



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:20 AM UTC

PDB ID : 1KEN / pdb_00001ken
Title : INFLUENZA VIRUS HEMAGGLUTININ COMPLEXED WITH AN AN-
TIBODY THAT PREVENTS THE HEMAGGLUTININ LOW PH FUSO-
GENIC TRANSITION
Authors : Barbey-Martin, C.; Gigant, B.; Bizebard, T.; Calder, L.J.; Wharto, S.A.;
Skehel, J.J.; Knossow, M.
Deposited on : 2001-11-16
Resolution : 3.50 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

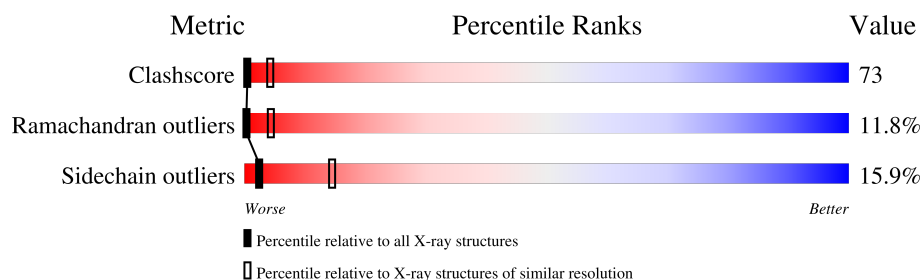
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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))
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	328	28% 52% 16% ..
1	C	328	27% 51% 17% ..
1	E	328	23% 55% 18% ..
2	B	175	16% 49% 30% 5%
2	D	175	15% 47% 35% .
2	F	175	14% 50% 33% .
3	L	213	19% 50% 27% .
3	U	213	17% 55% 25% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	H	221	
4	T	221	
5	G	3	
5	I	3	
5	J	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MAN	G	3	X	-	-	-
5	MAN	I	3	X	-	-	-
5	MAN	J	3	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18492 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 hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2472	1547	434	478	13			
1	C	320	Total	C	N	O	S	0	0	0
			2472	1547	434	478	13			
1	E	320	Total	C	N	O	S	0	0	0
			2472	1547	434	478	13			

- Molecule 2 is a protein called hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1421	882	250	283	6			
2	D	175	Total	C	N	O	S	0	0	0
			1421	882	250	283	6			
2	F	175	Total	C	N	O	S	0	0	0
			1421	882	250	283	6			

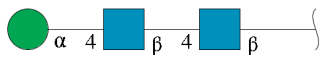
- Molecule 3 is a protein called influenza virus infectivity neutralizing antibody (light chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1638	1028	272	332	6			
3	U	213	Total	C	N	O	S	0	0	0
			1638	1028	272	332	6			

- Molecule 4 is a protein called influenza virus infectivity neutralizing antibody (heavy chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	221	Total	C	N	O	S	0	0	0
			1720	1102	272	340	6			
4	T	219	Total	C	N	O	S	0	0	0
			1700	1092	267	335	6			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



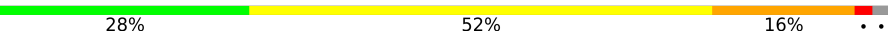
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	J	3	Total	C	N	O	0	0	0
			39	22	2	15			

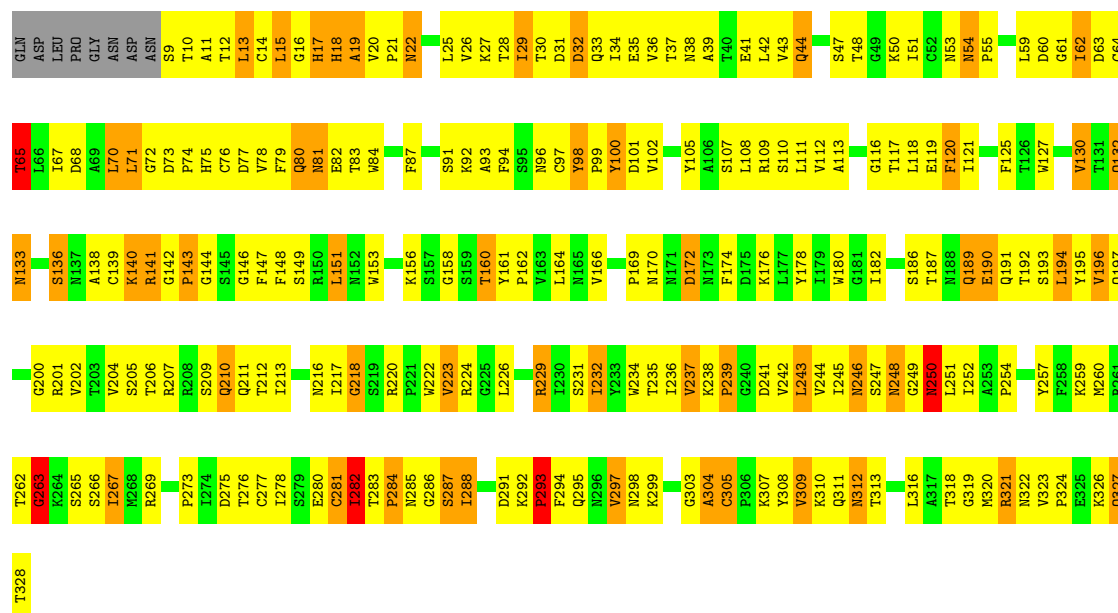
3 Residue-property plots

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

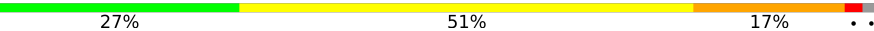
Note EDS was not executed.

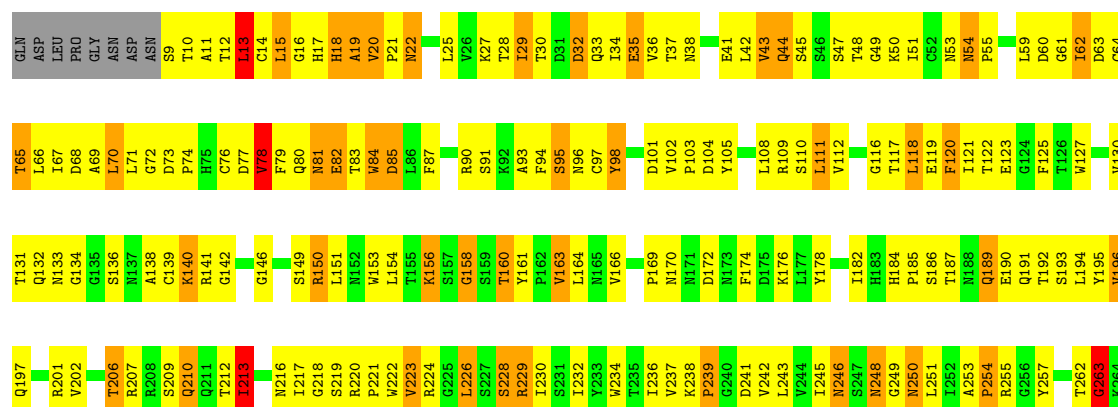
• Molecule 1: hemagglutinin HA1

Chain A: 



• Molecule 1: hemagglutinin HA1

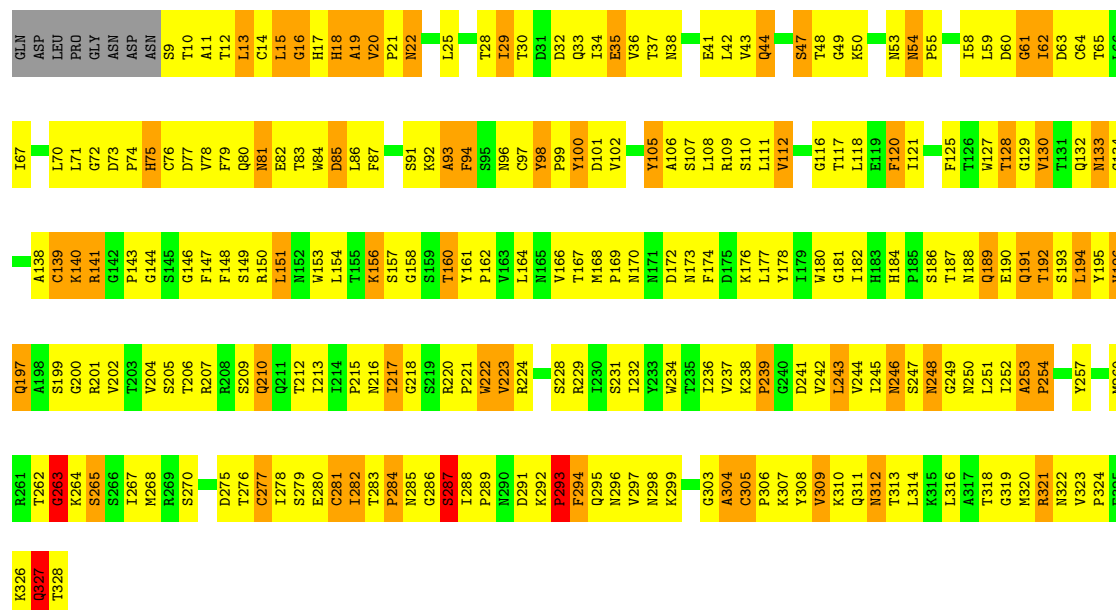
Chain C: 





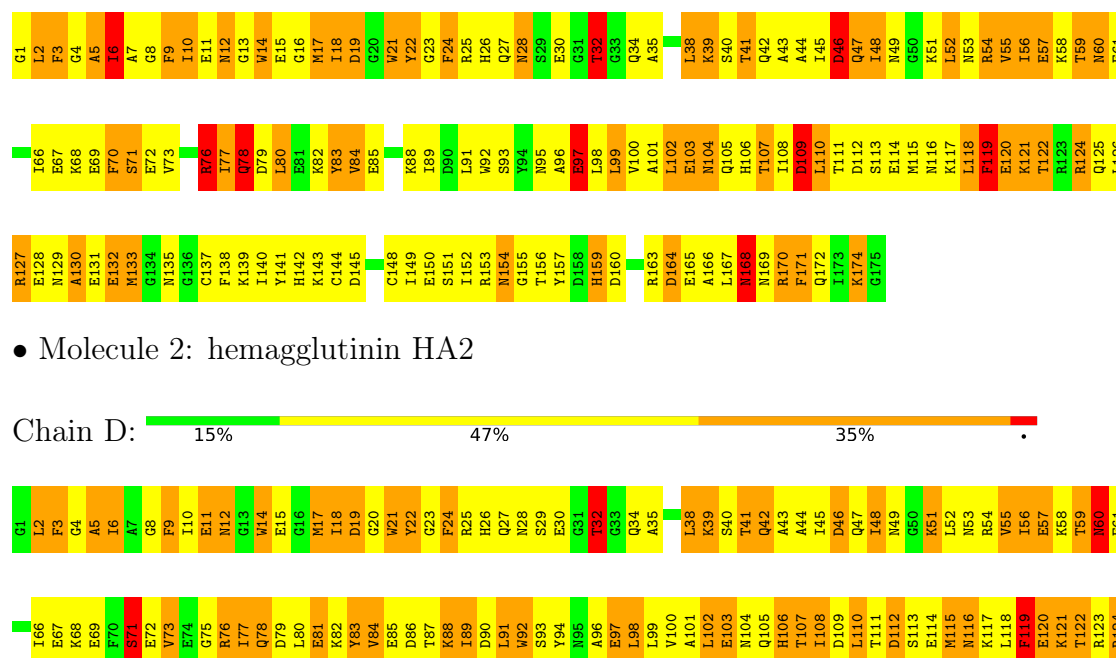
• Molecule 1: hemagglutinin HA1

Chain E: 23% 55% 18% ..



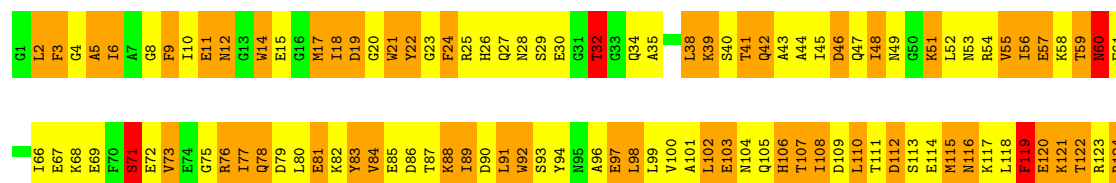
• Molecule 2: hemagglutinin HA2

Chain B: 16% 49% 30% 5%



• Molecule 2: hemagglutinin HA2

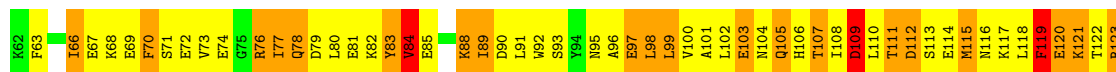
Chain D: 15% 47% 35%





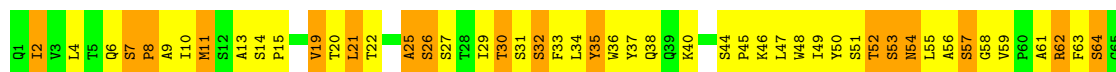
- Molecule 2: hemagglutinin HA2

Chain F: 14% 50% 33% .



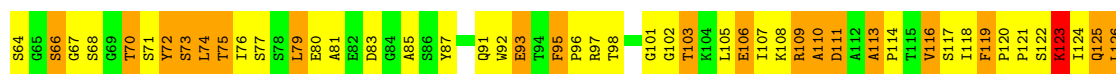
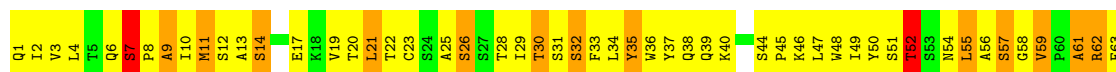
- Molecule 3: influenza virus infectivity neutralizing antibody (light chain)

Chain L: 19% 50% 27% .

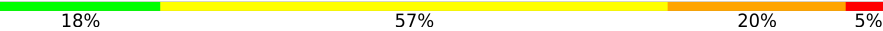


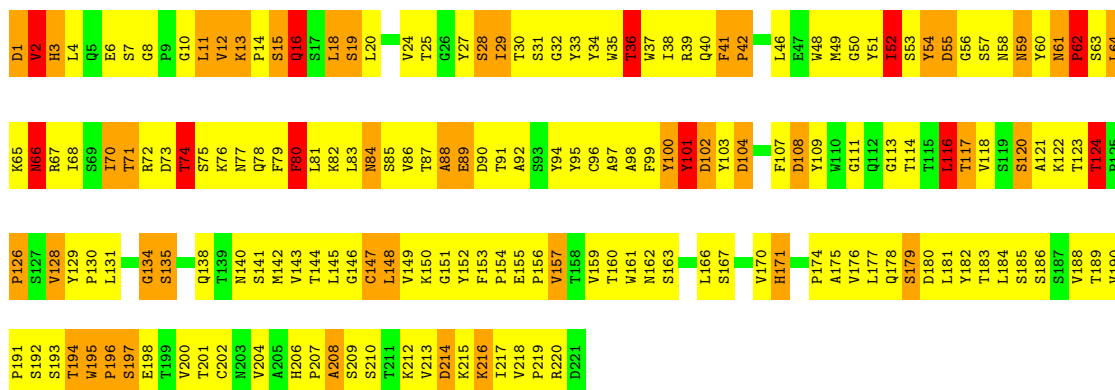
- Molecule 3: influenza virus infectivity neutralizing antibody (light chain)

Chain U: 17% 55% 25% .



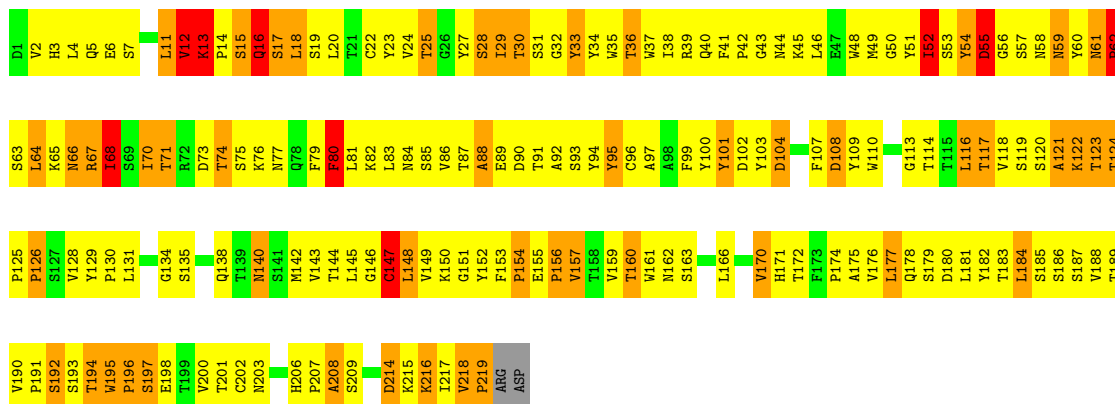
- Molecule 4: influenza virus infectivity neutralizing antibody (heavy chain)

Chain H:  18% 57% 20% 5%

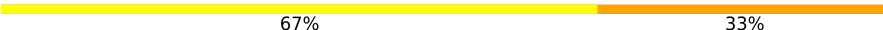


- Molecule 4: influenza virus infectivity neutralizing antibody (heavy chain)

Chain T:  17% 56% 23% 4%



- Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  67% 33%

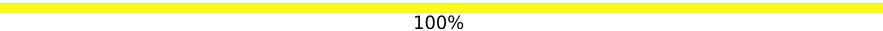


- Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 67%



- Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

MAG1
MAG2
MAG3

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	143.04Å 315.59Å 97.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.50	Depositor
% Data completeness (in resolution range)	91.8 (25.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.255 , 0.323	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18492	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.93	1/2528 (0.0%)	1.28	22/3443 (0.6%)
1	C	1.00	4/2528 (0.2%)	1.37	33/3443 (1.0%)
1	E	0.91	0/2528	1.33	31/3443 (0.9%)
2	B	0.92	3/1445 (0.2%)	1.26	20/1939 (1.0%)
2	D	0.91	0/1445	1.24	16/1939 (0.8%)
2	F	0.87	1/1445 (0.1%)	1.21	16/1939 (0.8%)
3	L	0.98	0/1679	1.44	34/2281 (1.5%)
3	U	0.95	2/1679 (0.1%)	1.42	24/2281 (1.1%)
4	H	1.04	5/1774 (0.3%)	1.41	25/2431 (1.0%)
4	T	0.94	1/1754 (0.1%)	1.37	22/2406 (0.9%)
All	All	0.95	17/18805 (0.1%)	1.34	243/25545 (1.0%)

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
3	L	0	1
3	U	0	1
4	H	0	1
4	T	0	2
All	All	0	5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	12	VAL	CA-CB	-9.47	1.48	1.55
2	B	77	ILE	CA-CB	-8.68	1.44	1.54
1	C	163	VAL	CA-CB	-8.23	1.43	1.54
2	F	77	ILE	CA-CB	-6.41	1.45	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	ASP	CB-CG	6.16	1.67	1.52
2	B	73	VAL	CA-CB	-6.15	1.46	1.54
1	C	206	THR	CA-CB	-5.91	1.46	1.53
4	H	2	VAL	CA-CB	5.66	1.62	1.54
4	H	2	VAL	N-CA	5.60	1.53	1.46
4	H	2	VAL	CA-C	5.59	1.59	1.52
3	U	28	THR	CA-CB	5.59	1.62	1.53
2	B	10	ILE	CA-CB	5.48	1.61	1.54
1	C	326	LYS	CA-C	5.44	1.58	1.52
3	U	109	ARG	CA-C	-5.38	1.45	1.52
1	C	78	VAL	CA-CB	-5.31	1.48	1.54
1	A	297	VAL	CA-CB	-5.11	1.47	1.54
4	T	68	ILE	CA-CB	5.03	1.61	1.53

All (243) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	111	ASP	N-CA-C	-12.39	84.40	110.80
2	B	99	LEU	N-CA-C	-11.12	97.76	111.11
2	D	2	LEU	N-CA-C	-10.28	97.24	112.04
2	B	119	PHE	N-CA-C	-10.00	100.38	111.28
2	D	119	PHE	N-CA-C	-9.97	100.40	111.07
4	H	70	ILE	N-CA-C	9.85	123.87	108.89
3	U	111	ASP	N-CA-C	-9.65	90.24	110.80
1	C	85	ASP	N-CA-C	-9.51	100.54	113.18
3	L	7	SER	N-CA-C	9.29	130.34	109.81
2	F	99	LEU	N-CA-C	-9.26	99.89	111.75
4	H	124	THR	CA-C-N	9.20	129.86	120.38
4	H	124	THR	C-N-CA	9.20	129.86	120.38
3	L	119	PHE	CA-C-N	9.09	126.21	119.66
3	L	119	PHE	C-N-CA	9.09	126.21	119.66
3	U	66	SER	N-CA-C	8.85	120.33	108.38
3	U	204	SER	CA-C-N	8.48	130.44	119.84
3	U	204	SER	C-N-CA	8.48	130.44	119.84
4	T	88	ALA	N-CA-C	-8.44	102.77	113.23
2	D	122	THR	N-CA-C	-8.36	102.16	111.28
3	L	138	ASN	N-CA-C	8.34	122.86	110.52
4	H	80	PHE	N-CA-C	8.32	121.67	109.69
3	U	95	PHE	N-CA-C	8.30	128.15	109.81
1	E	120	PHE	N-CA-C	8.23	124.24	107.69
2	F	119	PHE	N-CA-C	-8.03	102.48	111.71
3	U	113	ALA	N-CA-C	8.02	119.36	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	113	ALA	N-CA-C	7.88	119.20	110.13
1	C	305	CYS	N-CA-C	7.87	117.38	108.25
4	T	70	ILE	N-CA-C	7.84	121.22	108.99
4	T	54	TYR	N-CA-C	-7.82	102.84	112.38
4	T	68	ILE	N-CA-C	-7.81	98.39	108.93
2	B	107	THR	N-CA-C	-7.77	102.81	111.28
2	F	2	LEU	N-CA-C	-7.75	100.88	112.04
2	F	107	THR	N-CA-C	-7.72	102.95	111.36
4	T	122	LYS	N-CA-C	7.65	122.49	110.17
1	E	168	MET	CA-C-N	7.60	127.55	120.03
1	E	168	MET	C-N-CA	7.60	127.55	120.03
2	D	107	THR	N-CA-C	-7.54	103.15	111.36
4	H	88	ALA	N-CA-C	-7.51	103.91	113.23
2	B	2	LEU	N-CA-C	-7.50	102.02	112.45
3	U	200	LYS	N-CA-C	-7.44	103.47	112.54
4	T	64	LEU	CA-CB-CG	-7.41	90.37	116.30
4	H	36	THR	N-CA-C	7.39	121.12	109.81
2	B	46	ASP	N-CA-C	-7.34	103.21	111.14
1	E	281	CYS	N-CA-C	7.32	120.44	108.52
4	H	54	TYR	N-CA-C	-7.29	103.32	111.71
3	L	200	LYS	N-CA-C	-7.29	103.65	112.54
3	L	123	LYS	N-CA-C	-7.28	103.34	111.71
3	U	70	THR	N-CA-C	-7.23	104.47	112.72
1	A	120	PHE	N-CA-C	7.20	120.62	108.02
4	H	12	VAL	CB-CA-C	-7.17	105.00	111.74
4	T	80	PHE	N-CA-C	7.13	119.30	109.18
3	L	95	PHE	N-CA-C	7.10	125.50	109.81
3	U	113	ALA	CA-C-N	7.09	127.02	120.21
3	U	113	ALA	C-N-CA	7.09	127.02	120.21
4	H	64	LEU	CA-C-N	7.08	129.77	120.28
4	H	64	LEU	C-N-CA	7.08	129.77	120.28
3	L	199	HIS	N-CA-C	7.07	120.15	109.41
3	U	7	SER	N-CA-C	7.02	125.33	109.81
2	F	70	PHE	N-CA-C	7.01	120.60	108.76
1	A	305	CYS	N-CA-C	6.94	116.30	108.25
3	L	20	THR	N-CA-C	6.91	119.75	107.80
1	A	205	SER	N-CA-C	6.90	117.38	108.34
4	T	12	VAL	CB-CA-C	-6.86	105.30	111.74
2	B	71	SER	N-CA-C	6.81	121.34	112.89
1	E	223	VAL	N-CA-C	6.81	117.45	107.37
1	A	284	PRO	N-CA-C	-6.81	103.94	113.81
2	B	122	THR	N-CA-C	-6.74	103.86	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	123	LYS	N-CA-C	-6.73	104.01	111.82
3	U	199	HIS	N-CA-C	6.70	119.59	109.41
1	E	194	LEU	N-CA-C	6.69	121.75	112.45
1	E	139	CYS	N-CA-C	-6.67	100.41	109.54
1	A	281	CYS	N-CA-C	6.62	119.20	108.41
1	C	323	VAL	CA-C-N	6.59	126.55	119.76
1	C	323	VAL	C-N-CA	6.59	126.55	119.76
2	D	71	SER	N-CA-C	6.54	119.73	111.69
1	E	32	ASP	N-CA-C	-6.50	105.22	113.02
1	A	32	ASP	N-CA-C	-6.48	104.95	112.92
1	C	228	SER	N-CA-C	-6.48	100.35	109.69
3	L	187	TYR	N-CA-C	-6.48	103.44	112.45
3	L	152	ASP	N-CA-C	-6.46	105.42	113.55
3	U	188	GLU	N-CA-C	-6.45	104.43	113.20
2	D	59	THR	N-CA-C	6.44	124.52	110.80
2	F	159	HIS	N-CA-C	-6.42	105.43	113.20
4	H	108	ASP	N-CA-C	6.40	119.60	109.81
2	B	59	THR	N-CA-C	6.38	124.39	110.80
3	L	64	SER	N-CA-C	-6.38	100.47	110.36
3	L	204	SER	CA-C-N	6.37	127.81	119.84
3	L	204	SER	C-N-CA	6.37	127.81	119.84
2	F	59	THR	N-CA-C	6.35	124.33	110.80
1	E	61	GLY	N-CA-C	-6.34	106.48	114.16
1	C	69	ALA	N-CA-C	-6.34	104.28	111.07
1	C	160	THR	N-CA-C	6.30	117.80	108.60
3	L	188	GLU	N-CA-C	-6.27	104.68	113.20
1	C	194	LEU	N-CA-C	6.26	121.05	112.04
1	C	82	GLU	N-CA-C	6.26	118.40	110.33
1	A	282	ILE	N-CA-C	6.24	116.90	108.17
3	U	20	THR	N-CA-C	6.22	118.43	107.61
1	C	32	ASP	N-CA-C	-6.17	105.79	113.38
3	L	70	THR	N-CA-C	-6.17	105.69	112.72
1	A	160	THR	N-CA-C	6.16	117.59	108.60
3	L	115	THR	N-CA-C	-6.12	97.12	108.02
3	L	25	ALA	N-CA-C	6.12	118.13	107.49
1	C	151	LEU	N-CA-C	6.10	119.42	109.24
1	E	112	VAL	N-CA-C	-6.09	103.48	111.09
2	D	110	LEU	N-CA-C	-6.08	106.40	113.88
4	T	160	THR	N-CA-C	6.06	116.44	108.07
1	A	229	ARG	N-CA-C	6.06	116.56	108.38
2	B	60	ASN	N-CA-C	6.05	123.69	110.80
1	E	151	LEU	N-CA-C	6.04	119.05	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	84	VAL	N-CA-C	-6.01	105.27	110.74
2	D	108	ILE	N-CA-C	6.00	116.12	110.30
4	T	123	THR	N-CA-C	-5.99	101.31	110.30
4	T	219	PRO	N-CA-C	5.99	127.07	112.10
1	A	288	ILE	N-CA-C	5.99	115.78	109.01
3	L	57	SER	N-CA-C	5.98	123.54	110.80
1	C	111	LEU	N-CA-C	-5.97	105.66	113.12
1	C	223	VAL	N-CA-C	5.97	116.77	107.28
1	C	16	GLY	N-CA-C	5.95	120.40	111.42
2	D	159	HIS	N-CA-C	-5.93	105.80	113.16
1	E	160	THR	N-CA-C	5.91	117.84	108.79
3	U	116	VAL	N-CA-C	5.90	118.25	109.17
3	U	119	PHE	N-CA-C	5.89	119.19	109.58
1	C	131	THR	N-CA-C	5.88	117.88	108.41
1	C	105	TYR	N-CA-C	-5.88	104.79	111.14
1	A	151	LEU	N-CA-C	5.86	118.96	109.40
4	H	41	PHE	N-CA-C	5.86	118.62	110.07
1	E	238	LYS	CA-C-N	-5.83	113.75	119.76
1	E	238	LYS	C-N-CA	-5.83	113.75	119.76
4	T	68	ILE	N-CA-CB	5.82	117.18	110.49
2	D	32	THR	N-CA-C	5.79	115.89	108.24
1	C	281	CYS	N-CA-C	5.79	117.96	108.52
3	U	73	SER	N-CA-C	5.79	116.19	108.38
1	C	213	ILE	N-CA-C	5.79	116.81	108.48
4	H	10	GLY	N-CA-C	-5.79	106.63	115.66
1	C	223	VAL	CB-CA-C	-5.79	103.47	110.99
2	D	22	TYR	N-CA-C	5.79	115.74	108.45
1	C	318	THR	N-CA-C	-5.78	106.36	113.41
3	L	53	SER	N-CA-C	5.77	123.02	113.50
2	F	71	SER	N-CA-C	5.77	117.37	111.14
4	T	30	THR	N-CA-C	-5.76	104.79	113.89
4	T	11	LEU	N-CA-C	5.75	116.88	108.14
1	A	190	GLU	N-CA-C	-5.75	105.53	112.54
2	B	159	HIS	N-CA-C	-5.75	106.25	113.20
3	U	139	ASN	N-CA-C	5.74	123.02	110.80
4	T	177	LEU	N-CA-C	5.72	118.96	109.46
1	C	226	LEU	N-CA-C	5.68	118.08	110.35
2	F	22	TYR	N-CA-C	5.68	115.61	108.45
2	B	70	PHE	N-CA-C	5.68	118.74	108.69
1	E	284	PRO	N-CA-C	-5.68	105.58	113.81
1	A	194	LEU	N-CA-C	5.65	120.31	112.45
2	B	42	GLN	N-CA-C	-5.65	105.21	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	95	ASN	N-CA-C	-5.64	105.21	111.36
2	D	60	ASN	N-CA-C	5.64	122.82	110.80
1	C	13	LEU	N-CA-C	5.64	117.60	108.41
3	U	106	GLU	N-CA-C	-5.62	102.20	110.52
4	H	89	GLU	N-CA-C	-5.61	105.17	111.28
1	E	128	THR	N-CA-C	5.59	117.81	109.59
1	C	326	LYS	N-CA-C	5.59	117.34	107.61
3	L	212	ARG	N-CA-C	-5.55	101.02	108.19
1	C	213	ILE	CB-CA-C	-5.54	102.36	110.62
1	C	120	PHE	N-CA-C	5.54	117.55	108.52
4	T	64	LEU	CA-C-N	5.53	128.01	120.54
4	T	64	LEU	C-N-CA	5.53	128.01	120.54
4	T	128	VAL	N-CA-C	5.53	115.82	107.80
2	B	110	LEU	N-CA-C	-5.50	107.11	113.88
1	E	323	VAL	CA-C-N	5.50	125.42	119.76
1	E	323	VAL	C-N-CA	5.50	125.42	119.76
2	B	22	TYR	N-CA-C	5.49	115.49	108.24
1	E	327	GLN	N-CA-C	5.48	122.48	110.80
2	D	11	GLU	N-CA-C	5.48	122.47	110.80
4	H	64	LEU	CA-CB-CG	-5.48	97.13	116.30
3	L	95	PHE	CA-C-N	-5.47	113.00	119.84
3	L	95	PHE	C-N-CA	-5.47	113.00	119.84
2	B	80	LEU	N-CA-C	5.47	117.69	111.02
3	U	189	ARG	N-CA-C	-5.46	106.29	113.12
1	E	47	SER	N-CA-C	5.46	117.99	109.52
1	A	232	ILE	N-CA-C	5.46	116.10	108.89
2	F	46	ASP	N-CA-C	-5.45	105.25	111.14
4	H	116	LEU	N-CA-C	-5.44	101.01	109.72
2	B	47	GLN	N-CA-C	5.43	117.01	111.14
3	L	119	PHE	N-CA-C	5.43	118.98	109.48
1	E	253	ALA	CA-C-N	5.41	126.61	119.84
1	E	253	ALA	C-N-CA	5.41	126.61	119.84
4	H	100	TYR	N-CA-C	5.41	119.83	111.56
1	E	282	ILE	N-CA-C	5.38	115.70	108.17
4	T	108	ASP	N-CA-C	5.38	118.04	109.81
1	E	35	GLU	N-CA-C	5.36	117.94	108.24
2	D	51	LYS	N-CA-C	-5.32	105.59	111.71
2	D	73	VAL	N-CA-C	5.31	115.24	108.12
1	E	105	TYR	N-CA-C	-5.31	105.49	111.28
4	H	101	TYR	N-CA-C	5.31	122.11	110.80
2	D	42	GLN	N-CA-C	-5.30	105.41	111.14
3	L	110	ALA	CA-C-N	5.29	131.65	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	110	ALA	C-N-CA	5.29	131.65	121.54
1	E	75	HIS	N-CA-C	5.27	119.40	112.92
3	L	193	TYR	N-CA-C	5.26	117.23	107.60
2	F	60	ASN	N-CA-C	5.26	122.00	110.80
1	C	269	ARG	N-CA-C	-5.25	100.75	109.46
1	C	229	ARG	N-CA-C	5.23	114.74	107.73
1	A	224	ARG	N-CA-C	-5.23	104.20	111.52
1	A	142	GLY	CA-C-N	5.22	126.36	119.84
1	A	142	GLY	C-N-CA	5.22	126.36	119.84
2	F	66	ILE	N-CA-C	-5.22	102.20	109.45
1	E	16	GLY	N-CA-C	5.21	117.87	110.74
1	C	142	GLY	CA-C-N	5.21	126.35	119.84
1	C	142	GLY	C-N-CA	5.21	126.35	119.84
1	A	223	VAL	N-CA-C	5.20	115.54	107.28
4	H	171	HIS	CA-C-N	-5.19	115.74	123.11
4	H	171	HIS	C-N-CA	-5.19	115.74	123.11
1	E	263	GLY	N-CA-C	5.19	125.47	113.18
4	H	111	GLY	N-CA-C	5.18	118.62	110.91
1	A	263	GLY	N-CA-C	5.17	125.44	113.18
1	E	305	CYS	N-CA-C	5.17	114.78	108.11
1	A	65	THR	N-CA-C	-5.17	101.85	110.17
4	T	13	LYS	CA-C-N	5.16	126.30	119.84
4	T	13	LYS	C-N-CA	5.16	126.30	119.84
2	B	118	LEU	N-CA-C	-5.16	106.11	112.72
1	C	43	VAL	N-CA-C	5.15	114.19	106.42
3	L	19	VAL	N-CA-C	5.15	116.22	109.58
1	A	61	GLY	N-CA-C	-5.13	107.95	114.16
4	H	8	GLY	CA-C-N	5.13	125.41	119.92
4	H	8	GLY	C-N-CA	5.13	125.41	119.92
1	C	263	GLY	N-CA-C	5.13	125.33	113.18
3	U	61	ALA	N-CA-C	5.13	117.26	111.11
3	L	150	LYS	N-CA-C	5.12	119.15	112.13
1	E	294	PHE	N-CA-C	5.12	117.41	108.76
3	L	116	VAL	N-CA-C	5.12	117.05	109.17
2	F	111	THR	N-CA-C	-5.11	106.73	113.12
3	L	195	CYS	N-CA-C	-5.11	101.08	109.40
1	C	43	VAL	CB-CA-C	-5.11	106.07	111.23
1	C	35	GLU	N-CA-C	5.10	117.48	108.24
2	B	104	ASN	N-CA-C	5.08	116.63	111.14
4	H	176	VAL	CB-CA-C	-5.08	103.94	110.84
4	T	187	SER	N-CA-C	5.07	119.03	108.53
3	L	106	GLU	N-CA-C	-5.07	103.24	110.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	32	THR	N-CA-C	5.06	115.72	108.74
4	H	19	SER	N-CA-C	5.05	118.33	107.67
3	U	150	LYS	N-CA-C	5.04	119.06	111.96
2	F	14	TRP	N-CA-C	5.03	121.52	110.80
1	E	93	ALA	N-CA-C	5.01	117.70	110.28
2	F	11	GLU	N-CA-C	5.01	121.48	110.80
3	U	138	ASN	N-CA-C	5.01	116.99	110.53
1	A	218	GLY	N-CA-C	5.01	117.35	110.69

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	H	101	TYR	Sidechain
3	L	141	TYR	Sidechain
4	T	33	TYR	Sidechain
4	T	95	TYR	Sidechain
3	U	72	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	2472	0	2424	350	0
1	C	2472	0	2424	347	0
1	E	2472	0	2424	346	0
2	B	1421	0	1346	270	0
2	D	1421	0	1346	280	0
2	F	1421	0	1346	288	0
3	L	1638	0	1578	240	0
3	U	1638	0	1578	265	0
4	H	1720	0	1639	273	0
4	T	1700	0	1622	287	0
5	G	39	0	34	3	0
5	I	39	0	34	4	0
5	J	39	0	34	0	0
All	All	18492	0	17829	2649	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 73.

All (2649) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:PRO:HA	1:A:141:ARG:HH12	1.11	1.16
3:U:199:HIS:HB3	3:U:201:THR:HG22	1.28	1.11
3:U:134:VAL:HG22	3:U:179:THR:HG23	1.30	1.11
1:C:77:ASP:O	1:C:80:GLN:HG2	1.47	1.10
1:C:96:ASN:HD21	1:C:140:LYS:HE2	1.10	1.10
1:E:321:ARG:HG2	1:E:322:ASN:H	1.14	1.10
1:E:28:THR:HG22	2:F:104:ASN:HB3	1.23	1.09
2:B:25:ARG:HG2	2:B:34:GLN:HG2	1.31	1.09
2:D:3:PHE:HD2	2:D:113:SER:HA	1.14	1.09
1:A:54:ASN:HB3	1:A:278:ILE:HD13	1.35	1.08
2:B:3:PHE:HD2	2:B:113:SER:HA	1.10	1.08
4:T:18:LEU:HD12	4:T:19:SER:N	1.68	1.08
2:B:28:ASN:HD22	2:B:145:ASP:HA	1.12	1.08
1:E:14:CYS:HB2	2:F:25:ARG:HB2	1.32	1.06
1:A:28:THR:HG22	2:B:104:ASN:HB3	1.37	1.06
1:E:29:ILE:HD11	2:F:102:LEU:HD23	1.31	1.05
3:U:137:LEU:HD23	3:U:145:ILE:HD13	1.38	1.05
4:T:2:VAL:HB	4:T:109:TYR:CE2	1.93	1.04
1:A:186:SER:HA	1:A:218:GLY:O	1.56	1.03
1:E:102:VAL:HG22	1:E:232:ILE:HB	1.41	1.03
2:F:25:ARG:HG2	2:F:34:GLN:HG2	1.40	1.03
2:B:167:LEU:O	2:B:170:ARG:HB2	1.60	1.02
2:F:3:PHE:HD2	2:F:113:SER:HA	1.23	1.02
3:L:199:HIS:HB3	3:L:201:THR:HG22	1.42	1.02
1:C:14:CYS:HB2	2:D:25:ARG:HB2	1.40	1.02
4:T:2:VAL:HB	4:T:109:TYR:HE2	1.19	1.01
1:C:29:ILE:HD11	2:D:102:LEU:HD23	1.41	1.01
1:E:96:ASN:HD21	1:E:140:LYS:HE2	1.21	1.01
3:L:67:GLY:HA3	3:L:72:TYR:CD2	1.94	1.01
2:B:130:ALA:HB1	2:B:139:LYS:O	1.61	1.01
2:D:28:ASN:HD22	2:D:145:ASP:HA	1.19	1.01
2:F:28:ASN:HD22	2:F:145:ASP:HA	1.19	1.00
2:D:25:ARG:HG2	2:D:34:GLN:HG2	1.39	1.00
2:B:3:PHE:CD2	2:B:113:SER:HA	1.96	1.00
3:L:201:THR:HG23	3:L:202:SER:H	1.23	1.00
1:C:286:GLY:O	1:C:287:SER:HB2	1.62	1.00
3:L:199:HIS:CD2	3:L:200:LYS:H	1.80	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:151:ILE:HG22	3:L:152:ASP:N	1.76	0.99
1:A:216:ASN:HB3	1:C:212:THR:HG21	1.43	0.99
4:T:126:PRO:HB3	4:T:152:TYR:HB3	1.45	0.99
3:L:121:PRO:HB2	3:L:126:LEU:HD21	1.45	0.98
3:U:164:TRP:HE3	3:U:164:TRP:H	1.00	0.98
1:A:281:CYS:HB2	1:A:304:ALA:O	1.62	0.97
4:H:18:LEU:HD12	4:H:19:SER:N	1.77	0.97
1:A:22:ASN:HD22	1:A:22:ASN:H	1.10	0.97
1:A:18:HIS:HA	2:B:14:TRP:HB2	1.44	0.97
1:C:22:ASN:HD22	1:C:22:ASN:H	1.09	0.97
2:D:132:GLU:HA	2:D:138:PHE:HA	1.47	0.97
2:F:167:LEU:O	2:F:170:ARG:HB2	1.66	0.96
2:F:145:ASP:H	2:F:148:CYS:HB3	1.31	0.95
1:A:14:CYS:HB2	2:B:25:ARG:HB2	1.47	0.94
4:T:218:VAL:HG12	4:T:219:PRO:HD2	1.46	0.94
1:A:74:PRO:HA	1:A:141:ARG:NH1	1.82	0.94
1:A:77:ASP:O	1:A:80:GLN:HG2	1.67	0.94
3:U:14:SER:HA	3:U:108:LYS:HB2	1.49	0.94
1:A:111:LEU:HD12	1:A:112:VAL:N	1.82	0.94
2:B:132:GLU:HA	2:B:138:PHE:HA	1.49	0.94
1:C:18:HIS:HA	2:D:14:TRP:HB2	1.50	0.94
1:C:170:ASN:HB2	1:C:176:LYS:HE2	1.50	0.94
2:F:121:LYS:HZ1	2:F:122:THR:CG2	1.80	0.94
2:F:127:ARG:HB3	2:F:127:ARG:HH11	1.33	0.94
3:L:141:TYR:HB3	3:L:142:PRO:HD3	1.49	0.94
3:L:164:TRP:HE3	3:L:164:TRP:H	0.97	0.93
1:C:13:LEU:HD11	2:D:24:PHE:HB3	1.48	0.93
1:C:28:THR:HG22	2:D:104:ASN:HB3	1.48	0.93
4:H:63:SER:O	4:H:64:LEU:HG	1.68	0.93
1:A:54:ASN:HD22	1:A:55:PRO:HA	1.31	0.93
1:A:29:ILE:HD11	2:B:102:LEU:HD23	1.51	0.93
1:E:108:LEU:O	1:E:112:VAL:HG23	1.69	0.93
3:L:95:PHE:CZ	4:H:60:TYR:HB3	2.04	0.93
3:U:199:HIS:CD2	3:U:200:LYS:H	1.85	0.92
2:B:145:ASP:H	2:B:148:CYS:HB3	1.33	0.92
2:F:55:VAL:HG12	2:F:56:ILE:N	1.82	0.92
1:A:170:ASN:HB2	1:A:176:LYS:HE2	1.51	0.92
2:D:3:PHE:CD2	2:D:113:SER:HA	2.03	0.92
4:H:126:PRO:HB3	4:H:152:TYR:HB3	1.48	0.92
1:A:321:ARG:HG2	1:A:322:ASN:H	1.33	0.92
4:H:63:SER:C	4:H:64:LEU:HG	1.95	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ASP:HB3	1:A:174:PHE:CE2	2.05	0.91
1:C:84:TRP:CE2	1:C:116:GLY:HA2	2.05	0.91
4:H:52:ILE:HG23	4:H:52:ILE:O	1.67	0.91
4:H:191:PRO:HB2	4:H:194:THR:HB	1.53	0.91
3:U:137:LEU:HD23	3:U:145:ILE:CD1	2.01	0.91
1:A:9:SER:O	2:B:143:LYS:HE3	1.71	0.91
1:C:283:THR:HG22	1:C:287:SER:H	1.35	0.91
2:F:126:LEU:HD12	2:F:126:LEU:O	1.71	0.91
2:F:125:GLN:HE22	2:F:155:GLY:HA2	1.34	0.91
1:E:13:LEU:HD11	2:F:24:PHE:HB3	1.54	0.90
4:H:151:GLY:C	4:H:181:LEU:HD12	1.97	0.90
2:D:167:LEU:O	2:D:170:ARG:HB2	1.72	0.90
1:A:283:THR:HG23	1:A:286:GLY:N	1.86	0.90
1:A:283:THR:HG23	1:A:286:GLY:H	1.35	0.90
1:E:72:GLY:HA3	1:E:149:SER:OG	1.70	0.90
1:C:186:SER:HA	1:C:218:GLY:O	1.72	0.90
4:H:195:TRP:HB3	4:H:196:PRO:HD3	1.53	0.89
4:T:24:VAL:HG13	4:T:77:ASN:OD1	1.72	0.89
1:A:74:PRO:HG3	1:A:139:CYS:SG	2.11	0.89
1:E:18:HIS:HA	2:F:14:TRP:HB2	1.54	0.89
3:L:201:THR:HG23	3:L:202:SER:N	1.83	0.89
2:D:127:ARG:HB3	2:D:127:ARG:HH11	1.36	0.89
1:A:84:TRP:CZ2	1:A:116:GLY:HA2	2.07	0.89
4:T:18:LEU:HD12	4:T:19:SER:H	1.31	0.88
2:B:127:ARG:HB3	2:B:127:ARG:HH11	1.37	0.88
2:F:127:ARG:HB3	2:F:127:ARG:NH1	1.89	0.88
2:D:48:ILE:HD11	2:D:107:THR:HG23	1.54	0.88
1:C:96:ASN:ND2	1:C:140:LYS:HE2	1.88	0.88
2:F:3:PHE:CD2	2:F:113:SER:HA	2.08	0.87
3:L:151:ILE:O	3:L:192:SER:HB2	1.72	0.87
1:C:172:ASP:HB3	1:C:174:PHE:CE2	2.09	0.87
2:F:121:LYS:HZ1	2:F:122:THR:HG22	1.37	0.87
1:E:74:PRO:HD3	1:E:97:CYS:HB2	1.56	0.87
3:L:134:VAL:HG22	3:L:179:THR:HG23	1.57	0.87
1:A:17:HIS:HD2	2:B:6:ILE:HG23	1.40	0.87
3:U:121:PRO:HB2	3:U:126:LEU:HD21	1.55	0.87
4:H:34:TYR:CD2	4:H:53:SER:HB3	2.09	0.87
3:U:97:ARG:HB2	4:T:48:TRP:CD2	2.10	0.87
4:H:1:ASP:O	4:H:2:VAL:HG22	1.73	0.86
3:L:201:THR:CG2	3:L:202:SER:H	1.88	0.86
4:H:142:MET:HA	4:H:192:SER:HA	1.58	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:ARG:HB3	2:B:127:ARG:NH1	1.89	0.86
4:H:32:GLY:O	4:H:33:TYR:HB2	1.75	0.86
2:B:28:ASN:HD22	2:B:145:ASP:CA	1.88	0.86
4:H:18:LEU:HD12	4:H:19:SER:H	1.38	0.86
2:D:165:GLU:HA	2:D:168:ASN:HD21	1.39	0.86
3:L:48:TRP:O	3:L:49:ILE:HG13	1.75	0.86
3:L:151:ILE:HG22	3:L:152:ASP:H	1.37	0.86
1:E:307:LYS:HE2	2:F:60:ASN:ND2	1.90	0.85
1:E:321:ARG:HG2	1:E:322:ASN:N	1.90	0.85
2:F:165:GLU:HA	2:F:168:ASN:HD21	1.37	0.85
4:H:56:GLY:O	4:H:58:ASN:N	2.09	0.85
4:H:131:LEU:HB2	4:H:146:GLY:HA3	1.59	0.85
2:F:132:GLU:HA	2:F:138:PHE:HA	1.56	0.85
3:L:40:LYS:HD3	3:L:85:ALA:HB2	1.59	0.85
4:T:206:HIS:CE1	4:T:208:ALA:HB3	2.11	0.85
1:C:108:LEU:HD13	1:C:234:TRP:CE3	2.12	0.85
3:U:47:LEU:HD12	3:U:48:TRP:H	1.40	0.85
1:C:64:CYS:HB2	1:C:79:PHE:CE1	2.11	0.84
1:C:283:THR:HG23	1:C:286:GLY:N	1.92	0.84
3:L:97:ARG:HB2	4:H:48:TRP:CD2	2.11	0.84
2:D:100:VAL:HG23	2:D:101:ALA:H	1.42	0.84
1:A:28:THR:HB	2:B:105:GLN:HB2	1.58	0.84
1:A:176:LYS:HD2	1:A:257:TYR:CD2	2.13	0.84
2:F:28:ASN:HD22	2:F:145:ASP:CA	1.91	0.84
1:A:309:VAL:HG12	2:B:93:SER:HA	1.60	0.84
4:T:151:GLY:C	4:T:181:LEU:HD12	2.03	0.84
1:A:74:PRO:HD3	1:A:97:CYS:HB2	1.59	0.83
1:C:283:THR:HG23	1:C:286:GLY:H	1.38	0.83
3:U:201:THR:HG23	3:U:202:SER:H	1.43	0.83
1:E:17:HIS:HD2	2:F:6:ILE:HG23	1.43	0.83
1:E:77:ASP:O	1:E:80:GLN:HG2	1.78	0.83
1:A:11:ALA:O	2:B:140:ILE:HB	1.78	0.83
1:A:207:ARG:HG2	1:E:223:VAL:HG22	1.60	0.83
1:A:13:LEU:HD11	2:B:24:PHE:HB3	1.58	0.83
1:C:98:TYR:H	1:C:139:CYS:HB2	1.44	0.83
2:F:165:GLU:HA	2:F:168:ASN:ND2	1.93	0.83
4:T:142:MET:HA	4:T:192:SER:HA	1.59	0.83
1:A:212:THR:HG21	1:E:216:ASN:HB3	1.59	0.83
1:C:81:ASN:ND2	1:C:120:PHE:H	1.76	0.83
1:A:17:HIS:N	2:B:115:MET:HE1	1.92	0.83
3:L:9:ALA:N	3:L:103:THR:HG23	1.92	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:ASN:HD21	1:C:120:PHE:H	1.27	0.83
1:C:74:PRO:HD3	1:C:97:CYS:HB2	1.61	0.82
4:T:190:VAL:HG21	4:T:195:TRP:HB2	1.60	0.82
2:D:80:LEU:HD21	2:F:80:LEU:HD21	1.60	0.82
1:E:98:TYR:H	1:E:139:CYS:HB2	1.44	0.82
1:E:170:ASN:ND2	1:E:239:PRO:HA	1.94	0.82
2:D:28:ASN:HD22	2:D:145:ASP:CA	1.92	0.82
1:E:73:ASP:OD1	1:E:74:PRO:HD2	1.79	0.82
1:C:84:TRP:CZ2	1:C:116:GLY:HA2	2.14	0.82
2:D:125:GLN:HE22	2:D:155:GLY:HA2	1.43	0.82
1:E:74:PRO:HA	1:E:141:ARG:HH12	1.44	0.82
2:B:100:VAL:HG23	2:B:101:ALA:H	1.42	0.82
3:U:194:THR:HA	3:U:209:SER:HB2	1.59	0.82
3:L:164:TRP:N	3:L:164:TRP:CE3	2.47	0.82
1:A:22:ASN:HD22	1:A:22:ASN:N	1.76	0.81
4:T:63:SER:O	4:T:64:LEU:HG	1.80	0.81
2:D:171:PHE:HD2	2:F:167:LEU:HB3	1.43	0.81
4:H:162:ASN:ND2	4:H:201:THR:H	1.78	0.81
1:A:54:ASN:ND2	1:A:55:PRO:HA	1.94	0.81
2:D:131:GLU:O	2:D:139:LYS:HB3	1.78	0.81
3:L:9:ALA:H	3:L:103:THR:HG23	1.43	0.81
3:L:148:LYS:HD2	3:L:155:GLU:O	1.81	0.81
4:T:28:SER:O	4:T:30:THR:N	2.13	0.81
4:T:53:SER:OG	4:T:55:ASP:HB2	1.80	0.81
3:L:164:TRP:HE3	3:L:164:TRP:N	1.78	0.81
2:D:149:ILE:C	2:D:151:SER:H	1.86	0.81
1:E:108:LEU:HD13	1:E:234:TRP:CE3	2.16	0.81
4:H:122:LYS:HD3	4:H:123:THR:O	1.80	0.81
3:U:151:ILE:HG12	3:U:193:TYR:CD2	2.15	0.81
1:C:307:LYS:HE2	2:D:60:ASN:ND2	1.96	0.81
4:H:28:SER:C	4:H:30:THR:H	1.88	0.81
4:T:65:LYS:O	4:T:67:ARG:N	2.14	0.81
2:F:130:ALA:HB1	2:F:139:LYS:O	1.80	0.80
2:F:166:ALA:N	2:F:168:ASN:HD21	1.80	0.80
3:U:95:PHE:CE2	4:T:60:TYR:HB3	2.16	0.80
4:H:29:ILE:HG22	4:H:35:TRP:CE2	2.17	0.80
4:T:61:ASN:HB3	4:T:62:PRO:HD2	1.62	0.80
2:B:145:ASP:O	2:B:149:ILE:HG12	1.80	0.80
1:C:22:ASN:HD22	1:C:22:ASN:N	1.79	0.80
4:T:63:SER:C	4:T:64:LEU:HG	2.05	0.80
1:A:220:ARG:HH21	1:C:210:GLN:NE2	1.79	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:131:LEU:HB2	4:T:146:GLY:HA3	1.64	0.80
4:H:188:VAL:HG22	4:H:189:THR:N	1.97	0.80
1:A:237:VAL:HG12	1:A:241:ASP:HB3	1.64	0.80
3:U:141:TYR:HB3	3:U:142:PRO:HD3	1.62	0.80
4:T:86:VAL:HG23	4:T:90:ASP:HB2	1.63	0.80
1:C:42:LEU:O	1:C:293:PRO:HD2	1.80	0.79
4:T:81:LEU:HD12	4:T:82:LYS:H	1.46	0.79
4:T:218:VAL:CG1	4:T:219:PRO:HD2	2.11	0.79
3:U:118:ILE:HD13	3:U:195:CYS:HB2	1.63	0.79
1:A:72:GLY:HA3	1:A:149:SER:OG	1.82	0.79
2:F:121:LYS:HB3	2:F:121:LYS:HZ3	1.45	0.79
3:L:95:PHE:HZ	4:H:60:TYR:HB3	1.46	0.79
3:U:29:ILE:HD11	3:U:34:LEU:HB2	1.63	0.79
3:U:164:TRP:N	3:U:164:TRP:CE3	2.49	0.79
1:A:98:TYR:H	1:A:139:CYS:HB2	1.48	0.79
3:L:19:VAL:HG21	3:L:79:LEU:HD23	1.64	0.79
4:T:52:ILE:HG23	4:T:52:ILE:O	1.82	0.79
1:A:22:ASN:H	1:A:22:ASN:ND2	1.76	0.79
4:T:2:VAL:CG2	4:T:27:TYR:HB2	2.12	0.79
1:A:96:ASN:HD21	1:A:140:LYS:HE2	1.48	0.79
1:C:22:ASN:H	1:C:22:ASN:ND2	1.77	0.79
1:C:246:ASN:C	1:C:246:ASN:HD22	1.90	0.79
1:E:9:SER:O	2:F:143:LYS:HE3	1.82	0.79
4:H:24:VAL:HG13	4:H:77:ASN:OD1	1.83	0.79
2:B:121:LYS:HZ1	2:B:122:THR:HG22	1.48	0.79
2:F:110:LEU:O	2:F:110:LEU:HD13	1.82	0.79
1:E:11:ALA:O	2:F:140:ILE:HB	1.83	0.79
4:T:64:LEU:HD23	4:T:66:ASN:HD21	1.48	0.79
4:T:33:TYR:HD2	4:T:99:PHE:O	1.65	0.78
1:C:182:ILE:O	1:C:230:ILE:HG23	1.83	0.78
2:D:145:ASP:H	2:D:148:CYS:HB3	1.47	0.78
1:E:283:THR:HG23	1:E:286:GLY:N	1.96	0.78
3:U:14:SER:OG	3:U:108:LYS:HD2	1.84	0.78
2:B:167:LEU:HB3	2:F:171:PHE:HD2	1.46	0.78
3:L:48:TRP:CE2	3:L:59:VAL:HG13	2.19	0.78
1:E:186:SER:HA	1:E:218:GLY:O	1.84	0.78
4:H:28:SER:O	4:H:30:THR:N	2.17	0.78
4:T:195:TRP:HB3	4:T:196:PRO:HD3	1.64	0.78
3:U:151:ILE:HG12	3:U:193:TYR:CE2	2.19	0.78
1:A:147:PHE:CE2	1:A:153:TRP:HB2	2.18	0.78
2:B:125:GLN:HE22	2:B:155:GLY:HA2	1.49	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:MET:HA	2:D:111:THR:HG21	1.65	0.78
2:D:6:ILE:HG13	2:D:112:ASP:HA	1.66	0.78
3:U:116:VAL:HG12	3:U:117:SER:N	1.99	0.78
2:D:165:GLU:HA	2:D:168:ASN:ND2	1.98	0.77
3:U:201:THR:HG23	3:U:202:SER:N	1.98	0.77
1:C:320:MET:CA	2:D:111:THR:HG21	2.14	0.77
2:F:28:ASN:HB2	2:F:144:CYS:O	1.82	0.77
4:T:142:MET:SD	4:T:191:PRO:HA	2.24	0.77
2:B:55:VAL:HG12	2:B:56:ILE:N	2.00	0.77
4:H:37:TRP:CZ3	4:H:96:CYS:HB3	2.18	0.77
1:E:96:ASN:ND2	1:E:140:LYS:HE2	1.98	0.77
2:F:121:LYS:NZ	2:F:122:THR:CG2	2.47	0.77
3:L:194:THR:HA	3:L:209:SER:HB2	1.64	0.77
3:U:67:GLY:HA3	3:U:72:TYR:CD2	2.20	0.77
3:U:113:ALA:HB2	3:U:201:THR:OG1	1.83	0.77
2:B:28:ASN:ND2	2:B:145:ASP:HA	1.96	0.77
2:F:6:ILE:HG13	2:F:112:ASP:HA	1.66	0.77
4:H:97:ALA:HB1	4:H:109:TYR:O	1.85	0.77
1:C:283:THR:CG2	1:C:286:GLY:H	1.97	0.77
1:C:321:ARG:HG2	1:C:322:ASN:H	1.49	0.77
1:E:28:THR:HB	2:F:105:GLN:HB2	1.66	0.77
1:A:12:THR:HG23	2:B:138:PHE:O	1.86	0.76
1:E:170:ASN:HB2	1:E:176:LYS:HE2	1.66	0.76
2:F:129:ASN:ND2	2:F:159:HIS:HA	1.99	0.76
3:L:137:LEU:HD23	3:L:145:ILE:HD13	1.67	0.76
3:U:14:SER:CA	3:U:108:LYS:HB2	2.14	0.76
3:U:107:ILE:H	3:U:167:GLN:HE22	1.31	0.76
3:U:164:TRP:HE3	3:U:164:TRP:N	1.81	0.76
1:A:312:ASN:H	1:A:312:ASN:HD22	1.33	0.76
2:B:167:LEU:HD12	2:B:172:GLN:OE1	1.85	0.76
1:C:73:ASP:OD1	1:C:74:PRO:HD2	1.85	0.76
1:C:201:ARG:HG2	1:C:201:ARG:HH11	1.51	0.76
2:D:127:ARG:HB3	2:D:127:ARG:NH1	1.99	0.76
3:U:184:LYS:O	3:U:188:GLU:HG3	1.85	0.76
1:C:9:SER:O	2:D:143:LYS:HE3	1.85	0.76
1:C:29:ILE:HD13	2:D:101:ALA:HB1	1.67	0.76
1:C:87:PHE:HB3	1:C:267:ILE:HG13	1.67	0.76
2:F:115:MET:C	2:F:117:LYS:H	1.93	0.76
3:U:8:PRO:HG2	3:U:11:MET:HE3	1.66	0.76
2:F:100:VAL:HG23	2:F:101:ALA:H	1.49	0.76
1:A:47:SER:HB2	1:A:288:ILE:HG22	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:TRP:CE2	1:A:116:GLY:HA2	2.20	0.76
2:D:28:ASN:ND2	2:D:145:ASP:HA	1.99	0.76
1:E:28:THR:CG2	2:F:104:ASN:HB3	2.11	0.76
1:A:172:ASP:HB3	1:A:174:PHE:HE2	1.49	0.76
1:C:36:VAL:HG23	1:C:320:MET:O	1.86	0.76
2:D:130:ALA:HB1	2:D:139:LYS:O	1.85	0.76
1:E:141:ARG:HH11	1:E:141:ARG:HG3	1.50	0.76
3:U:48:TRP:CE2	3:U:59:VAL:HG13	2.21	0.76
2:F:17:MET:HE1	2:F:19:ASP:H	1.51	0.75
3:U:122:SER:O	3:U:126:LEU:HG	1.87	0.75
2:F:121:LYS:NZ	2:F:122:THR:HG22	2.01	0.75
1:A:81:ASN:ND2	1:A:120:PHE:H	1.85	0.75
1:E:10:THR:HG21	2:F:141:TYR:C	2.12	0.75
2:F:170:ARG:HB3	2:F:171:PHE:HD1	1.52	0.75
2:D:121:LYS:HZ3	2:D:122:THR:N	1.85	0.75
3:L:8:PRO:HG2	3:L:11:MET:HE3	1.68	0.75
4:H:121:ALA:HB3	4:H:153:PHE:CE2	2.22	0.75
1:E:64:CYS:HB2	1:E:79:PHE:CE1	2.22	0.75
4:H:32:GLY:HA2	4:H:54:TYR:CD2	2.22	0.75
4:H:88:ALA:O	4:H:91:THR:HG22	1.85	0.75
1:A:160:THR:HA	1:A:196:VAL:HG21	1.68	0.75
2:B:80:LEU:HD21	2:F:80:LEU:HD21	1.68	0.75
3:L:141:TYR:HB3	3:L:142:PRO:CD	2.16	0.75
2:F:111:THR:C	2:F:113:SER:H	1.93	0.75
2:D:121:LYS:HZ1	2:D:122:THR:HG22	1.52	0.74
4:H:170:VAL:HG12	4:H:188:VAL:HA	1.68	0.74
1:C:74:PRO:CD	1:C:97:CYS:HB2	2.18	0.74
1:C:80:GLN:O	1:C:82:GLU:N	2.21	0.74
1:A:25:LEU:HA	1:A:34:ILE:O	1.85	0.74
1:A:54:ASN:HB3	1:A:278:ILE:CD1	2.16	0.74
2:D:28:ASN:HB2	2:D:144:CYS:O	1.88	0.74
1:E:74:PRO:CD	1:E:97:CYS:HB2	2.15	0.74
2:F:149:ILE:C	2:F:151:SER:H	1.93	0.74
3:L:29:ILE:CD1	3:L:34:LEU:HB2	2.18	0.74
3:L:141:TYR:CB	3:L:142:PRO:HD3	2.17	0.74
3:L:201:THR:CG2	3:L:202:SER:N	2.49	0.74
3:U:148:LYS:HD2	3:U:155:GLU:O	1.87	0.74
3:U:125:GLN:HA	3:U:125:GLN:HE21	1.52	0.74
4:T:34:TYR:CD2	4:T:53:SER:HB3	2.22	0.74
1:A:47:SER:HB2	1:A:288:ILE:CG2	2.18	0.74
1:C:11:ALA:O	2:D:140:ILE:HB	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:THR:O	1:C:314:LEU:HD23	1.88	0.74
3:U:29:ILE:HD11	3:U:34:LEU:HD12	1.70	0.74
4:T:191:PRO:HB2	4:T:194:THR:HB	1.67	0.74
2:D:149:ILE:O	2:D:151:SER:N	2.19	0.74
1:E:286:GLY:O	1:E:287:SER:HB2	1.87	0.74
1:E:67:ILE:O	1:E:70:LEU:HB3	1.88	0.74
2:F:108:ILE:C	2:F:110:LEU:H	1.94	0.74
3:L:48:TRP:C	3:L:49:ILE:HG13	2.13	0.74
4:H:194:THR:O	4:H:194:THR:HG22	1.88	0.74
3:U:122:SER:HB3	3:U:125:GLN:HB3	1.68	0.74
1:A:62:ILE:HG22	1:A:63:ASP:H	1.51	0.74
1:C:10:THR:HG21	2:D:141:TYR:O	1.86	0.74
1:E:81:ASN:ND2	1:E:120:PHE:H	1.86	0.74
4:H:190:VAL:HG21	4:H:195:TRP:HB2	1.69	0.74
3:U:29:ILE:HD11	3:U:34:LEU:CD1	2.18	0.74
2:D:166:ALA:N	2:D:168:ASN:HD21	1.86	0.74
3:L:47:LEU:HD12	3:L:48:TRP:H	1.53	0.74
1:A:164:LEU:O	1:A:246:ASN:HA	1.87	0.73
3:U:95:PHE:CZ	4:T:60:TYR:HB3	2.23	0.73
1:A:73:ASP:OD1	1:A:74:PRO:HD2	1.88	0.73
3:U:14:SER:CB	3:U:108:LYS:HD2	2.19	0.73
1:E:29:ILE:HD13	2:F:101:ALA:HB1	1.68	0.73
1:A:293:PRO:O	1:A:294:PHE:HD2	1.71	0.73
1:E:84:TRP:CE2	1:E:116:GLY:HA2	2.22	0.73
2:F:149:ILE:O	2:F:151:SER:N	2.22	0.73
3:L:38:GLN:HG3	3:L:87:TYR:HE1	1.54	0.73
4:T:28:SER:C	4:T:30:THR:H	1.95	0.73
1:C:309:VAL:HG12	2:D:93:SER:HA	1.71	0.73
4:H:29:ILE:HG12	4:H:77:ASN:ND2	2.04	0.73
4:H:73:ASP:O	4:H:75:SER:N	2.22	0.73
4:T:195:TRP:O	4:T:196:PRO:C	2.31	0.73
2:B:28:ASN:HB2	2:B:144:CYS:O	1.87	0.73
2:B:117:LYS:HE3	2:F:4:GLY:HA2	1.69	0.73
2:F:115:MET:O	2:F:117:LYS:N	2.22	0.73
1:E:17:HIS:ND1	1:E:18:HIS:N	2.37	0.73
2:F:165:GLU:CA	2:F:168:ASN:HD21	2.01	0.73
3:U:48:TRP:C	3:U:49:ILE:HG13	2.13	0.73
2:B:47:GLN:OE1	2:B:110:LEU:HD21	1.89	0.72
2:D:154:ASN:HB3	2:D:156:THR:OG1	1.87	0.72
1:E:47:SER:HB2	1:E:288:ILE:CG2	2.19	0.72
3:L:150:LYS:O	3:L:151:ILE:HB	1.88	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:118:ILE:HG21	3:U:209:SER:HA	1.71	0.72
1:A:311:GLN:HE22	2:B:93:SER:HB3	1.53	0.72
2:B:108:ILE:C	2:B:110:LEU:H	1.96	0.72
3:L:36:TRP:HB2	3:L:49:ILE:HD12	1.70	0.72
1:C:17:HIS:HD2	2:D:6:ILE:HG23	1.54	0.72
3:U:141:TYR:HB3	3:U:142:PRO:CD	2.18	0.72
1:E:22:ASN:H	1:E:22:ASN:HD22	1.36	0.72
3:L:13:ALA:O	3:L:108:LYS:HG3	1.90	0.72
4:H:37:TRP:HB3	4:H:49:MET:CE	2.20	0.72
4:T:29:ILE:HG22	4:T:35:TRP:CE2	2.24	0.72
4:T:170:VAL:HG12	4:T:188:VAL:HA	1.69	0.72
2:B:78:GLN:O	2:B:79:ASP:C	2.32	0.72
2:D:28:ASN:HD21	2:D:30:GLU:HB2	1.55	0.72
2:D:131:GLU:HB2	2:F:127:ARG:HH21	1.52	0.72
4:H:100:TYR:O	4:H:101:TYR:HB3	1.90	0.72
1:A:81:ASN:HD21	1:A:120:PHE:H	1.34	0.72
3:L:51:SER:HB2	3:L:54:ASN:OD1	1.89	0.72
1:A:210:GLN:NE2	1:E:220:ARG:HH21	1.86	0.72
1:C:283:THR:CG2	1:C:286:GLY:N	2.53	0.72
2:D:170:ARG:HB3	2:D:171:PHE:HD1	1.53	0.72
4:H:56:GLY:C	4:H:58:ASN:H	1.98	0.72
3:U:51:SER:HB2	3:U:54:ASN:OD1	1.90	0.72
4:T:48:TRP:CZ2	4:T:50:GLY:HA2	2.25	0.72
4:T:177:LEU:HB2	4:T:182:TYR:CE1	2.24	0.72
1:E:294:PHE:CE1	2:F:96:ALA:HB1	2.24	0.72
4:H:86:VAL:HG23	4:H:90:ASP:HB2	1.72	0.72
3:U:47:LEU:HD12	3:U:48:TRP:N	2.04	0.72
1:C:87:PHE:O	1:C:267:ILE:HA	1.90	0.72
2:D:171:PHE:CD2	2:F:167:LEU:HB3	2.24	0.72
1:E:91:SER:C	1:E:93:ALA:H	1.97	0.72
3:U:183:THR:OG1	3:U:186:GLU:HB2	1.90	0.72
2:F:10:ILE:HD12	2:F:115:MET:HE3	1.72	0.71
2:F:89:ILE:H	2:F:89:ILE:HD12	1.53	0.71
4:T:206:HIS:HD2	4:T:209:SER:OG	1.72	0.71
4:H:37:TRP:HB3	4:H:49:MET:HE3	1.71	0.71
2:D:106:HIS:ND1	2:D:106:HIS:O	2.24	0.71
1:E:160:THR:HA	1:E:196:VAL:HG21	1.73	0.71
1:E:202:VAL:O	1:E:212:THR:HG23	1.91	0.71
3:L:125:GLN:HE21	3:L:125:GLN:HA	1.56	0.71
3:L:151:ILE:HG12	3:L:193:TYR:CE2	2.26	0.71
4:T:180:ASP:O	4:T:181:LEU:HD22	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:ALA:N	2:B:168:ASN:HD21	1.87	0.71
1:C:170:ASN:ND2	1:C:239:PRO:HA	2.05	0.71
3:L:126:LEU:O	3:L:128:SER:N	2.24	0.71
4:H:54:TYR:O	4:H:56:GLY:N	2.24	0.71
3:U:141:TYR:CB	3:U:142:PRO:HD3	2.21	0.71
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.72	0.71
2:B:2:LEU:HB2	2:B:109:ASP:OD1	1.91	0.71
2:D:141:TYR:CZ	2:D:170:ARG:HG2	2.26	0.71
2:F:10:ILE:O	2:F:12:ASN:N	2.23	0.71
3:U:29:ILE:CD1	3:U:34:LEU:HB2	2.20	0.71
1:C:50:LYS:O	1:C:286:GLY:O	2.09	0.71
1:E:172:ASP:HB3	1:E:174:PHE:CE2	2.26	0.71
2:D:68:LYS:HE2	2:D:85:GLU:CD	2.16	0.70
4:T:131:LEU:HG	4:T:147:CYS:H	1.55	0.70
1:A:172:ASP:CB	1:A:174:PHE:CE2	2.74	0.70
4:H:29:ILE:H	4:H:77:ASN:HD21	1.37	0.70
3:U:211:ASN:O	3:U:212:ARG:HG2	1.89	0.70
2:B:166:ALA:H	2:B:168:ASN:HD21	1.38	0.70
2:B:149:ILE:C	2:B:151:SER:H	2.00	0.70
2:D:84:VAL:HG12	2:D:85:GLU:N	2.06	0.70
2:D:141:TYR:CE2	2:D:170:ARG:HG2	2.26	0.70
1:E:191:GLN:O	1:E:194:LEU:N	2.24	0.70
1:E:295:GLN:OE1	1:E:297:VAL:HB	1.89	0.70
3:U:66:SER:OG	3:U:67:GLY:N	2.25	0.70
1:E:321:ARG:CG	1:E:322:ASN:H	1.96	0.70
3:U:126:LEU:C	3:U:128:SER:H	1.96	0.70
2:D:4:GLY:HA2	2:F:117:LYS:HE3	1.74	0.70
3:U:14:SER:OG	3:U:17:GLU:OE2	2.09	0.70
1:C:304:ALA:H	2:D:61:GLU:HG3	1.56	0.70
3:L:151:ILE:HG12	3:L:193:TYR:CD2	2.27	0.70
3:L:212:ARG:NH2	4:H:138:GLN:H	1.89	0.70
4:T:161:TRP:CE2	4:T:188:VAL:HB	2.27	0.70
3:L:21:LEU:HD21	3:L:87:TYR:CD2	2.27	0.70
3:L:199:HIS:HD2	3:L:200:LYS:H	1.37	0.70
1:A:74:PRO:CD	1:A:97:CYS:HB2	2.21	0.69
4:H:52:ILE:O	4:H:52:ILE:CG2	2.40	0.69
4:H:54:TYR:C	4:H:56:GLY:H	2.00	0.69
3:U:201:THR:CG2	3:U:202:SER:H	2.05	0.69
1:A:33:GLN:O	1:A:34:ILE:HG13	1.91	0.69
4:H:29:ILE:H	4:H:77:ASN:ND2	1.89	0.69
1:A:170:ASN:CB	1:A:176:LYS:HE2	2.22	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:LEU:HD22	1:C:33:GLN:OE1	1.90	0.69
3:L:97:ARG:HB2	4:H:48:TRP:CG	2.27	0.69
4:H:33:TYR:HD2	4:H:99:PHE:O	1.74	0.69
1:C:35:GLU:O	1:C:322:ASN:HB3	1.93	0.69
4:H:121:ALA:HB3	4:H:153:PHE:CZ	2.27	0.69
4:H:126:PRO:HB3	4:H:152:TYR:CB	2.19	0.69
4:H:142:MET:SD	4:H:191:PRO:HA	2.32	0.69
4:T:53:SER:H	4:T:58:ASN:HD21	1.40	0.69
1:A:206:THR:OG1	1:A:209:SER:HB3	1.93	0.69
1:A:9:SER:C	2:B:143:LYS:HE3	2.18	0.69
1:E:217:ILE:N	1:E:217:ILE:HD12	2.08	0.69
2:F:129:ASN:HD21	2:F:159:HIS:HA	1.58	0.69
3:L:167:GLN:HE21	3:L:172:SER:HB3	1.58	0.69
4:T:13:LYS:O	4:T:16:GLN:HG3	1.93	0.69
4:T:188:VAL:HG22	4:T:189:THR:N	2.07	0.69
2:D:166:ALA:H	2:D:168:ASN:HD21	1.40	0.69
1:E:59:LEU:HD21	1:E:82:GLU:HG3	1.75	0.69
2:F:96:ALA:O	2:F:98:LEU:N	2.25	0.69
3:L:95:PHE:CE2	4:H:60:TYR:HB3	2.27	0.69
1:A:10:THR:HG22	2:B:143:LYS:HD2	1.75	0.69
2:B:111:THR:C	2:B:113:SER:H	2.01	0.69
1:C:28:THR:HB	2:D:105:GLN:HB2	1.74	0.69
1:C:47:SER:HB2	1:C:288:ILE:CG2	2.23	0.69
2:D:108:ILE:C	2:D:110:LEU:H	1.99	0.69
4:T:102:ASP:O	4:T:103:TYR:HB2	1.93	0.69
3:L:118:ILE:HD13	3:L:195:CYS:HB2	1.74	0.69
3:U:193:TYR:O	3:U:209:SER:OG	2.10	0.69
1:C:54:ASN:HD22	1:C:55:PRO:HA	1.56	0.68
2:D:80:LEU:HD21	2:F:80:LEU:CD2	2.22	0.68
2:F:48:ILE:HD11	2:F:107:THR:HG23	1.73	0.68
3:L:151:ILE:CG2	3:L:152:ASP:N	2.50	0.68
3:U:106:GLU:HA	3:U:167:GLN:OE1	1.93	0.68
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.75	0.68
1:E:206:THR:HB	1:E:241:ASP:OD1	1.93	0.68
4:T:56:GLY:C	4:T:58:ASN:H	2.01	0.68
1:A:29:ILE:HD13	2:B:101:ALA:HB1	1.76	0.68
1:A:216:ASN:HB3	1:C:212:THR:CG2	2.21	0.68
1:A:294:PHE:CE1	2:B:96:ALA:HB1	2.28	0.68
3:U:48:TRP:O	3:U:49:ILE:HG13	1.91	0.68
3:U:141:TYR:CG	3:U:142:PRO:HD3	2.29	0.68
4:T:29:ILE:H	4:T:77:ASN:ND2	1.92	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:195:TRP:HZ2	4:T:217:ILE:HG22	1.57	0.68
2:B:100:VAL:O	2:B:104:ASN:HB2	1.94	0.68
1:E:12:THR:HB	2:F:27:GLN:HB3	1.73	0.68
1:A:321:ARG:HG2	1:A:322:ASN:N	2.04	0.68
1:C:12:THR:HB	2:D:27:GLN:HB3	1.75	0.68
1:C:18:HIS:O	1:C:19:ALA:HB2	1.93	0.68
4:H:58:ASN:O	4:H:60:TYR:N	2.22	0.68
4:H:131:LEU:HB2	4:H:146:GLY:CA	2.23	0.68
1:A:298:ASN:HD22	1:A:299:LYS:N	1.92	0.68
2:B:131:GLU:O	2:B:139:LYS:HB3	1.92	0.68
1:E:187:THR:C	1:E:189:GLN:H	2.00	0.68
1:E:191:GLN:OE1	1:E:195:TYR:HD1	1.77	0.68
4:H:58:ASN:HB2	4:H:60:TYR:CE2	2.29	0.68
1:C:295:GLN:OE1	1:C:297:VAL:HB	1.93	0.68
2:B:124:ARG:HH21	2:F:132:GLU:HB3	1.59	0.68
1:C:29:ILE:HD11	2:D:102:LEU:CD2	2.21	0.68
4:H:195:TRP:HH2	4:H:219:PRO:HA	1.58	0.68
4:T:184:LEU:HD12	4:T:185:SER:N	2.07	0.68
1:A:189:GLN:O	1:A:193:SER:OG	2.09	0.68
2:B:121:LYS:HZ3	2:B:122:THR:N	1.92	0.68
1:C:176:LYS:HE3	1:C:178:TYR:OH	1.94	0.68
3:L:167:GLN:NE2	3:L:172:SER:HB3	2.09	0.68
4:H:86:VAL:HG23	4:H:90:ASP:CB	2.25	0.67
1:A:252:ILE:HG22	1:A:252:ILE:O	1.92	0.67
2:B:17:MET:HE1	2:B:19:ASP:HB2	1.75	0.67
2:B:171:PHE:HZ	2:F:171:PHE:CE2	2.13	0.67
1:C:61:GLY:O	1:C:79:PHE:CZ	2.48	0.67
1:E:311:GLN:HE22	2:F:93:SER:HB3	1.59	0.67
2:F:166:ALA:H	2:F:168:ASN:HD21	1.40	0.67
3:L:141:TYR:O	3:L:142:PRO:C	2.37	0.67
3:L:199:HIS:CD2	3:L:200:LYS:N	2.59	0.67
4:H:13:LYS:HG3	4:H:120:SER:HA	1.76	0.67
1:C:98:TYR:HE2	1:C:229:ARG:HA	1.59	0.67
3:L:126:LEU:C	3:L:128:SER:H	2.02	0.67
3:U:13:ALA:O	3:U:108:LYS:N	2.28	0.67
4:T:51:TYR:HD1	4:T:52:ILE:N	1.92	0.67
1:A:54:ASN:CB	1:A:278:ILE:HD13	2.19	0.67
1:C:10:THR:HG22	2:D:143:LYS:HD2	1.77	0.67
3:U:35:TYR:HD2	3:U:50:TYR:HA	1.60	0.67
2:B:23:GLY:HA3	2:B:35:ALA:O	1.93	0.67
1:A:319:GLY:HA2	2:B:21:TRP:HH2	1.60	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:THR:HG21	2:D:141:TYR:C	2.20	0.67
2:D:23:GLY:HA3	2:D:35:ALA:O	1.95	0.67
1:E:37:THR:HG23	1:E:320:MET:O	1.95	0.67
1:E:246:ASN:HD22	1:E:246:ASN:C	2.03	0.67
2:F:96:ALA:C	2:F:98:LEU:H	2.02	0.67
4:H:61:ASN:HB3	4:H:62:PRO:HD2	1.77	0.67
1:A:91:SER:C	1:A:93:ALA:H	2.01	0.67
1:C:12:THR:HG23	2:D:138:PHE:O	1.96	0.67
2:D:115:MET:C	2:D:117:LYS:H	2.02	0.67
2:D:115:MET:O	2:D:117:LYS:N	2.27	0.67
2:D:126:LEU:HD12	2:D:126:LEU:O	1.95	0.67
3:U:80:GLU:O	3:U:81:ALA:C	2.38	0.67
1:A:41:GLU:HG3	1:A:43:VAL:H	1.61	0.66
2:B:3:PHE:HB2	2:B:112:ASP:O	1.94	0.66
1:E:94:PHE:CD1	1:E:94:PHE:C	2.72	0.66
3:U:32:SER:O	3:U:33:PHE:CD1	2.48	0.66
4:T:86:VAL:HG23	4:T:90:ASP:CB	2.25	0.66
1:A:77:ASP:O	1:A:80:GLN:CG	2.43	0.66
1:E:10:THR:HG21	2:F:141:TYR:O	1.95	0.66
1:E:319:GLY:HA2	2:F:21:TRP:HH2	1.59	0.66
3:U:168:ASP:OD1	3:U:171:ASP:HB2	1.96	0.66
4:T:162:ASN:ND2	4:T:201:THR:H	1.93	0.66
1:E:121:ILE:HG13	1:E:257:TYR:CZ	2.30	0.66
1:E:294:PHE:HB3	1:E:309:VAL:HG21	1.77	0.66
3:L:30:THR:O	3:L:32:SER:N	2.28	0.66
1:A:303:GLY:O	1:A:305:CYS:SG	2.53	0.66
1:A:310:LYS:HG3	2:B:93:SER:OG	1.94	0.66
1:C:47:SER:HB2	1:C:288:ILE:HG22	1.78	0.66
2:D:127:ARG:HG3	2:D:159:HIS:CG	2.31	0.66
3:U:119:PHE:CD2	4:T:131:LEU:HB3	2.30	0.66
2:D:28:ASN:ND2	2:D:30:GLU:HB2	2.11	0.66
1:E:102:VAL:HG22	1:E:232:ILE:CB	2.23	0.66
3:U:147:VAL:HA	3:U:196:GLU:O	1.96	0.66
3:U:151:ILE:O	3:U:192:SER:HB2	1.96	0.66
3:U:187:TYR:C	3:U:189:ARG:H	2.04	0.66
3:U:212:ARG:HA	3:U:212:ARG:HE	1.61	0.66
2:B:139:LYS:C	2:B:140:ILE:HD12	2.20	0.66
1:C:90:ARG:NH1	1:C:270:SER:O	2.29	0.66
1:E:125:PHE:HB2	1:E:127:TRP:NE1	2.10	0.66
3:L:116:VAL:HG12	3:L:117:SER:N	2.10	0.66
4:H:188:VAL:CG2	4:H:189:THR:N	2.58	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:8:PRO:O	3:U:10:ILE:N	2.27	0.66
1:C:77:ASP:O	1:C:80:GLN:CG	2.36	0.66
1:E:140:LYS:HD2	1:E:140:LYS:O	1.96	0.66
4:H:162:ASN:HD21	4:H:201:THR:H	1.41	0.66
2:B:25:ARG:CG	2:B:34:GLN:HG2	2.20	0.66
4:H:51:TYR:HD1	4:H:52:ILE:N	1.94	0.66
4:T:61:ASN:HB3	4:T:62:PRO:CD	2.26	0.66
1:A:36:VAL:HG23	1:A:320:MET:O	1.96	0.66
2:B:170:ARG:HB3	2:B:171:PHE:HD1	1.59	0.66
1:C:283:THR:HG22	1:C:287:SER:N	2.10	0.66
4:H:65:LYS:O	4:H:67:ARG:N	2.28	0.66
3:U:175:SER:HG	4:T:171:HIS:CE1	2.14	0.66
4:T:14:PRO:O	4:T:15:SER:CB	2.43	0.66
1:A:140:LYS:N	1:A:140:LYS:HD2	2.10	0.66
2:B:6:ILE:HG13	2:B:112:ASP:HA	1.77	0.66
2:B:51:LYS:O	2:B:54:ARG:HB2	1.96	0.66
1:C:36:VAL:HG22	1:C:37:THR:N	2.10	0.66
4:T:13:LYS:HG3	4:T:120:SER:HA	1.78	0.66
1:E:141:ARG:HG3	1:E:141:ARG:NH1	2.08	0.65
2:F:28:ASN:ND2	2:F:145:ASP:HA	2.02	0.65
3:L:25:ALA:O	3:L:26:SER:C	2.40	0.65
4:H:11:LEU:O	4:H:12:VAL:HG13	1.96	0.65
3:U:141:TYR:CB	3:U:142:PRO:CD	2.73	0.65
4:T:150:LYS:CB	4:T:183:THR:HG23	2.27	0.65
1:E:47:SER:HB2	1:E:288:ILE:HG22	1.78	0.65
3:L:38:GLN:HG3	3:L:87:TYR:CE1	2.30	0.65
1:C:318:THR:O	2:D:48:ILE:HG12	1.96	0.65
3:U:19:VAL:HG21	3:U:79:LEU:HD23	1.78	0.65
2:F:108:ILE:C	2:F:110:LEU:N	2.52	0.65
2:F:126:LEU:HA	2:F:159:HIS:HB3	1.77	0.65
4:H:18:LEU:HD22	4:H:116:LEU:CD1	2.27	0.65
4:H:195:TRP:CH2	4:H:219:PRO:HA	2.31	0.65
3:U:163:SER:HB2	4:T:174:PRO:HD2	1.77	0.65
4:T:131:LEU:HB2	4:T:146:GLY:CA	2.26	0.65
3:L:32:SER:HA	3:L:51:SER:HA	1.79	0.65
2:D:48:ILE:HD11	2:D:107:THR:CG2	2.27	0.65
2:F:44:ALA:HB2	2:F:114:GLU:HG3	1.77	0.65
4:T:6:GLU:OE1	4:T:95:TYR:HA	1.96	0.65
1:A:17:HIS:ND1	1:A:18:HIS:N	2.44	0.65
2:B:39:LYS:O	2:B:43:ALA:HB2	1.97	0.65
2:B:121:LYS:HZ1	2:B:122:THR:CG2	2.10	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:37:TRP:CB	4:H:49:MET:HE3	2.27	0.65
4:H:195:TRP:CZ2	4:H:219:PRO:HG3	2.31	0.65
2:B:141:TYR:CE2	2:B:170:ARG:HG2	2.32	0.65
3:U:118:ILE:HD11	3:U:149:TRP:CH2	2.32	0.65
1:A:59:LEU:HD12	1:A:60:ASP:N	2.12	0.65
3:L:91:GLN:HE21	3:L:93:GLU:HB3	1.62	0.65
1:C:41:GLU:HG3	1:C:43:VAL:H	1.61	0.65
4:H:13:LYS:HB2	4:H:16:GLN:OE1	1.97	0.65
3:U:125:GLN:HE21	3:U:125:GLN:CA	2.07	0.65
3:U:151:ILE:HG22	3:U:152:ASP:N	2.12	0.65
3:U:199:HIS:HD2	3:U:200:LYS:H	1.38	0.65
4:T:148:LEU:O	4:T:148:LEU:HD23	1.97	0.65
1:C:74:PRO:HG3	1:C:139:CYS:SG	2.37	0.64
1:C:111:LEU:HD12	1:C:112:VAL:N	2.11	0.64
2:D:38:LEU:C	2:D:40:SER:H	2.04	0.64
1:E:294:PHE:HB3	1:E:309:VAL:CG2	2.27	0.64
4:T:100:TYR:O	4:T:101:TYR:HB3	1.96	0.64
1:A:293:PRO:O	1:A:294:PHE:CD2	2.51	0.64
1:C:169:PRO:CA	1:C:242:VAL:HG23	2.27	0.64
1:E:54:ASN:HB3	1:E:278:ILE:HD13	1.79	0.64
1:E:9:SER:C	2:F:143:LYS:HE3	2.21	0.64
4:H:80:PHE:CD2	4:H:80:PHE:N	2.65	0.64
1:A:18:HIS:O	1:A:19:ALA:HB2	1.96	0.64
1:A:294:PHE:CE1	2:B:96:ALA:CB	2.80	0.64
1:E:97:CYS:O	1:E:98:TYR:C	2.41	0.64
3:L:8:PRO:HG2	3:L:11:MET:CE	2.28	0.64
3:U:116:VAL:HG12	3:U:117:SER:H	1.61	0.64
3:U:151:ILE:HA	3:U:192:SER:O	1.98	0.64
4:T:206:HIS:NE2	4:T:208:ALA:HB3	2.13	0.64
1:A:74:PRO:CG	1:A:139:CYS:SG	2.84	0.64
2:B:68:LYS:HE2	2:B:85:GLU:CD	2.23	0.64
1:C:18:HIS:HA	2:D:14:TRP:CB	2.24	0.64
1:E:187:THR:C	1:E:189:GLN:N	2.55	0.64
3:L:29:ILE:HD12	3:L:34:LEU:HB2	1.79	0.64
4:H:53:SER:OG	4:H:55:ASP:HB2	1.97	0.64
3:U:29:ILE:CD1	3:U:34:LEU:HD12	2.27	0.64
4:T:51:TYR:CD1	4:T:52:ILE:N	2.66	0.64
3:U:199:HIS:CD2	3:U:200:LYS:N	2.63	0.64
3:U:212:ARG:HG2	4:T:138:GLN:HE22	1.63	0.64
1:A:139:CYS:O	1:A:146:GLY:C	2.41	0.64
2:B:100:VAL:HG23	2:B:101:ALA:N	2.12	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:91:THR:OG1	4:T:117:THR:HA	1.97	0.64
1:A:216:ASN:ND2	1:C:212:THR:HB	2.12	0.64
4:T:67:ARG:HB3	4:T:84:ASN:HB2	1.80	0.64
2:D:98:LEU:O	2:D:99:LEU:C	2.37	0.64
3:L:141:TYR:CB	3:L:142:PRO:CD	2.75	0.64
3:L:187:TYR:C	3:L:189:ARG:H	2.05	0.64
3:U:149:TRP:O	3:U:154:SER:HB3	1.98	0.64
4:T:2:VAL:HG21	4:T:27:TYR:HB2	1.78	0.64
4:T:177:LEU:HD12	4:T:181:LEU:O	1.98	0.64
2:B:168:ASN:O	2:B:170:ARG:N	2.31	0.64
1:C:97:CYS:O	1:C:98:TYR:C	2.37	0.64
2:D:126:LEU:HA	2:D:159:HIS:HB3	1.80	0.64
2:D:165:GLU:CA	2:D:168:ASN:HD21	2.09	0.64
1:E:83:THR:O	1:E:84:TRP:HB3	1.97	0.64
1:C:61:GLY:O	1:C:79:PHE:HZ	1.81	0.63
1:C:283:THR:C	1:C:285:ASN:N	2.53	0.63
2:D:39:LYS:O	2:D:43:ALA:HB2	1.98	0.63
1:E:13:LEU:O	2:F:138:PHE:N	2.29	0.63
4:H:54:TYR:OH	5:I:2:NAG:H5	1.97	0.63
1:A:318:THR:O	2:B:48:ILE:HG21	1.98	0.63
1:C:117:THR:O	1:C:117:THR:HG23	1.98	0.63
1:E:303:GLY:O	1:E:305:CYS:SG	2.56	0.63
4:H:87:THR:O	4:H:118:VAL:HG11	1.97	0.63
3:U:133:VAL:HB	3:U:180:LEU:HB3	1.79	0.63
1:A:29:ILE:CD1	2:B:102:LEU:HD23	2.26	0.63
2:B:165:GLU:HA	2:B:168:ASN:HD21	1.62	0.63
4:T:155:GLU:OE2	4:T:156:PRO:HA	1.97	0.63
1:A:141:ARG:O	1:A:143:PRO:HD2	1.99	0.63
2:B:126:LEU:HA	2:B:159:HIS:HB3	1.79	0.63
1:C:13:LEU:O	2:D:138:PHE:N	2.30	0.63
2:D:25:ARG:HE	2:D:34:GLN:CD	2.07	0.63
1:E:222:TRP:CZ2	5:G:2:NAG:H61	2.34	0.63
4:T:58:ASN:O	4:T:59:ASN:HB2	1.98	0.63
1:A:80:GLN:O	1:A:82:GLU:N	2.31	0.63
2:B:47:GLN:OE1	2:B:110:LEU:HD11	1.98	0.63
2:D:21:TRP:HB2	2:D:41:THR:HG23	1.80	0.63
2:D:111:THR:C	2:D:113:SER:H	2.05	0.63
2:F:128:GLU:HA	2:F:170:ARG:NH2	2.13	0.63
3:L:19:VAL:CG2	3:L:79:LEU:HD23	2.29	0.63
4:H:87:THR:CG2	4:H:89:GLU:HB2	2.28	0.63
4:H:149:VAL:HB	4:H:184:LEU:HG	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:96:PRO:O	3:U:98:THR:HG23	1.98	0.63
1:A:119:GLU:OE2	1:A:259:LYS:HD2	1.98	0.63
4:H:13:LYS:O	4:H:16:GLN:HG3	1.99	0.63
3:U:14:SER:HB3	3:U:108:LYS:HD2	1.80	0.63
4:T:194:THR:HG22	4:T:194:THR:O	1.98	0.63
1:A:13:LEU:O	2:B:138:PHE:N	2.26	0.63
4:H:18:LEU:CD2	4:H:116:LEU:HD13	2.29	0.63
3:U:9:ALA:H	3:U:103:THR:HG23	1.63	0.63
2:D:170:ARG:HB3	2:D:171:PHE:CD1	2.34	0.63
3:L:163:SER:HB2	4:H:174:PRO:HD2	1.81	0.63
3:U:134:VAL:HG13	3:U:179:THR:OG1	1.99	0.63
4:T:120:SER:O	4:T:121:ALA:O	2.15	0.63
1:A:108:LEU:HD13	1:A:234:TRP:CE3	2.33	0.63
1:C:184:HIS:O	1:C:228:SER:HB2	1.98	0.63
2:D:129:ASN:O	2:D:130:ALA:HB2	1.98	0.63
3:U:4:LEU:HD12	3:U:4:LEU:N	2.14	0.63
1:C:19:ALA:O	1:C:20:VAL:HG13	1.99	0.62
3:L:2:ILE:HG12	3:L:2:ILE:O	1.97	0.62
3:U:8:PRO:HG2	3:U:11:MET:CE	2.29	0.62
1:A:321:ARG:CG	1:A:322:ASN:H	2.10	0.62
1:C:30:THR:HG23	2:D:105:GLN:HE22	1.64	0.62
1:E:62:ILE:HG22	1:E:63:ASP:H	1.64	0.62
3:U:9:ALA:N	3:U:103:THR:HG23	2.14	0.62
1:C:25:LEU:HD13	1:C:33:GLN:OE1	2.00	0.62
1:C:160:THR:HA	1:C:196:VAL:HG21	1.80	0.62
1:C:248:ASN:HD22	1:C:248:ASN:C	2.07	0.62
1:E:25:LEU:HD13	1:E:33:GLN:OE1	1.98	0.62
3:L:125:GLN:HE21	3:L:125:GLN:CA	2.11	0.62
1:A:109:ARG:HG2	1:A:109:ARG:HH11	1.64	0.62
1:E:319:GLY:HA2	2:F:21:TRP:CH2	2.35	0.62
3:L:122:SER:HB3	3:L:125:GLN:HB3	1.82	0.62
4:H:131:LEU:HG	4:H:147:CYS:H	1.64	0.62
3:U:118:ILE:CD1	3:U:195:CYS:HB2	2.29	0.62
4:T:97:ALA:HB1	4:T:109:TYR:O	1.99	0.62
4:T:195:TRP:CZ2	4:T:217:ILE:HG22	2.34	0.62
2:D:9:PHE:CD1	2:D:10:ILE:HG13	2.35	0.62
1:E:94:PHE:C	1:E:94:PHE:HD1	2.06	0.62
1:E:187:THR:O	1:E:190:GLU:N	2.25	0.62
4:H:18:LEU:HD22	4:H:116:LEU:HD13	1.81	0.62
3:U:38:GLN:HG3	3:U:87:TYR:HE1	1.65	0.62
3:U:153:GLY:O	3:U:154:SER:HB2	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:PHE:C	1:A:94:PHE:CD1	2.78	0.62
2:D:44:ALA:HB2	2:D:114:GLU:HG3	1.81	0.62
1:E:17:HIS:HB2	1:E:320:MET:SD	2.38	0.62
1:E:191:GLN:OE1	1:E:250:ASN:ND2	2.32	0.62
2:F:152:ILE:C	2:F:154:ASN:H	2.06	0.62
3:L:8:PRO:O	3:L:10:ILE:N	2.28	0.62
3:L:56:ALA:O	3:L:58:GLY:N	2.32	0.62
3:L:133:VAL:HB	3:L:180:LEU:HB3	1.80	0.62
4:H:67:ARG:HB3	4:H:84:ASN:HB2	1.80	0.62
1:A:29:ILE:HG23	2:D:103:GLU:OE1	1.99	0.62
1:A:91:SER:O	1:A:93:ALA:N	2.33	0.62
1:C:223:VAL:HG22	1:E:207:ARG:HG2	1.81	0.62
2:D:54:ARG:NH1	2:D:103:GLU:OE2	2.32	0.62
2:F:150:GLU:HG3	2:F:150:GLU:O	1.99	0.62
3:U:126:LEU:O	3:U:128:SER:N	2.33	0.62
1:A:108:LEU:HG	1:A:108:LEU:O	1.97	0.62
2:D:127:ARG:HG3	2:D:159:HIS:CD2	2.34	0.62
2:F:10:ILE:O	2:F:10:ILE:HG22	1.99	0.62
3:U:118:ILE:HD13	3:U:195:CYS:CB	2.30	0.62
3:U:201:THR:CG2	3:U:202:SER:N	2.63	0.62
4:T:18:LEU:HD22	4:T:116:LEU:HD13	1.81	0.62
2:B:3:PHE:CB	2:B:112:ASP:O	2.48	0.62
1:C:191:GLN:OE1	1:C:195:TYR:HD1	1.83	0.62
1:C:298:ASN:HD22	1:C:299:LYS:N	1.97	0.62
2:D:96:ALA:C	2:D:98:LEU:H	2.07	0.62
1:E:176:LYS:HE3	1:E:178:TYR:OH	2.00	0.62
1:E:283:THR:HG23	1:E:286:GLY:H	1.62	0.62
3:L:118:ILE:HD13	3:L:195:CYS:CB	2.30	0.62
3:U:7:SER:CB	3:U:8:PRO:HD3	2.30	0.62
4:T:29:ILE:H	4:T:77:ASN:HD21	1.44	0.62
1:A:10:THR:HG23	2:B:143:LYS:HZ2	1.64	0.62
1:A:138:ALA:O	1:A:140:LYS:NZ	2.33	0.62
2:B:108:ILE:O	2:B:110:LEU:N	2.33	0.62
1:C:176:LYS:HD2	1:C:257:TYR:CD2	2.35	0.62
1:C:318:THR:O	2:D:48:ILE:HG21	2.00	0.62
1:E:283:THR:HG22	1:E:287:SER:H	1.65	0.62
4:H:142:MET:CA	4:H:192:SER:HA	2.29	0.62
3:U:141:TYR:CD2	3:U:142:PRO:HD3	2.35	0.62
1:E:82:GLU:HA	1:E:82:GLU:OE2	2.00	0.61
3:U:21:LEU:HD13	3:U:21:LEU:N	2.15	0.61
1:A:29:ILE:HD11	2:B:102:LEU:CD2	2.28	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:THR:O	1:C:84:TRP:HB3	1.99	0.61
4:H:206:HIS:HD2	4:H:209:SER:OG	1.83	0.61
1:C:221:PRO:HG2	1:E:206:THR:HA	1.81	0.61
2:D:42:GLN:O	2:D:46:ASP:N	2.33	0.61
2:F:121:LYS:NZ	2:F:122:THR:N	2.48	0.61
1:A:207:ARG:HG2	1:E:223:VAL:CG2	2.30	0.61
2:D:141:TYR:OH	2:D:170:ARG:HG2	1.99	0.61
1:E:35:GLU:O	1:E:322:ASN:HB3	2.00	0.61
3:L:118:ILE:HG21	3:L:209:SER:HA	1.81	0.61
4:H:29:ILE:HG22	4:H:35:TRP:CZ2	2.35	0.61
3:U:6:GLN:OE1	3:U:87:TYR:O	2.18	0.61
1:A:12:THR:HB	2:B:27:GLN:HB3	1.83	0.61
1:C:25:LEU:HA	1:C:34:ILE:O	2.00	0.61
2:D:105:GLN:O	2:D:108:ILE:HB	2.00	0.61
3:U:21:LEU:N	3:U:21:LEU:CD1	2.63	0.61
1:A:246:ASN:C	1:A:246:ASN:HD22	2.09	0.61
2:B:130:ALA:CB	2:B:139:LYS:O	2.45	0.61
2:D:9:PHE:CE1	2:D:10:ILE:HG13	2.36	0.61
4:H:58:ASN:O	4:H:59:ASN:HB2	2.00	0.61
3:U:91:GLN:HE21	3:U:93:GLU:N	1.99	0.61
1:C:59:LEU:HD12	1:C:60:ASP:N	2.16	0.61
1:E:150:ARG:O	1:E:151:LEU:HD23	2.01	0.61
2:F:43:ALA:O	2:F:46:ASP:HB2	2.01	0.61
2:F:102:LEU:O	2:F:103:GLU:C	2.43	0.61
4:H:38:ILE:O	4:H:95:TYR:HB2	2.00	0.61
4:H:49:MET:O	4:H:62:PRO:HD3	2.00	0.61
3:U:2:ILE:HG22	3:U:4:LEU:CD1	2.30	0.61
1:C:51:ILE:HD11	1:C:272:ALA:HB3	1.82	0.61
1:C:64:CYS:HB2	1:C:79:PHE:HE1	1.63	0.61
3:L:62:ARG:O	3:L:76:ILE:HA	2.00	0.61
3:L:171:ASP:HB3	3:L:173:THR:HG23	1.81	0.61
4:H:122:LYS:HD3	4:H:124:THR:HG23	1.82	0.61
3:U:162:ASN:HA	3:U:177:SER:O	1.99	0.61
1:A:202:VAL:HG22	1:A:247:SER:HB2	1.83	0.61
1:C:209:SER:O	1:C:210:GLN:HB2	2.01	0.61
1:E:81:ASN:HD21	1:E:120:PHE:H	1.49	0.61
4:H:33:TYR:CE2	4:H:100:TYR:HB2	2.35	0.61
3:U:136:PHE:O	3:U:137:LEU:HD12	2.01	0.61
4:T:3:HIS:O	4:T:24:VAL:HA	2.01	0.61
1:A:18:HIS:HA	2:B:14:TRP:CB	2.27	0.61
1:A:27:LYS:HG3	1:A:32:ASP:HA	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:PHE:HB3	1:A:309:VAL:CG2	2.30	0.61
1:A:295:GLN:OE1	1:A:297:VAL:HB	2.01	0.61
2:B:149:ILE:O	2:B:151:SER:N	2.30	0.61
2:B:168:ASN:C	2:B:170:ARG:H	2.06	0.61
1:C:187:THR:O	1:C:190:GLU:N	2.34	0.61
1:E:73:ASP:OD1	1:E:75:HIS:CD2	2.54	0.61
4:H:40:GLN:HB3	4:H:46:LEU:HD23	1.83	0.61
1:A:96:ASN:ND2	1:A:140:LYS:HE2	2.13	0.60
1:C:221:PRO:HG2	1:E:206:THR:CA	2.31	0.60
1:E:109:ARG:HG2	1:E:109:ARG:HH11	1.66	0.60
1:E:184:HIS:O	1:E:228:SER:HB2	2.01	0.60
3:L:189:ARG:HB3	3:L:190:HIS:CE1	2.35	0.60
4:H:27:TYR:HE1	4:H:31:SER:O	1.84	0.60
4:T:38:ILE:O	4:T:95:TYR:HB2	2.01	0.60
1:A:293:PRO:C	1:A:294:PHE:CD2	2.79	0.60
1:E:43:VAL:HA	1:E:294:PHE:O	2.00	0.60
1:A:36:VAL:HG22	1:A:37:THR:N	2.16	0.60
1:E:80:GLN:O	1:E:82:GLU:N	2.34	0.60
3:U:97:ARG:HB2	4:T:48:TRP:CG	2.37	0.60
1:E:294:PHE:CE1	2:F:96:ALA:CB	2.84	0.60
2:F:57:GLU:O	2:F:58:LYS:HG2	2.00	0.60
4:H:100:TYR:CE1	5:I:1:NAG:H83	2.37	0.60
1:A:298:ASN:HD22	1:A:299:LYS:H	1.50	0.60
3:U:3:VAL:O	3:U:3:VAL:HG12	2.01	0.60
3:U:50:TYR:O	3:U:51:SER:C	2.44	0.60
4:T:32:GLY:O	4:T:33:TYR:HB2	2.01	0.60
4:T:87:THR:O	4:T:118:VAL:HG11	2.02	0.60
2:B:171:PHE:CD1	2:B:171:PHE:N	2.70	0.60
1:C:193:SER:HA	3:U:57:SER:HB2	1.83	0.60
3:L:191:ASN:HD22	3:L:191:ASN:N	2.00	0.60
3:L:29:ILE:HD11	3:L:34:LEU:HB2	1.83	0.60
3:U:6:GLN:NE2	3:U:101:GLY:O	2.35	0.60
3:U:107:ILE:H	3:U:167:GLN:NE2	1.97	0.60
1:A:148:PHE:HB2	1:A:151:LEU:HB2	1.83	0.60
2:B:44:ALA:HB2	2:B:114:GLU:HG3	1.84	0.60
1:C:18:HIS:CA	2:D:14:TRP:HB2	2.29	0.60
1:C:201:ARG:HG2	1:C:201:ARG:NH1	2.16	0.60
2:D:21:TRP:CE2	2:D:45:ILE:HD11	2.36	0.60
1:E:71:LEU:HD11	1:E:100:TYR:CE1	2.36	0.60
1:E:283:THR:CG2	1:E:286:GLY:N	2.65	0.60
4:H:51:TYR:CD1	4:H:52:ILE:N	2.69	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:87:THR:HG21	4:H:89:GLU:HB2	1.82	0.60
3:U:52:THR:HG23	3:U:72:TYR:CE2	2.36	0.60
1:A:247:SER:CB	1:A:251:LEU:HB2	2.32	0.60
1:C:19:ALA:C	1:C:20:VAL:HG22	2.26	0.60
2:F:23:GLY:HA3	2:F:35:ALA:O	2.01	0.60
3:U:36:TRP:CD2	3:U:74:LEU:HD23	2.37	0.60
4:T:65:LYS:C	4:T:67:ARG:N	2.60	0.60
4:T:130:PRO:HD3	4:T:215:LYS:HG2	1.84	0.60
1:C:41:GLU:HG3	1:C:42:LEU:N	2.17	0.60
1:C:108:LEU:O	1:C:112:VAL:HG23	2.01	0.60
3:U:14:SER:HB3	3:U:108:LYS:CB	2.32	0.60
4:T:86:VAL:CG2	4:T:87:THR:N	2.64	0.60
2:F:98:LEU:C	2:F:100:VAL:N	2.55	0.59
2:F:100:VAL:HG23	2:F:101:ALA:N	2.17	0.59
4:H:67:ARG:CB	4:H:84:ASN:HB2	2.31	0.59
3:U:61:ALA:O	3:U:63:PHE:N	2.36	0.59
2:B:108:ILE:C	2:B:110:LEU:N	2.59	0.59
1:C:220:ARG:HH21	1:E:210:GLN:NE2	2.00	0.59
1:C:293:PRO:O	1:C:294:PHE:CD2	2.55	0.59
2:D:30:GLU:OE2	2:D:145:ASP:HB2	2.02	0.59
1:E:91:SER:C	1:E:93:ALA:N	2.58	0.59
4:T:24:VAL:HG11	4:T:29:ILE:HG23	1.84	0.59
2:B:115:MET:C	2:B:117:LYS:H	2.08	0.59
2:B:141:TYR:HB3	2:B:165:GLU:HB3	1.83	0.59
1:C:123:GLU:O	1:C:255:ARG:O	2.21	0.59
2:D:121:LYS:NZ	2:D:122:THR:HG22	2.17	0.59
3:L:137:LEU:HD23	3:L:145:ILE:CD1	2.32	0.59
3:L:212:ARG:HG2	3:L:213:ASN:H	1.65	0.59
3:U:37:TYR:OH	4:T:99:PHE:HE2	1.83	0.59
3:U:165:THR:HG23	3:U:175:SER:O	2.03	0.59
4:T:80:PHE:N	4:T:80:PHE:CD2	2.69	0.59
1:A:312:ASN:H	1:A:312:ASN:ND2	1.99	0.59
1:C:68:ASP:OD2	1:C:95:SER:HB3	2.02	0.59
1:C:294:PHE:CE1	2:D:96:ALA:HB1	2.37	0.59
1:C:319:GLY:HA2	2:D:21:TRP:HH2	1.67	0.59
2:D:25:ARG:HG2	2:D:34:GLN:CG	2.25	0.59
1:E:169:PRO:CA	1:E:242:VAL:HG23	2.32	0.59
2:F:17:MET:CE	2:F:19:ASP:H	2.15	0.59
3:L:147:VAL:HA	3:L:196:GLU:O	2.03	0.59
4:H:6:GLU:OE1	4:H:95:TYR:HA	2.03	0.59
4:H:102:ASP:O	4:H:103:TYR:HB2	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ASP:OD2	1:A:292:LYS:N	2.35	0.59
1:C:17:HIS:HA	2:D:22:TYR:CD2	2.38	0.59
2:D:149:ILE:C	2:D:151:SER:N	2.57	0.59
2:D:151:SER:O	2:D:156:THR:N	2.33	0.59
2:F:85:GLU:O	2:F:89:ILE:HD13	2.02	0.59
2:B:129:ASN:HD21	2:B:159:HIS:HA	1.68	0.59
1:C:185:PRO:HB3	1:C:190:GLU:HG2	1.85	0.59
1:C:206:THR:OG1	1:C:209:SER:HB3	2.03	0.59
1:C:324:PRO:HB3	1:C:328:THR:HB	1.85	0.59
1:E:262:THR:O	1:E:263:GLY:O	2.21	0.59
2:F:170:ARG:HB3	2:F:171:PHE:CD1	2.34	0.59
2:B:141:TYR:CZ	2:B:170:ARG:HG2	2.37	0.59
2:F:2:LEU:HB2	2:F:109:ASP:OD1	2.02	0.59
1:A:17:HIS:HE1	2:B:13:GLY:HA2	1.67	0.59
1:C:94:PHE:CD1	1:C:94:PHE:C	2.79	0.59
1:E:74:PRO:HD2	1:E:96:ASN:O	2.02	0.59
2:F:48:ILE:HG22	2:F:49:ASN:N	2.17	0.59
2:F:166:ALA:N	2:F:168:ASN:ND2	2.50	0.59
3:U:167:GLN:HG2	3:U:172:SER:HA	1.85	0.59
1:A:10:THR:HG23	2:B:143:LYS:NZ	2.18	0.59
1:A:28:THR:O	1:A:30:THR:N	2.36	0.59
1:C:62:ILE:HG22	1:C:63:ASP:H	1.67	0.59
2:D:2:LEU:HB2	2:D:109:ASP:OD1	2.01	0.59
2:D:71:SER:HB2	2:D:72:GLU:OE2	2.03	0.59
2:D:96:ALA:O	2:D:98:LEU:N	2.35	0.59
1:E:309:VAL:CG1	2:F:93:SER:HA	2.33	0.59
2:F:121:LYS:NZ	2:F:122:THR:HG23	2.18	0.59
4:H:39:ARG:NH1	4:H:94:TYR:OH	2.35	0.59
4:T:146:GLY:O	4:T:147:CYS:HB3	2.01	0.59
1:A:108:LEU:O	1:A:112:VAL:HG23	2.02	0.59
1:A:166:VAL:HG22	1:A:245:ILE:HB	1.84	0.59
2:B:100:VAL:O	2:B:101:ALA:C	2.46	0.59
2:B:165:GLU:HA	2:B:168:ASN:ND2	2.18	0.59
1:E:281:CYS:HB2	1:E:304:ALA:O	2.03	0.59
1:A:10:THR:HG21	2:B:141:TYR:C	2.27	0.58
2:D:100:VAL:HG23	2:D:101:ALA:N	2.14	0.58
2:F:100:VAL:O	2:F:104:ASN:HB2	2.02	0.58
3:L:173:THR:C	3:L:174:TYR:CD2	2.81	0.58
4:T:142:MET:CA	4:T:192:SER:HA	2.33	0.58
2:B:26:HIS:ND1	2:B:26:HIS:O	2.36	0.58
1:E:293:PRO:C	1:E:294:PHE:CD2	2.81	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LEU:HD23	1:A:34:ILE:N	2.18	0.58
1:A:262:THR:O	1:A:263:GLY:O	2.21	0.58
2:B:3:PHE:HE2	2:B:113:SER:HG	1.49	0.58
1:C:169:PRO:HA	1:C:242:VAL:HG23	1.85	0.58
1:C:217:ILE:HD12	1:C:217:ILE:N	2.18	0.58
2:D:47:GLN:OE1	2:D:110:LEU:HD11	2.03	0.58
2:F:98:LEU:O	2:F:99:LEU:C	2.45	0.58
3:L:118:ILE:HD12	3:L:135:CYS:HB2	1.85	0.58
1:C:251:LEU:HD21	1:C:253:ALA:HB2	1.85	0.58
2:D:168:ASN:C	2:D:170:ARG:H	2.11	0.58
1:E:29:ILE:CD1	2:F:102:LEU:HD23	2.21	0.58
1:E:91:SER:O	1:E:93:ALA:N	2.37	0.58
2:F:108:ILE:O	2:F:110:LEU:N	2.36	0.58
3:L:21:LEU:HD21	3:L:87:TYR:HD2	1.66	0.58
4:H:195:TRP:HB3	4:H:196:PRO:CD	2.30	0.58
2:D:6:ILE:CG1	2:D:112:ASP:HA	2.32	0.58
4:H:13:LYS:N	4:H:16:GLN:OE1	2.30	0.58
3:U:6:GLN:NE2	3:U:102:GLY:HA2	2.19	0.58
3:U:125:GLN:HB2	4:T:129:TYR:CD2	2.37	0.58
2:B:171:PHE:HD2	2:D:167:LEU:HB3	1.69	0.58
1:C:17:HIS:HB2	1:C:320:MET:SD	2.43	0.58
3:L:7:SER:CB	3:L:8:PRO:HD3	2.33	0.58
4:H:146:GLY:O	4:H:147:CYS:CB	2.50	0.58
4:H:188:VAL:CG2	4:H:189:THR:H	2.16	0.58
3:U:32:SER:C	3:U:33:PHE:HD1	2.12	0.58
2:D:168:ASN:O	2:D:170:ARG:N	2.36	0.58
1:E:310:LYS:HG3	2:F:93:SER:OG	2.03	0.58
4:H:29:ILE:HG22	4:H:35:TRP:CD2	2.39	0.58
4:H:195:TRP:O	4:H:196:PRO:C	2.47	0.58
3:U:141:TYR:O	3:U:142:PRO:C	2.46	0.58
4:T:49:MET:O	4:T:62:PRO:HD3	2.03	0.58
2:D:6:ILE:CD1	2:D:112:ASP:HA	2.34	0.58
2:D:167:LEU:HD12	2:D:172:GLN:OE1	2.03	0.58
2:F:165:GLU:C	2:F:168:ASN:HD21	2.12	0.58
3:U:92:TRP:O	3:U:97:ARG:NH2	2.37	0.58
1:A:206:THR:HA	1:E:221:PRO:HG2	1.85	0.58
3:U:7:SER:HB2	3:U:8:PRO:HD3	1.86	0.58
3:U:119:PHE:O	3:U:133:VAL:HG13	2.03	0.58
1:A:53:ASN:OD1	1:A:276:THR:HA	2.04	0.58
2:B:168:ASN:C	2:B:170:ARG:N	2.62	0.58
1:C:166:VAL:CG2	1:C:245:ILE:HB	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:27:GLN:HG3	2:D:27:GLN:O	2.03	0.58
2:D:151:SER:HA	2:D:156:THR:O	2.04	0.58
1:E:17:HIS:HA	2:F:22:TYR:CD2	2.38	0.58
1:E:252:ILE:O	1:E:252:ILE:HG22	2.04	0.58
1:E:309:VAL:HG12	2:F:93:SER:HA	1.85	0.58
2:F:38:LEU:O	2:F:40:SER:N	2.37	0.58
4:T:75:SER:OG	4:T:76:LYS:N	2.35	0.58
4:T:149:VAL:HB	4:T:184:LEU:HG	1.84	0.58
4:T:162:ASN:HD21	4:T:201:THR:H	1.50	0.58
4:T:188:VAL:HG22	4:T:189:THR:H	1.67	0.58
1:A:37:THR:HG23	1:A:321:ARG:O	2.04	0.57
1:A:324:PRO:HB3	1:A:328:THR:HB	1.85	0.57
2:B:126:LEU:HD12	2:B:126:LEU:O	2.04	0.57
1:C:108:LEU:HA	1:C:111:LEU:HD21	1.85	0.57
1:A:17:HIS:CD2	2:B:6:ILE:HG23	2.29	0.57
1:A:44:GLN:HB3	1:A:295:GLN:CB	2.32	0.57
1:A:269:ARG:HH11	1:A:269:ARG:HG3	1.69	0.57
1:C:268:MET:SD	1:C:284:PRO:HG3	2.44	0.57
2:D:152:ILE:C	2:D:154:ASN:H	2.12	0.57
1:E:17:HIS:N	2:F:115:MET:HE1	2.19	0.57
3:U:199:HIS:HB3	3:U:201:THR:CG2	2.18	0.57
4:T:150:LYS:HB2	4:T:183:THR:HG23	1.85	0.57
4:T:160:THR:OG1	4:T:203:ASN:HB2	2.04	0.57
2:D:76:ARG:O	2:D:77:ILE:C	2.47	0.57
1:E:33:GLN:O	1:E:34:ILE:HG13	2.05	0.57
1:E:41:GLU:HG3	1:E:43:VAL:H	1.68	0.57
4:H:122:LYS:CD	4:H:124:THR:HG23	2.35	0.57
3:U:116:VAL:CG1	3:U:117:SER:N	2.67	0.57
1:E:18:HIS:O	1:E:19:ALA:HB2	2.04	0.57
1:E:41:GLU:HG3	1:E:42:LEU:N	2.18	0.57
1:E:148:PHE:HB2	1:E:151:LEU:HB2	1.86	0.57
2:F:141:TYR:CE2	2:F:170:ARG:HG2	2.40	0.57
4:H:91:THR:OG1	4:H:117:THR:HA	2.04	0.57
1:C:186:SER:CA	1:C:218:GLY:O	2.50	0.57
1:E:121:ILE:HG13	1:E:257:TYR:CE1	2.39	0.57
3:U:8:PRO:C	3:U:10:ILE:H	2.12	0.57
1:A:140:LYS:CD	1:A:140:LYS:H	2.15	0.57
1:C:59:LEU:HD12	1:C:59:LEU:C	2.28	0.57
2:F:166:ALA:H	2:F:168:ASN:ND2	2.01	0.57
3:U:21:LEU:HD21	3:U:87:TYR:CD2	2.40	0.57
4:T:17:SER:HA	4:T:84:ASN:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:THR:CG2	1:A:286:GLY:N	2.65	0.57
1:C:172:ASP:CB	1:C:174:PHE:CE2	2.87	0.57
1:C:220:ARG:HE	1:E:210:GLN:HG3	1.69	0.57
2:D:106:HIS:O	2:D:106:HIS:CG	2.58	0.57
1:E:291:ASP:OD2	1:E:292:LYS:N	2.38	0.57
2:F:89:ILE:HD12	2:F:89:ILE:N	2.19	0.57
3:L:8:PRO:C	3:L:10:ILE:H	2.10	0.57
3:L:174:TYR:CD2	3:L:174:TYR:N	2.73	0.57
3:U:3:VAL:H	3:U:26:SER:CB	2.18	0.57
3:U:40:LYS:HD3	3:U:85:ALA:HB2	1.84	0.57
1:A:191:GLN:OE1	1:A:195:TYR:HD1	1.86	0.57
2:B:27:GLN:HG3	2:B:27:GLN:O	2.05	0.57
2:D:98:LEU:C	2:D:100:VAL:N	2.58	0.57
2:F:47:GLN:OE1	2:F:110:LEU:HD11	2.05	0.57
2:F:89:ILE:H	2:F:89:ILE:CD1	2.17	0.57
1:A:91:SER:C	1:A:93:ALA:N	2.59	0.57
1:A:94:PHE:C	1:A:94:PHE:HD1	2.13	0.57
2:D:26:HIS:O	2:D:32:THR:HG22	2.04	0.57
4:H:87:THR:OG1	4:H:88:ALA:N	2.37	0.57
3:U:3:VAL:HB	3:U:26:SER:HB2	1.86	0.57
3:U:126:LEU:C	3:U:128:SER:N	2.61	0.57
1:A:64:CYS:HB2	1:A:79:PHE:CE1	2.40	0.57
1:A:283:THR:HG22	1:A:287:SER:H	1.69	0.57
2:B:17:MET:HE1	2:B:19:ASP:H	1.70	0.57
1:C:303:GLY:O	1:C:304:ALA:C	2.47	0.57
2:D:120:GLU:OE1	2:D:120:GLU:HA	2.04	0.57
1:E:25:LEU:HD22	1:E:33:GLN:OE1	2.05	0.57
2:F:141:TYR:CZ	2:F:170:ARG:HG2	2.39	0.57
4:T:146:GLY:O	4:T:147:CYS:CB	2.52	0.57
2:B:6:ILE:C	2:B:8:GLY:H	2.11	0.56
2:B:48:ILE:HD11	2:B:107:THR:HG23	1.86	0.56
1:C:36:VAL:HG22	1:C:37:THR:H	1.70	0.56
1:C:74:PRO:HD3	1:C:97:CYS:CB	2.34	0.56
2:D:78:GLN:O	2:D:79:ASP:C	2.46	0.56
1:E:187:THR:O	1:E:189:GLN:N	2.38	0.56
2:F:17:MET:SD	2:F:17:MET:C	2.88	0.56
4:H:1:ASP:C	4:H:2:VAL:HG22	2.30	0.56
4:T:131:LEU:HG	4:T:147:CYS:N	2.19	0.56
2:D:122:THR:O	2:D:126:LEU:HG	2.04	0.56
1:E:13:LEU:O	2:F:138:PHE:HB2	2.05	0.56
1:E:17:HIS:CG	1:E:18:HIS:H	2.23	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:139:LYS:C	2:F:140:ILE:HD12	2.29	0.56
4:H:91:THR:HB	4:H:118:VAL:H	1.70	0.56
4:T:14:PRO:O	4:T:15:SER:HB3	2.05	0.56
4:T:27:TYR:CE1	4:T:31:SER:HB2	2.40	0.56
1:A:38:ASN:HD22	1:A:318:THR:CG2	2.17	0.56
2:B:80:LEU:HD21	2:D:80:LEU:HD21	1.87	0.56
2:B:152:ILE:C	2:B:154:ASN:H	2.13	0.56
1:C:164:LEU:O	1:C:246:ASN:HA	2.05	0.56
2:D:3:PHE:CB	2:D:112:ASP:O	2.53	0.56
1:E:44:GLN:HB3	1:E:295:GLN:CB	2.35	0.56
1:E:209:SER:O	1:E:210:GLN:CB	2.53	0.56
2:F:38:LEU:C	2:F:40:SER:H	2.13	0.56
2:F:111:THR:C	2:F:113:SER:N	2.62	0.56
3:U:191:ASN:HD22	3:U:191:ASN:H	1.52	0.56
4:T:2:VAL:CB	4:T:109:TYR:HE2	2.06	0.56
4:T:18:LEU:HD12	4:T:18:LEU:C	2.29	0.56
4:T:86:VAL:HG22	4:T:87:THR:N	2.19	0.56
1:A:138:ALA:C	1:A:140:LYS:NZ	2.64	0.56
1:A:187:THR:C	1:A:189:GLN:H	2.12	0.56
1:C:37:THR:HG23	1:C:321:ARG:O	2.05	0.56
1:E:249:GLY:C	1:E:250:ASN:OD1	2.49	0.56
1:E:304:ALA:H	2:F:61:GLU:HG3	1.70	0.56
3:L:176:MET:HG2	3:L:177:SER:H	1.70	0.56
4:H:37:TRP:CH2	4:H:96:CYS:HB3	2.40	0.56
4:H:162:ASN:HD21	4:H:201:THR:N	2.02	0.56
1:A:200:GLY:HA3	1:A:250:ASN:OD1	2.05	0.56
1:C:248:ASN:C	1:C:248:ASN:ND2	2.63	0.56
3:L:184:LYS:O	3:L:188:GLU:HG3	2.05	0.56
3:U:14:SER:OG	3:U:108:LYS:CD	2.53	0.56
3:U:134:VAL:HG22	3:U:179:THR:CG2	2.20	0.56
4:T:3:HIS:HB3	4:T:25:THR:OG1	2.04	0.56
4:T:65:LYS:O	4:T:66:ASN:C	2.49	0.56
1:A:82:GLU:OE2	1:A:82:GLU:HA	2.06	0.56
1:A:182:ILE:HG22	1:A:231:SER:HB2	1.87	0.56
1:A:187:THR:C	1:A:189:GLN:N	2.62	0.56
2:B:21:TRP:HB2	2:B:41:THR:HG23	1.87	0.56
2:B:102:LEU:O	2:B:103:GLU:C	2.49	0.56
1:C:295:GLN:HG3	1:C:306:PRO:O	2.05	0.56
3:L:147:VAL:HG21	3:L:178:SER:OG	2.05	0.56
4:H:100:TYR:HE1	5:I:1:NAG:H83	1.69	0.56
4:T:159:VAL:HG22	4:T:160:THR:N	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:207:PRO:O	4:T:208:ALA:C	2.48	0.56
1:A:97:CYS:O	1:A:98:TYR:C	2.49	0.56
1:A:242:VAL:CG1	1:E:221:PRO:HB3	2.35	0.56
1:A:319:GLY:HA2	2:B:21:TRP:CH2	2.40	0.56
2:B:9:PHE:CD1	2:B:9:PHE:C	2.84	0.56
1:C:53:ASN:OD1	1:C:276:THR:HA	2.06	0.56
1:C:286:GLY:O	1:C:287:SER:CB	2.44	0.56
2:D:102:LEU:O	2:D:104:ASN:N	2.39	0.56
1:E:108:LEU:HD13	1:E:234:TRP:CD2	2.40	0.56
3:L:165:THR:OG1	3:L:166:ASP:N	2.37	0.56
3:L:199:HIS:HB3	3:L:201:THR:CG2	2.27	0.56
3:U:95:PHE:HE2	4:T:60:TYR:HB3	1.68	0.56
1:A:87:PHE:HB3	1:A:267:ILE:HG13	1.88	0.56
1:A:176:LYS:HD2	1:A:257:TYR:CE2	2.40	0.56
2:B:66:ILE:HG13	2:B:66:ILE:O	2.00	0.56
2:D:150:GLU:O	2:D:156:THR:OG1	2.24	0.56
1:E:140:LYS:HD2	1:E:140:LYS:N	2.21	0.56
2:F:27:GLN:HG3	2:F:27:GLN:O	2.06	0.56
2:B:68:LYS:HE2	2:B:85:GLU:OE2	2.06	0.56
2:D:118:LEU:O	2:D:122:THR:HG23	2.06	0.56
1:E:303:GLY:O	1:E:304:ALA:C	2.48	0.56
4:H:32:GLY:H	4:H:54:TYR:HB3	1.71	0.56
4:H:65:LYS:C	4:H:67:ARG:N	2.63	0.56
4:T:162:ASN:HD21	4:T:200:VAL:HA	1.71	0.56
1:C:138:ALA:O	1:C:140:LYS:NZ	2.39	0.56
1:C:254:PRO:HG2	1:C:254:PRO:O	2.06	0.56
2:D:166:ALA:N	2:D:168:ASN:ND2	2.54	0.56
3:U:168:ASP:CG	3:U:171:ASP:HB2	2.31	0.56
2:B:6:ILE:C	2:B:8:GLY:N	2.62	0.55
1:C:74:PRO:HA	1:C:141:ARG:HH12	1.70	0.55
1:E:153:TRP:O	1:E:154:LEU:HD23	2.06	0.55
4:H:33:TYR:HE2	4:H:100:TYR:HB2	1.71	0.55
4:T:201:THR:HG21	4:T:214:ASP:HB2	1.88	0.55
1:A:14:CYS:O	2:B:25:ARG:N	2.38	0.55
1:A:74:PRO:HD3	1:A:97:CYS:CB	2.31	0.55
1:A:180:TRP:CE2	1:A:204:VAL:HG21	2.41	0.55
2:B:105:GLN:O	2:B:108:ILE:HB	2.06	0.55
2:D:57:GLU:O	2:D:58:LYS:HG2	2.07	0.55
1:E:82:GLU:OE2	1:E:82:GLU:CA	2.54	0.55
1:E:293:PRO:O	1:E:294:PHE:HD2	1.89	0.55
2:F:52:LEU:O	2:F:53:ASN:C	2.45	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:4:LEU:HD23	3:L:89:CYS:SG	2.47	0.55
3:L:21:LEU:HB2	3:L:74:LEU:HB2	1.87	0.55
3:U:32:SER:HA	3:U:51:SER:HA	1.88	0.55
4:T:87:THR:CG2	4:T:89:GLU:HB2	2.37	0.55
1:A:283:THR:CG2	1:A:286:GLY:H	2.13	0.55
1:C:326:LYS:O	1:C:327:GLN:HB2	2.05	0.55
2:D:102:LEU:O	2:D:103:GLU:C	2.49	0.55
1:E:87:PHE:HB3	1:E:267:ILE:HG13	1.88	0.55
1:E:248:ASN:C	1:E:248:ASN:HD22	2.13	0.55
2:F:118:LEU:O	2:F:121:LYS:HB3	2.07	0.55
4:H:35:TRP:HB3	4:H:79:PHE:CZ	2.41	0.55
4:H:162:ASN:HD21	4:H:200:VAL:HA	1.71	0.55
3:U:149:TRP:HE1	3:U:178:SER:HB3	1.71	0.55
2:B:10:ILE:O	2:B:12:ASN:N	2.39	0.55
2:B:115:MET:O	2:B:117:LYS:N	2.36	0.55
1:C:82:GLU:OE2	1:C:83:THR:N	2.37	0.55
1:C:102:VAL:HG22	1:C:232:ILE:HB	1.88	0.55
1:E:74:PRO:HA	1:E:141:ARG:NH1	2.19	0.55
4:H:51:TYR:CE1	4:H:60:TYR:HB2	2.42	0.55
3:U:147:VAL:HG21	3:U:178:SER:OG	2.07	0.55
1:E:84:TRP:CZ2	1:E:116:GLY:HA2	2.42	0.55
2:F:163:ARG:O	2:F:164:ASP:C	2.50	0.55
4:H:15:SER:O	4:H:16:GLN:O	2.24	0.55
4:H:201:THR:HG23	4:H:215:LYS:C	2.31	0.55
3:U:80:GLU:O	3:U:83:ASP:N	2.39	0.55
3:U:116:VAL:HG13	3:U:136:PHE:O	2.07	0.55
3:U:171:ASP:HB3	3:U:173:THR:OG1	2.06	0.55
2:B:88:LYS:O	2:B:89:ILE:C	2.47	0.55
2:F:119:PHE:O	2:F:123:ARG:HB2	2.06	0.55
3:L:139:ASN:HA	3:L:174:TYR:O	2.06	0.55
4:H:142:MET:HA	4:H:192:SER:CA	2.35	0.55
4:H:177:LEU:HD12	4:H:181:LEU:O	2.07	0.55
3:U:113:ALA:HB2	3:U:201:THR:CB	2.37	0.55
4:T:190:VAL:HB	4:T:191:PRO:CD	2.36	0.55
2:B:25:ARG:HE	2:B:34:GLN:CD	2.15	0.55
2:B:170:ARG:HB3	2:B:171:PHE:CD1	2.41	0.55
2:D:91:LEU:O	2:D:92:TRP:C	2.46	0.55
1:E:138:ALA:O	1:E:140:LYS:NZ	2.40	0.55
3:L:44:SER:O	3:L:45:PRO:C	2.50	0.55
3:L:118:ILE:HD11	3:L:149:TRP:CH2	2.42	0.55
3:U:19:VAL:O	3:U:75:THR:HA	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:183:THR:OG1	3:U:186:GLU:CB	2.55	0.55
2:B:121:LYS:NZ	2:B:122:THR:N	2.55	0.55
1:C:36:VAL:CG2	1:C:320:MET:O	2.54	0.55
1:C:94:PHE:C	1:C:94:PHE:HD1	2.15	0.55
1:C:304:ALA:N	2:D:61:GLU:HG3	2.22	0.55
1:E:13:LEU:CD1	2:F:24:PHE:HB3	2.34	0.55
1:E:286:GLY:O	1:E:287:SER:CB	2.54	0.55
4:T:6:GLU:OE1	4:T:96:CYS:N	2.38	0.55
4:T:87:THR:OG1	4:T:88:ALA:N	2.36	0.55
4:T:190:VAL:HB	4:T:191:PRO:HD2	1.89	0.55
1:A:187:THR:OG1	1:A:189:GLN:HG2	2.06	0.55
1:A:295:GLN:HE22	1:A:308:TYR:HD1	1.54	0.55
2:D:128:GLU:HA	2:D:170:ARG:NH2	2.22	0.55
1:E:17:HIS:HE1	2:F:13:GLY:HA2	1.72	0.55
1:E:29:ILE:HB	2:F:105:GLN:NE2	2.22	0.55
3:L:175:SER:OG	4:H:171:HIS:CE1	2.60	0.55
4:H:24:VAL:HG11	4:H:29:ILE:HG23	1.88	0.55
4:H:27:TYR:CE1	4:H:31:SER:O	2.59	0.55
4:T:58:ASN:O	4:T:60:TYR:N	2.37	0.55
1:A:174:PHE:N	1:A:174:PHE:CD2	2.75	0.55
1:C:283:THR:O	1:C:284:PRO:C	2.49	0.55
2:D:38:LEU:O	2:D:40:SER:N	2.39	0.55
1:E:186:SER:CA	1:E:218:GLY:O	2.54	0.55
4:T:11:LEU:O	4:T:12:VAL:HG13	2.07	0.55
4:T:20:LEU:HD11	4:T:94:TYR:CB	2.37	0.55
2:B:126:LEU:CD2	2:B:152:ILE:HD11	2.37	0.54
1:E:64:CYS:HB2	1:E:79:PHE:HE1	1.72	0.54
4:H:195:TRP:O	4:H:197:SER:N	2.40	0.54
1:C:9:SER:C	2:D:143:LYS:HE3	2.32	0.54
2:D:18:ILE:C	2:D:20:GLY:H	2.15	0.54
2:F:131:GLU:O	2:F:139:LYS:HB3	2.07	0.54
2:D:166:ALA:H	2:D:168:ASN:ND2	2.04	0.54
1:E:22:ASN:H	1:E:22:ASN:ND2	2.03	0.54
1:E:106:ALA:O	1:E:109:ARG:HB3	2.06	0.54
2:F:47:GLN:OE1	2:F:110:LEU:HD21	2.07	0.54
3:L:19:VAL:HG21	3:L:79:LEU:CD2	2.35	0.54
4:H:15:SER:N	4:H:86:VAL:O	2.40	0.54
1:A:27:LYS:NZ	2:B:97:GLU:OE1	2.40	0.54
1:A:42:LEU:O	1:A:293:PRO:HD2	2.08	0.54
1:C:17:HIS:HA	2:D:22:TYR:HD2	1.72	0.54
1:C:121:ILE:HG13	1:C:257:TYR:CE1	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:TRP:C	1:E:154:LEU:HD23	2.33	0.54
1:E:292:LYS:HB3	1:E:293:PRO:HD2	1.89	0.54
4:H:201:THR:HG23	4:H:216:LYS:N	2.22	0.54
4:T:144:THR:O	4:T:145:LEU:HD23	2.07	0.54
2:D:76:ARG:HD2	2:F:81:GLU:OE2	2.06	0.54
1:E:42:LEU:O	1:E:293:PRO:HD2	2.07	0.54
3:L:47:LEU:HD12	3:L:48:TRP:N	2.21	0.54
4:H:150:LYS:HB2	4:H:183:THR:HG23	1.90	0.54
4:H:150:LYS:CB	4:H:183:THR:HG23	2.37	0.54
3:U:79:LEU:HD13	3:U:80:GLU:N	2.23	0.54
4:T:58:ASN:HB2	4:T:60:TYR:CE2	2.43	0.54
1:C:320:MET:CB	2:D:111:THR:HG21	2.37	0.54
4:T:41:PHE:HD1	4:T:92:ALA:HB2	1.72	0.54
1:A:169:PRO:CA	1:A:242:VAL:HG23	2.38	0.54
1:A:260:MET:HE1	2:F:73:VAL:HG21	1.89	0.54
2:B:121:LYS:HZ3	2:B:121:LYS:HB3	1.72	0.54
1:C:320:MET:HE1	2:D:22:TYR:CE2	2.42	0.54
2:D:6:ILE:C	2:D:8:GLY:N	2.63	0.54
2:D:52:LEU:O	2:D:53:ASN:C	2.51	0.54
1:E:44:GLN:N	1:E:294:PHE:O	2.37	0.54
3:L:191:ASN:HD22	3:L:191:ASN:H	1.55	0.54
4:H:56:GLY:O	4:H:58:ASN:OD1	2.26	0.54
4:H:65:LYS:O	4:H:66:ASN:C	2.50	0.54
4:H:217:ILE:O	4:H:219:PRO:HD3	2.08	0.54
1:C:43:VAL:O	1:C:43:VAL:HG12	2.06	0.54
2:D:108:ILE:C	2:D:110:LEU:N	2.62	0.54
1:E:307:LYS:HE2	2:F:60:ASN:HD22	1.71	0.54
2:F:115:MET:C	2:F:117:LYS:N	2.61	0.54
3:L:58:GLY:O	3:L:59:VAL:C	2.50	0.54
3:U:150:LYS:O	3:U:151:ILE:HB	2.08	0.54
3:U:205:PRO:O	3:U:206:ILE:C	2.50	0.54
4:T:61:ASN:CB	4:T:62:PRO:HD2	2.37	0.54
1:A:17:HIS:HA	2:B:22:TYR:CD2	2.43	0.54
1:A:109:ARG:NH2	1:A:267:ILE:HD13	2.22	0.54
1:A:206:THR:HB	1:A:241:ASP:OD1	2.08	0.54
2:B:9:PHE:C	2:B:9:PHE:HD1	2.16	0.54
1:C:44:GLN:HB3	1:C:295:GLN:CB	2.37	0.54
1:E:313:THR:O	1:E:314:LEU:HD23	2.07	0.54
3:L:149:TRP:HE1	3:L:178:SER:HB3	1.73	0.54
4:T:145:LEU:HB2	4:T:188:VAL:CG1	2.38	0.54
1:C:80:GLN:O	1:C:81:ASN:C	2.51	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:88:LYS:O	2:D:89:ILE:C	2.51	0.54
1:E:74:PRO:HG3	1:E:139:CYS:SG	2.48	0.54
1:E:102:VAL:HB	1:E:105:TYR:HD2	1.73	0.54
3:L:168:ASP:CG	3:L:169:SER:N	2.66	0.54
3:U:91:GLN:NE2	3:U:93:GLU:N	2.56	0.54
3:U:151:ILE:HA	3:U:193:TYR:HA	1.90	0.54
1:A:17:HIS:HD2	2:B:6:ILE:CG2	2.15	0.53
2:B:83:TYR:CD2	2:D:66:ILE:HG23	2.43	0.53
2:D:10:ILE:O	2:D:10:ILE:HG22	2.09	0.53
1:E:140:LYS:H	1:E:140:LYS:CD	2.20	0.53
3:L:81:ALA:O	3:L:107:ILE:HD11	2.07	0.53
3:L:118:ILE:CD1	3:L:195:CYS:HB2	2.37	0.53
4:T:29:ILE:HG22	4:T:35:TRP:CZ2	2.43	0.53
4:T:73:ASP:O	4:T:75:SER:N	2.41	0.53
1:A:59:LEU:HD12	1:A:59:LEU:C	2.32	0.53
2:B:129:ASN:ND2	2:B:159:HIS:HA	2.24	0.53
1:C:221:PRO:HG2	1:E:206:THR:C	2.34	0.53
2:D:106:HIS:ND1	2:D:106:HIS:C	2.65	0.53
1:E:109:ARG:HG2	1:E:109:ARG:NH1	2.23	0.53
3:L:116:VAL:HG13	3:L:136:PHE:O	2.08	0.53
1:A:38:ASN:HD22	1:A:318:THR:HB	1.74	0.53
2:B:76:ARG:O	2:B:77:ILE:C	2.49	0.53
3:U:52:THR:CG2	3:U:72:TYR:HE2	2.21	0.53
3:U:123:LYS:H	3:U:123:LYS:HD2	1.72	0.53
1:A:38:ASN:ND2	1:A:318:THR:HB	2.23	0.53
1:A:294:PHE:HB3	1:A:309:VAL:HG21	1.90	0.53
2:D:168:ASN:C	2:D:170:ARG:N	2.67	0.53
3:U:14:SER:CB	3:U:108:LYS:HB2	2.39	0.53
4:T:87:THR:HG21	4:T:89:GLU:HB2	1.91	0.53
1:A:117:THR:HG23	1:A:117:THR:O	2.09	0.53
1:A:187:THR:HB	1:A:189:GLN:OE1	2.09	0.53
1:C:67:ILE:O	1:C:70:LEU:HB3	2.08	0.53
3:L:52:THR:HG23	3:L:72:TYR:CE2	2.44	0.53
3:L:123:LYS:HB3	3:L:123:LYS:NZ	2.24	0.53
3:L:183:THR:O	3:L:184:LYS:C	2.49	0.53
4:H:11:LEU:HB2	4:H:117:THR:O	2.08	0.53
4:T:195:TRP:HB3	4:T:196:PRO:CD	2.37	0.53
2:D:129:ASN:ND2	2:D:159:HIS:HA	2.23	0.53
1:E:44:GLN:OE1	1:E:289:PRO:HG2	2.08	0.53
1:E:222:TRP:CD1	5:G:2:NAG:H2	2.43	0.53
2:F:149:ILE:C	2:F:151:SER:N	2.64	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:56:ALA:O	3:L:59:VAL:HG23	2.09	0.53
3:L:67:GLY:HA2	3:L:72:TYR:HA	1.90	0.53
3:U:38:GLN:HG3	3:U:87:TYR:CE1	2.41	0.53
3:U:167:GLN:CG	3:U:172:SER:HA	2.38	0.53
1:A:17:HIS:CG	1:A:18:HIS:H	2.26	0.53
1:A:283:THR:C	1:A:285:ASN:N	2.63	0.53
1:C:76:CYS:O	1:C:77:ASP:C	2.52	0.53
2:D:80:LEU:O	2:D:81:GLU:C	2.51	0.53
2:F:21:TRP:CE2	2:F:45:ILE:HD11	2.43	0.53
2:F:39:LYS:O	2:F:43:ALA:HB2	2.08	0.53
3:L:113:ALA:HB1	3:L:114:PRO:HD2	1.91	0.53
4:H:35:TRP:N	4:H:35:TRP:CD1	2.77	0.53
4:T:54:TYR:C	4:T:56:GLY:H	2.17	0.53
4:T:180:ASP:C	4:T:181:LEU:HD22	2.32	0.53
1:A:223:VAL:HG22	1:C:207:ARG:HG2	1.90	0.53
1:A:275:ASP:CG	1:A:276:THR:N	2.67	0.53
1:C:291:ASP:OD2	1:C:292:LYS:N	2.42	0.53
1:C:293:PRO:O	1:C:294:PHE:HD2	1.89	0.53
2:D:17:MET:HE1	2:D:19:ASP:HB2	1.91	0.53
2:F:9:PHE:CD1	2:F:9:PHE:C	2.87	0.53
4:T:125:PRO:HG3	4:T:209:SER:HB2	1.89	0.53
4:T:194:THR:HG23	4:T:198:GLU:OE2	2.09	0.53
2:B:149:ILE:C	2:B:151:SER:N	2.65	0.53
1:E:10:THR:HG22	2:F:142:HIS:C	2.34	0.53
1:E:25:LEU:HA	1:E:34:ILE:O	2.09	0.53
3:U:149:TRP:CD1	3:U:160:VAL:HG11	2.44	0.53
1:A:250:ASN:OD1	1:A:250:ASN:N	2.41	0.53
1:C:275:ASP:CG	1:C:276:THR:N	2.67	0.53
1:C:298:ASN:ND2	1:C:299:LYS:N	2.56	0.53
3:L:141:TYR:O	3:L:142:PRO:O	2.27	0.53
3:U:19:VAL:CG2	3:U:79:LEU:HD23	2.38	0.53
1:A:111:LEU:HD12	1:A:111:LEU:C	2.33	0.52
2:B:48:ILE:HG22	2:B:49:ASN:N	2.24	0.52
1:C:303:GLY:O	1:C:305:CYS:SG	2.68	0.52
1:E:36:VAL:HG22	1:E:37:THR:N	2.25	0.52
4:H:179:SER:O	4:H:180:ASP:HB2	2.08	0.52
4:T:62:PRO:HG2	4:T:64:LEU:H	1.75	0.52
1:A:220:ARG:HE	1:C:210:GLN:HE21	1.57	0.52
2:B:121:LYS:NZ	2:B:122:THR:CG2	2.73	0.52
2:F:3:PHE:HB2	2:F:112:ASP:OD2	2.09	0.52
2:F:88:LYS:O	2:F:89:ILE:C	2.52	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:145:ASP:N	2:F:148:CYS:HB3	2.13	0.52
3:L:61:ALA:O	3:L:63:PHE:N	2.43	0.52
3:L:167:GLN:CG	3:L:172:SER:HA	2.40	0.52
3:U:39:GLN:HB2	3:U:45:PRO:HA	1.92	0.52
4:T:24:VAL:O	4:T:25:THR:HG23	2.08	0.52
4:T:201:THR:HG23	4:T:216:LYS:N	2.23	0.52
1:A:87:PHE:O	1:A:267:ILE:HA	2.09	0.52
1:A:312:ASN:HD22	1:A:312:ASN:N	1.96	0.52
1:A:320:MET:HA	2:B:111:THR:HG21	1.91	0.52
1:C:166:VAL:HG22	1:C:245:ILE:HB	1.92	0.52
2:D:127:ARG:H	2:D:159:HIS:HB2	1.74	0.52
1:E:169:PRO:HA	1:E:242:VAL:HA	1.91	0.52
2:F:5:ALA:HB1	2:F:115:MET:HG2	1.91	0.52
3:L:95:PHE:HA	3:L:97:ARG:NH1	2.24	0.52
3:L:156:ARG:O	3:L:158:ASN:OD1	2.27	0.52
3:U:32:SER:C	3:U:33:PHE:CD1	2.88	0.52
4:T:6:GLU:O	4:T:7:SER:HB2	2.09	0.52
2:B:96:ALA:C	2:B:98:LEU:H	2.17	0.52
1:C:55:PRO:HG3	1:C:280:GLU:CD	2.34	0.52
1:E:177:LEU:CD1	1:E:236:ILE:HG22	2.40	0.52
1:E:202:VAL:HG22	1:E:247:SER:OG	2.09	0.52
2:F:17:MET:HE1	2:F:19:ASP:HB2	1.90	0.52
3:L:95:PHE:HZ	4:H:60:TYR:CB	2.20	0.52
1:C:74:PRO:HD2	1:C:96:ASN:O	2.10	0.52
1:C:249:GLY:C	1:C:250:ASN:OD1	2.52	0.52
2:D:67:GLU:C	2:D:68:LYS:HG3	2.35	0.52
1:E:283:THR:C	1:E:285:ASN:N	2.66	0.52
2:F:145:ASP:O	2:F:149:ILE:N	2.40	0.52
3:L:116:VAL:HG12	3:L:117:SER:H	1.73	0.52
4:H:131:LEU:HG	4:H:147:CYS:N	2.24	0.52
4:T:35:TRP:CD1	4:T:35:TRP:H	2.27	0.52
4:T:56:GLY:C	4:T:58:ASN:N	2.67	0.52
1:A:38:ASN:HD22	1:A:318:THR:CB	2.23	0.52
1:A:83:THR:O	1:A:84:TRP:HB3	2.08	0.52
1:A:102:VAL:HB	1:A:105:TYR:HD2	1.74	0.52
1:C:299:LYS:HA	1:C:308:TYR:CD1	2.44	0.52
1:E:17:HIS:CD2	2:F:6:ILE:HG23	2.34	0.52
2:F:154:ASN:HB3	2:F:156:THR:OG1	2.09	0.52
1:A:307:LYS:HE2	2:B:60:ASN:ND2	2.25	0.52
2:B:6:ILE:O	2:B:8:GLY:N	2.43	0.52
1:E:201:ARG:HG2	1:E:201:ARG:HH11	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:155:GLU:OE2	4:H:156:PRO:HA	2.09	0.52
4:H:184:LEU:HD12	4:H:185:SER:N	2.24	0.52
1:A:42:LEU:HD22	2:B:55:VAL:HG11	1.91	0.52
2:B:3:PHE:HB2	2:B:112:ASP:OD2	2.10	0.52
2:B:110:LEU:HD13	2:B:110:LEU:O	2.10	0.52
1:C:294:PHE:HB3	1:C:309:VAL:CG2	2.40	0.52
3:L:52:THR:O	3:L:52:THR:HG22	2.10	0.52
3:L:141:TYR:CG	3:L:142:PRO:HD3	2.44	0.52
3:U:30:THR:O	3:U:32:SER:N	2.40	0.52
3:U:173:THR:C	3:U:174:TYR:CD2	2.88	0.52
4:T:56:GLY:O	4:T:58:ASN:OD1	2.27	0.52
1:A:316:LEU:HD12	2:B:104:ASN:OD1	2.09	0.52
1:C:250:ASN:OD1	1:C:250:ASN:N	2.42	0.52
1:C:319:GLY:HA2	2:D:21:TRP:CH2	2.44	0.52
2:D:66:ILE:O	2:D:66:ILE:HG13	2.02	0.52
1:E:222:TRP:CG	5:G:2:NAG:H2	2.44	0.52
2:F:51:LYS:O	2:F:54:ARG:HB2	2.10	0.52
3:U:91:GLN:HE21	3:U:93:GLU:HB3	1.74	0.52
3:U:116:VAL:CG1	3:U:117:SER:H	2.22	0.52
4:T:33:TYR:CD2	4:T:99:PHE:O	2.55	0.52
1:A:238:LYS:HE2	2:F:72:GLU:HG3	1.92	0.52
2:D:100:VAL:O	2:D:104:ASN:HB2	2.09	0.52
1:E:127:TRP:CE3	1:E:164:LEU:HD23	2.45	0.52
1:E:298:ASN:HD22	1:E:299:LYS:N	2.07	0.52
2:F:6:ILE:C	2:F:8:GLY:H	2.18	0.52
3:L:32:SER:O	3:L:33:PHE:CD1	2.62	0.52
4:H:206:HIS:CE1	4:H:208:ALA:HB3	2.44	0.52
3:U:91:GLN:HE21	3:U:93:GLU:CB	2.23	0.52
1:A:209:SER:OG	1:A:210:GLN:N	2.42	0.51
1:E:62:ILE:HG22	1:E:63:ASP:N	2.25	0.51
2:F:67:GLU:C	2:F:68:LYS:HG3	2.35	0.51
4:H:162:ASN:O	4:H:163:SER:HB2	2.10	0.51
4:T:18:LEU:O	4:T:82:LYS:O	2.28	0.51
4:T:195:TRP:O	4:T:197:SER:N	2.43	0.51
1:A:320:MET:CA	2:B:111:THR:HG21	2.41	0.51
2:B:4:GLY:O	2:B:8:GLY:HA3	2.09	0.51
2:D:129:ASN:HD21	2:D:159:HIS:HA	1.75	0.51
2:F:42:GLN:O	2:F:46:ASP:N	2.43	0.51
2:F:171:PHE:HD1	2:F:171:PHE:H	1.55	0.51
3:L:96:PRO:O	3:L:98:THR:HG23	2.10	0.51
4:H:34:TYR:O	4:H:36:THR:HG22	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:67:ARG:HD2	4:H:83:LEU:O	2.09	0.51
3:U:52:THR:HG23	3:U:72:TYR:HE2	1.73	0.51
4:T:32:GLY:H	4:T:54:TYR:HB3	1.74	0.51
1:A:109:ARG:HG2	1:A:109:ARG:NH1	2.25	0.51
1:A:211:GLN:NE2	1:A:235:THR:OG1	2.44	0.51
2:B:3:PHE:CZ	2:F:2:LEU:O	2.63	0.51
2:B:91:LEU:HD21	2:D:92:TRP:NE1	2.25	0.51
1:A:326:LYS:O	1:A:327:GLN:HB2	2.09	0.51
1:C:163:VAL:HG22	1:C:248:ASN:HB3	1.91	0.51
3:L:21:LEU:CD2	3:L:87:TYR:CD2	2.93	0.51
3:L:167:GLN:HG3	3:L:172:SER:HA	1.91	0.51
4:T:56:GLY:O	4:T:58:ASN:N	2.43	0.51
1:A:169:PRO:HA	1:A:242:VAL:HG23	1.93	0.51
2:B:57:GLU:O	2:B:58:LYS:HG2	2.11	0.51
2:B:108:ILE:HG22	2:B:109:ASP:N	2.26	0.51
2:B:129:ASN:O	2:B:130:ALA:HB2	2.11	0.51
2:D:9:PHE:CD1	2:D:9:PHE:C	2.89	0.51
1:E:12:THR:HG23	2:F:138:PHE:O	2.10	0.51
1:E:172:ASP:CB	1:E:174:PHE:CE2	2.94	0.51
1:E:283:THR:HG23	1:E:285:ASN:C	2.35	0.51
2:F:9:PHE:HD1	2:F:10:ILE:N	2.09	0.51
4:H:61:ASN:HB3	4:H:62:PRO:CD	2.41	0.51
4:H:194:THR:HG23	4:H:198:GLU:OE2	2.10	0.51
1:A:143:PRO:HG2	1:A:144:GLY:H	1.75	0.51
1:E:132:GLN:O	1:E:133:ASN:C	2.53	0.51
2:F:67:GLU:O	2:F:68:LYS:HG3	2.11	0.51
3:L:36:TRP:CD2	3:L:74:LEU:HD23	2.45	0.51
4:H:128:VAL:HG11	4:H:204:VAL:HG21	1.92	0.51
1:A:25:LEU:HD23	1:A:34:ILE:C	2.36	0.51
1:A:125:PHE:HB2	1:A:127:TRP:NE1	2.26	0.51
3:L:124:ILE:O	3:L:125:GLN:C	2.54	0.51
4:T:20:LEU:CD1	4:T:94:TYR:HB3	2.40	0.51
4:T:49:MET:HE1	4:T:81:LEU:HD21	1.93	0.51
1:C:209:SER:O	1:C:210:GLN:CB	2.59	0.51
1:C:283:THR:C	1:C:285:ASN:H	2.17	0.51
1:E:217:ILE:HG22	1:E:218:GLY:N	2.26	0.51
1:E:248:ASN:C	1:E:248:ASN:ND2	2.69	0.51
1:E:294:PHE:HE1	2:F:96:ALA:HB1	1.71	0.51
3:L:29:ILE:HD11	3:L:34:LEU:HD13	1.92	0.51
3:U:141:TYR:CG	3:U:142:PRO:CD	2.93	0.51
4:T:33:TYR:CE2	4:T:100:TYR:HB2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:64:LEU:O	4:T:66:ASN:OD1	2.28	0.51
2:B:151:SER:O	2:B:156:THR:N	2.44	0.51
1:E:186:SER:O	1:E:218:GLY:O	2.29	0.51
2:F:96:ALA:C	2:F:98:LEU:N	2.68	0.51
2:F:168:ASN:C	2:F:170:ARG:H	2.19	0.51
3:L:119:PHE:CD2	4:H:131:LEU:HB3	2.45	0.51
1:C:108:LEU:O	1:C:108:LEU:HG	2.10	0.51
1:C:140:LYS:HD2	1:C:140:LYS:N	2.26	0.51
1:E:288:ILE:HG21	1:E:297:VAL:HG21	1.91	0.51
4:H:161:TRP:CZ3	4:H:202:CYS:HB3	2.45	0.51
3:U:25:ALA:O	3:U:26:SER:C	2.54	0.51
1:A:121:ILE:HG13	1:A:257:TYR:CZ	2.46	0.50
1:C:320:MET:HB3	2:D:111:THR:HG21	1.93	0.50
3:L:126:LEU:C	3:L:128:SER:N	2.65	0.50
4:H:195:TRP:CB	4:H:196:PRO:HD3	2.34	0.50
3:U:174:TYR:CD2	3:U:174:TYR:N	2.79	0.50
4:T:33:TYR:HD2	4:T:99:PHE:C	2.19	0.50
4:T:161:TRP:HB3	4:T:166:LEU:HB2	1.93	0.50
1:A:38:ASN:HD22	1:A:318:THR:HG21	1.76	0.50
1:A:294:PHE:HE1	2:B:96:ALA:HB1	1.72	0.50
1:C:29:ILE:O	2:F:51:LYS:HA	2.11	0.50
1:C:127:TRP:CZ3	1:C:164:LEU:HD23	2.46	0.50
1:C:166:VAL:HG23	1:C:166:VAL:O	2.12	0.50
1:C:283:THR:O	1:C:285:ASN:N	2.44	0.50
1:E:54:ASN:HB2	1:E:277:CYS:O	2.10	0.50
1:E:316:LEU:HD12	2:F:104:ASN:OD1	2.11	0.50
2:F:26:HIS:O	2:F:32:THR:HA	2.11	0.50
3:L:187:TYR:C	3:L:189:ARG:N	2.68	0.50
4:H:58:ASN:O	4:H:59:ASN:CB	2.58	0.50
4:T:4:LEU:HD12	4:T:110:TRP:O	2.12	0.50
1:A:187:THR:O	1:A:190:GLU:N	2.44	0.50
1:A:320:MET:HE3	2:B:21:TRP:CE3	2.46	0.50
2:B:3:PHE:CD2	2:B:113:SER:CA	2.85	0.50
1:C:15:LEU:N	1:C:15:LEU:HD23	2.26	0.50
1:C:294:PHE:HB3	1:C:309:VAL:HG21	1.92	0.50
1:E:10:THR:HG22	2:F:143:LYS:HD2	1.94	0.50
1:E:43:VAL:O	1:E:43:VAL:HG12	2.10	0.50
3:L:107:ILE:N	3:L:167:GLN:OE1	2.40	0.50
3:L:125:GLN:HB2	4:H:129:TYR:CD2	2.45	0.50
4:H:14:PRO:O	4:H:15:SER:CB	2.59	0.50
4:H:177:LEU:HB2	4:H:182:TYR:CE1	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:29:ILE:HG22	4:T:35:TRP:CD2	2.45	0.50
4:T:35:TRP:CD1	4:T:35:TRP:N	2.80	0.50
1:A:191:GLN:HE22	1:A:250:ASN:HD21	1.58	0.50
2:B:79:ASP:O	2:B:82:LYS:HB2	2.10	0.50
1:C:13:LEU:O	2:D:138:PHE:HB2	2.10	0.50
1:C:66:LEU:HD11	1:C:118:LEU:HD21	1.93	0.50
2:D:76:ARG:O	2:D:78:GLN:N	2.44	0.50
1:E:72:GLY:CA	1:E:149:SER:OG	2.52	0.50
1:E:201:ARG:O	1:E:247:SER:HA	2.12	0.50
1:E:285:ASN:HD22	1:E:298:ASN:HB2	1.75	0.50
2:F:40:SER:OG	2:F:114:GLU:HB3	2.12	0.50
3:L:183:THR:OG1	3:L:186:GLU:HB2	2.11	0.50
1:A:16:GLY:C	2:B:115:MET:HE1	2.36	0.50
2:B:127:ARG:HG3	2:B:159:HIS:CG	2.47	0.50
1:C:283:THR:HG23	1:C:283:THR:O	2.12	0.50
2:D:56:ILE:HG12	2:D:57:GLU:HG3	1.93	0.50
2:F:9:PHE:C	2:F:9:PHE:HD1	2.19	0.50
3:L:8:PRO:HB2	3:L:103:THR:CG2	2.41	0.50
3:L:209:SER:OG	3:L:210:PHE:CD1	2.64	0.50
1:C:43:VAL:O	1:C:45:SER:N	2.45	0.50
1:E:196:VAL:O	1:E:197:GLN:C	2.54	0.50
2:F:127:ARG:HH11	2:F:127:ARG:CB	2.16	0.50
3:L:153:GLY:O	3:L:154:SER:HB2	2.10	0.50
4:H:76:LYS:O	4:H:77:ASN:C	2.52	0.50
3:U:74:LEU:O	3:U:75:THR:HB	2.12	0.50
3:U:113:ALA:HB1	3:U:114:PRO:HD2	1.94	0.50
4:T:28:SER:O	4:T:31:SER:N	2.39	0.50
1:A:283:THR:O	1:A:284:PRO:C	2.54	0.50
2:D:6:ILE:C	2:D:8:GLY:H	2.18	0.50
2:D:21:TRP:CD2	2:D:45:ILE:HD11	2.45	0.50
1:E:19:ALA:O	1:E:20:VAL:HG13	2.12	0.50
1:E:191:GLN:O	1:E:192:THR:C	2.53	0.50
4:H:128:VAL:CG1	4:H:204:VAL:HG21	2.41	0.50
4:T:12:VAL:O	4:T:118:VAL:HA	2.12	0.50
1:A:64:CYS:SG	1:A:75:HIS:CE1	3.04	0.50
1:A:140:LYS:HD2	1:A:140:LYS:H	1.70	0.50
1:A:140:LYS:HD2	1:A:140:LYS:O	2.11	0.50
1:C:251:LEU:CD2	1:C:253:ALA:HB2	2.41	0.50
1:C:312:ASN:O	1:C:313:THR:HB	2.12	0.50
2:D:85:GLU:O	2:D:86:ASP:C	2.55	0.50
3:L:141:TYR:CD2	3:L:142:PRO:HD3	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:168:ASP:CG	3:L:169:SER:H	2.20	0.50
4:H:145:LEU:HB2	4:H:188:VAL:CG1	2.42	0.50
3:U:136:PHE:C	3:U:137:LEU:HD12	2.37	0.50
4:T:3:HIS:ND1	4:T:4:LEU:N	2.60	0.50
2:B:128:GLU:HA	2:B:170:ARG:NH2	2.26	0.50
1:E:41:GLU:OE2	1:E:314:LEU:N	2.41	0.50
1:E:320:MET:O	1:E:321:ARG:O	2.30	0.50
2:F:102:LEU:O	2:F:104:ASN:N	2.45	0.50
3:L:66:SER:OG	3:L:67:GLY:N	2.42	0.50
4:H:190:VAL:CG2	4:H:195:TRP:HB2	2.42	0.50
3:U:186:GLU:HG3	3:U:189:ARG:CZ	2.42	0.50
4:T:37:TRP:CZ3	4:T:96:CYS:HB3	2.47	0.50
1:A:62:ILE:HG22	1:A:63:ASP:N	2.22	0.49
1:A:212:THR:CG2	1:E:216:ASN:HB3	2.37	0.49
2:B:166:ALA:H	2:B:168:ASN:ND2	2.09	0.49
1:E:17:HIS:HA	2:F:22:TYR:HD2	1.77	0.49
2:F:38:LEU:C	2:F:40:SER:N	2.68	0.49
3:L:118:ILE:CD1	3:L:135:CYS:HB2	2.42	0.49
4:T:61:ASN:CB	4:T:62:PRO:CD	2.90	0.49
4:T:195:TRP:O	4:T:198:GLU:N	2.45	0.49
2:B:38:LEU:C	2:B:40:SER:H	2.19	0.49
2:D:38:LEU:C	2:D:40:SER:N	2.66	0.49
1:E:117:THR:C	1:E:118:LEU:HD23	2.37	0.49
1:E:147:PHE:CE2	1:E:153:TRP:HB2	2.47	0.49
1:E:169:PRO:HA	1:E:242:VAL:HG23	1.94	0.49
2:F:6:ILE:CG1	2:F:112:ASP:HA	2.38	0.49
2:F:110:LEU:HD13	2:F:110:LEU:C	2.37	0.49
3:L:29:ILE:HD11	3:L:34:LEU:CD1	2.42	0.49
4:H:114:THR:O	4:H:114:THR:HG23	2.12	0.49
3:U:191:ASN:HD22	3:U:191:ASN:N	2.09	0.49
4:T:4:LEU:HA	4:T:23:TYR:O	2.12	0.49
1:E:217:ILE:N	1:E:217:ILE:CD1	2.75	0.49
4:H:3:HIS:O	4:H:24:VAL:HA	2.11	0.49
4:H:129:TYR:HB2	4:H:148:LEU:CD2	2.42	0.49
4:H:159:VAL:HG11	4:H:186:SER:HB2	1.93	0.49
3:U:4:LEU:N	3:U:4:LEU:CD1	2.75	0.49
1:A:197:GLN:H	1:A:197:GLN:CD	2.19	0.49
1:C:161:TYR:N	1:C:196:VAL:HG21	2.28	0.49
1:E:138:ALA:HB1	1:E:224:ARG:HG2	1.93	0.49
2:F:78:GLN:O	2:F:79:ASP:C	2.54	0.49
2:F:152:ILE:C	2:F:154:ASN:N	2.71	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:125:GLN:HB2	4:H:129:TYR:CG	2.48	0.49
4:H:20:LEU:HB2	4:H:81:LEU:HB3	1.95	0.49
4:H:56:GLY:C	4:H:58:ASN:N	2.64	0.49
3:U:187:TYR:C	3:U:189:ARG:N	2.69	0.49
4:T:37:TRP:HB3	4:T:49:MET:HE3	1.95	0.49
2:B:98:LEU:O	2:B:99:LEU:C	2.55	0.49
1:C:226:LEU:HD21	4:T:104:ASP:CB	2.42	0.49
2:D:68:LYS:HE2	2:D:85:GLU:OE2	2.12	0.49
2:D:110:LEU:O	2:D:110:LEU:HD13	2.12	0.49
2:F:24:PHE:CE1	2:F:153:ARG:HG3	2.48	0.49
2:F:125:GLN:OE1	2:F:152:ILE:HG23	2.13	0.49
3:L:127:THR:HG22	3:L:127:THR:O	2.12	0.49
3:U:14:SER:HB3	3:U:108:LYS:HB2	1.94	0.49
3:U:137:LEU:CD2	3:U:145:ILE:HD13	2.26	0.49
3:U:151:ILE:CA	3:U:192:SER:O	2.60	0.49
4:T:161:TRP:CB	4:T:166:LEU:HB2	2.42	0.49
2:B:51:LYS:NZ	2:B:106:HIS:ND1	2.58	0.49
1:C:312:ASN:ND2	1:C:313:THR:HG22	2.28	0.49
1:E:29:ILE:HD11	2:F:102:LEU:CD2	2.23	0.49
3:L:32:SER:C	3:L:33:PHE:CD1	2.90	0.49
4:T:6:GLU:O	4:T:7:SER:CB	2.61	0.49
1:A:39:ALA:HA	1:A:316:LEU:O	2.13	0.49
1:C:10:THR:CG2	2:D:141:TYR:O	2.60	0.49
1:C:136:SER:OG	4:T:104:ASP:OD1	2.23	0.49
2:D:159:HIS:C	2:D:159:HIS:ND1	2.70	0.49
2:F:122:THR:C	2:F:124:ARG:N	2.71	0.49
3:L:151:ILE:HA	3:L:192:SER:O	2.12	0.49
3:U:96:PRO:HA	4:T:48:TRP:CZ3	2.47	0.49
1:A:50:LYS:O	1:A:286:GLY:O	2.31	0.49
1:A:121:ILE:HG13	1:A:257:TYR:CE1	2.47	0.49
2:B:48:ILE:HD11	2:B:107:THR:CG2	2.43	0.49
1:C:74:PRO:CG	1:C:139:CYS:SG	3.00	0.49
1:C:82:GLU:OE2	1:C:82:GLU:CA	2.59	0.49
1:C:283:THR:HG23	1:C:285:ASN:CA	2.42	0.49
1:E:37:THR:HG23	1:E:321:ARG:O	2.12	0.49
2:F:122:THR:C	2:F:124:ARG:H	2.18	0.49
3:L:124:ILE:O	3:L:127:THR:N	2.46	0.49
3:U:134:VAL:HA	3:U:179:THR:HA	1.94	0.49
1:A:19:ALA:HB1	1:A:322:ASN:OD1	2.12	0.49
1:C:191:GLN:O	1:C:192:THR:C	2.55	0.49
2:D:24:PHE:CE1	2:D:153:ARG:HG3	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:29:ILE:HA	3:L:93:GLU:OE1	2.13	0.49
3:L:82:GLU:C	3:L:84:GLY:H	2.21	0.49
4:H:190:VAL:HB	4:H:191:PRO:CD	2.42	0.49
3:U:166:ASP:O	3:U:167:GLN:C	2.55	0.49
1:A:82:GLU:OE2	1:A:82:GLU:CA	2.61	0.49
1:A:139:CYS:SG	1:A:147:PHE:O	2.70	0.49
2:B:117:LYS:HE3	2:F:4:GLY:CA	2.42	0.49
1:C:111:LEU:HD12	1:C:111:LEU:C	2.37	0.49
1:C:321:ARG:HG2	1:C:322:ASN:N	2.24	0.49
2:D:9:PHE:C	2:D:9:PHE:HD1	2.21	0.49
2:D:67:GLU:O	2:D:68:LYS:HG3	2.13	0.49
2:D:127:ARG:HD2	2:D:159:HIS:CE1	2.48	0.49
2:D:150:GLU:O	2:D:150:GLU:HG3	2.12	0.49
2:F:70:PHE:HD1	2:F:82:LYS:HE3	1.77	0.49
4:T:188:VAL:CG2	4:T:189:THR:N	2.74	0.49
1:A:311:GLN:H	1:A:311:GLN:CD	2.21	0.48
2:F:55:VAL:HG12	2:F:56:ILE:H	1.71	0.48
3:L:63:PHE:HE1	3:L:76:ILE:HD11	1.78	0.48
3:L:137:LEU:O	3:L:140:PHE:HE1	1.96	0.48
3:U:33:PHE:CZ	4:T:101:TYR:HE1	2.31	0.48
3:U:74:LEU:O	3:U:75:THR:CB	2.60	0.48
1:A:248:ASN:C	1:A:248:ASN:HD22	2.20	0.48
1:A:307:LYS:HD3	2:B:92:TRP:CZ2	2.48	0.48
1:C:36:VAL:CG2	1:C:37:THR:N	2.77	0.48
1:C:43:VAL:HA	1:C:294:PHE:O	2.13	0.48
2:D:127:ARG:C	2:D:129:ASN:H	2.21	0.48
1:E:12:THR:HB	2:F:27:GLN:CB	2.40	0.48
1:E:14:CYS:HA	2:F:137:CYS:HA	1.95	0.48
1:E:170:ASN:OD1	1:E:176:LYS:HD3	2.12	0.48
2:F:171:PHE:CD1	2:F:171:PHE:N	2.73	0.48
3:L:124:ILE:O	3:L:126:LEU:N	2.46	0.48
4:H:35:TRP:CD1	4:H:35:TRP:H	2.31	0.48
2:B:38:LEU:O	2:B:40:SER:N	2.47	0.48
1:C:61:GLY:O	1:C:62:ILE:HB	2.14	0.48
1:E:130:VAL:HG13	1:E:162:PRO:HD2	1.95	0.48
1:E:138:ALA:C	1:E:140:LYS:NZ	2.71	0.48
1:E:283:THR:HG22	1:E:287:SER:N	2.28	0.48
2:F:89:ILE:O	2:F:90:ASP:C	2.56	0.48
2:F:107:THR:O	2:F:110:LEU:HB3	2.13	0.48
3:L:97:ARG:CB	4:H:48:TRP:CG	2.96	0.48
3:L:116:VAL:HG13	3:L:137:LEU:HD12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:162:ASN:HA	3:L:177:SER:O	2.14	0.48
3:L:162:ASN:HB3	3:L:176:MET:HE3	1.95	0.48
4:H:27:TYR:CE1	4:H:31:SER:HB2	2.48	0.48
4:H:51:TYR:C	4:H:59:ASN:O	2.56	0.48
3:U:131:ALA:O	3:U:181:THR:HA	2.13	0.48
4:T:159:VAL:CG2	4:T:160:THR:N	2.76	0.48
4:T:184:LEU:HD12	4:T:184:LEU:C	2.38	0.48
1:C:17:HIS:ND1	1:C:18:HIS:N	2.60	0.48
1:C:54:ASN:ND2	1:C:55:PRO:HA	2.23	0.48
4:H:149:VAL:O	4:H:183:THR:HA	2.13	0.48
1:A:18:HIS:CA	2:B:14:TRP:HB2	2.31	0.48
2:B:21:TRP:CE2	2:B:45:ILE:HD11	2.49	0.48
2:B:56:ILE:HG12	2:B:57:GLU:HG3	1.94	0.48
2:B:124:ARG:NH2	2:F:132:GLU:HB3	2.26	0.48
2:B:140:ILE:HD12	2:B:140:ILE:N	2.27	0.48
2:B:167:LEU:HB3	2:F:171:PHE:CD2	2.37	0.48
2:B:170:ARG:NH1	2:D:127:ARG:HH22	2.10	0.48
1:C:320:MET:HB3	2:D:111:THR:CG2	2.44	0.48
2:D:121:LYS:NZ	2:D:122:THR:CG2	2.76	0.48
2:F:17:MET:HE2	2:F:17:MET:HA	1.96	0.48
2:F:108:ILE:HG22	2:F:109:ASP:N	2.27	0.48
2:F:121:LYS:HZ1	2:F:122:THR:CA	2.27	0.48
2:F:122:THR:O	2:F:124:ARG:N	2.33	0.48
3:L:81:ALA:O	3:L:107:ILE:CD1	2.61	0.48
3:L:122:SER:O	3:L:126:LEU:HG	2.14	0.48
4:H:13:LYS:O	4:H:14:PRO:C	2.55	0.48
4:H:18:LEU:HD12	4:H:18:LEU:C	2.36	0.48
4:H:130:PRO:C	4:H:131:LEU:HD23	2.38	0.48
3:U:137:LEU:O	3:U:175:SER:HA	2.14	0.48
3:U:162:ASN:HB3	3:U:176:MET:HE3	1.94	0.48
2:B:85:GLU:OE1	2:F:83:TYR:OH	2.27	0.48
1:C:72:GLY:HA3	1:C:149:SER:OG	2.13	0.48
1:C:176:LYS:HD2	1:C:257:TYR:CG	2.49	0.48
1:C:236:ILE:O	1:C:236:ILE:HG13	2.13	0.48
2:D:10:ILE:O	2:D:12:ASN:N	2.44	0.48
2:D:91:LEU:O	2:D:93:SER:N	2.46	0.48
1:E:108:LEU:O	1:E:108:LEU:HG	2.13	0.48
3:U:2:ILE:HG22	3:U:4:LEU:HD12	1.96	0.48
3:U:44:SER:O	3:U:45:PRO:C	2.57	0.48
3:U:141:TYR:CG	3:U:142:PRO:N	2.81	0.48
4:T:184:LEU:HD12	4:T:185:SER:CA	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ILE:CG1	1:A:257:TYR:CE1	2.96	0.48
2:D:83:TYR:OH	2:F:85:GLU:OE1	2.24	0.48
1:E:22:ASN:HD22	1:E:22:ASN:N	2.01	0.48
4:T:2:VAL:HB	4:T:109:TYR:CD2	2.47	0.48
1:A:17:HIS:CG	1:A:18:HIS:N	2.80	0.48
1:C:160:THR:C	1:C:196:VAL:HG21	2.38	0.48
1:C:186:SER:O	1:C:218:GLY:O	2.31	0.48
1:C:191:GLN:OE1	1:C:250:ASN:ND2	2.45	0.48
2:D:89:ILE:HD12	2:D:89:ILE:H	1.79	0.48
3:L:149:TRP:O	3:L:154:SER:HB3	2.14	0.48
4:H:146:GLY:O	4:H:161:TRP:HH2	1.97	0.48
4:T:161:TRP:CD1	4:T:170:VAL:HG11	2.47	0.48
1:A:10:THR:CG2	2:B:143:LYS:HD2	2.41	0.48
2:B:4:GLY:O	2:B:5:ALA:O	2.31	0.48
2:D:3:PHE:HB3	2:D:112:ASP:O	2.14	0.48
2:D:43:ALA:O	2:D:46:ASP:HB2	2.13	0.48
2:D:165:GLU:C	2:D:168:ASN:HD21	2.22	0.48
1:E:54:ASN:HD22	1:E:55:PRO:HA	1.79	0.48
1:E:164:LEU:O	1:E:246:ASN:HA	2.14	0.48
2:F:26:HIS:O	2:F:26:HIS:ND1	2.47	0.48
2:F:76:ARG:O	2:F:77:ILE:C	2.55	0.48
3:L:121:PRO:HB2	3:L:126:LEU:CD2	2.32	0.48
4:H:177:LEU:HD12	4:H:178:GLN:H	1.79	0.48
4:T:201:THR:OG1	4:T:216:LYS:HA	2.13	0.48
1:A:13:LEU:CD1	2:B:24:PHE:HB3	2.38	0.48
1:A:176:LYS:HE3	1:A:178:TYR:OH	2.14	0.48
1:C:202:VAL:O	1:C:212:THR:HG23	2.13	0.48
1:C:309:VAL:CG1	2:D:93:SER:HA	2.40	0.48
1:E:18:HIS:HA	2:F:14:TRP:CB	2.36	0.48
1:E:182:ILE:HG22	1:E:231:SER:HB2	1.95	0.48
3:L:91:GLN:HE21	3:L:93:GLU:CB	2.27	0.48
3:L:91:GLN:C	3:L:91:GLN:CD	2.81	0.48
2:B:28:ASN:CB	2:B:144:CYS:O	2.58	0.47
2:B:82:LYS:O	2:B:84:VAL:N	2.47	0.47
1:E:36:VAL:HG23	1:E:320:MET:O	2.14	0.47
1:E:318:THR:O	2:F:48:ILE:HG21	2.13	0.47
2:F:6:ILE:C	2:F:8:GLY:N	2.71	0.47
3:L:63:PHE:CE1	3:L:76:ILE:HD11	2.48	0.47
3:U:207:VAL:O	3:U:208:LYS:HG2	2.14	0.47
4:T:201:THR:HG22	4:T:202:CYS:O	2.14	0.47
1:A:117:THR:C	1:A:118:LEU:HD23	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:LEU:CD1	1:C:234:TRP:CE3	2.92	0.47
2:D:94:TYR:CE2	2:F:95:ASN:HB3	2.48	0.47
1:E:48:THR:HG23	1:E:49:GLY:N	2.29	0.47
1:E:98:TYR:HE2	1:E:229:ARG:HA	1.78	0.47
1:E:318:THR:O	1:E:318:THR:HG22	2.13	0.47
3:L:19:VAL:O	3:L:75:THR:HA	2.14	0.47
3:L:107:ILE:HG22	3:L:108:LYS:H	1.79	0.47
4:H:6:GLU:CD	4:H:113:GLY:HA2	2.39	0.47
4:H:87:THR:HG23	4:H:90:ASP:H	1.78	0.47
4:H:188:VAL:HG22	4:H:189:THR:H	1.69	0.47
3:U:97:ARG:N	4:T:48:TRP:CE3	2.82	0.47
3:U:186:GLU:O	3:U:189:ARG:HB2	2.14	0.47
4:T:5:GLN:OE1	4:T:5:GLN:HA	2.14	0.47
4:T:188:VAL:CG2	4:T:189:THR:H	2.27	0.47
4:T:194:THR:HG23	4:T:198:GLU:CD	2.39	0.47
1:A:13:LEU:O	2:B:138:PHE:HB2	2.15	0.47
1:A:36:VAL:CG2	1:A:320:MET:O	2.62	0.47
1:A:73:ASP:OD1	1:A:75:HIS:CD2	2.68	0.47
1:A:153:TRP:CD1	1:A:153:TRP:C	2.91	0.47
1:A:283:THR:HG22	1:A:287:SER:N	2.29	0.47
2:B:9:PHE:CE1	2:B:10:ILE:HG13	2.50	0.47
1:C:33:GLN:O	1:C:34:ILE:HG13	2.13	0.47
1:C:38:ASN:HD22	1:C:318:THR:HB	1.79	0.47
1:C:109:ARG:HG2	1:C:109:ARG:HH11	1.79	0.47
1:E:242:VAL:HG22	1:E:243:LEU:N	2.29	0.47
2:F:140:ILE:HD12	2:F:140:ILE:N	2.28	0.47
3:U:150:LYS:HB2	3:U:194:THR:OG1	2.13	0.47
1:A:248:ASN:C	1:A:248:ASN:ND2	2.73	0.47
2:B:26:HIS:CE1	2:B:32:THR:C	2.92	0.47
2:B:91:LEU:O	2:B:92:TRP:C	2.56	0.47
1:C:44:GLN:N	1:C:294:PHE:O	2.45	0.47
1:C:81:ASN:ND2	1:C:119:GLU:HA	2.29	0.47
1:C:220:ARG:HH21	1:E:210:GLN:HE21	1.63	0.47
2:D:119:PHE:C	2:D:121:LYS:H	2.22	0.47
4:T:86:VAL:HG22	4:T:87:THR:O	2.13	0.47
4:T:91:THR:HB	4:T:118:VAL:H	1.80	0.47
1:A:266:SER:OG	1:A:267:ILE:N	2.47	0.47
2:B:145:ASP:N	2:B:148:CYS:HB3	2.16	0.47
2:D:3:PHE:HB2	2:D:112:ASP:O	2.13	0.47
2:D:57:GLU:O	2:D:58:LYS:CG	2.62	0.47
2:D:129:ASN:O	2:D:130:ALA:CB	2.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:LYS:O	1:E:286:GLY:O	2.32	0.47
1:E:324:PRO:HB3	1:E:328:THR:HB	1.96	0.47
2:F:26:HIS:O	2:F:32:THR:HG22	2.14	0.47
4:H:41:PHE:HD1	4:H:92:ALA:HB2	1.80	0.47
4:T:22:CYS:HB3	4:T:79:PHE:CE1	2.49	0.47
4:T:174:PRO:O	4:T:175:ALA:C	2.57	0.47
2:B:163:ARG:O	2:B:164:ASP:C	2.57	0.47
2:D:86:ASP:O	2:D:87:THR:C	2.56	0.47
2:D:100:VAL:O	2:D:101:ALA:C	2.57	0.47
1:E:182:ILE:HD11	1:E:215:PRO:HD3	1.95	0.47
1:E:187:THR:HB	1:E:189:GLN:CD	2.40	0.47
2:F:10:ILE:C	2:F:12:ASN:H	2.20	0.47
2:F:25:ARG:HE	2:F:34:GLN:CD	2.22	0.47
2:F:39:LYS:O	2:F:39:LYS:HG2	2.15	0.47
2:F:120:GLU:OE1	2:F:120:GLU:HA	2.14	0.47
3:L:35:TYR:HD2	3:L:50:TYR:HA	1.78	0.47
3:L:95:PHE:HD1	3:L:97:ARG:HH12	1.63	0.47
4:H:126:PRO:CB	4:H:152:TYR:HB3	2.34	0.47
3:U:141:TYR:O	3:U:142:PRO:O	2.32	0.47
3:U:164:TRP:CG	3:U:176:MET:HG3	2.49	0.47
4:T:28:SER:HA	4:T:77:ASN:ND2	2.30	0.47
4:T:88:ALA:O	4:T:91:THR:HG22	2.14	0.47
4:T:146:GLY:O	4:T:161:TRP:HH2	1.96	0.47
1:A:32:ASP:O	1:A:33:GLN:NE2	2.46	0.47
2:B:103:GLU:OE1	1:E:29:ILE:HG23	2.14	0.47
2:B:125:GLN:OE1	2:B:152:ILE:HG23	2.15	0.47
1:C:35:GLU:HG2	1:C:322:ASN:HD22	1.79	0.47
1:C:54:ASN:HB3	1:C:278:ILE:HD13	1.95	0.47
1:C:117:THR:O	1:C:117:THR:CG2	2.62	0.47
1:C:312:ASN:HD22	1:C:312:ASN:N	2.11	0.47
2:D:28:ASN:CB	2:D:144:CYS:O	2.59	0.47
1:E:13:LEU:C	1:E:13:LEU:HD13	2.40	0.47
1:E:54:ASN:CB	1:E:278:ILE:HD13	2.44	0.47
1:E:176:LYS:HD2	1:E:257:TYR:CD2	2.49	0.47
2:F:85:GLU:HG3	2:F:89:ILE:HD13	1.96	0.47
2:F:141:TYR:OH	2:F:170:ARG:HG2	2.15	0.47
3:L:35:TYR:N	3:L:35:TYR:CD1	2.81	0.47
3:L:74:LEU:O	3:L:75:THR:CB	2.63	0.47
3:L:74:LEU:O	3:L:75:THR:HB	2.15	0.47
3:U:11:MET:O	3:U:105:LEU:HA	2.14	0.47
3:U:125:GLN:HB2	4:T:129:TYR:CG	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:53:SER:HG	4:T:55:ASP:HB2	1.75	0.47
2:B:17:MET:SD	2:B:17:MET:C	2.98	0.47
2:B:117:LYS:CE	2:F:4:GLY:HA2	2.42	0.47
1:C:13:LEU:HD13	1:C:14:CYS:N	2.30	0.47
2:D:17:MET:HE2	2:D:17:MET:HA	1.97	0.47
1:E:251:LEU:HD21	1:E:253:ALA:HB2	1.97	0.47
1:E:270:SER:HB2	1:E:284:PRO:HA	1.97	0.47
3:L:32:SER:C	3:L:33:PHE:HD1	2.23	0.47
3:L:123:LYS:CD	3:L:124:ILE:HG13	2.45	0.47
4:H:20:LEU:HD23	4:H:20:LEU:HA	1.63	0.47
4:T:126:PRO:HB3	4:T:152:TYR:CB	2.32	0.47
1:A:35:GLU:O	1:A:322:ASN:HB3	2.14	0.47
2:B:21:TRP:CD2	2:B:45:ILE:HD11	2.50	0.47
1:C:15:LEU:HD11	2:D:119:PHE:HB2	1.97	0.47
1:C:174:PHE:N	1:C:174:PHE:CD2	2.83	0.47
1:C:209:SER:OG	1:C:210:GLN:N	2.41	0.47
1:C:295:GLN:OE1	1:C:297:VAL:N	2.46	0.47
1:E:139:CYS:O	1:E:146:GLY:C	2.58	0.47
1:A:41:GLU:HG3	1:A:42:LEU:N	2.29	0.47
2:B:2:LEU:O	2:D:3:PHE:CZ	2.68	0.47
1:C:294:PHE:CE1	2:D:96:ALA:CB	2.97	0.47
2:D:130:ALA:CB	2:D:139:LYS:O	2.59	0.47
1:E:14:CYS:O	2:F:25:ARG:N	2.48	0.47
1:E:141:ARG:HH11	1:E:141:ARG:CG	2.21	0.47
4:T:40:GLN:HB3	4:T:46:LEU:HD23	1.97	0.47
4:T:54:TYR:O	4:T:56:GLY:N	2.48	0.47
4:T:123:THR:HA	4:T:154:PRO:HD3	1.96	0.47
1:A:70:LEU:O	1:A:71:LEU:C	2.58	0.46
2:B:67:GLU:O	2:B:68:LYS:HG3	2.15	0.46
2:B:111:THR:C	2:B:113:SER:N	2.70	0.46
1:C:121:ILE:HG13	1:C:257:TYR:CZ	2.50	0.46
1:C:323:VAL:HA	1:C:324:PRO:HD3	1.79	0.46
2:D:48:ILE:HG22	2:D:49:ASN:N	2.30	0.46
4:H:67:ARG:O	4:H:68:ILE:C	2.57	0.46
4:H:177:LEU:HD12	4:H:178:GLN:N	2.30	0.46
4:H:180:ASP:C	4:H:181:LEU:HD22	2.40	0.46
1:A:29:ILE:CG2	2:D:103:GLU:OE1	2.62	0.46
2:B:30:GLU:OE2	2:B:145:ASP:HB2	2.15	0.46
1:C:298:ASN:ND2	1:C:298:ASN:C	2.71	0.46
2:D:119:PHE:O	2:D:123:ARG:HB2	2.15	0.46
1:E:87:PHE:O	1:E:267:ILE:HA	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:SER:CB	1:E:251:LEU:HB2	2.46	0.46
2:F:145:ASP:O	2:F:149:ILE:HG12	2.14	0.46
3:L:63:PHE:CE1	3:L:76:ILE:CD1	2.98	0.46
4:H:218:VAL:O	4:H:219:PRO:C	2.56	0.46
3:U:118:ILE:HD11	3:U:149:TRP:CZ3	2.51	0.46
3:U:133:VAL:N	3:U:180:LEU:O	2.32	0.46
4:T:2:VAL:HG13	4:T:24:VAL:HG23	1.97	0.46
4:T:177:LEU:HD12	4:T:178:GLN:N	2.31	0.46
2:B:165:GLU:CA	2:B:168:ASN:HD21	2.29	0.46
2:B:166:ALA:N	2:B:168:ASN:ND2	2.59	0.46
1:C:17:HIS:N	2:D:115:MET:HE1	2.30	0.46
1:E:70:LEU:HD22	1:E:112:VAL:HG21	1.97	0.46
1:E:283:THR:HG23	1:E:283:THR:O	2.14	0.46
2:F:106:HIS:O	2:F:106:HIS:CG	2.68	0.46
2:F:121:LYS:HZ1	2:F:122:THR:N	2.12	0.46
2:F:132:GLU:HG3	2:F:137:CYS:O	2.16	0.46
1:A:118:LEU:HD23	1:A:118:LEU:N	2.30	0.46
2:B:4:GLY:O	2:B:5:ALA:C	2.59	0.46
1:C:13:LEU:HD13	1:C:13:LEU:C	2.41	0.46
1:C:85:ASP:HA	1:C:265:SER:HB3	1.96	0.46
2:D:48:ILE:CD1	2:D:107:THR:HG23	2.36	0.46
1:E:312:ASN:H	1:E:312:ASN:ND2	2.14	0.46
3:L:79:LEU:HD13	3:L:80:GLU:N	2.30	0.46
4:H:84:ASN:HB3	4:H:85:SER:H	1.42	0.46
4:H:201:THR:HG21	4:H:214:ASP:HB2	1.97	0.46
4:T:62:PRO:HG2	4:T:63:SER:N	2.29	0.46
1:A:222:TRP:CG	5:I:2:NAG:H2	2.50	0.46
1:C:121:ILE:CG1	1:C:257:TYR:CE1	2.98	0.46
2:D:80:LEU:O	2:D:82:LYS:N	2.49	0.46
2:D:171:PHE:HD1	2:D:171:PHE:H	1.56	0.46
1:E:53:ASN:OD1	1:E:276:THR:HA	2.16	0.46
1:E:167:THR:HG23	1:E:167:THR:O	2.13	0.46
1:E:195:TYR:O	1:E:196:VAL:HB	2.15	0.46
1:E:268:MET:SD	1:E:284:PRO:HG3	2.56	0.46
2:F:68:LYS:HE2	2:F:85:GLU:CD	2.41	0.46
3:L:25:ALA:O	3:L:27:SER:O	2.34	0.46
4:H:87:THR:HG23	4:H:89:GLU:HB2	1.97	0.46
3:U:175:SER:OG	4:T:171:HIS:ND1	2.49	0.46
4:T:67:ARG:CB	4:T:84:ASN:HB2	2.45	0.46
1:A:237:VAL:CG1	1:A:241:ASP:HB3	2.41	0.46
2:D:89:ILE:HD12	2:D:89:ILE:N	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:89:ILE:H	2:D:89:ILE:CD1	2.28	0.46
1:E:15:LEU:HD11	2:F:119:PHE:HB2	1.97	0.46
1:E:29:ILE:HG12	2:F:101:ALA:O	2.15	0.46
1:E:48:THR:HG23	1:E:49:GLY:H	1.81	0.46
1:E:217:ILE:HD12	1:E:217:ILE:H	1.79	0.46
1:E:312:ASN:N	1:E:312:ASN:HD22	2.13	0.46
2:F:129:ASN:O	2:F:130:ALA:HB2	2.14	0.46
3:L:34:LEU:HD22	3:L:72:TYR:CD2	2.50	0.46
4:H:107:PHE:HE1	4:H:109:TYR:HE1	1.63	0.46
3:U:66:SER:HB3	3:U:73:SER:OG	2.15	0.46
4:T:142:MET:HA	4:T:192:SER:CA	2.37	0.46
4:T:143:VAL:O	4:T:189:THR:HG23	2.16	0.46
1:A:17:HIS:CE1	2:B:13:GLY:HA2	2.48	0.46
1:A:84:TRP:HZ2	1:A:113:ALA:HA	1.80	0.46
1:A:191:GLN:OE1	1:A:250:ASN:ND2	2.48	0.46
2:B:5:ALA:O	2:B:8:GLY:N	2.47	0.46
2:B:16:GLY:O	2:B:18:ILE:HG23	2.16	0.46
1:C:98:TYR:CZ	1:C:226:LEU:HD13	2.50	0.46
1:C:103:PRO:O	1:C:104:ASP:C	2.59	0.46
2:D:76:ARG:O	2:D:79:ASP:N	2.48	0.46
2:D:145:ASP:O	2:D:149:ILE:HG12	2.16	0.46
2:F:168:ASN:O	2:F:170:ARG:N	2.48	0.46
4:H:128:VAL:O	4:H:215:LYS:HE3	2.16	0.46
4:H:216:LYS:HE2	4:T:194:THR:OG1	2.15	0.46
4:T:33:TYR:HE2	4:T:100:TYR:HB2	1.80	0.46
1:A:15:LEU:C	2:B:14:TRP:CZ2	2.94	0.46
1:A:201:ARG:HH12	1:A:246:ASN:ND2	2.12	0.46
1:A:206:THR:CA	1:E:221:PRO:HG2	2.46	0.46
1:A:209:SER:O	1:A:210:GLN:CB	2.64	0.46
2:B:51:LYS:HA	1:E:29:ILE:O	2.15	0.46
1:C:15:LEU:HD23	1:C:15:LEU:H	1.80	0.46
1:C:170:ASN:CB	1:C:176:LYS:HE2	2.33	0.46
2:D:6:ILE:N	2:D:112:ASP:OD1	2.49	0.46
1:E:209:SER:O	1:E:210:GLN:HB2	2.15	0.46
2:F:100:VAL:O	2:F:101:ALA:C	2.59	0.46
4:H:41:PHE:O	4:H:42:PRO:C	2.58	0.46
3:U:11:MET:O	3:U:105:LEU:HD12	2.16	0.46
3:U:38:GLN:NE2	3:U:48:TRP:CZ2	2.84	0.46
3:U:76:ILE:O	3:U:77:SER:C	2.57	0.46
4:T:51:TYR:CE1	4:T:60:TYR:HB2	2.51	0.46
1:A:55:PRO:HG3	1:A:280:GLU:OE1	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:CYS:O	1:A:77:ASP:C	2.56	0.46
1:A:139:CYS:O	1:A:146:GLY:O	2.34	0.46
2:B:1:GLY:HA2	2:B:112:ASP:CG	2.41	0.46
2:B:5:ALA:O	2:B:6:ILE:C	2.58	0.46
2:B:43:ALA:O	2:B:46:ASP:HB2	2.15	0.46
1:C:15:LEU:C	2:D:14:TRP:CZ2	2.94	0.46
2:D:127:ARG:HG3	2:D:159:HIS:CE1	2.51	0.46
2:F:4:GLY:O	2:F:8:GLY:HA3	2.16	0.46
2:F:105:GLN:O	2:F:108:ILE:HB	2.16	0.46
3:L:205:PRO:O	3:L:206:ILE:C	2.59	0.46
4:T:130:PRO:C	4:T:131:LEU:HD23	2.41	0.46
4:T:140:ASN:HD22	4:T:140:ASN:HA	1.64	0.46
2:B:40:SER:HA	2:B:43:ALA:HB3	1.97	0.46
1:C:44:GLN:HG3	1:C:44:GLN:O	2.16	0.46
1:C:136:SER:CB	4:T:104:ASP:OD1	2.64	0.46
1:E:85:ASP:O	1:E:265:SER:HA	2.16	0.46
2:F:168:ASN:C	2:F:170:ARG:N	2.71	0.46
4:H:41:PHE:HB3	4:H:42:PRO:HD2	1.97	0.46
4:H:144:THR:O	4:H:145:LEU:HD23	2.16	0.46
3:U:12:SER:HA	3:U:106:GLU:O	2.17	0.46
3:U:32:SER:O	3:U:33:PHE:HD1	1.98	0.46
4:T:15:SER:N	4:T:86:VAL:O	2.49	0.46
4:T:162:ASN:HD21	4:T:201:THR:N	2.14	0.46
1:A:174:PHE:CE1	1:A:259:LYS:HG3	2.51	0.45
1:A:298:ASN:ND2	1:A:299:LYS:N	2.61	0.45
2:D:14:TRP:CH2	2:D:23:GLY:O	2.69	0.45
2:F:24:PHE:O	2:F:34:GLN:HA	2.16	0.45
2:F:127:ARG:HG3	2:F:159:HIS:CG	2.51	0.45
3:L:48:TRP:CZ2	3:L:59:VAL:HG13	2.51	0.45
3:L:185:ASP:O	3:L:188:GLU:N	2.49	0.45
4:H:67:ARG:NH1	4:H:90:ASP:OD1	2.47	0.45
4:T:154:PRO:O	4:T:155:GLU:C	2.58	0.45
4:T:155:GLU:HG2	4:T:182:TYR:CE2	2.51	0.45
1:A:98:TYR:CD2	1:A:99:PRO:HD2	2.51	0.45
1:A:170:ASN:ND2	1:A:239:PRO:HA	2.32	0.45
2:B:28:ASN:HD21	2:B:30:GLU:HB2	1.81	0.45
1:C:300:ILE:HD11	2:D:69:GLU:HG3	1.98	0.45
4:H:58:ASN:HB2	4:H:60:TYR:CD2	2.51	0.45
4:H:175:ALA:HB2	4:H:184:LEU:HB3	1.98	0.45
3:U:3:VAL:H	3:U:26:SER:HB3	1.82	0.45
3:U:61:ALA:O	3:U:62:ARG:C	2.58	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:201:THR:HG22	4:T:202:CYS:N	2.31	0.45
1:A:178:TYR:CE1	1:A:243:LEU:HG	2.51	0.45
2:B:89:ILE:H	2:B:89:ILE:HD12	1.81	0.45
4:T:193:SER:O	4:T:196:PRO:HD2	2.16	0.45
4:T:201:THR:HG23	4:T:215:LYS:C	2.42	0.45
1:A:187:THR:HB	1:A:189:GLN:CD	2.41	0.45
1:C:18:HIS:O	1:C:19:ALA:CB	2.60	0.45
1:C:81:ASN:HD22	1:C:119:GLU:HA	1.80	0.45
1:C:283:THR:HG23	1:C:285:ASN:N	2.32	0.45
2:D:83:TYR:CG	2:F:66:ILE:HG23	2.51	0.45
1:E:67:ILE:HG13	1:E:105:TYR:CE2	2.52	0.45
1:E:170:ASN:ND2	1:E:239:PRO:CA	2.75	0.45
3:L:132:SER:HA	3:L:180:LEU:O	2.17	0.45
4:H:59:ASN:OD1	4:H:61:ASN:OD1	2.34	0.45
4:H:141:SER:O	4:H:192:SER:HA	2.15	0.45
4:H:151:GLY:CA	4:H:181:LEU:HD12	2.45	0.45
4:T:177:LEU:HD12	4:T:178:GLN:H	1.81	0.45
1:A:44:GLN:HB3	1:A:295:GLN:HA	1.97	0.45
1:C:82:GLU:OE2	1:C:82:GLU:HA	2.16	0.45
1:C:195:TYR:O	1:C:196:VAL:HB	2.17	0.45
1:E:10:THR:HB	1:E:11:ALA:H	1.57	0.45
2:F:51:LYS:NZ	2:F:106:HIS:ND1	2.64	0.45
4:T:2:VAL:HG21	4:T:27:TYR:CB	2.46	0.45
1:A:17:HIS:HB2	1:A:320:MET:SD	2.57	0.45
1:C:14:CYS:O	2:D:25:ARG:N	2.49	0.45
1:C:283:THR:CG2	1:C:283:THR:O	2.64	0.45
1:C:293:PRO:C	1:C:294:PHE:CD2	2.95	0.45
2:D:5:ALA:HB1	2:D:115:MET:HG2	1.98	0.45
2:D:159:HIS:C	2:D:159:HIS:HD1	2.25	0.45
3:L:90:HIS:ND1	3:L:98:THR:O	2.49	0.45
4:H:28:SER:C	4:H:30:THR:N	2.55	0.45
4:H:73:ASP:O	4:H:74:THR:C	2.60	0.45
1:A:138:ALA:C	1:A:140:LYS:HZ3	2.23	0.45
1:C:42:LEU:C	1:C:293:PRO:HD2	2.42	0.45
1:C:176:LYS:HD2	1:C:257:TYR:CE2	2.51	0.45
2:D:167:LEU:N	2:D:167:LEU:HD23	2.32	0.45
1:E:13:LEU:HD13	1:E:14:CYS:N	2.32	0.45
1:E:164:LEU:N	1:E:164:LEU:HD12	2.31	0.45
1:E:181:GLY:C	1:E:252:ILE:HB	2.41	0.45
1:E:204:VAL:HA	1:E:244:VAL:O	2.17	0.45
3:L:21:LEU:N	3:L:21:LEU:CD1	2.79	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:64:LEU:HD23	4:H:64:LEU:HA	1.82	0.45
3:U:7:SER:CB	3:U:8:PRO:CD	2.94	0.45
3:U:14:SER:CB	3:U:108:LYS:CD	2.94	0.45
3:U:95:PHE:CD1	3:U:97:ARG:NH1	2.85	0.45
2:B:17:MET:HE1	2:B:19:ASP:CB	2.44	0.45
2:B:24:PHE:O	2:B:34:GLN:HA	2.16	0.45
2:B:82:LYS:O	2:B:83:TYR:C	2.59	0.45
1:C:108:LEU:HD12	1:C:111:LEU:HD21	1.98	0.45
1:E:73:ASP:OD1	1:E:75:HIS:HD2	2.00	0.45
2:F:130:ALA:CB	2:F:139:LYS:O	2.60	0.45
3:L:55:LEU:HB3	3:L:59:VAL:HB	1.99	0.45
3:L:74:LEU:HB3	3:L:75:THR:H	1.58	0.45
3:L:119:PHE:HA	3:L:120:PRO:HD3	1.71	0.45
1:A:176:LYS:HD2	1:A:257:TYR:CG	2.52	0.45
1:A:191:GLN:OE1	1:A:195:TYR:CD1	2.68	0.45
2:B:71:SER:C	2:B:72:GLU:CD	2.85	0.45
1:C:138:ALA:C	1:C:140:LYS:NZ	2.75	0.45
1:C:150:ARG:N	1:C:150:ARG:CD	2.79	0.45
1:C:275:ASP:CG	1:C:276:THR:H	2.25	0.45
4:H:37:TRP:CE3	4:H:96:CYS:HB3	2.50	0.45
4:H:53:SER:H	4:H:58:ASN:HD21	1.65	0.45
4:H:216:LYS:HD2	4:H:216:LYS:H	1.81	0.45
3:U:55:LEU:HD21	3:U:63:PHE:O	2.17	0.45
4:T:70:ILE:CG2	4:T:71:THR:N	2.79	0.45
4:T:71:THR:O	4:T:79:PHE:HB2	2.16	0.45
1:A:191:GLN:NE2	1:A:250:ASN:HD21	2.15	0.45
2:B:17:MET:HA	2:B:17:MET:HE2	1.98	0.45
2:B:52:LEU:O	2:B:53:ASN:C	2.59	0.45
2:B:77:ILE:HD13	2:B:77:ILE:HA	1.52	0.45
2:B:118:LEU:O	2:B:122:THR:HG23	2.16	0.45
1:C:248:ASN:HD22	1:C:248:ASN:H	1.65	0.45
1:E:61:GLY:O	1:E:79:PHE:CZ	2.70	0.45
3:L:36:TRP:CZ2	3:L:73:SER:O	2.70	0.45
3:L:120:PRO:HG2	4:H:220:ARG:NH2	2.32	0.45
3:L:124:ILE:C	3:L:126:LEU:N	2.71	0.45
4:H:76:LYS:HD2	4:H:76:LYS:HA	1.76	0.45
4:H:146:GLY:O	4:H:147:CYS:HB2	2.15	0.45
4:H:190:VAL:HB	4:H:191:PRO:HD2	1.99	0.45
3:U:2:ILE:HG22	3:U:4:LEU:HD11	1.98	0.45
4:T:195:TRP:C	4:T:197:SER:N	2.74	0.45
1:C:184:HIS:CE1	1:C:216:ASN:ND2	2.85	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:163:ARG:O	2:D:164:ASP:C	2.59	0.44
1:E:200:GLY:HA3	1:E:250:ASN:OD1	2.17	0.44
3:L:92:TRP:O	3:L:97:ARG:NH2	2.50	0.44
3:L:141:TYR:CG	3:L:142:PRO:N	2.83	0.44
4:H:76:LYS:HA	4:H:76:LYS:CE	2.46	0.44
3:U:14:SER:HB3	3:U:108:LYS:CD	2.45	0.44
4:T:20:LEU:CD1	4:T:94:TYR:CB	2.96	0.44
4:T:52:ILE:O	4:T:52:ILE:CG2	2.54	0.44
4:T:172:THR:HA	4:T:186:SER:HA	1.99	0.44
1:C:43:VAL:HG23	1:C:314:LEU:HB2	1.99	0.44
1:C:298:ASN:HD22	1:C:299:LYS:H	1.61	0.44
3:L:182:LEU:HA	3:L:182:LEU:HD23	1.77	0.44
3:L:210:PHE:C	3:L:212:ARG:H	2.25	0.44
4:H:6:GLU:OE1	4:H:96:CYS:N	2.41	0.44
4:H:35:TRP:CE3	4:H:98:ALA:HB2	2.52	0.44
3:U:127:THR:O	3:U:127:THR:HG22	2.18	0.44
1:A:10:THR:HG21	2:B:141:TYR:O	2.17	0.44
1:A:36:VAL:HG22	1:A:37:THR:H	1.80	0.44
1:C:28:THR:HG22	2:D:105:GLN:N	2.32	0.44
1:E:42:LEU:O	1:E:294:PHE:HB2	2.17	0.44
1:E:209:SER:OG	1:E:210:GLN:N	2.45	0.44
3:L:38:GLN:CG	3:L:87:TYR:HE1	2.27	0.44
3:L:116:VAL:CG1	3:L:117:SER:N	2.80	0.44
3:U:2:ILE:HD13	3:U:2:ILE:HA	1.67	0.44
3:U:114:PRO:HD3	3:U:140:PHE:CB	2.48	0.44
4:T:39:ARG:HB2	4:T:93:SER:O	2.18	0.44
1:C:96:ASN:O	1:C:97:CYS:HB2	2.17	0.44
1:C:153:TRP:CD1	1:C:153:TRP:C	2.93	0.44
1:C:306:PRO:O	1:C:307:LYS:C	2.60	0.44
2:D:111:THR:C	2:D:113:SER:N	2.72	0.44
1:E:16:GLY:HA2	2:F:115:MET:SD	2.58	0.44
2:F:48:ILE:HD11	2:F:107:THR:CG2	2.43	0.44
4:H:7:SER:O	4:H:20:LEU:HD22	2.17	0.44
4:H:134:GLY:HA3	4:H:220:ARG:HE	1.82	0.44
4:T:149:VAL:O	4:T:184:LEU:N	2.45	0.44
4:T:195:TRP:CB	4:T:196:PRO:CD	2.96	0.44
1:A:71:LEU:CD1	1:A:100:TYR:CE1	3.00	0.44
1:A:136:SER:C	1:A:138:ALA:H	2.24	0.44
1:A:292:LYS:HB3	1:A:293:PRO:HD2	1.99	0.44
2:B:9:PHE:HD1	2:B:10:ILE:N	2.16	0.44
2:B:121:LYS:NZ	2:B:122:THR:HG22	2.24	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:GLN:C	1:C:82:GLU:N	2.76	0.44
2:D:82:LYS:O	2:D:84:VAL:N	2.51	0.44
2:D:130:ALA:HB2	2:D:140:ILE:HA	1.99	0.44
1:E:10:THR:CG2	2:F:141:TYR:O	2.62	0.44
3:L:6:GLN:HE22	3:L:88:PHE:HA	1.83	0.44
4:H:86:VAL:HG22	4:H:87:THR:O	2.18	0.44
4:T:34:TYR:O	4:T:36:THR:HG22	2.18	0.44
4:T:58:ASN:O	4:T:59:ASN:CB	2.60	0.44
4:T:152:TYR:CE2	4:T:157:VAL:HG22	2.52	0.44
1:A:17:HIS:HA	2:B:22:TYR:HD2	1.81	0.44
1:A:136:SER:HB2	4:H:104:ASP:OD1	2.18	0.44
1:C:14:CYS:HA	2:D:137:CYS:HA	1.99	0.44
2:D:91:LEU:HD13	2:F:91:LEU:HD13	1.99	0.44
2:D:103:GLU:O	2:D:107:THR:OG1	2.20	0.44
1:E:121:ILE:HG13	1:E:257:TYR:OH	2.17	0.44
1:E:121:ILE:CG1	1:E:257:TYR:CE1	3.01	0.44
2:F:28:ASN:HD21	2:F:30:GLU:HB2	1.83	0.44
2:F:146:ASN:O	2:F:149:ILE:HB	2.18	0.44
3:L:4:LEU:HD12	3:L:4:LEU:N	2.32	0.44
3:L:185:ASP:C	3:L:187:TYR:N	2.74	0.44
3:L:186:GLU:HG3	3:L:189:ARG:CZ	2.48	0.44
4:H:20:LEU:HD11	4:H:94:TYR:CB	2.47	0.44
3:U:49:ILE:HA	3:U:54:ASN:O	2.17	0.44
4:T:67:ARG:O	4:T:68:ILE:C	2.57	0.44
1:A:65:THR:HG23	1:A:68:ASP:OD2	2.18	0.44
1:A:127:TRP:CZ3	1:A:166:VAL:HG11	2.53	0.44
1:A:147:PHE:CG	1:A:148:PHE:N	2.85	0.44
1:A:226:LEU:HD21	4:H:104:ASP:HB2	1.98	0.44
2:B:3:PHE:HZ	2:F:2:LEU:O	2.00	0.44
2:D:55:VAL:HG12	2:D:56:ILE:N	2.33	0.44
1:E:283:THR:HG23	1:E:285:ASN:CA	2.48	0.44
2:F:84:VAL:HG12	2:F:85:GLU:N	2.32	0.44
4:H:72:ARG:O	4:H:72:ARG:HG3	2.18	0.44
4:T:97:ALA:CB	4:T:109:TYR:O	2.65	0.44
1:A:18:HIS:CE1	1:A:320:MET:SD	3.11	0.44
1:C:139:CYS:O	1:C:146:GLY:C	2.61	0.44
2:D:3:PHE:CD2	2:D:113:SER:CA	2.90	0.44
2:D:4:GLY:CA	2:F:117:LYS:HE3	2.46	0.44
2:D:6:ILE:HG13	2:D:112:ASP:OD1	2.18	0.44
1:E:283:THR:HG23	1:E:285:ASN:N	2.33	0.44
3:L:194:THR:HG22	3:L:209:SER:CB	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:51:TYR:HE1	4:T:58:ASN:HD22	1.65	0.44
4:T:54:TYR:C	4:T:56:GLY:N	2.74	0.44
4:T:59:ASN:OD1	4:T:61:ASN:OD1	2.35	0.44
4:T:206:HIS:CD2	4:T:209:SER:OG	2.60	0.44
1:A:74:PRO:HD3	1:A:97:CYS:SG	2.58	0.44
1:E:13:LEU:HB3	2:F:138:PHE:HB2	1.99	0.44
2:F:9:PHE:CE1	2:F:10:ILE:HG13	2.52	0.44
2:F:74:GLU:HB2	2:F:78:GLN:HB2	2.00	0.44
3:L:95:PHE:CD1	3:L:97:ARG:NH1	2.86	0.44
3:L:204:SER:HA	3:L:205:PRO:HD2	1.65	0.44
3:U:122:SER:HB3	3:U:125:GLN:CB	2.43	0.44
3:U:122:SER:OG	3:U:124:ILE:HG13	2.17	0.44
1:A:191:GLN:O	1:A:192:THR:C	2.60	0.43
2:B:28:ASN:ND2	2:B:30:GLU:HB2	2.33	0.43
2:B:132:GLU:HG3	2:B:137:CYS:O	2.18	0.43
1:C:326:LYS:O	1:C:327:GLN:CB	2.66	0.43
2:D:9:PHE:HD1	2:D:10:ILE:N	2.15	0.43
2:D:98:LEU:O	2:D:100:VAL:N	2.51	0.43
4:H:54:TYR:HA	4:H:72:ARG:HH22	1.81	0.43
3:U:35:TYR:CD2	3:U:50:TYR:HA	2.46	0.43
3:U:56:ALA:O	3:U:58:GLY:N	2.45	0.43
3:U:95:PHE:HD1	3:U:97:ARG:HH12	1.66	0.43
3:U:194:THR:HG22	3:U:209:SER:CB	2.47	0.43
4:T:40:GLN:HA	4:T:45:LYS:O	2.18	0.43
4:T:114:THR:O	4:T:114:THR:HG23	2.18	0.43
1:A:18:HIS:O	1:A:19:ALA:CB	2.63	0.43
1:A:38:ASN:ND2	1:A:318:THR:CB	2.81	0.43
1:A:209:SER:O	1:A:210:GLN:HB2	2.18	0.43
2:B:153:ARG:O	2:B:153:ARG:HG2	2.18	0.43
2:B:159:HIS:C	2:B:159:HIS:ND1	2.76	0.43
2:B:171:PHE:CZ	2:F:171:PHE:CE2	3.00	0.43
1:C:13:LEU:CD1	2:D:24:PHE:HB3	2.34	0.43
1:C:182:ILE:O	1:C:230:ILE:CG2	2.60	0.43
1:C:223:VAL:O	1:C:223:VAL:HG12	2.17	0.43
1:C:311:GLN:HE22	2:D:93:SER:HB3	1.82	0.43
1:E:12:THR:CB	2:F:27:GLN:HB3	2.45	0.43
1:E:73:ASP:CG	1:E:74:PRO:HD2	2.43	0.43
1:E:173:ASN:C	1:E:239:PRO:HG2	2.43	0.43
1:E:205:SER:HB3	1:E:210:GLN:HA	1.99	0.43
2:F:6:ILE:CD1	2:F:112:ASP:HA	2.49	0.43
2:F:56:ILE:O	2:F:58:LYS:HG3	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:165:THR:HG23	3:L:175:SER:O	2.18	0.43
4:H:155:GLU:HG2	4:H:182:TYR:CE2	2.53	0.43
3:U:74:LEU:HB3	3:U:75:THR:H	1.52	0.43
1:A:25:LEU:HD22	1:A:33:GLN:OE1	2.18	0.43
1:A:229:ARG:HE	1:A:229:ARG:HB3	1.61	0.43
1:A:286:GLY:O	1:A:287:SER:CB	2.65	0.43
1:C:288:ILE:HG21	1:C:297:VAL:HG21	1.99	0.43
2:F:132:GLU:O	2:F:133:MET:C	2.61	0.43
3:L:82:GLU:O	3:L:84:GLY:N	2.52	0.43
4:H:86:VAL:CG2	4:H:90:ASP:HB2	2.45	0.43
4:H:206:HIS:CD2	4:H:209:SER:OG	2.66	0.43
3:U:96:PRO:HA	4:T:48:TRP:HZ3	1.84	0.43
4:T:53:SER:H	4:T:58:ASN:ND2	2.10	0.43
1:A:323:VAL:HA	1:A:324:PRO:HD3	1.88	0.43
1:C:196:VAL:O	1:C:197:GLN:C	2.62	0.43
1:E:19:ALA:C	1:E:20:VAL:HG22	2.43	0.43
1:E:134:GLY:HA3	1:E:153:TRP:HB3	2.00	0.43
3:L:36:TRP:CE3	3:L:74:LEU:HD23	2.53	0.43
3:U:109:ARG:O	3:U:110:ALA:C	2.62	0.43
3:U:121:PRO:HG3	3:U:132:SER:C	2.43	0.43
3:U:125:GLN:CA	3:U:125:GLN:NE2	2.79	0.43
3:U:193:TYR:C	3:U:209:SER:OG	2.61	0.43
1:A:130:VAL:HG13	1:A:162:PRO:HD2	2.00	0.43
2:B:102:LEU:CD1	2:F:102:LEU:HD11	2.48	0.43
2:B:127:ARG:H	2:B:159:HIS:HB2	1.84	0.43
2:B:165:GLU:HA	2:B:165:GLU:OE1	2.18	0.43
1:C:108:LEU:HD13	1:C:234:TRP:CD2	2.52	0.43
1:C:140:LYS:HD2	1:C:140:LYS:O	2.18	0.43
1:E:108:LEU:HA	1:E:108:LEU:HD12	1.70	0.43
2:F:3:PHE:CB	2:F:112:ASP:OD2	2.66	0.43
2:F:14:TRP:CH2	2:F:25:ARG:HG3	2.53	0.43
3:U:55:LEU:H	3:U:55:LEU:HG	1.65	0.43
3:U:119:PHE:HA	3:U:120:PRO:HD3	1.82	0.43
4:T:32:GLY:HA2	4:T:54:TYR:CD2	2.53	0.43
4:T:53:SER:C	4:T:55:ASP:N	2.73	0.43
1:A:31:ASP:CG	1:A:34:ILE:HD11	2.44	0.43
1:A:216:ASN:CG	1:C:212:THR:HB	2.43	0.43
2:B:44:ALA:O	2:B:47:GLN:N	2.52	0.43
1:C:262:THR:O	1:C:263:GLY:O	2.36	0.43
2:D:80:LEU:C	2:D:82:LYS:N	2.75	0.43
3:L:171:ASP:HB3	3:L:173:THR:CG2	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:134:GLY:O	4:H:135:SER:C	2.61	0.43
3:U:79:LEU:HD13	3:U:79:LEU:C	2.43	0.43
3:U:212:ARG:HA	3:U:212:ARG:NE	2.32	0.43
1:A:42:LEU:HD22	2:B:55:VAL:CG1	2.49	0.43
1:A:249:GLY:C	1:A:250:ASN:OD1	2.61	0.43
1:C:27:LYS:HG3	1:C:32:ASP:HA	2.00	0.43
1:C:109:ARG:CZ	1:C:269:ARG:NH2	2.82	0.43
1:E:37:THR:OG1	1:E:38:ASN:N	2.51	0.43
1:E:127:TRP:HE3	1:E:164:LEU:HD23	1.84	0.43
1:E:140:LYS:N	1:E:140:LYS:CD	2.79	0.43
1:E:254:PRO:O	1:E:254:PRO:HG2	2.19	0.43
3:L:75:THR:HG22	3:L:76:ILE:N	2.34	0.43
3:L:191:ASN:N	3:L:191:ASN:ND2	2.65	0.43
4:H:20:LEU:CD1	4:H:94:TYR:HB3	2.49	0.43
3:U:91:GLN:HE21	3:U:93:GLU:H	1.64	0.43
1:A:143:PRO:HG2	1:A:144:GLY:N	2.34	0.43
1:A:210:GLN:HE21	1:E:220:ARG:HE	1.65	0.43
1:C:187:THR:C	1:C:189:GLN:N	2.72	0.43
2:D:117:LYS:HB3	2:D:117:LYS:HE2	1.88	0.43
1:E:253:ALA:HB1	1:E:254:PRO:HD2	2.00	0.43
1:E:307:LYS:HD3	2:F:92:TRP:CZ2	2.53	0.43
1:E:320:MET:C	1:E:321:ARG:O	2.61	0.43
2:F:21:TRP:CD2	2:F:45:ILE:HD11	2.54	0.43
3:L:25:ALA:O	3:L:27:SER:N	2.52	0.43
4:H:76:LYS:HA	4:H:76:LYS:HE3	2.01	0.43
4:H:161:TRP:HB3	4:H:166:LEU:HB2	2.01	0.43
4:T:64:LEU:HB2	4:T:68:ILE:CD1	2.48	0.43
4:T:84:ASN:HB3	4:T:85:SER:H	1.43	0.43
1:C:27:LYS:HE2	2:F:54:ARG:HD2	2.00	0.43
1:C:127:TRP:CH2	1:C:166:VAL:HG21	2.53	0.43
1:C:308:TYR:C	1:C:308:TYR:CD2	2.96	0.43
1:E:264:LYS:HD2	2:F:63:PHE:CE2	2.54	0.43
2:F:104:ASN:O	2:F:107:THR:N	2.50	0.43
4:T:20:LEU:HB2	4:T:81:LEU:HB3	2.00	0.43
4:T:216:LYS:H	4:T:216:LYS:HD2	1.82	0.43
1:A:98:TYR:HE2	1:A:229:ARG:HA	1.83	0.43
1:A:309:VAL:CG1	2:B:93:SER:HA	2.38	0.43
2:B:3:PHE:HD1	2:B:3:PHE:HA	1.67	0.43
2:B:171:PHE:CD2	2:D:167:LEU:HB3	2.50	0.43
2:D:89:ILE:O	2:D:90:ASP:C	2.61	0.43
1:E:11:ALA:HB2	2:F:28:ASN:HA	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:70:THR:O	3:L:70:THR:OG1	2.36	0.43
3:L:137:LEU:O	3:L:175:SER:HA	2.19	0.43
4:H:41:PHE:HB3	4:H:42:PRO:CD	2.49	0.43
3:U:1:GLN:HG2	3:U:1:GLN:O	2.19	0.43
3:U:137:LEU:O	3:U:140:PHE:CE1	2.72	0.43
3:U:207:VAL:HG22	3:U:208:LYS:N	2.33	0.43
1:A:42:LEU:HD11	1:A:316:LEU:HB2	2.01	0.42
1:A:67:ILE:HD13	1:A:67:ILE:HA	1.89	0.42
1:A:204:VAL:HA	1:A:244:VAL:O	2.19	0.42
2:B:72:GLU:HG3	1:C:238:LYS:HE2	2.01	0.42
2:B:106:HIS:ND1	2:B:106:HIS:C	2.77	0.42
1:C:28:THR:HG21	2:D:105:GLN:HA	2.00	0.42
1:C:74:PRO:HA	1:C:141:ARG:NH1	2.34	0.42
2:D:167:LEU:HG	2:D:168:ASN:N	2.34	0.42
1:E:15:LEU:N	1:E:15:LEU:HD23	2.33	0.42
4:H:37:TRP:O	4:H:49:MET:HB2	2.20	0.42
4:T:81:LEU:HD12	4:T:82:LYS:N	2.23	0.42
4:T:122:LYS:O	4:T:123:THR:C	2.60	0.42
1:A:10:THR:HG22	2:B:142:HIS:C	2.44	0.42
1:A:54:ASN:O	1:A:278:ILE:HA	2.18	0.42
1:C:29:ILE:HG23	2:F:103:GLU:OE1	2.19	0.42
1:C:206:THR:HB	1:C:241:ASP:OD1	2.19	0.42
2:D:58:LYS:HB3	2:D:58:LYS:HE2	1.86	0.42
2:D:132:GLU:O	2:D:133:MET:C	2.61	0.42
2:D:171:PHE:CD1	2:D:171:PHE:N	2.77	0.42
1:E:132:GLN:HA	1:E:154:LEU:CD2	2.49	0.42
2:F:66:ILE:O	2:F:66:ILE:HG13	2.12	0.42
3:U:21:LEU:HD22	3:U:74:LEU:HG	2.00	0.42
1:A:18:HIS:CG	1:A:19:ALA:N	2.86	0.42
2:B:3:PHE:HE2	2:B:113:SER:OG	2.00	0.42
1:C:47:SER:OG	1:C:48:THR:N	2.53	0.42
1:C:54:ASN:CB	1:C:278:ILE:HD13	2.49	0.42
1:E:304:ALA:N	2:F:61:GLU:HG3	2.34	0.42
1:E:306:PRO:O	1:E:307:LYS:C	2.62	0.42
4:H:180:ASP:O	4:H:181:LEU:HD22	2.20	0.42
4:H:218:VAL:O	4:H:218:VAL:HG13	2.19	0.42
3:U:34:LEU:HD22	3:U:72:TYR:CD2	2.55	0.42
4:T:13:LYS:HA	4:T:14:PRO:HD3	1.81	0.42
4:T:150:LYS:HG3	4:T:183:THR:OG1	2.19	0.42
1:A:80:GLN:O	1:A:81:ASN:C	2.62	0.42
1:C:189:GLN:HE21	1:C:189:GLN:HB3	1.57	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:ILE:HD12	1:C:217:ILE:H	1.85	0.42
2:D:140:ILE:HD12	2:D:140:ILE:N	2.35	0.42
1:E:58:ILE:CD1	1:E:86:LEU:HB3	2.49	0.42
1:E:111:LEU:HD12	1:E:112:VAL:N	2.33	0.42
1:E:283:THR:HG21	1:E:297:VAL:HG11	2.01	0.42
3:L:82:GLU:C	3:L:84:GLY:N	2.77	0.42
4:H:161:TRP:CB	4:H:166:LEU:HB2	2.49	0.42
4:H:195:TRP:CB	4:H:196:PRO:CD	2.90	0.42
4:T:49:MET:HE1	4:T:81:LEU:CD2	2.49	0.42
4:T:215:LYS:O	4:T:216:LYS:C	2.62	0.42
1:A:291:ASP:OD2	1:A:292:LYS:HG2	2.19	0.42
1:A:303:GLY:O	1:A:304:ALA:C	2.63	0.42
2:B:151:SER:HB2	2:B:157:TYR:HB2	2.02	0.42
1:C:111:LEU:H	1:C:111:LEU:HG	1.73	0.42
1:E:28:THR:HA	2:F:101:ALA:HA	2.01	0.42
3:U:34:LEU:HD13	3:U:72:TYR:CD1	2.54	0.42
3:U:194:THR:HG22	3:U:209:SER:HB2	2.02	0.42
3:U:209:SER:OG	3:U:210:PHE:CD1	2.71	0.42
4:T:122:LYS:HG3	4:T:124:THR:HG23	2.01	0.42
4:T:150:LYS:CA	4:T:183:THR:HG23	2.49	0.42
4:T:217:ILE:O	4:T:218:VAL:HG22	2.20	0.42
1:A:212:THR:HG22	1:A:213:ILE:N	2.33	0.42
2:B:80:LEU:CD2	2:F:80:LEU:HD21	2.44	0.42
1:C:36:VAL:CG2	1:C:37:THR:H	2.31	0.42
1:C:50:LYS:C	1:C:286:GLY:O	2.63	0.42
1:C:109:ARG:NH2	1:C:267:ILE:HD13	2.35	0.42
1:C:127:TRP:CE3	1:C:164:LEU:HD23	2.54	0.42
1:C:281:CYS:HB2	1:C:304:ALA:O	2.20	0.42
2:D:132:GLU:HG3	2:D:137:CYS:O	2.19	0.42
4:H:70:ILE:CG2	4:H:71:THR:N	2.81	0.42
4:H:212:LYS:C	4:H:213:VAL:HG13	2.44	0.42
3:U:14:SER:CB	3:U:108:LYS:CB	2.96	0.42
4:T:119:SER:HB3	4:T:153:PHE:HZ	1.84	0.42
1:A:29:ILE:CG1	2:B:102:LEU:HD23	2.49	0.42
1:C:17:HIS:CG	1:C:18:HIS:H	2.36	0.42
1:E:98:TYR:CD2	1:E:99:PRO:HD2	2.55	0.42
1:E:172:ASP:O	1:E:239:PRO:HB3	2.20	0.42
1:E:275:ASP:CG	1:E:276:THR:N	2.78	0.42
2:F:3:PHE:CB	2:F:112:ASP:O	2.67	0.42
2:F:91:LEU:O	2:F:92:TRP:C	2.63	0.42
3:L:97:ARG:HB2	4:H:48:TRP:CE2	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:175:SER:OG	4:T:171:HIS:CE1	2.71	0.42
4:T:6:GLU:CD	4:T:113:GLY:HA2	2.45	0.42
4:T:65:LYS:C	4:T:67:ARG:H	2.26	0.42
4:T:152:TYR:CE1	4:T:182:TYR:HB3	2.55	0.42
1:A:22:ASN:N	1:A:22:ASN:ND2	2.46	0.42
1:A:191:GLN:O	1:A:194:LEU:N	2.53	0.42
1:C:37:THR:OG1	1:C:319:GLY:HA3	2.19	0.42
2:D:21:TRP:CE3	2:D:45:ILE:HG13	2.55	0.42
1:E:28:THR:O	1:E:30:THR:N	2.52	0.42
1:E:177:LEU:HB2	1:E:260:MET:SD	2.60	0.42
2:F:42:GLN:O	2:F:46:ASP:HB2	2.19	0.42
2:F:121:LYS:HB3	2:F:121:LYS:NZ	2.24	0.42
3:L:51:SER:O	3:L:53:SER:N	2.53	0.42
4:H:18:LEU:O	4:H:82:LYS:O	2.37	0.42
4:H:73:ASP:OD1	4:H:75:SER:OG	2.38	0.42
4:T:37:TRP:O	4:T:49:MET:HB2	2.20	0.42
1:A:25:LEU:HD13	1:A:33:GLN:OE1	2.20	0.42
1:A:47:SER:CB	1:A:288:ILE:HG22	2.45	0.42
1:A:55:PRO:HG3	1:A:280:GLU:CD	2.45	0.42
1:A:166:VAL:CG2	1:A:245:ILE:HB	2.47	0.42
1:A:176:LYS:O	1:A:236:ILE:HA	2.19	0.42
2:B:10:ILE:C	2:B:12:ASN:H	2.26	0.42
2:B:127:ARG:HH21	2:F:131:GLU:HB2	1.85	0.42
1:C:65:THR:O	1:C:66:LEU:C	2.60	0.42
1:C:309:VAL:HG12	2:D:93:SER:CA	2.44	0.42
2:D:51:LYS:O	2:D:54:ARG:HB2	2.19	0.42
1:E:15:LEU:C	2:F:14:TRP:CZ2	2.98	0.42
1:E:187:THR:HB	1:E:189:GLN:HG2	2.02	0.42
1:E:318:THR:O	1:E:318:THR:CG2	2.68	0.42
3:L:2:ILE:HG23	3:L:98:THR:HG21	2.02	0.42
3:L:8:PRO:HB3	3:L:11:MET:HB3	2.01	0.42
4:H:167:SER:O	4:H:170:VAL:HG22	2.20	0.42
3:U:3:VAL:N	3:U:26:SER:HB2	2.34	0.42
3:U:35:TYR:HB3	3:U:49:ILE:O	2.20	0.42
3:U:156:ARG:O	3:U:158:ASN:OD1	2.38	0.42
4:T:73:ASP:O	4:T:76:LYS:N	2.53	0.42
4:T:153:PHE:CG	4:T:154:PRO:HA	2.54	0.42
1:A:29:ILE:O	2:D:51:LYS:HA	2.19	0.42
1:A:80:GLN:HE21	1:A:80:GLN:HB3	1.63	0.42
1:A:308:TYR:CD2	2:B:89:ILE:HG13	2.54	0.42
2:B:40:SER:OG	2:B:114:GLU:HB3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:LYS:HE2	2:B:85:GLU:OE1	2.19	0.42
1:C:226:LEU:HD21	4:T:104:ASP:HB2	2.02	0.42
2:F:48:ILE:C	2:F:50:GLY:H	2.28	0.42
2:F:68:LYS:HE2	2:F:85:GLU:OE2	2.20	0.42
2:F:141:TYR:HB3	2:F:165:GLU:HB3	2.02	0.42
3:L:149:TRP:CD1	3:L:160:VAL:HG11	2.55	0.42
3:L:190:HIS:ND1	3:L:190:HIS:N	2.67	0.42
3:U:55:LEU:HB3	3:U:59:VAL:HB	2.02	0.42
3:U:61:ALA:C	3:U:63:PHE:N	2.76	0.42
3:U:160:VAL:O	3:U:161:LEU:HD23	2.19	0.42
1:A:308:TYR:CD2	1:A:308:TYR:C	2.98	0.41
2:B:54:ARG:NH1	2:B:103:GLU:OE2	2.53	0.41
1:C:246:ASN:C	1:C:246:ASN:ND2	2.63	0.41
2:D:68:LYS:HE2	2:D:85:GLU:OE1	2.20	0.41
1:E:17:HIS:H	2:F:115:MET:HE1	1.85	0.41
1:E:71:LEU:CD1	1:E:100:TYR:CE1	3.03	0.41
1:E:130:VAL:HG21	1:E:164:LEU:HD21	2.02	0.41
1:E:180:TRP:CE2	1:E:204:VAL:HG21	2.55	0.41
1:E:280:GLU:HB3	1:E:304:ALA:HB3	2.02	0.41
2:F:165:GLU:OE1	2:F:168:ASN:ND2	2.53	0.41
3:L:136:PHE:C	3:L:137:LEU:HD12	2.45	0.41
4:H:58:ASN:C	4:H:60:TYR:N	2.77	0.41
4:T:18:LEU:CD2	4:T:116:LEU:HD13	2.48	0.41
4:T:29:ILE:HG12	4:T:77:ASN:ND2	2.34	0.41
1:A:50:LYS:HG2	1:A:273:PRO:HG2	2.03	0.41
1:A:141:ARG:HH11	1:A:141:ARG:HG3	1.85	0.41
1:C:67:ILE:HD13	1:C:67:ILE:HA	1.92	0.41
1:C:212:THR:C	1:C:213:ILE:HD13	2.44	0.41
2:D:6:ILE:O	2:D:8:GLY:N	2.54	0.41
1:E:176:LYS:CE	1:E:178:TYR:OH	2.68	0.41
1:E:196:VAL:O	1:E:197:GLN:O	2.38	0.41
3:L:4:LEU:N	3:L:4:LEU:CD1	2.84	0.41
3:L:6:GLN:NE2	3:L:102:GLY:HA2	2.35	0.41
4:H:67:ARG:NH1	4:H:85:SER:O	2.53	0.41
4:H:107:PHE:CE1	4:H:109:TYR:HE1	2.38	0.41
4:H:193:SER:O	4:H:196:PRO:HD2	2.20	0.41
4:T:108:ASP:C	4:T:108:ASP:OD1	2.63	0.41
4:T:154:PRO:C	4:T:155:GLU:O	2.63	0.41
1:A:111:LEU:HD12	1:A:112:VAL:CA	2.48	0.41
1:A:246:ASN:C	1:A:246:ASN:ND2	2.75	0.41
2:B:102:LEU:O	2:B:104:ASN:N	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:LEU:HD23	2:B:152:ILE:HD11	2.02	0.41
1:C:70:LEU:O	1:C:71:LEU:C	2.62	0.41
1:C:140:LYS:CD	1:C:140:LYS:H	2.34	0.41
2:D:17:MET:HE1	2:D:19:ASP:H	1.85	0.41
2:D:132:GLU:O	2:D:134:GLY:N	2.53	0.41
2:F:167:LEU:HG	2:F:168:ASN:N	2.36	0.41
3:L:123:LYS:HG2	3:L:124:ILE:N	2.35	0.41
3:L:125:GLN:NE2	4:H:129:TYR:CE2	2.88	0.41
4:H:51:TYR:O	4:H:70:ILE:HD12	2.20	0.41
4:H:159:VAL:HG22	4:H:160:THR:N	2.34	0.41
3:U:3:VAL:O	3:U:25:ALA:HA	2.20	0.41
3:U:137:LEU:O	3:U:140:PHE:HE1	2.03	0.41
3:U:204:SER:HA	3:U:205:PRO:HD2	1.57	0.41
4:T:41:PHE:O	4:T:42:PRO:C	2.62	0.41
4:T:43:GLY:O	4:T:44:ASN:HB2	2.20	0.41
1:A:51:ILE:CG2	1:A:282:ILE:HD13	2.50	0.41
1:A:238:LYS:O	1:A:239:PRO:C	2.62	0.41
1:A:294:PHE:CE1	2:B:96:ALA:HB2	2.54	0.41
1:A:304:ALA:H	2:B:61:GLU:HG3	1.85	0.41
1:C:18:HIS:CG	1:C:19:ALA:N	2.88	0.41
2:D:44:ALA:C	2:D:46:ASP:N	2.76	0.41
1:E:143:PRO:HG2	1:E:144:GLY:H	1.85	0.41
1:E:293:PRO:C	1:E:294:PHE:HD2	2.24	0.41
2:F:142:HIS:ND1	2:F:142:HIS:N	2.68	0.41
4:H:34:TYR:CE2	4:H:53:SER:HB3	2.53	0.41
4:H:86:VAL:HG22	4:H:87:THR:N	2.34	0.41
3:U:118:ILE:HD12	3:U:135:CYS:HB2	2.01	0.41
4:T:107:PHE:CE1	4:T:109:TYR:HE1	2.39	0.41
4:T:130:PRO:HB2	4:T:217:ILE:HD13	2.02	0.41
2:B:5:ALA:HB1	2:B:115:MET:HG2	2.02	0.41
2:B:26:HIS:HE1	2:B:32:THR:C	2.29	0.41
2:B:171:PHE:HD1	2:B:171:PHE:H	1.57	0.41
1:C:44:GLN:HB3	1:C:295:GLN:HB3	2.01	0.41
1:C:48:THR:HG23	1:C:49:GLY:H	1.83	0.41
1:C:53:ASN:CG	1:C:276:THR:HA	2.45	0.41
1:C:141:ARG:HH11	1:C:141:ARG:HG3	1.86	0.41
1:C:223:VAL:O	1:C:224:ARG:HB3	2.20	0.41
2:D:131:GLU:HB3	2:F:127:ARG:HE	1.85	0.41
1:E:164:LEU:HB2	1:E:247:SER:O	2.21	0.41
1:E:298:ASN:HD22	1:E:299:LYS:H	1.68	0.41
1:E:308:TYR:CD2	1:E:308:TYR:C	2.98	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:326:LYS:O	1:E:327:GLN:HB2	2.20	0.41
3:L:37:TYR:OH	4:H:99:PHE:HE2	2.03	0.41
3:L:141:TYR:CG	3:L:142:PRO:CD	3.03	0.41
3:L:151:ILE:HA	3:L:193:TYR:HA	2.02	0.41
4:H:4:LEU:CD1	4:H:97:ALA:HA	2.51	0.41
1:A:269:ARG:HG3	1:A:269:ARG:NH1	2.34	0.41
2:B:69:GLU:O	2:B:70:PHE:CD2	2.73	0.41
1:C:78:VAL:HG13	1:C:79:PHE:N	2.36	0.41
1:C:191:GLN:OE1	1:C:195:TYR:CD1	2.69	0.41
1:C:313:THR:O	1:C:313:THR:HG23	2.19	0.41
2:D:91:LEU:C	2:D:93:SER:N	2.79	0.41
2:D:108:ILE:O	2:D:110:LEU:N	2.53	0.41
2:D:152:ILE:C	2:D:154:ASN:N	2.78	0.41
2:D:167:LEU:HA	2:D:171:PHE:CE1	2.56	0.41
1:E:189:GLN:O	1:E:193:SER:OG	2.31	0.41
2:F:121:LYS:HZ3	2:F:122:THR:N	2.18	0.41
4:H:15:SER:C	4:H:16:GLN:O	2.62	0.41
4:H:33:TYR:CD2	4:H:99:PHE:O	2.65	0.41
4:H:160:THR:O	4:H:202:CYS:HA	2.21	0.41
4:T:150:LYS:HG3	4:T:183:THR:CG2	2.50	0.41
1:A:25:LEU:C	1:A:26:VAL:HG13	2.46	0.41
1:A:71:LEU:HD11	1:A:100:TYR:CE1	2.56	0.41
2:B:96:ALA:O	2:B:98:LEU:N	2.50	0.41
2:B:132:GLU:O	2:B:133:MET:C	2.63	0.41
1:C:254:PRO:O	1:C:254:PRO:CG	2.68	0.41
1:C:308:TYR:CD2	2:D:89:ILE:HG13	2.56	0.41
1:E:59:LEU:HD12	1:E:60:ASP:N	2.36	0.41
1:E:76:CYS:O	1:E:77:ASP:C	2.63	0.41
1:E:151:LEU:HD23	1:E:151:LEU:HA	1.87	0.41
2:F:28:ASN:ND2	2:F:146:ASN:N	2.68	0.41
3:U:3:VAL:CB	3:U:26:SER:HB2	2.50	0.41
3:U:29:ILE:HD12	3:U:34:LEU:HB2	2.01	0.41
4:T:51:TYR:HE1	4:T:58:ASN:ND2	2.18	0.41
1:A:13:LEU:HD13	1:A:14:CYS:N	2.36	0.41
1:A:102:VAL:HG22	1:A:232:ILE:CB	2.46	0.41
1:A:309:VAL:HG12	2:B:93:SER:CA	2.39	0.41
1:C:63:ASP:O	1:C:93:ALA:HB1	2.21	0.41
2:D:100:VAL:CG2	2:D:101:ALA:H	2.22	0.41
1:E:74:PRO:HD3	1:E:97:CYS:CB	2.38	0.41
2:F:127:ARG:NH1	2:F:128:GLU:HG2	2.36	0.41
3:L:8:PRO:C	3:L:10:ILE:N	2.72	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:83:LEU:HD21	4:T:90:ASP:OD1	2.21	0.41
4:T:87:THR:HG23	4:T:90:ASP:H	1.85	0.41
4:T:129:TYR:HB2	4:T:148:LEU:CD2	2.51	0.41
4:T:193:SER:OG	4:T:194:THR:N	2.54	0.41
1:A:67:ILE:O	1:A:70:LEU:HB3	2.20	0.41
1:A:172:ASP:HB3	1:A:174:PHE:CD2	2.53	0.41
1:A:247:SER:OG	1:A:249:GLY:O	2.39	0.41
2:B:17:MET:CE	2:B:19:ASP:H	2.31	0.41
2:B:120:GLU:OE1	2:B:120:GLU:HA	2.21	0.41
1:C:72:GLY:O	1:C:73:ASP:C	2.63	0.41
1:C:140:LYS:N	1:C:140:LYS:CD	2.84	0.41
1:C:154:LEU:N	1:C:154:LEU:HD23	2.36	0.41
2:D:26:HIS:O	2:D:32:THR:HA	2.21	0.41
2:D:39:LYS:O	2:D:39:LYS:HG2	2.20	0.41
1:E:107:SER:C	1:E:109:ARG:N	2.78	0.41
1:E:129:GLY:O	1:E:157:SER:HB3	2.21	0.41
1:E:161:TYR:CE2	1:E:249:GLY:HA2	2.56	0.41
1:E:247:SER:OG	1:E:251:LEU:HB2	2.21	0.41
2:F:69:GLU:O	2:F:70:PHE:CD2	2.74	0.41
2:F:77:ILE:HD13	2:F:77:ILE:HA	1.80	0.41
2:F:145:ASP:O	2:F:146:ASN:C	2.63	0.41
3:L:139:ASN:CA	3:L:174:TYR:O	2.69	0.41
3:L:167:GLN:HG3	3:L:172:SER:CA	2.51	0.41
4:H:73:ASP:N	4:H:78:GLN:O	2.50	0.41
4:H:84:ASN:HD22	4:H:84:ASN:HA	1.66	0.41
4:H:195:TRP:C	4:H:197:SER:N	2.78	0.41
4:T:159:VAL:HG11	4:T:172:THR:OG1	2.20	0.41
1:A:13:LEU:HD13	1:A:13:LEU:C	2.46	0.41
2:B:24:PHE:CD1	2:B:24:PHE:N	2.89	0.41
2:D:56:ILE:O	2:D:58:LYS:HG3	2.21	0.41
1:E:177:LEU:HD12	1:E:236:ILE:HG22	2.02	0.41
1:E:246:ASN:C	1:E:246:ASN:ND2	2.70	0.41
3:L:142:PRO:C	3:L:144:ASP:N	2.79	0.41
4:H:48:TRP:CZ2	4:H:50:GLY:HA2	2.56	0.41
4:T:64:LEU:HD23	4:T:64:LEU:HA	1.74	0.41
4:T:195:TRP:O	4:T:198:GLU:O	2.39	0.41
1:A:59:LEU:HD21	1:A:82:GLU:HG3	2.03	0.40
1:C:91:SER:C	1:C:93:ALA:H	2.27	0.40
1:C:158:GLY:O	3:U:59:VAL:O	2.39	0.40
1:C:283:THR:HG23	1:C:285:ASN:C	2.43	0.40
2:D:115:MET:HB3	2:D:116:ASN:H	1.65	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:VAL:HG22	1:E:245:ILE:HB	2.02	0.40
1:E:212:THR:O	1:E:213:ILE:HD13	2.20	0.40
1:E:312:ASN:ND2	1:E:312:ASN:N	2.68	0.40
3:L:137:LEU:HD21	3:L:147:VAL:CG1	2.50	0.40
4:H:72:ARG:HD3	4:H:74:THR:HG22	2.02	0.40
4:H:141:SER:C	4:H:192:SER:HA	2.46	0.40
4:H:148:LEU:HD23	4:H:148:LEU:O	2.22	0.40
3:U:52:THR:CG2	3:U:72:TYR:CE2	3.00	0.40
4:T:190:VAL:CG2	4:T:195:TRP:HB2	2.41	0.40
1:A:25:LEU:HD23	1:A:34:ILE:H	1.85	0.40
1:A:51:ILE:HA	1:A:287:SER:OG	2.21	0.40
1:A:107:SER:O	1:A:111:LEU:HG	2.20	0.40
1:A:161:TYR:CZ	1:A:249:GLY:HA2	2.57	0.40
2:B:2:LEU:O	2:D:3:PHE:HZ	2.04	0.40
2:B:9:PHE:CD1	2:B:10:ILE:HG13	2.56	0.40
1:C:28:THR:CG2	2:D:105:GLN:N	2.84	0.40
1:C:160:THR:CA	1:C:196:VAL:HG21	2.49	0.40
2:D:5:ALA:O	2:D:8:GLY:N	2.54	0.40
1:E:125:PHE:HB2	1:E:127:TRP:HE1	1.80	0.40
3:L:7:SER:HB2	3:L:8:PRO:HD3	2.04	0.40
4:H:3:HIS:CG	4:H:4:LEU:N	2.88	0.40
3:U:8:PRO:HB2	3:U:11:MET:HG2	2.03	0.40
3:U:107:ILE:HG13	3:U:167:GLN:NE2	2.37	0.40
4:T:67:ARG:NH1	4:T:90:ASP:OD1	2.49	0.40
4:T:162:ASN:O	4:T:163:SER:HB2	2.21	0.40
1:A:13:LEU:HB3	2:B:138:PHE:HB2	2.03	0.40
1:A:326:LYS:O	1:A:327:GLN:CB	2.70	0.40
2:B:106:HIS:O	2:B:106:HIS:CG	2.72	0.40
2:D:165:GLU:OE1	2:D:168:ASN:ND2	2.55	0.40
2:F:158:ASP:C	2:F:160:ASP:H	2.28	0.40
3:L:35:TYR:HB3	3:L:49:ILE:O	2.22	0.40
4:H:73:ASP:O	4:H:76:LYS:N	2.51	0.40
3:U:6:GLN:CD	3:U:102:GLY:HA2	2.47	0.40
3:U:145:ILE:HG12	3:U:146:ASN:N	2.36	0.40
4:T:39:ARG:NH1	4:T:94:TYR:OH	2.53	0.40
4:T:150:LYS:HA	4:T:183:THR:HG23	2.02	0.40
1:A:15:LEU:HD11	2:B:119:PHE:HB2	2.03	0.40
1:A:132:GLN:HB3	1:A:133:ASN:H	1.65	0.40
2:B:52:LEU:O	2:B:55:VAL:N	2.55	0.40
2:B:80:LEU:HD21	2:D:80:LEU:CD2	2.51	0.40
2:D:107:THR:O	2:D:110:LEU:HB3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:LEU:HD13	1:E:14:CYS:O	2.22	0.40
1:E:296:ASN:ND2	1:E:309:VAL:O	2.55	0.40
2:F:88:LYS:O	2:F:91:LEU:N	2.54	0.40
2:F:122:THR:OG1	2:F:123:ARG:N	2.53	0.40
2:F:170:ARG:CB	2:F:171:PHE:CD1	3.02	0.40
3:L:6:GLN:OE1	3:L:87:TYR:O	2.39	0.40
3:L:79:LEU:HD13	3:L:79:LEU:C	2.47	0.40
3:L:180:LEU:HD12	3:L:181:THR:N	2.36	0.40
4:H:14:PRO:O	4:H:15:SER:OG	2.33	0.40
4:H:108:ASP:OD1	4:H:108:ASP:C	2.63	0.40
4:H:207:PRO:O	4:H:208:ALA:C	2.64	0.40
3:U:113:ALA:HB2	3:U:201:THR:HG21	2.02	0.40
3:U:125:GLN:NE2	4:T:129:TYR:CE2	2.88	0.40
1:A:308:TYR:HD2	2:B:89:ILE:HG13	1.86	0.40
2:B:166:ALA:O	2:B:167:LEU:C	2.65	0.40
1:C:125:PHE:HB2	1:C:127:TRP:NE1	2.37	0.40
1:C:232:ILE:HD12	1:C:232:ILE:HG23	1.71	0.40
1:C:308:TYR:CD2	1:C:309:VAL:N	2.89	0.40
2:D:96:ALA:C	2:D:98:LEU:N	2.76	0.40
1:E:94:PHE:HD1	1:E:94:PHE:O	2.03	0.40
2:F:28:ASN:HD22	2:F:145:ASP:C	2.30	0.40
2:F:98:LEU:HD23	2:F:102:LEU:HG	2.03	0.40
3:L:149:TRP:HE1	3:L:178:SER:CB	2.34	0.40
3:L:212:ARG:NH2	4:H:138:GLN:N	2.63	0.40
4:H:53:SER:C	4:H:55:ASP:N	2.78	0.40
4:H:97:ALA:CB	4:H:109:TYR:O	2.63	0.40
4:H:152:TYR:CZ	4:H:157:VAL:HG22	2.57	0.40
4:H:212:LYS:O	4:H:213:VAL:HG13	2.21	0.40
4:H:217:ILE:HD12	4:H:217:ILE:HG23	1.86	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	318/328 (97%)	247 (78%)	43 (14%)	28 (9%)	0	7
1	C	318/328 (97%)	241 (76%)	53 (17%)	24 (8%)	1	9
1	E	318/328 (97%)	250 (79%)	41 (13%)	27 (8%)	0	7
2	B	173/175 (99%)	96 (56%)	44 (25%)	33 (19%)	0	1
2	D	173/175 (99%)	89 (51%)	48 (28%)	36 (21%)	0	1
2	F	173/175 (99%)	89 (51%)	49 (28%)	35 (20%)	0	1
3	L	211/213 (99%)	141 (67%)	46 (22%)	24 (11%)	0	5
3	U	211/213 (99%)	139 (66%)	51 (24%)	21 (10%)	0	6
4	H	219/221 (99%)	158 (72%)	38 (17%)	23 (10%)	0	5
4	T	217/221 (98%)	147 (68%)	47 (22%)	23 (11%)	0	5
All	All	2331/2377 (98%)	1597 (68%)	460 (20%)	274 (12%)	0	4

All (274) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ILE
1	A	81	ASN
1	A	210	GLN
1	A	263	GLY
1	A	287	SER
1	A	304	ALA
2	B	5	ALA
2	B	11	GLU
2	B	55	VAL
2	B	56	ILE
2	B	59	THR
2	B	116	ASN
2	B	154	ASN
2	B	168	ASN
2	B	170	ARG
1	C	44	GLN
1	C	70	LEU
1	C	81	ASN
1	C	156	LYS
1	C	210	GLN
1	C	263	GLY
1	C	287	SER
2	D	5	ALA
2	D	11	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	15	GLU
2	D	55	VAL
2	D	59	THR
2	D	97	GLU
2	D	116	ASN
2	D	127	ARG
2	D	150	GLU
2	D	164	ASP
2	D	168	ASN
2	D	170	ARG
1	E	44	GLN
1	E	81	ASN
1	E	156	LYS
1	E	210	GLN
1	E	263	GLY
1	E	287	SER
1	E	321	ARG
2	F	5	ALA
2	F	11	GLU
2	F	14	TRP
2	F	15	GLU
2	F	55	VAL
2	F	56	ILE
2	F	59	THR
2	F	97	GLU
2	F	116	ASN
2	F	127	ARG
2	F	150	GLU
2	F	168	ASN
2	F	170	ARG
2	F	174	LYS
3	L	26	SER
3	L	31	SER
3	L	32	SER
3	L	57	SER
3	L	93	GLU
3	L	127	THR
3	L	141	TYR
3	L	142	PRO
3	L	206	ILE
3	L	209	SER
4	H	2	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	H	16	GLN
4	H	29	ILE
4	H	52	ILE
4	H	55	ASP
4	H	57	SER
4	H	66	ASN
4	H	74	THR
4	H	135	SER
4	H	147	CYS
4	H	194	THR
4	H	195	TRP
3	U	31	SER
3	U	57	SER
3	U	62	ARG
3	U	93	GLU
3	U	111	ASP
3	U	127	THR
3	U	139	ASN
3	U	141	TYR
3	U	142	PRO
4	T	29	ILE
4	T	52	ILE
4	T	66	ASN
4	T	74	THR
4	T	121	ALA
4	T	135	SER
4	T	147	CYS
4	T	195	TRP
1	A	19	ALA
1	A	44	GLN
1	A	70	LEU
1	A	92	LYS
1	A	133	ASN
1	A	321	ARG
2	B	7	ALA
2	B	14	TRP
2	B	15	GLU
2	B	28	ASN
2	B	39	LYS
2	B	57	GLU
2	B	83	TYR
2	B	97	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	109	ASP
2	B	127	ARG
2	B	150	GLU
2	B	164	ASP
2	B	169	ASN
2	B	174	LYS
1	C	19	ALA
1	C	62	ILE
1	C	132	GLN
1	C	133	ASN
1	C	277	CYS
1	C	304	ALA
1	C	327	GLN
2	D	14	TRP
2	D	39	LYS
2	D	56	ILE
2	D	57	GLU
2	D	75	GLY
2	D	77	ILE
2	D	83	TYR
2	D	102	LEU
2	D	103	GLU
2	D	115	MET
2	D	130	ALA
2	D	132	GLU
2	D	133	MET
2	D	154	ASN
2	D	169	ASN
2	D	174	LYS
1	E	29	ILE
1	E	92	LYS
1	E	133	ASN
1	E	191	GLN
1	E	197	GLN
1	E	279	SER
2	F	39	LYS
2	F	57	GLU
2	F	83	TYR
2	F	89	ILE
2	F	132	GLU
2	F	154	ASN
2	F	164	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	169	ASN
3	L	62	ARG
3	L	75	THR
3	L	111	ASP
3	L	139	ASN
3	L	151	ILE
3	L	205	PRO
4	H	15	SER
4	H	62	PRO
4	H	134	GLY
3	U	110	ALA
3	U	151	ILE
3	U	154	SER
3	U	205	PRO
3	U	206	ILE
3	U	209	SER
4	T	15	SER
4	T	16	GLN
4	T	55	ASP
4	T	57	SER
4	T	61	ASN
4	T	62	PRO
4	T	194	THR
1	A	21	PRO
1	A	172	ASP
1	A	327	GLN
2	B	78	GLN
2	B	102	LEU
2	B	132	GLU
1	C	18	HIS
1	C	29	ILE
1	C	279	SER
1	C	293	PRO
1	C	313	THR
2	D	92	TRP
2	D	124	ARG
1	E	19	ALA
1	E	110	SER
1	E	192	THR
1	E	196	VAL
1	E	277	CYS
1	E	304	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	88	LYS
2	F	103	GLU
2	F	109	ASP
2	F	133	MET
3	L	83	ASP
3	L	154	SER
3	L	169	SER
3	L	201	THR
4	H	102	ASP
4	H	208	ALA
4	H	210	SER
3	U	9	ALA
3	U	26	SER
3	U	75	THR
4	T	134	GLY
4	T	192	SER
4	T	197	SER
1	A	18	HIS
1	A	62	ILE
1	A	80	GLN
1	A	132	GLN
1	A	158	GLY
1	A	196	VAL
1	A	250	ASN
1	A	277	CYS
1	A	313	THR
2	B	103	GLU
2	B	124	ARG
2	B	133	MET
1	C	21	PRO
1	C	158	GLY
2	D	19	ASP
2	D	81	GLU
2	D	88	LYS
2	D	112	ASP
1	E	18	HIS
1	E	21	PRO
1	E	62	ILE
1	E	327	GLN
2	F	28	ASN
2	F	54	ARG
2	F	112	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	124	ARG
2	F	130	ALA
3	L	52	THR
4	H	3	HIS
4	H	197	SER
3	U	52	THR
4	T	208	ALA
1	A	71	LEU
1	A	98	TYR
1	A	293	PRO
2	B	6	ILE
2	B	19	ASP
2	B	76	ARG
2	B	130	ALA
1	C	84	TRP
1	C	196	VAL
1	E	98	TYR
1	E	188	ASN
1	E	293	PRO
2	F	115	MET
2	F	123	ARG
2	F	153	ARG
3	L	125	GLN
4	H	101	TYR
4	H	196	PRO
4	T	179	SER
1	A	143	PRO
2	D	89	ILE
2	D	91	LEU
1	E	158	GLY
2	F	76	ARG
3	L	110	ALA
3	U	32	SER
4	T	101	TYR
3	U	7	SER
4	T	196	PRO
1	C	98	TYR
4	H	61	ASN
3	L	15	PRO
4	T	156	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/289 (98%)	250 (89%)	32 (11%)	5	25
1	C	282/289 (98%)	247 (88%)	35 (12%)	4	22
1	E	282/289 (98%)	250 (89%)	32 (11%)	5	25
2	B	149/149 (100%)	121 (81%)	28 (19%)	1	9
2	D	149/149 (100%)	117 (78%)	32 (22%)	1	6
2	F	149/149 (100%)	122 (82%)	27 (18%)	2	10
3	L	187/187 (100%)	147 (79%)	40 (21%)	1	6
3	U	187/187 (100%)	150 (80%)	37 (20%)	1	7
4	H	196/196 (100%)	164 (84%)	32 (16%)	2	14
4	T	194/196 (99%)	161 (83%)	33 (17%)	2	12
All	All	2057/2080 (99%)	1729 (84%)	328 (16%)	2	14

All (328) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	15	LEU
1	A	17	HIS
1	A	20	VAL
1	A	22	ASN
1	A	48	THR
1	A	54	ASN
1	A	65	THR
1	A	78	VAL
1	A	100	TYR
1	A	101	ASP
1	A	110	SER
1	A	130	VAL
1	A	136	SER
1	A	140	LYS
1	A	141	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	156	LYS
1	A	189	GLN
1	A	217	ILE
1	A	237	VAL
1	A	239	PRO
1	A	243	LEU
1	A	246	ASN
1	A	248	ASN
1	A	250	ASN
1	A	254	PRO
1	A	265	SER
1	A	267	ILE
1	A	282	ILE
1	A	293	PRO
1	A	309	VAL
1	A	312	ASN
2	B	3	PHE
2	B	6	ILE
2	B	9	PHE
2	B	12	ASN
2	B	17	MET
2	B	18	ILE
2	B	21	TRP
2	B	24	PHE
2	B	32	THR
2	B	38	LEU
2	B	41	THR
2	B	46	ASP
2	B	48	ILE
2	B	52	LEU
2	B	54	ARG
2	B	76	ARG
2	B	78	GLN
2	B	84	VAL
2	B	97	GLU
2	B	109	ASP
2	B	119	PHE
2	B	120	GLU
2	B	121	LYS
2	B	135	ASN
2	B	160	ASP
2	B	168	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	171	PHE
2	B	174	LYS
1	C	13	LEU
1	C	15	LEU
1	C	20	VAL
1	C	22	ASN
1	C	54	ASN
1	C	65	THR
1	C	78	VAL
1	C	95	SER
1	C	101	ASP
1	C	110	SER
1	C	118	LEU
1	C	122	THR
1	C	130	VAL
1	C	140	LYS
1	C	150	ARG
1	C	156	LYS
1	C	189	GLN
1	C	213	ILE
1	C	219	SER
1	C	222	TRP
1	C	237	VAL
1	C	239	PRO
1	C	243	LEU
1	C	246	ASN
1	C	248	ASN
1	C	250	ASN
1	C	254	PRO
1	C	265	SER
1	C	267	ILE
1	C	282	ILE
1	C	287	SER
1	C	288	ILE
1	C	293	PRO
1	C	309	VAL
1	C	312	ASN
2	D	3	PHE
2	D	6	ILE
2	D	9	PHE
2	D	12	ASN
2	D	17	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	18	ILE
2	D	21	TRP
2	D	24	PHE
2	D	29	SER
2	D	32	THR
2	D	38	LEU
2	D	41	THR
2	D	46	ASP
2	D	48	ILE
2	D	60	ASN
2	D	71	SER
2	D	73	VAL
2	D	76	ARG
2	D	78	GLN
2	D	84	VAL
2	D	97	GLU
2	D	98	LEU
2	D	106	HIS
2	D	119	PHE
2	D	120	GLU
2	D	121	LYS
2	D	124	ARG
2	D	135	ASN
2	D	160	ASP
2	D	168	ASN
2	D	171	PHE
2	D	174	LYS
1	E	13	LEU
1	E	15	LEU
1	E	20	VAL
1	E	22	ASN
1	E	54	ASN
1	E	65	THR
1	E	78	VAL
1	E	85	ASP
1	E	94	PHE
1	E	100	TYR
1	E	101	ASP
1	E	128	THR
1	E	130	VAL
1	E	140	LYS
1	E	141	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	156	LYS
1	E	189	GLN
1	E	199	SER
1	E	217	ILE
1	E	222	TRP
1	E	237	VAL
1	E	239	PRO
1	E	243	LEU
1	E	246	ASN
1	E	248	ASN
1	E	254	PRO
1	E	265	SER
1	E	282	ILE
1	E	287	SER
1	E	293	PRO
1	E	309	VAL
1	E	312	ASN
2	F	3	PHE
2	F	6	ILE
2	F	9	PHE
2	F	17	MET
2	F	18	ILE
2	F	21	TRP
2	F	24	PHE
2	F	32	THR
2	F	41	THR
2	F	46	ASP
2	F	48	ILE
2	F	52	LEU
2	F	78	GLN
2	F	84	VAL
2	F	97	GLU
2	F	98	LEU
2	F	105	GLN
2	F	109	ASP
2	F	119	PHE
2	F	120	GLU
2	F	121	LYS
2	F	135	ASN
2	F	156	THR
2	F	158	ASP
2	F	160	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	171	PHE
2	F	174	LYS
3	L	2	ILE
3	L	8	PRO
3	L	11	MET
3	L	14	SER
3	L	21	LEU
3	L	22	THR
3	L	30	THR
3	L	35	TYR
3	L	46	LYS
3	L	54	ASN
3	L	64	SER
3	L	68	SER
3	L	70	THR
3	L	71	SER
3	L	74	LEU
3	L	79	LEU
3	L	94	THR
3	L	103	THR
3	L	107	ILE
3	L	123	LYS
3	L	125	GLN
3	L	126	LEU
3	L	134	VAL
3	L	139	ASN
3	L	151	ILE
3	L	154	SER
3	L	155	GLU
3	L	164	TRP
3	L	165	THR
3	L	166	ASP
3	L	170	LYS
3	L	171	ASP
3	L	174	TYR
3	L	185	ASP
3	L	189	ARG
3	L	190	HIS
3	L	191	ASN
3	L	192	SER
3	L	203	THR
3	L	204	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	H	2	VAL
4	H	11	LEU
4	H	13	LYS
4	H	16	GLN
4	H	18	LEU
4	H	25	THR
4	H	28	SER
4	H	36	THR
4	H	42	PRO
4	H	52	ILE
4	H	59	ASN
4	H	62	PRO
4	H	66	ASN
4	H	71	THR
4	H	74	THR
4	H	80	PHE
4	H	84	ASN
4	H	104	ASP
4	H	116	LEU
4	H	117	THR
4	H	120	SER
4	H	124	THR
4	H	126	PRO
4	H	128	VAL
4	H	140	ASN
4	H	143	VAL
4	H	148	LEU
4	H	154	PRO
4	H	157	VAL
4	H	179	SER
4	H	214	ASP
4	H	216	LYS
3	U	11	MET
3	U	14	SER
3	U	21	LEU
3	U	22	THR
3	U	23	CYS
3	U	30	THR
3	U	35	TYR
3	U	46	LYS
3	U	52	THR
3	U	55	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	U	59	VAL
3	U	64	SER
3	U	68	SER
3	U	70	THR
3	U	71	SER
3	U	74	LEU
3	U	79	LEU
3	U	103	THR
3	U	123	LYS
3	U	125	GLN
3	U	126	LEU
3	U	134	VAL
3	U	154	SER
3	U	155	GLU
3	U	164	TRP
3	U	165	THR
3	U	166	ASP
3	U	170	LYS
3	U	171	ASP
3	U	183	THR
3	U	185	ASP
3	U	189	ARG
3	U	190	HIS
3	U	191	ASN
3	U	192	SER
3	U	203	THR
3	U	204	SER
4	T	12	VAL
4	T	13	LYS
4	T	16	GLN
4	T	17	SER
4	T	18	LEU
4	T	25	THR
4	T	28	SER
4	T	36	THR
4	T	52	ILE
4	T	55	ASP
4	T	59	ASN
4	T	62	PRO
4	T	67	ARG
4	T	68	ILE
4	T	71	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	T	74	THR
4	T	80	PHE
4	T	104	ASP
4	T	116	LEU
4	T	117	THR
4	T	124	THR
4	T	126	PRO
4	T	140	ASN
4	T	147	CYS
4	T	148	LEU
4	T	154	PRO
4	T	157	VAL
4	T	170	VAL
4	T	176	VAL
4	T	184	LEU
4	T	214	ASP
4	T	216	LYS
4	T	218	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	22	ASN
1	A	38	ASN
1	A	54	ASN
1	A	80	GLN
1	A	81	ASN
1	A	96	ASN
1	A	170	ASN
1	A	188	ASN
1	A	189	GLN
1	A	191	GLN
1	A	210	GLN
1	A	211	GLN
1	A	216	ASN
1	A	246	ASN
1	A	248	ASN
1	A	250	ASN
1	A	296	ASN
1	A	298	ASN
1	A	312	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	27	GLN
2	B	28	ASN
2	B	49	ASN
2	B	60	ASN
2	B	78	GLN
2	B	95	ASN
2	B	125	GLN
2	B	142	HIS
2	B	154	ASN
2	B	168	ASN
1	C	17	HIS
1	C	22	ASN
1	C	38	ASN
1	C	54	ASN
1	C	81	ASN
1	C	96	ASN
1	C	170	ASN
1	C	188	ASN
1	C	189	GLN
1	C	210	GLN
1	C	211	GLN
1	C	216	ASN
1	C	248	ASN
1	C	296	ASN
1	C	298	ASN
1	C	311	GLN
1	C	312	ASN
1	C	322	ASN
2	D	28	ASN
2	D	49	ASN
2	D	60	ASN
2	D	125	GLN
2	D	129	ASN
2	D	154	ASN
2	D	168	ASN
1	E	22	ASN
1	E	38	ASN
1	E	44	GLN
1	E	54	ASN
1	E	75	HIS
1	E	81	ASN
1	E	96	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	188	ASN
1	E	189	GLN
1	E	210	GLN
1	E	246	ASN
1	E	248	ASN
1	E	285	ASN
1	E	290	ASN
1	E	296	ASN
1	E	298	ASN
1	E	312	ASN
2	F	27	GLN
2	F	28	ASN
2	F	49	ASN
2	F	60	ASN
2	F	78	GLN
2	F	105	GLN
2	F	125	GLN
2	F	168	ASN
3	L	6	GLN
3	L	39	GLN
3	L	91	GLN
3	L	191	ASN
3	L	199	HIS
4	H	40	GLN
4	H	61	ASN
4	H	77	ASN
4	H	78	GLN
4	H	84	ASN
4	H	112	GLN
4	H	140	ASN
4	H	162	ASN
4	H	206	HIS
3	U	1	GLN
3	U	6	GLN
3	U	38	GLN
3	U	91	GLN
3	U	191	ASN
3	U	199	HIS
3	U	213	ASN
4	T	61	ASN
4	T	77	ASN
4	T	78	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	T	84	ASN
4	T	112	GLN
4	T	138	GLN
4	T	140	ASN
4	T	162	ASN
4	T	206	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

9 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	NAG	G	1	5,1	14,14,15	0.68	0	17,19,21	1.43	2 (11%)
5	NAG	G	2	5	14,14,15	0.52	0	17,19,21	0.97	1 (5%)
5	MAN	G	3	5	11,11,12	1.00	1 (9%)	15,15,17	0.87	1 (6%)
5	NAG	I	1	5,1	14,14,15	0.66	0	17,19,21	1.07	2 (11%)
5	NAG	I	2	5	14,14,15	0.72	0	17,19,21	0.99	1 (5%)
5	MAN	I	3	5	11,11,12	1.15	2 (18%)	15,15,17	0.98	1 (6%)
5	NAG	J	1	5,1	14,14,15	0.82	0	17,19,21	1.30	2 (11%)
5	NAG	J	2	5	14,14,15	1.23	1 (7%)	17,19,21	1.37	4 (23%)
5	MAN	J	3	5	11,11,12	0.89	0	15,15,17	1.01	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	G	2	5	-	3/6/23/26	0/1/1/1
5	MAN	G	3	5	1/1/4/5	1/2/19/22	0/1/1/1
5	NAG	I	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	3/6/23/26	0/1/1/1
5	MAN	I	3	5	1/1/4/5	2/2/19/22	0/1/1/1
5	NAG	J	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	MAN	J	3	5	1/1/4/5	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	2	NAG	C1-C2	-3.35	1.47	1.52
5	G	3	MAN	C4-C5	2.18	1.57	1.53
5	I	3	MAN	C4-C5	2.05	1.57	1.53
5	I	3	MAN	C6-C5	2.05	1.58	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	1	NAG	C2-N2-C7	-3.97	117.58	122.90
5	G	1	NAG	C4-C3-C2	-3.21	106.31	111.02
5	I	3	MAN	C6-C5-C4	2.87	120.06	113.02
5	J	2	NAG	C4-C3-C2	2.81	115.14	111.02
5	J	2	NAG	C2-N2-C7	-2.70	119.29	122.90
5	I	2	NAG	C2-N2-C7	-2.69	119.30	122.90
5	J	3	MAN	C6-C5-C4	2.68	119.61	113.02
5	G	2	NAG	C2-N2-C7	-2.56	119.46	122.90
5	J	1	NAG	C2-N2-C7	-2.50	119.55	122.90
5	J	1	NAG	C4-C3-C2	-2.40	107.51	111.02
5	I	1	NAG	C2-N2-C7	-2.39	119.69	122.90
5	G	3	MAN	C6-C5-C4	2.37	118.84	113.02
5	J	2	NAG	C1-C2-N2	-2.37	106.71	110.43
5	I	1	NAG	C4-C3-C2	-2.36	107.56	111.02
5	J	2	NAG	O5-C1-C2	-2.02	108.17	111.29

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	3	MAN	C1
5	I	3	MAN	C1
5	J	3	MAN	C1

All (18) torsion outliers are listed below:

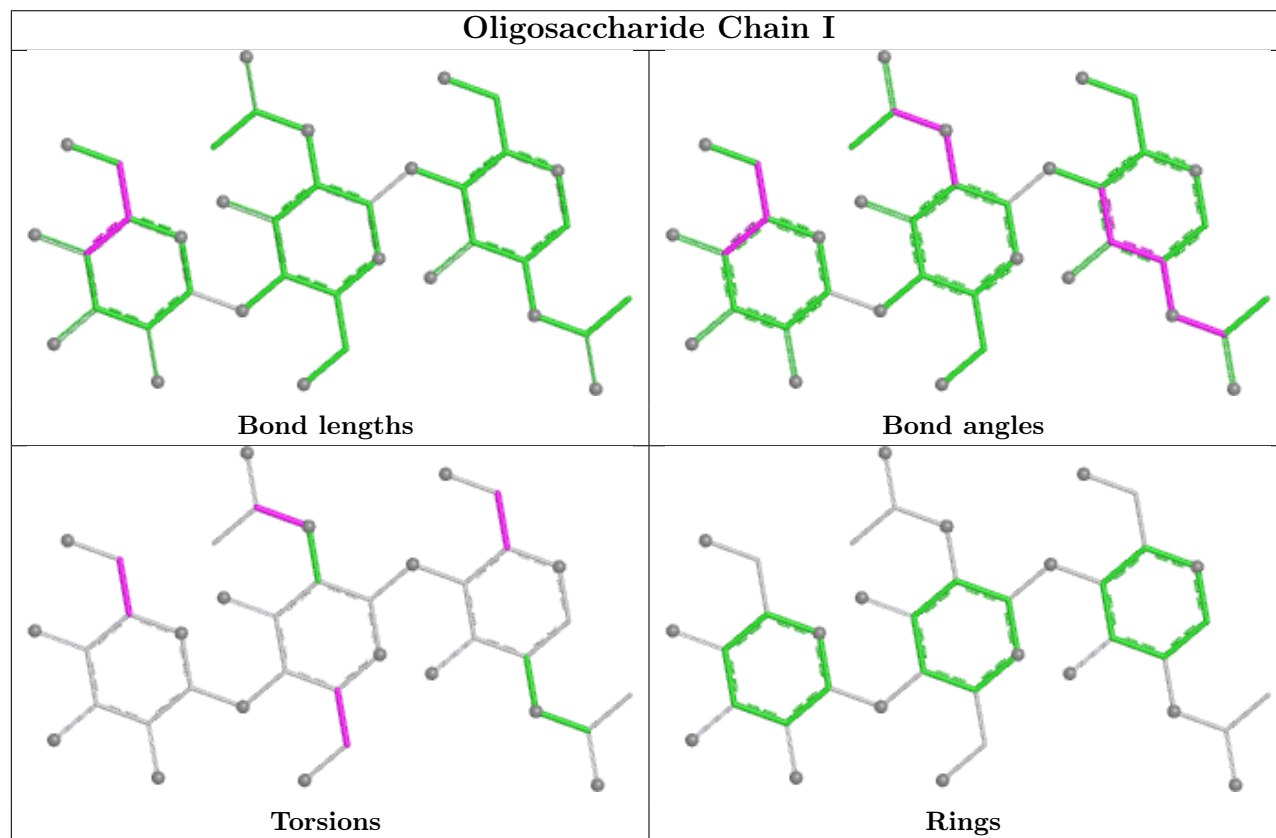
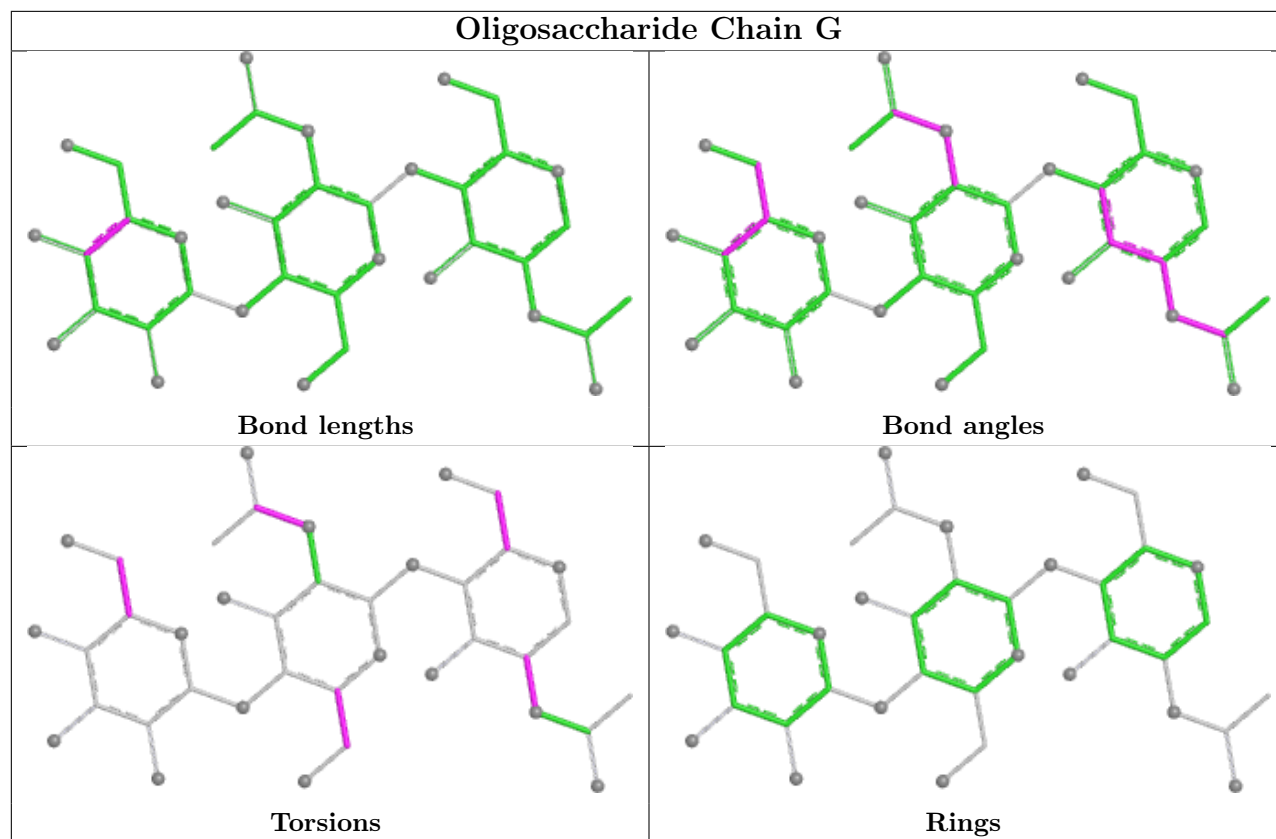
Mol	Chain	Res	Type	Atoms
5	J	1	NAG	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	J	2	NAG	C8-C7-N2-C2
5	J	1	NAG	C4-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
5	G	2	NAG	C8-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2
5	G	1	NAG	O5-C5-C6-O6
5	I	3	MAN	O5-C5-C6-O6
5	G	2	NAG	O7-C7-N2-C2
5	I	2	NAG	C8-C7-N2-C2
5	G	1	NAG	C4-C5-C6-O6
5	I	3	MAN	C4-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
5	I	2	NAG	O7-C7-N2-C2
5	G	2	NAG	O5-C5-C6-O6
5	G	1	NAG	C1-C2-N2-C7
5	G	3	MAN	O5-C5-C6-O6

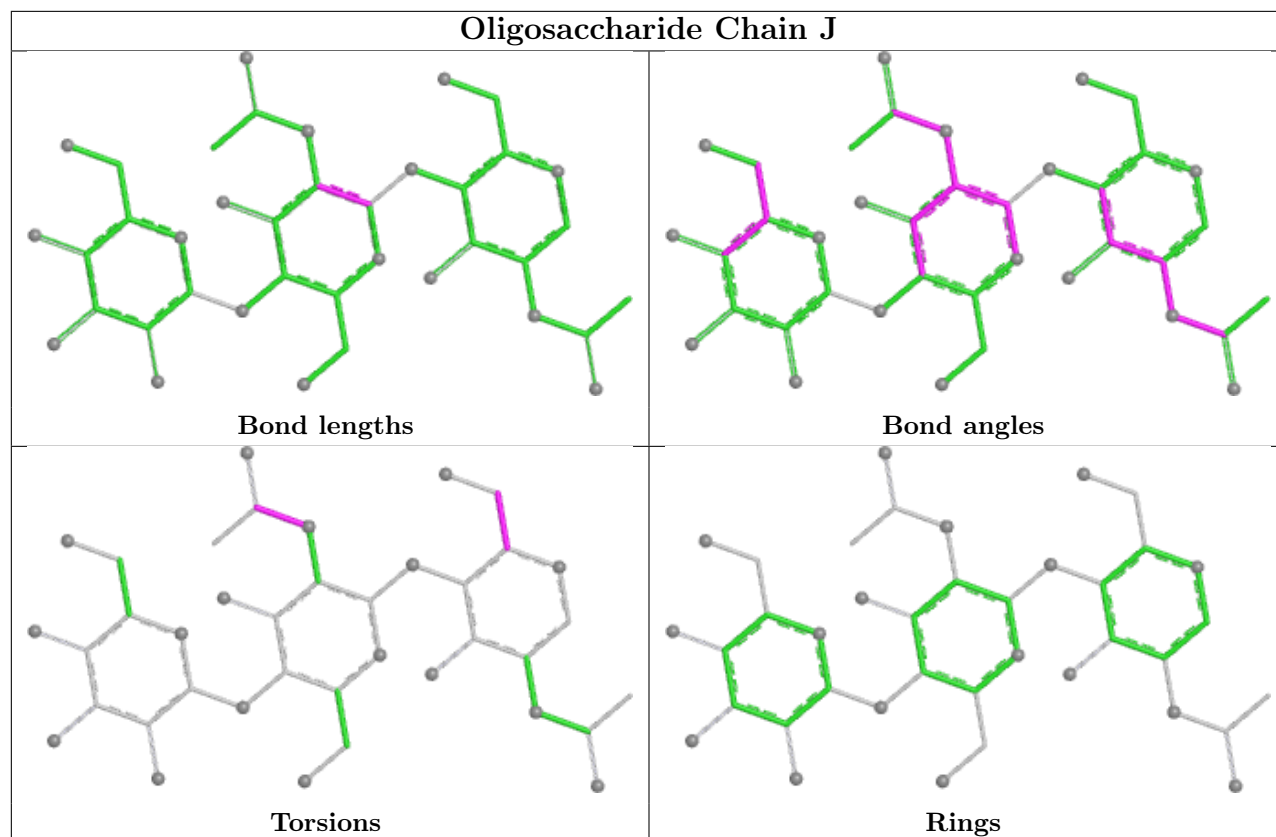
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	2	NAG	2	0
5	I	1	NAG	2	0
5	G	2	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.