	186	SER
1	B	201	TYR
1	B	236	LEU
1	B	275	ILE
1	B	286	THR
1	B	347	LEU
1	B	349	VAL
1	B	351	LEU
1	B	362	LEU
1	B	363	GLU
1	B	369	ASP
1	B	370	ARG
1	B	372	ILE
1	B	380	ARG
1	B	387	ASP
1	B	429	ARG
1	C	32	ILE
1	C	34	ASN
1	C	36	GLU
1	C	41	GLN
1	C	49	LYS
1	C	61	VAL
1	C	68	MET
1	C	73	ASP
1	C	94	CYS
1	C	96	ILE
1	C	112	LEU
1	C	120	GLU
1	C	129	LEU
1	C	142	GLU
1	C	153	LYS
1	C	161	PRO
1	C	163	ASP
1	C	183	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	194	GLN
1	C	201	TYR
1	C	224	LYS
1	C	252	LYS
1	C	255	VAL
1	C	264	ASP
1	C	286	THR
1	C	308	TYR
1	C	312	SER
1	C	347	LEU
1	C	351	LEU
1	C	368	ILE
1	C	371	ASN
1	C	373	TYR
1	C	382	GLU
1	C	409	LEU
1	C	429	ARG
1	C	431	GLN
1	C	437	ARG
1	C	441	MET
1	D	5	THR
1	D	6	ARG
1	D	15	GLU
1	D	26	THR
1	D	28	ILE
1	D	34	ASN
1	D	35	VAL
1	D	40	SER
1	D	70	LEU
1	D	82	TRP
1	D	91	ARG
1	D	94	CYS
1	D	112	LEU
1	D	126	ASP
1	D	129	LEU
1	D	151	ASN
1	D	159	LEU
1	D	161	PRO
1	D	163	ASP
1	D	164	LEU
1	D	177	GLU
1	D	183	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	207	SER
1	D	221	ILE
1	D	265	LEU
1	D	295	SER
1	D	308	TYR
1	D	314	GLN
1	D	319	LEU
1	D	328	ILE
1	D	331	ARG
1	D	332	VAL
1	D	337	VAL
1	D	359	LYS
1	D	378	GLU
1	D	383	ASN
1	D	387	ASP
1	D	394	GLU
1	D	429	ARG
1	D	443	GLN
1	E	5	THR
1	E	7	GLU
1	E	11	LYS
1	E	12	LEU
1	E	16	GLU
1	E	35	VAL
1	E	51	MET
1	E	61	VAL
1	E	62	ARG
1	E	70	LEU
1	E	85	GLU
1	E	91	ARG
1	E	96	ILE
1	E	105	GLU
1	E	109	ARG
1	E	110	ASN
1	E	126	ASP
1	E	129	LEU
1	E	148	LEU
1	E	149	GLU
1	E	161	PRO
1	E	164	LEU
1	E	172	ILE
1	E	183	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	201	TYR
1	E	223	ARG
1	E	230	THR
1	E	262	ASN
1	E	264	ASP
1	E	273	HIS
1	E	285	PHE
1	E	289	THR
1	E	294	ASN
1	E	322	ILE
1	E	326	ARG
1	E	328	ILE
1	E	349	VAL
1	E	369	ASP
1	E	370	ARG
1	E	373	TYR
1	E	381	MET
1	E	391	THR
1	E	412	HIS
1	E	436	GLU
1	E	441	MET
1	F	14	LYS
1	F	28	ILE
1	F	29	LEU
1	F	31	THR
1	F	32	ILE
1	F	34	ASN
1	F	36	GLU
1	F	40	SER
1	F	41	GLN
1	F	61	VAL
1	F	70	LEU
1	F	82	TRP
1	F	98	ASN
1	F	105	GLU
1	F	112	LEU
1	F	126	ASP
1	F	129	LEU
1	F	148	LEU
1	F	150	LEU
1	F	153	LYS
1	F	159	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	161	PRO
1	F	189	GLU
1	F	206	ARG
1	F	218	VAL
1	F	219	LYS
1	F	236	LEU
1	F	239	VAL
1	F	299	LEU
1	F	308	TYR
1	F	328	ILE
1	F	342	ASN
1	F	349	VAL
1	F	351	LEU
1	F	370	ARG
1	F	378	GLU
1	F	387	ASP
1	F	398	GLU
1	F	423	ILE
1	F	437	ARG
1	F	439	GLN
1	G	12	LEU
1	G	34	ASN
1	G	41	GLN
1	G	63	ILE
1	G	64	GLU
1	G	70	LEU
1	G	78	VAL
1	G	88	LYS
1	G	91	ARG
1	G	95	ASP
1	G	117	LYS
1	G	122	LEU
1	G	129	LEU
1	G	161	PRO
1	G	168	CYS
1	G	169	ARG
1	G	174	LEU
1	G	177	GLU
1	G	183	ILE
1	G	198	ASP
1	G	199	PHE
1	G	201	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	216	LEU
1	G	221	ILE
1	G	223	ARG
1	G	224	LYS
1	G	250	LEU
1	G	251	PHE
1	G	258	PHE
1	G	273	HIS
1	G	315	ASN
1	G	316	ARG
1	G	335	ARG
1	G	337	VAL
1	G	342	ASN
1	G	350	LEU
1	G	351	LEU
1	G	363	GLU
1	G	370	ARG
1	G	373	TYR
1	G	385	ILE
1	G	387	ASP
1	G	409	LEU
1	G	427	MET
1	G	442	SER
1	H	7	GLU
1	H	19	LYS
1	H	21	ILE
1	H	28	ILE
1	H	29	LEU
1	H	32	ILE
1	H	34	ASN
1	H	35	VAL
1	H	70	LEU
1	H	74	LEU
1	H	94	CYS
1	H	105	GLU
1	H	112	LEU
1	H	126	ASP
1	H	143	LYS
1	H	158	ASP
1	H	159	LEU
1	H	161	PRO
1	H	166	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	201	TYR
1	H	239	VAL
1	H	240	ASN
1	H	273	HIS
1	H	283	THR
1	H	321	ARG
1	H	328	ILE
1	H	350	LEU
1	H	351	LEU
1	H	359	LYS
1	H	362	LEU
1	H	370	ARG
1	H	372	ILE
1	H	381	MET
1	H	401	SER
1	H	418	ILE
1	H	419	GLU
1	I	7	GLU
1	I	28	ILE
1	I	32	ILE
1	I	34	ASN
1	I	40	SER
1	I	49	LYS
1	I	58	GLU
1	I	70	LEU
1	I	86	LYS
1	I	91	ARG
1	I	94	CYS
1	I	100	ASP
1	I	109	ARG
1	I	110	ASN
1	I	112	LEU
1	I	114	ARG
1	I	129	LEU
1	I	158	ASP
1	I	159	LEU
1	I	161	PRO
1	I	164	LEU
1	I	169	ARG
1	I	174	LEU
1	I	199	PHE
1	I	207	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	216	LEU
1	I	217	VAL
1	I	239	VAL
1	I	248	LEU
1	I	261	GLU
1	I	300	VAL
1	I	328	ILE
1	I	349	VAL
1	I	351	LEU
1	I	370	ARG
1	I	372	ILE
1	I	373	TYR
1	I	391	THR
1	I	409	LEU
1	I	434	PRO
1	I	441	MET
1	J	5	THR
1	J	12	LEU
1	J	34	ASN
1	J	35	VAL
1	J	36	GLU
1	J	37	ILE
1	J	49	LYS
1	J	58	GLU
1	J	66	SER
1	J	70	LEU
1	J	85	GLU
1	J	91	ARG
1	J	94	CYS
1	J	105	GLU
1	J	112	LEU
1	J	117	LYS
1	J	125	SER
1	J	126	ASP
1	J	129	LEU
1	J	142	GLU
1	J	161	PRO
1	J	167	ASN
1	J	169	ARG
1	J	200	LYS
1	J	206	ARG
1	J	212	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	216	LEU
1	J	223	ARG
1	J	224	LYS
1	J	236	LEU
1	J	250	LEU
1	J	262	ASN
1	J	265	LEU
1	J	270	THR
1	J	272	LYS
1	J	285	PHE
1	J	286	THR
1	J	308	TYR
1	J	347	LEU
1	J	349	VAL
1	J	350	LEU
1	J	363	GLU
1	J	373	TYR
1	J	385	ILE
1	J	387	ASP
1	K	24	GLN
1	K	34	ASN
1	K	36	GLU
1	K	58	GLU
1	K	65	GLU
1	K	94	CYS
1	K	109	ARG
1	K	142	GLU
1	K	153	LYS
1	K	159	LEU
1	K	164	LEU
1	K	166	GLU
1	K	169	ARG
1	K	174	LEU
1	K	197	ILE
1	K	199	PHE
1	K	223	ARG
1	K	239	VAL
1	K	270	THR
1	K	273	HIS
1	K	283	THR
1	K	285	PHE
1	K	298	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	315	ASN
1	K	316	ARG
1	K	326	ARG
1	K	337	VAL
1	K	360	ASN
1	K	363	GLU
1	K	373	TYR
1	K	374	VAL
1	K	375	MET
1	K	382	GLU
1	K	391	THR
1	K	411	GLU
1	K	426	ASP
1	K	436	GLU
1	K	442	SER
1	L	11	LYS
1	L	14	LYS
1	L	21	ILE
1	L	32	ILE
1	L	34	ASN
1	L	40	SER
1	L	65	GLU
1	L	75	ASN
1	L	78	VAL
1	L	91	ARG
1	L	102	THR
1	L	105	GLU
1	L	109	ARG
1	L	122	LEU
1	L	129	LEU
1	L	149	GLU
1	L	162	THR
1	L	164	LEU
1	L	174	LEU
1	L	178	GLU
1	L	183	ILE
1	L	189	GLU
1	L	194	GLN
1	L	201	TYR
1	L	236	LEU
1	L	262	ASN
1	L	285	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	321	ARG
1	L	325	SER
1	L	328	ILE
1	L	349	VAL
1	L	351	LEU
1	L	362	LEU
1	L	363	GLU
1	L	372	ILE
1	L	375	MET
1	L	378	GLU
1	L	385	ILE
1	L	443	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (200) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	24	GLN
1	A	41	GLN
1	A	110	ASN
1	A	128	ASN
1	A	167	ASN
1	A	188	HIS
1	A	194	GLN
1	A	247	ASN
1	A	253	ASN
1	A	281	HIS
1	A	314	GLN
1	A	315	ASN
1	A	383	ASN
1	A	431	GLN
1	A	443	GLN
1	B	17	ASN
1	B	41	GLN
1	B	98	ASN
1	B	128	ASN
1	B	167	ASN
1	B	194	GLN
1	B	225	HIS
1	B	245	HIS
1	B	247	ASN
1	B	262	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	266	GLN
1	B	281	HIS
1	B	290	ASN
1	B	294	ASN
1	B	315	ASN
1	B	342	ASN
1	B	371	ASN
1	B	383	ASN
1	B	431	GLN
1	B	443	GLN
1	C	24	GLN
1	C	34	ASN
1	C	98	ASN
1	C	110	ASN
1	C	151	ASN
1	C	194	GLN
1	C	225	HIS
1	C	228	HIS
1	C	245	HIS
1	C	266	GLN
1	C	290	ASN
1	C	314	GLN
1	C	315	ASN
1	C	416	HIS
1	C	431	GLN
1	C	443	GLN
1	D	75	ASN
1	D	111	ASN
1	D	128	ASN
1	D	151	ASN
1	D	187	HIS
1	D	194	GLN
1	D	225	HIS
1	D	228	HIS
1	D	240	ASN
1	D	262	ASN
1	D	273	HIS
1	D	281	HIS
1	D	290	ASN
1	D	314	GLN
1	D	383	ASN
1	D	433	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	439	GLN
1	D	443	GLN
1	E	17	ASN
1	E	34	ASN
1	E	41	GLN
1	E	110	ASN
1	E	151	ASN
1	E	195	HIS
1	E	225	HIS
1	E	247	ASN
1	E	262	ASN
1	E	281	HIS
1	E	290	ASN
1	E	314	GLN
1	E	342	ASN
1	E	360	ASN
1	E	412	HIS
1	E	416	HIS
1	E	431	GLN
1	F	17	ASN
1	F	24	GLN
1	F	41	GLN
1	F	98	ASN
1	F	151	ASN
1	F	167	ASN
1	F	187	HIS
1	F	194	GLN
1	F	225	HIS
1	F	228	HIS
1	F	240	ASN
1	F	266	GLN
1	F	281	HIS
1	F	290	ASN
1	F	314	GLN
1	F	342	ASN
1	F	360	ASN
1	F	383	ASN
1	F	439	GLN
1	G	98	ASN
1	G	110	ASN
1	G	151	ASN
1	G	167	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	194	GLN
1	G	225	HIS
1	G	228	HIS
1	G	247	ASN
1	G	253	ASN
1	G	262	ASN
1	G	266	GLN
1	G	281	HIS
1	G	314	GLN
1	G	342	ASN
1	G	360	ASN
1	G	383	ASN
1	G	416	HIS
1	G	431	GLN
1	G	443	GLN
1	H	17	ASN
1	H	41	GLN
1	H	98	ASN
1	H	128	ASN
1	H	194	GLN
1	H	228	HIS
1	H	240	ASN
1	H	245	HIS
1	H	281	HIS
1	H	290	ASN
1	H	315	ASN
1	H	360	ASN
1	H	383	ASN
1	H	431	GLN
1	I	128	ASN
1	I	151	ASN
1	I	187	HIS
1	I	194	GLN
1	I	240	ASN
1	I	245	HIS
1	I	247	ASN
1	I	253	ASN
1	I	262	ASN
1	I	266	GLN
1	I	281	HIS
1	I	290	ASN
1	I	383	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	416	HIS
1	I	433	HIS
1	I	439	GLN
1	J	17	ASN
1	J	34	ASN
1	J	98	ASN
1	J	110	ASN
1	J	111	ASN
1	J	128	ASN
1	J	194	GLN
1	J	245	HIS
1	J	281	HIS
1	J	290	ASN
1	J	371	ASN
1	J	416	HIS
1	J	433	HIS
1	J	439	GLN
1	K	98	ASN
1	K	110	ASN
1	K	128	ASN
1	K	194	GLN
1	K	212	GLN
1	K	245	HIS
1	K	262	ASN
1	K	281	HIS
1	K	290	ASN
1	K	315	ASN
1	K	342	ASN
1	K	360	ASN
1	K	383	ASN
1	K	431	GLN
1	L	24	GLN
1	L	41	GLN
1	L	98	ASN
1	L	110	ASN
1	L	111	ASN
1	L	128	ASN
1	L	151	ASN
1	L	167	ASN
1	L	194	GLN
1	L	228	HIS
1	L	247	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	266	GLN
1	L	281	HIS
1	L	290	ASN
1	L	360	ASN
1	L	402	ASN
1	L	431	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 25 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	F	503	-	4,4,4	0.37	0	6,6,6	0.10	0
3	SO4	D	504	-	4,4,4	0.37	0	6,6,6	0.08	0
3	SO4	D	501	-	4,4,4	0.35	0	6,6,6	0.12	0
3	SO4	E	503	-	4,4,4	0.39	0	6,6,6	0.06	0
3	SO4	H	501	-	4,4,4	0.36	0	6,6,6	0.06	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	439/443 (99%)	-1.48	0 100 100	38, 61, 115, 125	0
1	B	439/443 (99%)	-1.46	0 100 100	34, 61, 114, 124	0
1	C	438/443 (98%)	-1.50	0 100 100	30, 61, 114, 126	0
1	D	439/443 (99%)	-1.46	0 100 100	38, 63, 116, 130	0
1	E	438/443 (98%)	-1.46	0 100 100	39, 64, 118, 126	0
1	F	437/443 (98%)	-1.48	0 100 100	40, 60, 114, 130	0
1	G	438/443 (98%)	-1.47	0 100 100	35, 60, 116, 124	0
1	H	437/443 (98%)	-1.45	0 100 100	35, 60, 115, 127	0
1	I	436/443 (98%)	-1.48	0 100 100	39, 62, 118, 132	0
1	J	438/443 (98%)	-1.46	0 100 100	40, 63, 118, 126	0
1	K	438/443 (98%)	-1.48	0 100 100	39, 63, 116, 127	0
1	L	440/443 (99%)	-1.48	0 100 100	32, 59, 116, 126	0
All	All	5257/5316 (98%)	-1.47	0 100 100	30, 62, 116, 132	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	D	504	5/5	0.96	0.04	154,154,154,155	0
3	SO4	F	503	5/5	0.97	0.05	181,181,182,182	0
3	SO4	E	503	5/5	0.98	0.04	158,159,159,159	0
2	MG	B	503	1/1	0.98	0.12	92,92,92,92	0
2	MG	F	502	1/1	0.99	0.04	22,22,22,22	0
2	MG	G	502	1/1	0.99	0.04	19,19,19,19	0
2	MG	I	501	1/1	0.99	0.03	18,18,18,18	0
2	MG	J	501	1/1	0.99	0.05	30,30,30,30	0
2	MG	J	502	1/1	0.99	0.08	27,27,27,27	0
2	MG	K	502	1/1	0.99	0.04	39,39,39,39	0
2	MG	L	501	1/1	0.99	0.06	30,30,30,30	0
3	SO4	D	501	5/5	0.99	0.07	131,131,132,132	0
2	MG	C	501	1/1	0.99	0.04	27,27,27,27	0
2	MG	C	502	1/1	0.99	0.05	34,34,34,34	0
2	MG	E	502	1/1	0.99	0.04	39,39,39,39	0
3	SO4	H	501	5/5	0.99	0.03	169,169,169,169	0
2	MG	H	503	1/1	1.00	0.03	35,35,35,35	0
2	MG	B	501	1/1	1.00	0.03	21,21,21,21	0
2	MG	I	502	1/1	1.00	0.03	39,39,39,39	0
2	MG	D	502	1/1	1.00	0.02	7,7,7,7	0
2	MG	D	503	1/1	1.00	0.03	32,32,32,32	0
2	MG	K	501	1/1	1.00	0.02	13,13,13,13	0
2	MG	E	501	1/1	1.00	0.05	22,22,22,22	0
2	MG	B	502	1/1	1.00	0.04	23,23,23,23	0
2	MG	L	502	1/1	1.00	0.03	29,29,29,29	0
2	MG	F	501	1/1	1.00	0.01	32,32,32,32	0
2	MG	A	501	1/1	1.00	0.02	10,10,10,10	0
2	MG	G	501	1/1	1.00	0.04	24,24,24,24	0
2	MG	A	502	1/1	1.00	0.01	19,19,19,19	0
2	MG	H	502	1/1	1.00	0.03	16,16,16,16	0

6.5 Other polymers

There are no such residues in this entry.